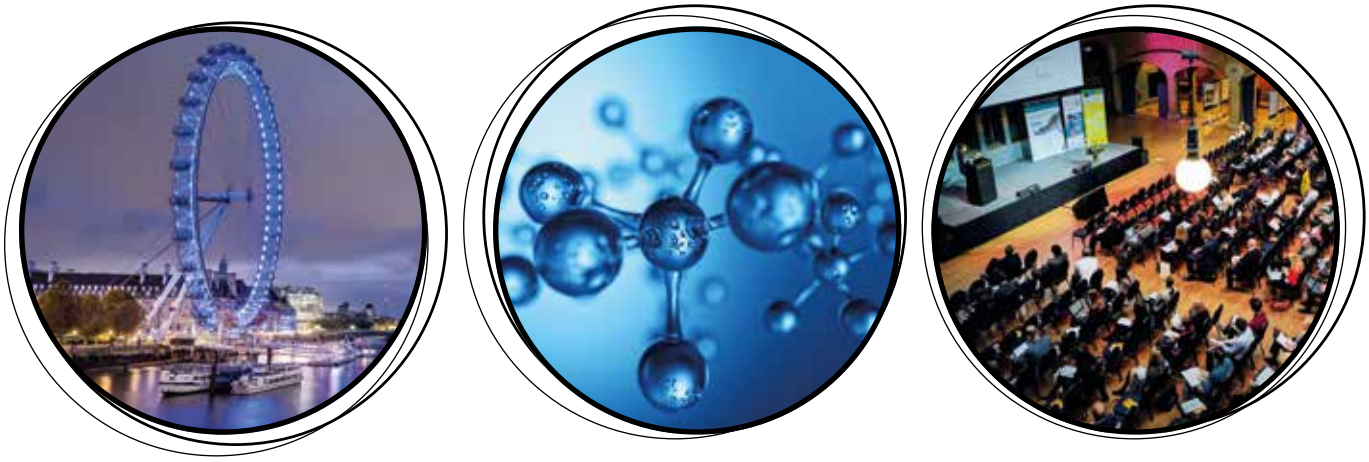
Global Engage

# GLOBAL MEDICINAL CHEMISTRY & GPCR LEADERS SUMMIT: EUROPE

## — LONDON, UK —

27-28 November 2017



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## **WARM** WELCOME

Global Engage

Global Engage are pleased to announce as part of their Drug Discovery Series of events, the **Global Medicinal Chemistry Leaders Summit**, which will be held on November 27-28 2017 in London, UK. The meeting will be co-located with the GPCR Congress 2017 whose presentations will compliment this summit.

Designed to attract experts working in all areas of medicinal chemistry the Summit has four tracks focusing on key issues and such as optimising hit to lead quality and timescale, protein degradation, DNA Encoded libraries, small molecule Immuno-oncology research, FBDD, SBDD, CADD as well as best strategies for partnerships, collaborations, outsourcing and integration of research. The summit will provide a forum to network, learn and engage with senior representatives of leading pharmaceutical and biotech companies worldwide.

## **EXPERT SPEAKERS** Include:

**EMMA PARMEE**
Associate VP, Head of Chemistry Capabilities and Screening, Merck Sharp & Dohme

**LAURENT SCHIO**
Head of France Medicinal Chemistry, Lead Optimization, Sanofi

**IAN CHURCHER**
Head, Protein Degradation Discovery Performance Unit, GSK

**GARRY PAIRAUDEAU**
Head of External Sciences, AstraZeneca

**FIONA MARSHALL**
Founder, Director & CSO, Heptares Therapeutics

**JULIE SELKIRK**
Associate Director, Biology, Celgene

# CONFERENCE SYNOPSIS

## DAY 1 – TRACK 1

**Medicinal Chemistry Strategies**

- Drug Discovery Chemistry – where are we heading
- Artificial Intelligence for medicinal chemistry
- Target (In)validation using medicinal chemistry tools
- Optimising hit to lead optimization quality and timescale
  - ► Best Practice Case Studies
  - ► CADD / Cheminformatics
  - ► Data for decision making
  - ► Virtual screening for identifying hits
- Panel Discussion – Future of Medicinal Chemistry

## DAY 1 – TRACK 2

**Enabling Technologies - Degraded Chemistry & DNA Encoded Libraries**

- Targeted protein degradation / PROTACs
- DNA encoded libraries
- Integrated synthesis platforms
- Oher enabling technologies
- Panel Discussion – Protein Degradation – the possibilities

## DAY 1 – TRACK 3

**GPCR - Addressing complex pharmacology and signalling**

- Allosteric Modulation approaches and development
- Signalling / Biased signalling
- Drug Discovery case studies

## DAY 2 – TRACK 1

**Integrating Medicinal Chemistry into the drug discovery process**

- ADCs – Targeted delivery
- Small molecule Immuno-oncology research
- Methods to Reducing Toxicity
- Molecules with predictable in vivo and safety profiles
- Phenotypic screening

**Fragment Based Drug Discovery**

- When FBDD should be used
- Best practice case studies

**Structure Based Drug Design**

- SBDD Case studies
- GPCR targets
- Macrocyclic compounds

## DAY 2 – TRACK 2

**Partnerships, Collaborations & Outsourcing**

- Identifying & choosing a partner for a productive partnership
  - ► CRO v partnership
  - ► True benefits to outsourcing
  - ► Risk sharing business models
  - ► Managing the partnership – communication, data exchange, measuring quality & success
- What and when to outsource
  - ► Integrating outsourced research to internal products
  - ► Keeping to budget – Optimizing ROI
  - ► Risk and rewards
- What worked well and what didn't – Lessons learned and tips for success
- Open Innovation / Pre-competitive activity
- Panel Discussion – Best methods to identify, choose and manage your partnership

## PANEL & ROUNDTABLE DISCUSSIONS

**Panel Discussions**

1. Future of Medicinal Chemistry
2. Targeted Protein Degradation
3. Best methods to identify, choose and manage your outsourcing partner

**One Hour Roundtable Discussions**

1. Targeted Protein Degradation
2. Optimising hit to lead optimization
3. Optimising Outsourcing activities
4. DNA Encoded Libraries
5. Fragment Based Drug Discovery
6. GPCR – Biased Signalling

# CONFIRMED SPEAKERS

**EMMA PARMEE**
Associate VP, Head of Chemistry Capabilities and Screening, Merck Sharp & Dohme

**DAVID WILSON**
Senior Director and Head, Global Oncology Chemistry, IMED Oncology, AstraZeneca

**STEVAN DJURIC**
Distinguished Research Fellow, Senior Director Discovery Chemistry and Technology, Abbvie

**LAURENT SCHIO**
Head of France Medicinal Chemistry, Lead Optimization, Sanofi

**THOMAS FRANCH**
CSO Nuevolution A/S

**ANDREAS LERCHNER**
Senior Investigator, Project Team Leader, Novartis Institutes for Biomedical Research

**ANDREAS BRUNSCHWEIGER**
Independent Group Leader, TU Dortmund

**MARK BOYS**
Principal Research Investigator, Array BioPharma

**FIONA MARSHALL**
Founder, Director & CSO, Heptares Therapeutics

**NICK TERRETT**
Scientific Associate Vice President, European Chemistry Lead, Merck Sharp and Dohme

**IAN CHURCHER**
Head, Protein Degradation Discovery Performance Unit, GSK

**GEORGE BURSLEM**
Research Fellow, Crews Lab, Yale University

**DARREN GREEN**
Director Molecular Design, GSK

**GARRY PAIRAUDEAU**
Head of External Sciences, AstraZeneca

**ALLEYN PLOWRIGHT**
Head of Integrated Drug Discovery Germany, Sanofi

**TAKASHI ICHIKAWA**
Senior Director, Head of Drug Discovery Chemistry Laboratories, CNS Drug Discovery Unit, Research, Takeda Pharmaceutical Company

**LAWRENCE HAMANN**
Vice President, Chemistry, Celgene

**GISBERT SCHNEIDER**
Professor, Computer-Assisted Drug Design at the Institute of Pharmaceutical Sciences in the Department of Chemistry and Applied Biosciences, ETH Zurich


**ALESSIO CIULLI**
Professor of Chemical & Structural Biology, Division of Biological Chemistry and Drug Discovery, School of Life Sciences, University of Dundee

**ALEXANDER ALANINE**
Chief Operating Officer, Bactevo

**XIAOPENG BAI**
Investigator, GSK


**STEPHEN SHUTTLEWORTH**
Chief Operating Officer & Chief Scientific Officer, Karus Therapeutics Ltd

**NICHOLAS CARRUTHERS**
Senior Director, Neuroscience, Janssen, Pharmaceutical Companies of Johnson and Johnson

**EDUARD FELDER**
Director, Head of Chemical Core Technologies, Oncology Research, Nerviano Medical Sciences

**DAVID POWELL**
Director, Chemistry, Inception Sciences Canada


**DARREN MCKERRECHER**
Director Medicinal Chemistry, AstraZeneca

**MATTHIAS ZENTGRAF**
Head of Computational Chemistry, Boehringer-Ingelheim

**JONATHAN MASON**
Senior Research Fellow & Head of CADD, Heptares Therapeutics (UK)


**CRAIG JOHNSTONE**
Executive Vice President, Head of Chemistry and Directeur General, Evotec (France) SAS

**JULIE SELKIRK**
Associate Director, Biology, Celgene

**JEFF REAGAN**
Scientific Director, CardioMetabolic Disorders, Amgen

**ANDREW ALT**
Associate Director, Biology, Arvinas

**AYLIN HANYALOGLU**
Senior Lecturer, Institute of Reproductive and Developmental Biology, Department of Surgery and Cancer, Faculty of Medicine, Imperial College London

**METTE ROSENKILDE**
Professor, Laboratory for Molecular Pharmacology, Department of Biomedical Sciences, Faculty of Health and Medical Sciences, University of Copenhagen

**ADAM WEINGLASS**
Director, Screening & Compound Profiling, MSD

08:00-08:50 | Room: Lindbergh & Aviators Lobby | Registration & Refreshments

08:50-09:00 | Room: Lindbergh 2&3 | **Global Engage Welcome Address and Morning Chair's Opening Remarks**

09:00-09:35

## KEYNOTE ADDRESS:
## EMMA PARMEE

Associate VP, Head of Chemistry Capabilities and Screening, Merck Sharp & Dohme

**Novel Strategies for Design Cycle Enhancement in Medicinal Chemistry**

This presentation will highlight several strategic elements adopted at Merck aimed at accelerating the molecular optimization "design cycle" used by medicinal chemists. The talk will describe our efforts to capitalize on advances in structure based drug design and our ability to integrate datasets and leverage predictive tools. Most importantly, recent breakthroughs in high throughput experimentation technology pioneered at Merck will be described. This latter topic is also part of our strategy to ensure a continued focus on the crucial role synthetic chemistry plays in enabling and inspiring design in Drug Discovery.

09:35-10:15

## KEYNOTE ADDRESS:
## NICHOLAS CARRUTHERS

Senior Director, Neuroscience, Janssen, Pharmaceutical Companies of Johnson and Johnson

**Targeting Protein-Protein Interactions of AMPA Channels**

Glutamate mediates the majority of fast synaptic transmission in the central nervous system (CNS) via activation of ionotropic α-amino-3-hydroxy-5-methyl-4-isoxazolepropionic acid (AMPA) receptors. Although AMPA receptors (AMPARs) are widely expressed throughout the CNS, their activity can be modulated by numerous auxiliary proteins including transmembrane regulatory proteins (TARPs), which are often localized in distinct brain regions. In particular, TARP-γ8 is expressed primarily in the hippocampus, a key component of the limbic system. By selectively inhibiting neurotransmission within this brain region, negative modulators of TARP-γ8 dependent AMPARs exhibit strong anticonvulsant effects in rodent seizure models without the motor impairment associated with nonselective AMPAR antagonists. The preclinical pharmacology for JNJ-55511118 an AMPA receptor negative modulator with exquisite selectivity for TARP-γ8 together with a second-generation series of 5-pyridyloxindoles will be presented.

10:15-10:45

## SOLUTION PROVIDER PRESENTATION:
## SENIOR REPRESENTATIVE

WuXi AppTec

10:45-11:55 | Room: Lindbergh & Aviators Lobby | Morning Refreshments / Poster Presentations / One-to-One Networking Meetings

## Room: Lindbergh 2&3

ENABLING TECHNOLOGIES - DEGRADED CHEMISTRY & DNA ENCODED LIBRARIES

11:55-12:25

### STEVAN DJURIC

Distinguished Research Fellow, Senior Director Discovery Chemistry and Technology, Abbvie

**Enabling Chemistry Technologies – Accelerators of Drug Discovery**

Drug Discovery has recently been described as a race by diMasi et al. As such, it is imperative to develop chemistry related technology that can reduce cycle time, cost of goods and improve PoS. To this end, we will describe our efforts in the chemistry technology area with a focus on integrated synthesis-purification-bioassay, photochemistry and high temperature chemistry platforms.

12:25-12:55

### SOLUTION PROVIDER PRESENTATION: SENIOR REPRESENTATIVE

Hitgen

12:55-13:25

### THOMAS FRANCH

CSO Nuevolution A/S

**DNA-encoded Library Technology: From Hits to clinical Candidate**

Identification of attractive hit matter is imperative as starting point for small molecule lead discovery efforts. The recent advancement of DNA-encoding technologies has enabled the encoding of fragments and combinatorial chemistry libraries at a massive scale comprising billions of compounds to aid the screening of drug targets supporting lead discovery. The principle of the DNA encoding technology will be illustrated including library designs and properties as well as screening data from multiple targets across epigenetic targets, proteases and "tough-to-drug" protein-protein interactions. Case stories on the BET bromodomains and the RORyt NHR will be presented showing the application of the technology and program data from initial hit finding through lead optimization to preclinical candidate identification.

## Room: Lindbergh 1

MEDICINAL CHEMISTRY STRATEGIES

11:55-12:25

### DAVID WILSON

Senior Director and Head, Global Oncology Chemistry, IMED Oncology, AstraZeneca

**Successful strategies to drug protein-protein interactions: Discovery of AZD5991, a potent and selective inhibitor of Mcl-1**

This presentation will highlight the challenges faced by medicinal chemists in successfully 'drugging' protein-protein interactions (PPIs) and will focus on how macrocyclization has been used successfully as a strategy in lead optimization. Mcl-1, a member of the Bcl/Mcl family, is a key protein involved in evasion of apoptosis in a wide variety of tumors. Its amplification and overexpression have also been implicated in innate and acquired resistance to anticancer drugs. AZD5991 is a rationally designed macrocycle with sub-nanomolar affinity for Mcl-1. It demonstrates all the hallmarks of a true Mcl-1 inhibitor and is active in vivo, with complete (100%) tumor regression demonstrated in several mouse xenograft models after a single tolerated dose.

12:25-12:55

### SOLUTION PROVIDER PRESENTATION: CRAIG JOHNSTONE

Executive Vice President, Head of Chemistry and Directeur General, Evotec (France) SAS

12:55-13:25

### LAURENT SCHIO

Head of France Medicinal Chemistry, Lead Optimization, Sanofi

**Drug Design: Beyond a Static Vision**

3D structures elucidation of target-ligand complexes has often provided valuable information in the way to design more potent inhibitors or agonists. However the comparison of apo vs natural substrate and ligand binding structures usually highlights protein segments shifts, so called induced fits and transient pockets formation which weaken the standard and rigid lock-key model. Over the last years several reports have pointed out the productive effect of considering the role of water molecules located in the binding site regarding ligand affinity improvement. Long run molecular dynamics simulations as well as free energy perturbation calculations are methodologies that are now accessible and could be applied to better predict new compound affinity or to rationalize observed structure activities relationships. Several case studies will be shown.

## Bleriot Suite

GPCR: ADDRESSING COMPLEX PHARMACOLOGY AND SIGNALLING

11:55-12:25

### JULIE SELKIRK

Associate Director, Biology, Celgene

**Ozanimod: A novel sphingosine 1 phosphate receptor modulator for the treatment of relapsing and remitting multiple sclerosis**

Ozanimod is a novel sphingosine 1 phosphate receptor (S1PR) modulator with demonstrated selectivity for S1PR1 and S1PR5. Ozanimod was specifically developed to treat relapsing and remitting multiple sclerosis by targeting multiple critical control points in the progression of the disease, acting both peripherally to reduce lymphocyte exit from the lymph nodes and centrally vial S1PR1/5 expressed on neural cells. Ozanimod was developed in an expedited manner and has demonstrated clinical efficacy in Phase III clinical trials in patients with relapsing and remitting multiple sclerosis. The presentation will highlight the project flow scheme, pharmacological characterization, and clinical data of this efficacious modulator.

12:25-12:55

**SOLUTION PROVIDER PRESENTATION**

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12:55-13:25

### JEFF REAGAN

Scientific Director, CardioMetabolic Disorders, Amgen

**Allosteric Modulation of the Calcium Sensing Receptor: A History of Calcimimetics**

Calcimimetics are positive allosteric modulators to the calcium sensing receptor (CaSR) which are used clinically to treat primary and secondary hyperparathyroidism. This presentation will discuss.

- Brief history of cinacalcet, a first generation calcimimetic
- Application of an operational model of allosteric modulation to aid in the design of second generation calcimimetics
- Evaluation of calcimimetics to treat patients suffering from hypercalcemia as a consequence of inactivating mutations in the CaSR.

13:25-14:20 | Room: Lindbergh & Aviators Lobby | Lunch / One-to-One Networking Meetings

14:20-14:50

## ANDREAS BRUNSCHWEIGER

Independent Group Leader, TU Dortmund

**Accessing genetically tagged heterocycle libraries via a chemoresistant DNA sequence**

DNA-encoded compound libraries (DELs) have found widespread use in drug research as screening technology. Tagging compounds with genetic information allows for handling them as complex mixtures. Bioactive compounds are efficiently identified from these mixtures by selection and DNA-sequencing. However, the chemical space of DELs is biased by the requirement to employ DNA-compatible synthesis methods in library synthesis. We observed that a hexathymidine DNA oligonucleotide "hexT" tolerated a surprisingly broad spectrum of catalysts, thus we use it as an adapter in the initial step of DEL synthesis. Testimony of the remarkable chemoresistance of the hexT sequence was the synthesis of hexT-pyrazole conjugates through a Au(I)-mediated three-component reaction in glacial acetic acid. The hexT-heterocycle conjugates were readily ligated to coding DNA sequences giving rise to encoded libraries.

14:50-15:20

**SOLUTION PROVIDER PRESENTATION**

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13:10-13:35

## ANDREAS LERCHNER

Senior Investigator, Project Team Leader, Novartis Institutes for Biomedical Research

**Is CLK a valid target for Phelan-McDermid syndrome?**

SHANK3 haploinsufficiency is causative for Phelan-McDermid syndrome (PMDS), a neurodevelopmental condition leading to Autism Spectrum Disorder. Recent results demonstrated that down-regulation of Akt/mTORC1 signaling resulted from enhanced phosphorylation and activation of PP2A regulatory subunit, B56β, due to increased steady-state levels of its kinase, Cdc2-like kinase 2 (CLK2) (Bidinosti et al. Science 2016). Based on this evidence, a 30k biochemical CLK2 HTS was performed, and a very potent and selective CLK inhibitor series was identified via SAR by archive. Efficacy of the most advanced CLK inhibitors was shown in a Shank3 kd mouse brain slice assay on synaptogenesis and assessment of the best tool compounds in a human primary lymphocytes MNT was performed to judge the suitability of CLK as a possible target for PMDS.

14:50-15:20

**SOLUTION PROVIDER PRESENTATION**

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13:10-13:35

## ANDREW ALT

Associate Director, Biology, Arvinas

**Positive Allosteric Modulators of Opioid Receptors: A Novel Approach for Future Pain Medications**

- Positive Allosteric Modulators (PAMs) of opioid receptors block pain by amplifying the activity of endogenous opioid agonists which are naturally released in pain states
- Opioid PAMs do not directly activate opioid receptors, and have no effect in tissues where agonists are not present
- Therefore, opioid PAMs may exhibit significantly improved side effect and abuse liability profiles compared to current opioid medications
- The current preclinical data supporting a rationale for developing opioid receptor PAMs as novel pain medications will be presented

14:50-15:20

**SOLUTION PROVIDER PRESENTATION**

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15:20-15:45

**FREDERIC BERST** (Reserved)
Senior Investigator, Program Team Leader, Head DNA Encoded Library Chemistry Team, Novartis Institutes for Biomedical Research
**DNA Encoded Libraries – Title TBC**

15:45-16:10

**XIAOPENG BAI**
Investigator, GSK
**DNA-encoded Library Technology (ELT) at GSK: Hit Identification and Beyond**
DNA-encoded Library Technologies (ELT) has evolved into important screening platforms in pharmaceutical industry. The recent advancement in the ELT platform at GSK will be discussed together with several case studies on how the technology has impacted the drug discovery programs. In addition, the application of ELT on parallel screening of large sets of proteins will also be presented to demonstrate its potential on the identification and prioritization of therapeutic targets.

15:20-16:10

**50 MINUTE EXECUTIVE PANEL DISCUSSION:**
**Future of Medicinal Chemistry**

**TAKASHI ICHIKAWA**
Senior Director, Head of Drug Discovery Chemistry Laboratories, CNS Drug Discovery Unit, Research, Takeda Pharmaceutical Company

**DAVID POWELL**
Director, Chemistry, Inception Sciences Canada

**DARREN MCKERRECHER**
Director Medicinal Chemistry, AstraZeneca

**Reserved:**
**Giles Brown**
Director of Medicinal Chemistry, Heptares

**Nick Carruthers**
Senior Director, Janssen, Pharmaceutical Companies of Johnson and Johnson

15:20-15:45

**ADAM WEINGLASS**
Director, Screening & Compound Profiling, MSD
**Structural basis for the cooperative allosteric activation of the free fatty acid receptor GPR40**
Agonists of GPR40 enhance glucose-dependent insulin secretion and represent a potential mechanism for the treatment of type-2 diabetes mellitus. Pharmacologic studies indicate that partial and full allosteric agonists (AgoPAM's) bind distinct sites on GPR40 eliciting differentiated pre-clinical efficacy. Here, we present the path to a ternary complex structure with partial and full allosteric agonists bound, and evidence supporting an identified novel, lipid-facing AgoPAM binding pocket.

15:45-16:10

**AYLIN HANYALOGLU**
Senior Lecturer, Institute of Reproductive and Developmental Biology, Department of Surgery and Cancer, Faculty of Medicine, Imperial College London
**Multi-dimensional programming of GPCR signalling via the endocytic pathway; functional and therapeutic applications**

- Recent studies have not only demonstrated that membrane trafficking of GPCRs is critical for temporal control of cell surface signalling, but that signalling can also be reactivated or continue to signal from highly distinct endocytic compartments.
- GPCRs are divergently organized within the endocytic system and our recent work demonstrates that compartmental bias in signalling occurs is tightly regulated by location
- across a complex inter-endosomal communication system.
- Examples of how spatially encoded GPCR signalling is critical for physiological function and potentially perturbed in disease

16:10-17:00 | Room: Lindbergh & Aviators Lobby | Afternoon Refreshments / Poster Presentations / One-to-One Networking Meetings

17:00-17:30

**IAN CHURCHER**
Head, Protein Degradation Discovery Performance Unit, GSK
**Protein degradation in drug discovery – where next?**
In this presentation I will introduce the concepts around using targeted protein degradation in drug discovery and briefly review some of the key published progress. The talk will go on to highlight opportunities where protein degradation approaches could give unique ways to identify new medicines and will also discuss outstanding challenges in the area

17:00-17:30

**NICK TERRETT**
Scientific Associate Vice President, European Chemistry Lead, Merck Sharp and Dohme
**Cell permeability with beyond 'Rule of 5' modalities – do we understand how this works?**

- The talk will describe the considerable growth in interest in beyond 'Rule of 5' drug molecules, but there are significant challenges in achieving cell penetration
- We are beginning to understand the factors that can influence cell permeability but the picture is still complex with multiple mechanisms in play
- The talk will describe the need to distinguish between classes of molecules that can enter cells by passive permeation vs. endocytosis

15:45-16:10

**JEAN-LUC GALZI** (Reserved)
Research Director, School of Biotechnology, CNRS, University of Strasbourg
**Biased Signalling – Title TBC**

17:30-18:00

## GEORGE BURSLEM

Research Fellow, Crews Lab, Yale University

**PROTACs: Inducing Protein Degradation as a Therapeutic Strategy**

For the last 15 years, the Crews lab has focused on developing Proteolysis Targeting Chimera (PROTAC), a technology that overcomes the limitations of the current inhibitor pharmacological paradigm. PROTACs offer a mechanism to irreversibly inhibit protein function by destruction of the target proteins. This approach employs heterobifunctional molecules to recruit target proteins to the cellular quality control machinery, thus leading to their degradation. We have demonstrated the ability to degrade a wide variety of targets. This talk will highlight some of our key findings in the field of protein degradation and demonstrate the advantages of degradation over inhibition.

17:30-18:00

## ALEXANDER ALANINE

Chief Operating Officer, Bactevo

**Next generation drug discovery: T.I.M.E. an integrated micro-droplet based platform'**

Bactevo has developed a tightly integrated set of game-changing proprietary technologies which radically disrupt current methods of creating new medicines. Our Totally Integrated Medicines Engine (T.I.M.E.) has been devised to address the needs of drug discovery and development scientists. Integrating the latest generation of microfluidics enabling ultra-fast phenotypic assaying, next-generation encoded synthetic libraries, natural products, in vitro profiling and in silico machine learning to create new therapeutics, TIME provides a paradigm shift in the speed, efficiency and quality of drug discovery. Bactevo is applying its TIME platform to create a portfolio of therapeutics for the treatment of diseases involving defects in mitochondrial function, with an internal focus on rare diseases.

17:30-18:00

## METTE ROSENKILDE

Professor, Laboratory for Molecular Pharmacology, Department of Biomedical Sciences, Faculty of Health and Medical Sciences, University of Copenhagen

**Development of GIP receptor antagonists to reveal the role of GIP in normal physiology and during diseases like obesity and T2D**

Family B has the conserved 7TM domain and is distinguished from other families by the large N-terminal extracellular domain (ECD) for which structural information is available. Recently, increased interest for the structure of the 7TM domain of family B GPCRs has resulted in novel crystal structures. Glucose-dependent insulinotropic polypeptide (GIP) is an incretin hormone secreted from enteroendocrine K-cells in the postprandial state in parallel with GLP1, secreted from L-cells. Both stimulate insulin secretion when blood glucose is high. Yet only GIP stimulates glucagon secretion during hypoglycemia and also inhibits bone resorption and stimulates fat deposition. I present the discovery of the first GIPR antagonist with efficacy in humans designed to reveal the role of GIP in pathophysiological conditions like obesity and T2D.

18:00-18:30


## ALESSIO CIULLI

Professor of Chemical & Structural Biology, Division of Biological Chemistry and Drug Discovery, School of Life Sciences, University of Dundee

**Targeted protein degradation with small molecules: How PROTACs work.**

Targeted protein degradation is a new modality of pharmacological intervention onto biological systems with therapeutic potential. One approach is to design bivalent degrader molecules (also called PROTACs) that comprise of a ligand for the target protein, and a ligand for an E3 ubiquitin ligase, joined by a linker. Formation of a ternary complex between the degrader, the ligase and the target triggers target polyubiquitylation and subsequent degradation by the proteasome. I will describe research that led to the structure-guided design of VH298, a potent and selective ligand for the E3 ligase VHL, a discovery that opened the door to the development of increasingly 'drug-like' molecules. Our first crystal structure of a PROTAC bound to its ligase and target protein has shone new light into how PROTACs work.

17:30-18:00

## HORST HEMMERLE (Reserved)

Executive Director, Lead Generation, Novartis

**Lead generation Strategies**

17:30-18:00

## ROCHDI BOUHELAL (Reserved)

Senior Investigator, Novartis

**Title TBC**

| | |
|---|---|
| 18:25 | Chair's Closing Remarks / End of Day One |
| 18:25-19:25 | Room: Lindbergh & Aviators Lobby — Networking Drinks Reception |

08:00-08:40 | Room: Lindbergh & Aviators Lobby | Refreshments / One-to-One Partnering Meetings

08:40-09:15

## KEYNOTE ADDRESS:
## FIONA MARSHALL

Founder, Director & CSO, Heptares Therapeutics

**Structure based drug design applied to allosteric modulators of GPCRs**

- Heptares Therapeutics have applied it's StaR® technology platform to generate over 150 GPCR ligand co-structures
- Many of these structures have revealed a diverse range of unexpected allosteric binding sites throughout the GPCR protein
- These novel allosteric binding sites may be exploited for the design of novel drugs targeting the GPCR superfamily

### Room: Lindbergh 2&3

**INTEGRATING MEDICINAL CHEMISTRY INTO THE DRUG DISCOVERY PROCESS**

09:15-09:45

## DARREN GREEN

Director Molecular Design, GSK

**Automation, Analytics and AI: what is and what should never be**

This presentation will describe how data-driven chemoinformatics methods may automate much of what has historically been done by a medicinal chemist. It will explore what is reasonable to expect "AI" approaches might achieve, and what is best left with a human expert.

09:45-10:15

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### Room: Lindbergh 1

**PARTNERSHIPS, COLLABORATIONS & OUTSOURCING**

09:15-09:45

## GARRY PAIRAUDEAU

Head of External Sciences, AstraZeneca

**Open Innovation at Astrazeneca - Title TBC**

09:45-10:15

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10:15-11:25 | Room: Lindbergh & Aviators Lobby | Morning Refreshments / Poster Presentation Sessions / One-to-One Partnering Meetings

11:25-11:55

## GISBERT SCHNEIDER

Professor, Computer-Assisted Drug Design at the Institute of Pharmaceutical Sciences in the Department of Chemistry and Applied Biosciences, ETH Zurich

**Automating drug discovery**

- Artificial intelligence methods for molecular design
- Target prediction and hit de-orphaning
- Robotic synthesis and testing

11:55-12:25

**SOLUTION PROVIDER PRESENTATION**

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Faizel Ismail at faizel@globalengage.co.uk

12:25-12:50

## MATTHIAS ZENTGRAF

Head of Computational Chemistry, Boehringer-Ingelheim

**eDesign – The next generation molecular design platform**

Excellence in molecular design is a key business capability of every research driven Pharma Company. Boehringer Ingelheim has recently implemented a molecular design platform to provide scientists live access to contextual experimental data and in-silico predictions during their molecular design sessions and idea prioritization discussions. It facilitates molecular designs of an even higher quality and a more stringent prioritization of compounds for synthesis.

12:50-13:15

## ALLEYN PLOWRIGHT

Head of Integrated Drug Discovery Germany, Sanofi

**Applications of New Synthetic Modalities in Drug Discovery**

- Opportunities and applications with New Modalities in Drug Discovery
- Natural peptidic frameworks for peptide therapeutics
- Mixed modalities for half-life extension and tissue targeting
- Optimization of physicochemical and biophysical properties

11:25-11:55

## MARK BOYS

Principal Research Investigator, Array BioPharma

**Partnering and outsourcing, experiences from a small company perspective**

Throughout its almost 20 years of existence Array BioPharma has a rich history of partnerships. Many IND's have been generated for partners, a significant number of these experimental drugs are still active in various stages of clinical development. Some of these partnerships will be discussed with reference to the deal structure, what worked well and what were important learnings or pitfalls. More recently Array has moved to a flexible business model with more impetus behind strategic outsourcing and contingency resources. Key learnings from these endeavours will be discussed.

11:55-12:25

**SOLUTION PROVIDER PRESENTATION**

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Faizel Ismail at faizel@globalengage.co.uk

12:25-13:15

## 50 MINUTE EXECUTIVE PANEL DISCUSSION:

**Best methods to identify, choose and manage your partner**

**GARRY PAIRAUDEAU**
Head of External Sciences, AstraZeneca


**CRAIG JOHNSTONE**
Executive Vice President, Head of Chemistry and Directeur General, Evotec (France) SAS

**Senior Representatives x2**

13:15-14:15 | Room: Lindbergh & Aviators Lobby | Lunch / One-to-One Partnering Meetings

14:15-14:45

## STEPHEN SHUTTLEWORTH

Chief Operating Officer & Chief Scientific Officer, Karus Therapeutics Ltd

**Small Molecule Immuno-oncology – Title TBC**

14:15-14:45

## TAKASHI ICHIKAWA

Senior Director, Head of Drug Discovery Chemistry Laboratories, CNS Drug Discovery Unit, Research, Takeda Pharmaceutical Company Limited

**Driving External Chemistry Optimization at Takeda - Management of Chemistry CRO**

The exploration of new business models to effectively utilize contract research organizations (CROs) would be common topic in the Pharma Industries. Especially in the synthetic chemistry arena, the Pharma industries can increasingly leverage external synthetic execution capabilities as long as the management effort to conduct daily research activities can be streamlined to maximize efficiency and output. Takeda has developed an interface with IT for this purpose, which we call Takeda Outsourcing Management Interface (TOMi). TOMi has the following IT functions without email; communication board, compound shipping tracking, individual and team productivity data, final report posting, and sharing document. I will show you detail about that. In addition, I would like to discuss how to manage CRO's productivity.

14:45-15:15

## JONATHAN MASON

Senior Research Fellow & Head of CADD, Heptares Therapeutics (UK)

**High End GPCR SBDD: The Revolution in GPCR Ligand Design from Multiple Co-Crystal X-Ray Structures**

- Unexpected binding modes of ligands for GPCR targets revealed from new X-ray structures
- Key role of water molecules in ligand binding and selectivity
- Implications of these new experimental findings for all ligand identification & design/optimisation

14:40-15:10

## DON KYLE (Reserved)

Vice President, Discovery Research and Non-Clinical Development, Purdue Pharma

**IP Analysis – Title TBC**

15:15-15:45

## BRADLEY MORGAN (Reserved)

Vice President, Cytokinetics

**Modulation of Muscle Contractility**

Overview of over 15 years of discovery efforts that have resulted in two compounds currently in phase 3 clinical trials, omecamtive mercarbil for heart failure and tirsemtiv for ALS

15:45-16:15

## EDUARD FELDER

Director, Head of Chemical Core Technologies, Oncology Research, Nerviano Medical Sciences

**The systematic use of highly profiled antitumor agents in probing the sensitivity contexts of cancer cells and assessing the validity of target combinations**

A diligently assembled panel of annotated chemical probes, broadly profiled antitumor agents, including active ingredients of oncology drugs, is used recurrently for the identification of targets and target combinations associated with specific cancer sensitivity contexts. This cell-based screening approach is part of our purinome platform developed in house, addressing structurally diverse ATP-binding targets such as kinases and ATPases. Cellular inhibitory activity is cross-referenced with biochemical data to identify candidate targets. Our results on six different Chordoma cell lines show Afatinib, an FDA approved EGFR inhibitor, being broadly active across all lines, unlike other biochemically equipotent EGFR inhibitors. Other applications range from the characterization of MELK as a novel survival marker in particular carcinomas to the documentation of the polypharmacology effects of clinically relevant kinase inhibitors.

15:15-16:15

## ONE HOUR ROUNDTABLE DISCUSSIONS:

**1) Targeted Protein Degradation**

**LAWRENCE HAMANN**

Vice President, Chemistry, Celgene

**2) Optimising hit to lead optimization**

**DARREN MCKERRECHER**

Director Medicinal Chemistry, AstraZeneca

**3) Optimising Outsourcing activities**

**4) DNA Encoded Libraries**

**5) Fragment Based Drug Discovery**

**6) GPCR – Biased Signalling**

16:15 | Conference Close

## MAKING A POSTER PRESENTATION

Poster presentation sessions will take place in breaks and alongside the other bkout sessions of the conference. Your presentation will be displayed in a dedicated area, with the other accepted posters from industry and academic presenters. We also issue a poster eBook to all attendees with your full abstract in and can share your poster as a PDF after the meeting if you desire (optional). Whether looking for funding, employment opportunities or simply wanting to share your work with a like-minded and focused group, these are an excellent way to join the heart of this congress.

In order to present a poster at the congress you need to be registered as a delegate. Please note that there is limited space available and poster space is assigned on a first come first served basis (subject to checks and successful registration). We charge an admin fee of £100 to industry delegates to present, that goes towards the shared cost of providing the poster presentation area and display boards, guides etc.  This fee is waived for those representing academic institutions and not for profit organisations.


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