4TH MEDICINAL CHEMISTRY & PROTEIN DEGRADATION SUMMIT

Co-located with the 3RD GLOBAL PHARMA R&D INFORMATICS & AI CONGRESS

— LONDON UK —
28-29 October 2019

#MedChemSummit

www.global-engage.com
Global Engage is pleased to announce the 4th Medicinal Chemistry & Protein Degradation Summit confirmed to be held on 28th-29th October 2019 in London, UK. It will once again be co-located with our 3rd Global Pharma R&D Informatics & AI Congress providing a forum to network, learn, and engage with senior representatives of leading pharmaceutical, biotech and universities worldwide.

This Summit will focus its attention to some of the leading issues in Medicinal Chemistry today. The conference has expanded its coverage on Protein Degradation and now has a day dedicated to the cutting edge research taking place in this exciting area. Presentations are already confirmed from The Crews Lab, University of Dundee, Dana Faber, Fimecs and Cullgen among others. The integration of AI and machine learning into the medicinal chemistry process is tackled in another track at the meeting with numerous case studies of how this developing technology is being utilized. This compliments the co-located informatics and AI meeting, which can be attended at any time, which examines artificial Intelligence in other parts of the drug discovery timeline. Finally the case studies track looks into how the druggable target landscape is being expanded through small molecule targeting of RNA, as well as talks on protein-protein interactions and small molecule Immuno-oncology.

Feedback has shown that delegates enjoy a diverse way of both learning and networking and during the comprehensive two-day conference. The summit will therefore contain:-

- 30+ expert-led presentations
- Interactive panel discussion
- Hour long roundtable discussions
- Poster presentations
- Exhibition room
- Ample networking time
- Drinks reception
- Networking dinner

We look forward to meeting you in October and hope you take advantage of the early bird, and 3 for 2 registration offers so that your team can participate and benefit.

EXPERT SPEAKERS INCLUDE:

ALEXANDER HILLISCH  
Director of Medicinal Chemistry, Bayer AG

MALIN LEMURELL  
Head of Medicinal Chemistry, Research and Early Development Cardiovascular, Renal and Metabolism, BioPharmaceuticals R&D, AstraZeneca

GEORGE BURSLEM  
Research Fellow, Crews Lab, University of Yale

YUSUKE TOMINARI  
CEO & CSO, FIMECS Ltd
Implementing Artificial Intelligence into Medicinal Chemistry
- Drug Discovery Chemistry – where are we heading
- Artificial Intelligence in Medicinal Chemistry
- Target (In)validation using Medicinal Chemistry tools
- Optimizing hit to lead optimization quality and timescale
- Panel – Artificial Intelligence: The Future of Medicinal Chemistry?

Medicinal Chemistry Case Studies
- Small-molecule targeting of RNAs
- Small-molecule immuno-oncology
- Protein-protein Interactions
- DNA encoded libraries
- ADCs – targeted delivery
- Macrocycles

Protein Degradation
- Targeted protein degradation/ PROTACs
- Challenges/limitations, and how to overcome them
- Case studies

Table 1: Optimising Outsourcing Activities
Table 2: Hit to Lead Optimization
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CONFIRMED SPEAKERS

MIKE GENIN
Vice President of Chemistry, Recursion Pharmaceuticals

ALEXANDER HILLISCH
VP, Head of Computational Molecular Design, Wuppertal, Bayer AG

VID STOJEVIC
Co-Founder and CTO, GTN

ROLF JAUTELAT
Director, Medicinal Chemistry, Bayer

JOHN GRIFFIN
CSO, Numerate

DARREN GREEN
Director of Molecular Design, GSK

MALIN LEMURELL
Head of Medicinal Chemistry, Research and Early Development Cardiovascular, Renal and Metabolism, BioPharmaceuticals R&D, AstraZeneca

MEIZHONG JIN
Senior Director Chemistry, Arrakis Therapeutics

GEORGE BURSLEM
Research Fellow, Crews Lab, University of Yale

SCOTT HUGHES
Senior Biologist, Alessio Ciulli Lab, University of Dundee

MICHAEL PLEWE
VP of Medicinal Chemistry, Cullgen

TINGHU ZHANG
Lead Scientist, Nathanael Gray Lab, Cancer Biology, Dana-Farber Cancer Institute

YUSUKE TOMINARI
CEO & CSO, FIMECS Ltd.

TAKESHI YURA
Vice President, Head of Medicinal Chemistry and Site Head, Jublant Biosys

OMAR AHMAD (Chair)
Senior Scientist II, Medicinal Chemistry Group, Blueprint Medicines

GREG MAKARA
ChemPass Ltd

WILLEM VAN HOORN
Chief Decision Scientist, Exscientia

YUGAL SHARMA
Sr. Director, CAS, A Division of the American Chemical Society

PAUL COLBON
CEO, Liverpool Chirochem Ltd

VICKY STEADMAN
GM & Business Line Leader, Integrated Drug Discovery, Eurofins Integrated Discovery UK Ltd, Eurofins Discovery

CHRIS YATES
Associate Director of Chemistry, Kymera Therapeutics

STEPHANOS IOANNIDIS
VP, Head of Chemistry, H3 Biomedicine

SAMANTHA HUGHES
Samantha Hughes, Associate Director, Medicinal Chemistry, R&D Oncology, AstraZeneca, UK

JONATHAN MASON
Senior Research Fellow CADD & Scientific Advisor, Sosei Heptares, UK

JOHN KARANICOLAS
Associate Professor, Molecular Therapeutics Group, Fox Chase Cancer Center USA

PETER ETTMAYER
Scientific Director, Cancer Research, Boehringer Ingelheim RCV GmbH & Co KG

ROBERT LAW
Investigator – Medicinal Chemistry, GSK

SHABNAM SHAABANI
Post-Doc. Faculty of Science and Engineering, University of Groningen

ALEXANDER DÖMLING
Professor and Chair, Department of Drug Design, University of Groningen

ANDREAS BRUNSCHWEIGER
Independent Group Leader, University of Dortmund, Germany

4TH MEDICINAL CHEMISTRY & PROTEIN DEGRADATION SUMMIT 2019
artificial intelligence (AI) and machine learning (ML) toward the development of robust predictive models of small molecule ADMET. Our efforts to couple traditional and high content data with algorithmic approaches will greatly accelerate lead optimization efforts. Access to computational methods tailored descriptors are essential to achieve predictive models. In addition, protein-structure based ADMET predictions will be presented. Certain combinations of tools and scenarios to predict drug-like properties and to guide hit-to-lead and lead optimization will be discussed. Application examples will be shown and an analysis of the tool's impact will be presented.

Two main reasons for the failure of many chemical series pre-clinically are undesirable ADME and toxicity properties. SAR toward the resolution of CYP inhibitory and/or hERG blocking properties often involve lengthy campaigns and at times, even after much effort, dead ends are encountered in a chemical series that prevent advancement to the clinic. Overall this problem adds significant time and costs to preclinical discovery efforts. Recursion has embarked on a journey to develop robust predictive models of small molecule ADMET. Our efforts to couple traditional and high content data with artificial intelligence (AI) and machine learning (ML) toward the development of such models will be discussed.
RI Revitalises Drug Discovery & Drives AI: GPCR Structures Reveal the Critical Importance of Water Molecules in Binding, Selectivity, and Kinetics

Full structure-based drug design is now possible for GPCRs including

- Full structure-based drug design is now possible for GPCRs including binding affinity prediction.
- Critical role of waters and lipophilic hotspots for binding, selectivity & kinetics delineated.
- Real Intelligence drives Artificial Intelligence / Machine Learning algorithms? Often times, these challenges are driven by low signal-to-noise ratios – where under sampling and unbalanced ratios result in poor predictions. The solution? Better quality data, yet quality data is both time-consuming and difficult to find. Join us to learn how we improved prediction accuracy of ligand biological activity by over 31% percent just by improving the quality of the data.

- Computational prediction of relative ligand binding affinity is now finally possible using Free-Energy Perturbation (FEP) methods, but for GPCRs not using default settings and with water sampling during the simulation critical.

The lessons learnt from the multiple ligand GPCR structures have implications for all targets and commonly used design approaches such as those using pharmacophores, and provide real intelligence to drive artificial intelligence / machine learning methods.

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**Panel Discussion:**

*Artificial Intelligence: The Future of Medicinal Chemistry?*

- **Integration**
  - **Overcoming barriers**

**Track Chair:** Rolf Jautelat, Director, Medicinal Chemistry, Bayer

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**Evolution of Contract Research Organisations to Contract Innovation Organisations?**

Historically, CROs were employed by their customer to carry out certain pre-designated tasks. However, CROs evolved to provide solutions to customer’s challenges and now are evolving further to provide innovation in the form of project ideas. Collaborative partnerships on integrated drug discovery projects are now common in the drug discovery landscape. Eurofins Discovery will present DiscoveryOneTM, their integrated drug discovery platform, and a successful case history which led to pre-clinical candidates for a pharma partner on a challenging target.

**Track Chair:** Frank Böckler, University Professor, Eberhard Karls University Tübingen

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**Vector Efficiency: A Quantitative Assessment of the Molecular Shape and Functionality of Fragment-Based Chemical Libraries**

This presentation introduces the development of a new parameter, Vector Efficiency (VE), that guides considerations of vector space within the fragment library design process. This quantitative parameter measures the vector space coverage of the key functionalities (e.g. HBD’s, HBA’s, lipophilic groups) within a fragment library. Optimally designed libraries achieve the broadest coverage of vector space from the smallest number of compounds.

**Track Chair:** Paul Colbon, CEO, Liverpool Chirochem Ltd

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**ARTIFICIAL INTELLIGENCE: THE FUTURE OF MEDICINAL CHEMISTRY?**

**PANEL DISCUSSION:**

*AI-assisted lead optimization with SynSpace*

High failure rates, increasing cost of drug discovery, and extended research and development timelines hinder the development of medicines. Due to these challenges there has been an increasing need for substantial innovations in the pharmaceutical sector. ChemPass has developed a purpose-made, rule-based AI technology that can produce novel, synthetically-enabled lead analogues and scaffold hopping designs around lead structures leading to real reduction of the lead optimization timeline. Thus, SynSpace is a valuable addition to the medicinal chemistry toolbox. In addition, we have also been developing an automated AI-assisted lead optimization platform – utilizing the design capability of SynSpace – that can automatically carry out scaffold hopping and lead analogue idea generation, on-target and off-target binding predictions and MPO scoring.

**Track Chair:** Mike Burden, Director, Conference Production, Global Engage

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**Targeting the Spliceosome: Phenotypic hit to the discovery of H3B-8800, a novel, orally bioavailable, splice modulator**

Genomic analyses of cancer have identified recurrent point mutations in the RNA splicing factors SF3B1, U2AF1, and SRSF2 that confer an alteration of function. Although cells bearing these mutations are preferentially dependent on wild-type (WT) spliceosome function, the use of an SF3b modulator can act as protein-RNA disrupter, causing preferential lethality in these spliceosome mutant cells and providing a way to therapeutically target these cancers. Here we describe the discovery of the clinical splice–modulator H3B-8800, starting from phenotypic screening and optimized for preferential lethality in spliceosome mutant cells and some recent MOA advances in spliceosome structural biology for further investigation of the approach.

**Track Chair:** Yugal Sharma, Sr. Director, CAS, A Division of the American Chemical Society

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**The Critical Role of Data**

Are you struggling with less than ideal prediction results for your AI and machine learning algorithms? Often times, these challenges are driven by low signal-to-noise ratios – where under sampling and unbalanced ratios result in poor predictions. The solution? Better quality data, yet quality data is both time-consuming and difficult to find. Join us to learn how we improved prediction accuracy of ligand biological activity by over 31% percent just by improving the quality of the data.

Discover why human curated data is so valuable, the complexity required for proper data modeling, and the unique insights only highly connected human curated data can provide.

**Track Chair:** Paul Colbon, CEO, Liverpool Chirochem Ltd

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**Artificial Intelligence: The Future of Medicinal Chemistry?**

**Panel Chair:** Rolf Jautelat, Director, Medicinal Chemistry, Bayer

I will discuss three discovery stories for the discovery of small molecule protein/protein interaction antagonists from my lab:
SUMMIT on a nanomole scale in an automated and miniaturized fashion and fast quality control to screen efficiency of synthetic reactions waste and can deliver products in shorter time frames. Here, we chemistry in the 21st century as it helps to reduce resources and chemistry, nL dispensing, acoustic-MS, uHTS and artificial preclinical drug discovery and development by blending instant and hit-to-lead campaigns using mostly traditional technologies. Here, we introduce a fundamentally novel approach towards problems can be attributed to the preclinical drug discovery and development costs of drugs are skyrocketing while the introduction revenues per year. Each day not on the market corresponds to a loss of $2.7 million. Multiple benchmark reports suggest of novel drugs is decreasing or at best stagnating. Part of the breakthroughs and are ideal antibody drug conjugate (ADC) payloads. agents that are capable of promoting double-strand DNA breaks and are ideal antibody drug conjugate (ADC) payloads. Harnessing the reactivity of these natural products has been critical for the design and development of calicheamicin-based ADCs. The structural complexity poses a significant challenge to understanding the chemistry of these molecules. For the development of next generation calicheamicin ADCs, our work has focused on refining the linker chemistry and the method and site of conjugation, as well as understanding the reactivity and SAR of the payload itself, with the goals of improving efflux, efficacy and more importantly, selectivity. These modifications led to a more efficacious and safer conjugate that overcame hepatotoxicity observed with first and second generation calicheamicin ADCs.

- p53/mdm2: A computational pharmacophore method (ANCHOR.QUERY) was developed and has led to the discovery of multiple novel scaffolds.
- PD1/PDL1: Structural biology methods helped to understand this b-sheet mediated very flat PPI.
- IL17a/IL17r: Artificial intelligence methods were instrumental to discovery high affinity IL17a antagonists.

ANDREAS BRUNSCHEIGER
Independent Group Leader, University of Dortmund, Germany
DNA Encoded Library case study
Initiating encoded library synthesis with a solid support-based strategy DNA-encoded compound libraries are firmly embedded in the arsenal of small molecule screening technologies. They are commonly synthesized by solution phase combinatorial chemistry giving rise to large screening compound collections. This approach uses a limited scope of chemistry for compound synthesis due to the need to perform reactions in aqueous solvents and to consider DNA reactivity. I will discuss an alternative barcoding strategy based on initiating encoded library synthesis with solid phase-coupled nucleobase-protected DNA barcodes. This approach allowed for DNA-tagged small molecule synthesis in freely selectable organic solvents, and nucleobase-protection provided greater stability of the barcode against chemical degradation. Thus, several heterocycle-forming reactions could be translated to the DNA-encoded format.

**ROUNDTABLE DISCUSSIONS:**

**Table 1: Integrating AI Into Med Chem**

<table>
<thead>
<tr>
<th>Moderator</th>
<th>Expertise</th>
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<tbody>
<tr>
<td>SAMANTHA HUGHES</td>
<td>Associate Director, Medicinal Chemistry, R&amp;D Oncology, AstraZeneca, UK</td>
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<td>JOHN GRIFFIN</td>
<td>CSO, Numerate</td>
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<td>Senior Scientist II, Medicinal Chemistry Group, Blueprint Medicines</td>
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<td>JOHN KARANICOLAS</td>
<td>Associate Professor, Molecular Therapeutics Group, Fox Chase Cancer Center USA</td>
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**Table 2: Fuel and fulcrum for AI-driven drug discovery**

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SHABNAM SHAABANI
Post-Doc. Faculty of Science and Engineering, University of Groningen
Miniaturized, automated and accelerated chemistry
A blockbuster drug generates > $1 billion revenues per year. Each day not on the market corresponds to a loss of > $2.7 million. Multiple benchmark reports suggest development costs of drugs are skyrocketing while the introduction of novel drugs is decreasing or at best stagnating. Part of the problems can be attributed to the preclinical drug discovery and development involving expensive high throughput screening (HTS) and hit-to-lead campaigns using mostly traditional technologies. Here, we introduce a fundamentally novel approach towards preclinical drug discovery and development by blending instant chemistry, nL dispensing, acoustic-MS, uHTS and artificial intelligence. Automated, miniaturized and accelerated synthesis for efficient property optimization is a formidable challenge for chemistry in the 21st century as it helps to reduce resources and waste and can deliver products in shorter time frames. Here, we used for the first-time acoustic droplet ejection (ADE) technology and fast quality control to screen efficacy of synthetic reactions on a nanomole scale in an automated and miniaturized fashion
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<th>Time</th>
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<tbody>
<tr>
<td>18:20</td>
<td>Chair’s Closing Remarks / End of Day One</td>
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<td>18:20-19:20</td>
<td>Networking Drinks Reception</td>
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<td>19:20</td>
<td>Room: Lindbergh 3 Gala Dinner</td>
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**VID STOJEVIC**
Co-Founder and CTO, GTN

*Drug Discovery Disrupted - Quantum Physics Meets Machine Learning*

- How AI, in particular machine learning, is impacting drug discovery
- Driving efficiency in Hit to Lead
- Using Deep Learning to open up new areas of chemical space.

**Approaches to discovery?**
- Would open-source/pre-competitive data sets be helpful to the field? Which ones?
<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Speaker</th>
<th>Topic</th>
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<tr>
<td>08:30</td>
<td>Refreshments</td>
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<tr>
<td>09:00</td>
<td>Keynote Address</td>
<td>Chris Yates</td>
<td>Targeted Protein Degradation to explore novel biology</td>
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<td></td>
<td>• Overview of Kymera’s target protein degradation platform and approaches</td>
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<td>• Novel therapeutic hypotheses resulting from degradation of proteins of interest</td>
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<td>• How do we turn degraders into drugs</td>
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<tr>
<td>09:40</td>
<td>Protein Degradation</td>
<td>Yusuke Tominari</td>
<td>Drug Discovery on IRAK-M degrader for cancer-immunotherapy</td>
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<td>• Targeted IRAK-M degradation as a novel and efficacious cancer-immunotherapy</td>
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<td>• Effective degrader drug discovery platform RaPPIDS (TM).</td>
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<td></td>
<td>• Don’t you need to optimize not the linkers but also the E3 ligase binders depends on target of interest?</td>
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<tr>
<td>10:40</td>
<td>Morning Refreshments / One-to-One Meetings</td>
<td>George Burslem</td>
<td>PROTACs: Inducing Protein Degradation as a Therapeutic Strategy</td>
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<td>For the past two decades, the Crews lab has focused on developing Protolysis 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, particularly for hematologic malignancies.</td>
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<tr>
<td>12:20</td>
<td>Lunch</td>
<td>Michael Plewe</td>
<td>Ubiquitin mediated small molecule induced target elimination (uSMITE) for cancer</td>
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<td>Targeted protein degradation using bifunctional molecules to remove specific proteins by hijacking the ubiquitin proteasome system has emerged as a novel drug discovery approach. Several challenges remain in designing optimal degraders that also show efficacy in vivo. We will present case studies from our ongoing efforts in the design and biological evaluation of novel degraders for selected oncology targets that display in vivo activity in mouse models.</td>
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<tr>
<td>09:00</td>
<td>Panel Discussion:</td>
<td>Peter Ettmayer</td>
<td>Overcoming Challenges in Protein Degradation</td>
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<td>(Chair) Boehringer Ingelheim</td>
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<td>• Selectively targeting CDK has been a challenge with a small molecule inhibitor</td>
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<td>• Bifunctional PROTAC is a viable strategy for selective degradation of CDKs</td>
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<tr>
<td>13:30</td>
<td>Lunch</td>
<td>Tingshu Zhang</td>
<td>A selective degradation of CDK protein with PROTAC molecules</td>
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SCOTT HUGHES
Senior Biologist, Alessio Ciulli Lab, University of Dundee
Structural and Biophysical Characterization of PROTAC Ternary Complexes
- PROTACs and molecular glues represent a fascinating new therapeutic modality, capable of targeting any binding site and driven by ternary complex formation.
- Recent developments in techniques (SPR, FP) designed to interrogate the thermodynamic and kinetic properties of ternary systems have enhanced our understanding of the interplay between degradation and biophysical properties
  - The elucidation of ternary complex structures have revealed extensive inter- and intramolecular interactions formed by the bound ligand, the analysis of which has enabled the design of PROTACs with optimized properties and degradation profiles

PETER ETTMAYER
Scientific Director, Cancer Research, Boehringer Ingelheim RCV GmbH & Co KG
Structure guided and co-operativity driven optimization towards potent SMARCA PROTACs
- Current PROTAC design is driven by screening exit vectors and linkers until a suitable degrader is identified. Based on our recently published SMARCA PROTACs an alternative rational PROTAC optimization utilizing high-resolution ternary complex crystal structures and cooperativity considerations will be presented. The case study will exemplify a successful structure driven campaign to degrade targets previously considered undruggable and pave the way towards new therapeutics for the treatment of genetically-defined tumors.

ROBERT LAW
Investigator – Medicinal Chemistry, GSK
Discovery and Optimisation of PROTACs Targeting Focal Adhesion Kinase (FAK)
Focal adhesion kinase (FAK/PTK2) is a non-receptor kinase that integrates growth factor and cell adhesion signalling through its kinase domain and non-kinase scaffolding functions. FAK acts as a mechanosensor, linking the extracellular matrix to DNA, and is crucial for cell migration and invasion. Increased expression of FAK in solid tumours correlates with poor prognosis, however FAK kinase inhibitors have shown limited clinical efficacy in oncology. We sought to investigate the targeted degradation of FAK using a Proteolysis Targeting Chimera (PROTAC) strategy, and optimised a lead series to obtain potent and selective molecules capable of in vivo degradation of FAK. Representative FAK-PROTAC-E3 ligase ternary complex structures have been further characterized by X-Ray crystallography, and the corresponding PROTACs show differentiated biology compared to FAK inhibitors.

MAKING A POSTER PRESENTATION
Poster presentation sessions will take place in breaks and alongside the other breakout 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.

VENUE INFORMATION
London Heathrow Marriott Hotel
Bath Road, Heathrow Airport Hayes, UB3 5AN, United Kingdom
Located less than half a mile away from the Heathrow Airport, this four-star deluxe hotel offers comfortable, noise-free accommodations and is near attractions such as Legoland and Windsor Castle. Modern and vibrant, discover the culinary delights and more in the London Heathrow Marriott.
DON’T DELAY, BOOK YOUR PLACE TODAY!
Places are limited and are based on a first come, first served basis so to avoid disappointment contact us today to reserve your place at Global Engage’s 4th Medicinal Chemistry & Protein Degradation Summit on the 28th-29th October 2019.

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maria@globalengage.co.uk
Our conference team will make all the necessary arrangements.

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Visit the website to book your place

THE CONGRESS PACKAGE INCLUDES:
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Networking Drinks Reception
Conference Workbook
E-Document Pack

HOTEL ACCOMMODATION
Hotel accommodation will be available at a group rate.

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For updates on the 4th Medicinal Chemistry & Protein Degradation Summit, plus free resources and reports, as and when our speakers authorise their release dates, check for updates at:
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