

## Key Discovery Strategies

- Strategies for target selection and phenotypic drug discovery
- Drug repositions and repurposing
- New target classes and modalities
- Accelerated target based discovery using genomic technologies

## Screening & Assays: Enabling Technologies

- Developing a successful phenotypic screening strategy
- Developing a physiologically relevant cell assay system
- Efficient target identification after a phenotypic screen
- Capitalizing on patient genetic information
- Phenotypic screening strategies using primary cells and in cell binding experiments

## Discovery Chemistry & Drug Design

- Drug discovery toxicology case studies
- New computational tools for drug design
- Epigenetic drug discovery
- How to build increasing molecular complexity into drug design
- Fragment based drug discovery

## Supporting Innovation with Informatics Tools

- Bioinformatics challenges in clinical genomics
- Using Big Data to identify potential new therapies
- Translational & biomarker strategies for chronic viral infections
- Data-mining and analysis of databases

## Meet Senior Decision Makers

Over 150 VPs, Directors & Global Heads from leading pharmaceutical organisations, biotech companies and academic institutions will

Drug discovery  
Medicinal chemistry  
Discovery chemistry

Screening technologies  
Drug design  
Fragment based discovery

Structure based discovery  
Target identification  
Target validation

Discovery informatics  
Assay development  
Lead optimisation

## Discover New Solutions

Formal and informal meeting opportunities offer delegates the chance to discuss key solutions with leading service providers. Services to be discussed include:

Lead generation  
Candidate analysis  
Target based screening

Phenotypic screening  
Library optimisation  
Stem cell technology

Biologics discovery  
Predictive technologies  
Informatics

Data analysis  
Knowledge management  
Compound profiling

## Benefits to Attending

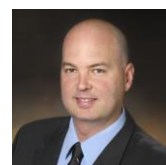
- ✓ **Hear from and meet with the key innovators in drug discovery and medicinal chemistry.** Attendees last year included VP's and Directors from: Pfizer, Janssen, Merck, Shire, Sanofi, Takeda, Genentech, UCB, AstraZeneca, Roche, Bristol-Myers Squibb, Ra Pharma and more
- ✓ **Discover collaborative solutions to drug discovery challenges.** Our Congress brings together drug discovery and medicinal chemistry experts to discuss new approaches to open innovation, successful phenotypic screening strategies, finding physiologically relevant cell assays, epigenetic drug discovery and high content analysis
- ✓ **Discuss the latest innovations in discovery technology,** including computer aided drug design, compound libraries, 3D screening tools, flow cytometry, novel bioinformatics tools, and tools for data modelling, simulations and improved data visualisation
- ✓ **Unparalleled networking opportunities.** The two-day congress format combines dedicated networking breaks, pre-organised 1-2-1 meetings and our popular drinks reception.
- ✓ **A high quality programme devised with the help of our esteemed advisory board.** Presentations will cover areas including drug design, discovery informatics and discovery data, computational chemistry, open innovation and external research strategies
- ✓ **Co-located with our Biomarkers USA Congress**

Register to attend our complimentary pre-congress webinar "Advances in Drug Discovery- Fragmented-based Drug Discovery", 1st September 2016, 4pm GMT, email [marketing@oxfordglobal.co.uk](mailto:marketing@oxfordglobal.co.uk)

## 2016 Speakers Include...



**Lisa Mendoza**  
Bayer



**Christopher Winrow**  
Merck

For booking details & registration fees please refer to the last page or visit:

[www.discoveryusa-congress.com/marketing](http://www.discoveryusa-congress.com/marketing)


## Speakers 2016:

- Vincent Stoll, Associate Director, Structural Biology, AbbVie
- Jennifer Riggs-Sauthier, Vice-President, Chemistry, Nektar Therapeutics
- Hicham Alaoui, Director, Biochemical & Cellular Pharmacology, Genentech
- Thomas Höberg, Senior Scientific Advisor, LEO Pharma
- James Brown, Director & Senior Research Fellow, Computational Biology, GlaxoSmithKline
- Lidio Meireles, Research Scientist II, Vertex Pharmaceuticals
- Arijit Chakravarty, Director, Modeling & Simulation (DMPK), Takeda Pharmaceutical
- Paul Greenspan, Senior Director of Discovery Chemistry, Takeda
- Radu Dobrin, Associate Director, J&J
- Michael Letavic, Scientific Director and Fellow, Janssen
- Christopher Winrow, Director, Neurology & Insomnia, Merck Research Laboratories
- Michael Jackson, Center Director Senior Vice President, Drug Discovery and Development Adjunct Associate Professor, Sanford Burnham Prebys Medical Discovery Institute
- Chris Gibson, Chief Executive Officer, Recursion Pharmaceuticals
- Asim Siddiqui, CTO, NuMedii
- Mark Currie, Senior Vice President, Chief Scientific Officer & President of R&D, Ironwood Pharmaceuticals
- Thazha P. Prakash, Director, Medicinal Chemistry, Ionis Pharmaceuticals, Inc
- Scott Davis, Manager, Screening & Assay Development, Regulus Therapeutics
- Huijun Wang, Associate Principle Scientist, Merck
- Derek Ostertag, Director R&D Diagnostics, Tocagen Inc.
- Svetlana Belyanskaya, Manager, GlaxoSmithKline
- Dean Brown, Director of External Chemistry, AstraZeneca Pharmaceuticals
- C. B. Gurumurthy, Assistant Professor, Developmental Neuroscience, Director, Mouse Genome Engineering Core Facility, University of Nebraska Medical Center
- Daniel McMasters, Director, Modeling & Informatics, Vertex Pharmaceuticals
- Brian Gerstenberger, Principal Scientist, Medicinal Chemistry, Pfizer
- Adeela Kamal, Senior Director, Therapeutic Area Head for Urology and Translational Research Ferring Research Institute Inc
- Gerard Rosse, Associate Director, Structure Guided Chemistry, Dart Neuroscience LLC
- Adam Pavlicek, Senior Director, Discovery Technologies and Orphan Diseases, Regulus Therapeutics Inc
- Huifen Chen, Senior Scientist, Discovery Chemistry, Genentech
- Scott Davis, Manager, Screening & Assay Development, Regulus Therapeutics
- Jim Brown, Director & Senior Research Fellow, Computational Biology, GlaxoSmithKline
- Philippe Diaz, CSO, DermaXon, Associate Professor, Department of Biomedical Sciences, University of Montana


## 2016 Sponsors Include:



**3<sup>rd</sup> Annual Drug Discovery USA Congress**  
**Day 1 – 3<sup>rd</sup> October 2016**

07.30 – 08.20	<b>Registration: Cortez Prefunction</b>	
	<b>Conference Room: North Park 1</b>	
08.20 – 08.25	<b>Oxford Global's Welcome Address</b>	
08.25 – 08.30	<b>Chairperson's Opening Address: Vincent Stoll, Research Fellow, Associate Director of Structural Biology, AbbVie</b>	
08.30 – 09.00	<b>Keynote Address:</b> <b>Structure-Based Drug Design Of Bcl-2 Selective, ABT-199</b> This talk will go through the history and learnings from the development of fragment-based drug discovery to the structure-based design of Bcl-2 selective ABT-199. ABT-199 has recently been FDA approved and is on the market known as Venclexta.  <b>Vincent Stoll, Research Fellow, Associate Director of Structural Biology, AbbVie</b>	
09.00 – 09.30	<b>Can Physiological Relevance Enhance Target Validation and Lead Optimization? A Tale Of Two Kinases</b> <ul style="list-style-type: none"> <li>• In vitro physiologically relevant systems such as primary human cells, 3D tissues, and iPSC-derived cells are increasingly being used throughout the drug discovery process</li> <li>• Recent scientific advancements and emerging technologies make these systems more accessible and are thus being applied earlier and earlier in lead discovery and optimization</li> <li>• Given the potential species differences in biologies between rodent and humans, these systems are now being deployed also for target discovery and validation</li> <li>• Two case studies will be discussed where primary human immune cells have been used</li> <li>• In the first example, the role the T cell kinase ITK plays in Th2 cytokine regulation was investigated in primary human Th2 cells</li> <li>• The second case study will discuss how a NIK small molecule lead optimization program was accelerated using a combination of primary human B cells and primary human hepatocytes to assess whole blood potency and in vitro clearance, respectively, with the goal to estimate human dose projections early in the discovery cascade</li> </ul> <b>Hicham Alaoui, Director, Biochemical &amp; Cellular Pharmacology, Genentech</b>	
09.30 – 10.00	<b>Drug Discovery At Selvita – Case Studies</b>  <b>Milosz Gruca, Director of Biology and Member of the Management Board, Selvita S.A.</b>  	
10.00 – 11.20	<b>Exhibition Room: Cortez Ballroom</b> <b>Coffee &amp; Refreshments, One to One Meetings x4, Poster Presentation Sessions</b>	
	<b>Conference Room: North Park 1</b>	<b>Conference Room: Hillcrest 1</b>
	<b>Key Discovery Strategies, Target Based Discovery, Translation And Phenotypic Screening</b>	<b>Screening And Assays: Enabling Technologies</b>
	<b>Stream Chair: Vincent Stoll, Research Fellow, Associate Director of Structural Biology, AbbVie</b>	<b>Stream Chair: Scott Davis, Manager, Screening &amp; Assay Development, Regulus Therapeutics</b>
11.20 – 11.50	<b>Modern Approaches To Maximize Efficiency In Drug Discovery</b> <ul style="list-style-type: none"> <li>• Innovative technologies to make better compounds and make them faster</li> <li>• Value of an industrial approach to produce small molecules</li> <li>• Changing the landscape of Super Critical Fluid Chromatography within modern medicinal chemistry</li> </ul> <b>Gerard Rosse, Associate Director, Structure Guided Chemistry, Dart NeuroScience LLC</b>	<b>Optimization Of An In Vitro Screening Cascade For Prioritization Of Anti-miR Compounds</b> <ul style="list-style-type: none"> <li>• Overview of Regulus Therapeutics, microRNAs, and anti-miR technology</li> <li>• Creation of screening cascade efficient and robust in enriching for safe, active, and stable anti-miR compounds</li> </ul> <b>Scott Davis, Manager, Screening &amp; Assay Development, Regulus Therapeutics</b>
11.50 – 12.20	<b>Chemical And Biological Studies Of Ingenol Esters For Treatment Of Non-Melanoma Skin Cancers</b> <ul style="list-style-type: none"> <li>• Multifactorial SAR studies supported by molecular modelling</li> <li>• Reducing acyl migration to improve chemical stability</li> <li>• PKC-mediated cell growth arrest and induction of pro-inflammatory responses</li> <li>• Acute induction of cell death (necrosis)</li> <li>• Anti-tumor effects in mouse models</li> </ul> <b>Thomas Högberg, Senior Scientific Adviser, LEO Pharma</b>	<b>DNA Encoded Library: A Platform For Lead Discovery</b> <ul style="list-style-type: none"> <li>• Overview of DNA Encoded Library technology at GSK</li> <li>• Recent platform advances</li> <li>• Platform application for the identification of potent and specific inhibitors to the Therapeutic Targets from different target classes</li> </ul> <b>Svetlana Belyanskaya, Senior Scientific Investigator, GlaxoSmithKline</b>

**3<sup>rd</sup> Annual Drug Discovery USA Congress  
Day 1 – 3<sup>rd</sup> October 2016**

	<b>Conference Room: North Park 1</b>	<b>Conference Room: Hillcrest 1</b>
	<b>Key Discovery Strategies, Target Based Discovery, Translation and Phenotypic Screening</b>	<b>Screening and Assays: Enabling Technologies</b>
<b>12.20 – 12.50</b>	<p><b>CRISPR/Cas System: Basics, Advances And Paradigm-shifts In Animal Genome Editing Approaches</b></p> <ul style="list-style-type: none"> <li>• Introduction to the long-used traditional animal transgenic technologies, using mouse as a model organism.</li> <li>• Newer technical breakthroughs in transgenic technologies that have been possible because of the CRISPR/Cas9 system</li> <li>• The CRISPR strategies for developing designer animal models for basic, translational and pharmaceutical research</li> </ul> <p><b>C. B. Gurumurthy, Assistant Professor, Developmental Neuroscience, Director, Mouse Genome Engineering Core Facility, University of Nebraska Medical Center</b></p>	<p><b>Using Predictive Models To Prioritize Experimental Screening</b></p> <ul style="list-style-type: none"> <li>• Quantitative Structure–Activity Relationship (QSAR) models can provide the probability a given molecule will have a particular undesired off-target activity</li> <li>• These predictions can be used to prioritize experimental derisking of predicted liabilities</li> <li>• Applying this “fail fast; fail cheap” approach to molecules in lead optimization saves significant experimental resources</li> </ul> <p><b>Daniel McMasters, Director, Modeling &amp; Informatics, Vertex Pharmaceuticals</b></p>
<b>12.50 – 13.50</b>	<b>Exhibition Room: Cortez Ballroom Lunch, One to One Meetings x2</b>	
<b>13.50 – 14.20</b>	<p><b>Massive Parallelization Of Rare Disease Drug Discovery</b></p> <ul style="list-style-type: none"> <li>• The complex molecular biology of many rare diseases is poorly understood, making traditional target-based drug discovery approaches difficult</li> <li>• Target agnostic approaches, which circumvent the lack of molecular understanding, may be a useful alternative strategy</li> <li>• A number of target-agnostic approaches will be discussed, along with a detailed discussion of work being done at Recursion Pharmaceuticals to use complex and subtle phenotypic signatures at the level of individual cells as the basis for broad drug discovery approaches</li> </ul> <p><b>Chris Gibson, Chief Executive Officer, Recursion Pharmaceuticals</b></p>	<p><b>Screening Technologies: Modelling</b></p> <p><b>Arijit Chakravarty, Director, Modeling &amp; Simulation (DMPK), Takeda Pharmaceutical</b></p>
<b>14.20 – 14.50</b>	<p><b>Phenotypic Screening Of Patient Derived Cells: Balancing Throughput With Relevance</b></p> <ul style="list-style-type: none"> <li>• Screening higher order functions of iPSC-derived cellular cultures</li> </ul> <p><b>Michael Jackson, Senior Vice President, Drug Discovery &amp; Development, Sanford Burnham Prebys Medical Discovery Institute</b></p>	<p><b>Tumor Heterogeneity, Retroviral Replicating Vectors, And Biomarkers: Predicting Response In Recurrent High Grade Glioma Clinical Trials</b></p> <p><b>Derek Ostertag, Director R&amp;D Diagnostics, Tocagen Inc.</b></p>
	<b>Conference Room: North Park 1</b>	
<b>14.50 – 15.20</b>	<p><b>Presenting Advanced Software Solutions And Strategies For The Biophysical Analysis of Ligand-Receptor Interactions With Isothermal Titration Calorimetry</b></p> <ul style="list-style-type: none"> <li>• AFFINImeter: filling the gaps existing in other existing software packages</li> <li>• Exploiting the full potential of Isothermal Titration Calorimetry with AFFINImeter: presenting the tools KinTC, for the kinetic characterization of interactions, and the model builder, for the thermodynamic analysis of complex binding</li> <li>• AFFINImeter in Drug discovery &amp; Development</li> </ul> <p><b>Juan Sabin, Co-Founder and Sales Director, AFFINImeter</b></p> <div align="center">  <p><b>AFFINIMETER</b></p> </div>	

**3<sup>rd</sup> Annual Drug Discovery USA Congress  
Day 1 – 3<sup>rd</sup> October 2016**

	<b>Conference Room: North Park 1</b>
<b>15.20 – 15.50</b>	<p><b>Microbe-Host Interactions</b></p> <ul style="list-style-type: none"> <li>• Traditionally, infectious pathogens and chronic diseases have been separate research disciplines. However, recent advances in genomics and bioinformatics are rapidly opening a deeper dialogue between these fields</li> <li>• The human body supports dynamic and complex ecosystems of microbiota across different body sites, such as the gut and lung. Understanding the diversity of the microbiome in human populations and its role in human health could provide new therapeutic paradigms for many chronic diseases</li> <li>• In addition, high throughput genomics platforms are providing new insights into the interplay between human and pathogens – the so-called host-pathogen interactome</li> <li>• This presentation will discuss the opportunities and challenges in translating both the microbiome and interactome from basic science into clinical therapies using specific examples from our drug discovery efforts in infectious, metabolic and respiratory diseases</li> </ul> <p><b>Jim Brown, Director &amp; Senior Research Fellow, Computational Biology, GlaxoSmithKline</b></p>
<b>15.50 – 16.30</b>	<p><b>Exhibition Room: Cortez Ballroom</b> <b>Afternoon Refreshments, One to One Meetings x2, Poster Presentation Sessions</b></p>
<b>16.30 – 17.00</b>	<p><b>Linaclotide: The Journey From The Discovery To The Market Of This Orally Active Peptide</b></p> <ul style="list-style-type: none"> <li>• The challenges of developing the first all-natural amino acid peptide</li> <li>• Characterization of the actions of linaclotide in the GI system</li> <li>• Advancing a First in Class Peptide into Development, Approval, and Commercialization</li> </ul> <p><b>Mark Currie, Senior Vice President, Chief Scientific Officer &amp; President of R&amp;D, Ironwood Pharmaceuticals</b></p>
<b>17.00 – 17.30</b>	<p><b>Potent And Selective Substrate-based Inhibitors Of Retinoic Acid Catabolizing Enzymes For The Treatment Of Ichthyosis</b></p> <p>Ichthyosis is a family of rare genetic disorders characterized by persistently dry and scaly skin. Current treatments do not adequately address patient needs, presenting significant efficacy or tolerability concerns. Retinoic acid is the most efficient topical treatment for ichthyosis. However, retinoic acid induces its own clearance and adverse effects in humans. We have identified a novel class of substrate-based CYP26 inhibitors acting through retinoic acid metabolism inhibition as a novel class of therapeutic agents for the treatment of ichthyosis. We will report the effects of our CYP26 inhibitors in skin cells and discuss about the therapeutic effect of this novel class of compounds.</p> <p><b>Philippe Diaz, CSO, DermaXon, Associate Professor, Department of Biomedical Sciences, University of Montana</b></p>
<b>17.30 – 18.00</b>	<i>Delegates are welcome to attend co-located presentations</i>
<b>18.00</b>	<p><b>Exhibition Room: Cortez Ballroom</b> <b>Networking Drinks, End of Day One</b></p>



**3<sup>rd</sup> Annual Drug Discovery USA Congress  
Day 2 – 4<sup>th</sup> October 2016**

<b>08.00- 08.25</b>	<b>Registration: Cortez Prefunction</b>	
	<b>Conference Room: North Park 1</b>	<b>Conference Room: Hillcrest 1</b>
	<b>Discovery Chemistry &amp; Drug Design</b>	<b>Supporting Innovation With Informatics Tools</b>
	<b>Stream Chair: Dean Brown, Director of External Chemistry, AstraZeneca Pharmaceuticals</b>	<b>Stream Chair: Radu Dobrin, Associate Director, J&amp;J</b>
<b>09.00 – 09.30</b>	<p><b>Progress Towards The Identification Of Brain Penetrant P2X7 Antagonists Useful For The Treatment Of Depression</b></p> <ul style="list-style-type: none"> <li>The P2X7 receptor is an ATP gated ion channel that is expressed peripherally in monocytes and in the CNS in glial cells. Activation of P2X7 leads to the secretion of IL-1 <math>\beta</math> and IL-1 <math>\beta</math> release is hypothesized to participate in neuroinflammatory processes and likely contributes to a number of CNS disorders. For this reason, we became interested in the identification of P2X7 antagonists suitable for testing the hypothesis that antagonism of P2X7 is a viable approach for the treatment of CNS disorders, and in particular, depression</li> <li>Towards that end, we have discovered numerous chemotypes of potent P2X7 antagonists that distribute into the CNS and we have demonstrated target engagement in rat. In addition, we have shown that these compounds are capable of suppressing the release of IL-1 <math>\beta</math> after activation of the P2X7 receptor with benzoyl-ATP using microdialysis in the brains of anesthetized rats</li> <li>This presentation will focus on the medicinal chemistry efforts that led to useful probe compounds that helped validate P2X7 as a target for depression and then describe our efforts that led to a clinical candidate that can be used to test this hypothesis in humans. A synopsis of Phase I clinical data for one of our clinical candidates will also be presented</li> </ul> <p><b>Michael Letavic, Scientific Director &amp; Fellow, Janssen</b></p>	<p><b>Using Big Data To Accelerate Drug Discovery</b></p> <ul style="list-style-type: none"> <li>The growth of biological data has enabled us to answer questions in silico that were not previously accessible</li> <li>Integrating and correctly interpreting this dataset requires specific knowledge and skills.</li> <li>How we have applied this approach to drug discovery</li> </ul> <p><b>Asim Siddiqui, CTO, NuMedii</b></p>
<b>09.30 – 10.00</b>	<p><b>NKTR 181 – A Novel Oral Opioid Analgesic Designed With Slow Entry Into The CNS Resulting In Markedly Reduced CNS Side Effects And Inherently Low Abuse Potential</b></p> <ul style="list-style-type: none"> <li>NKTR-181 is a novel mu opioid receptor agonist that was specifically designed using medicinal chemistry and polymer to conjugation to have a reduced rate of entry into the central nervous system (CNS) and is currently in Phase 3 clinical studies for chronic lower back pain</li> <li>The unique CNS entry kinetics and bio-distribution of NKTR-181 are inherent characteristics of the molecule, and have been shown to reduce central side-effects as well as abuse potential (demonstrated in preclinical and Phase 1 human studies), while retaining strong analgesic efficacy in preclinical studies of acute visceral pain</li> </ul> <p><b>Jennifer Riggs-Sauthier, Vice-President, Chemistry, Nektar Therapeutics</b></p>	<p><b>Computational Approaches For Drug Target Identification: A Benchmark Study</b></p> <ul style="list-style-type: none"> <li>Target identification using protein sequence, structure and 2D/3D ligand similarity</li> <li>3D binding site comparison</li> <li>Relationship between pocket shape and ligand shape</li> </ul> <p><b>Lidio Meireles, Research Scientist II, Vertex Pharmaceuticals</b></p>
<b>10.00 – 11.00</b>	<b>Exhibition Room: Cortez Ballroom</b>	
	<b>Morning Coffee, One to One Meetings x3, Poster Presentation Sessions</b>	
<b>11.00 – 11.30</b>	<i>Delegates are welcome to attend co-located presentations</i>	<i>Delegates are welcome to attend co-located presentations</i>

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	<b>Conference Room: North Park 1</b>	<b>Conference Room: Hillcrest 1</b>
<b>11.30 – 12.00</b>	<p><b>Inhibition Of Autoimmune Pathways With Dual Inhibition Of JAK1 And TYK2: Discovery Of PF-06700841</b></p> <p>The Janus (JAK) kinases are a family of four non-receptor tyrosine kinases that modulate cytokine signaling through the Signal and Transduction of Transcription (STAT) pathways. The JAK kinases (JAK1, JAK2, JAK3 and TYK2) are important in both the innate and adaptive immune system, in a variety of cell types. The current work describes the discovery of a series of selective JAK1/ TYK2 inhibitors for a range of inflammatory disorders such as inflammatory bowel disease, systemic lupus erythematosus and psoriasis. Balancing the in-family kinase selectivity is important to optimize the inhibition of pathogenic cytokines while limiting immune suppression, as well as to limit effects driven by JAK2 signaling through EPO and other molecules important in hematopoietic cell differentiation. The lead is a well behaved molecule with excellent <i>in-vitro</i> potency and a superior off-target poly-pharmacology profile. PF-06700841 is currently in Phase 1 clinical study.</p> <p><b>Brian Gerstenberger, Principal Scientist - Medicinal Chemistry, Pfizer</b></p>	<p><b>Competitive Intelligence Workbench – Getting Access To Information For Decision Making</b></p> <p>Pharmaceutical Companies have a large past generated and continue enlarged data collection. Meanwhile, there is rich information available externally due to the new techniques. Information is vital to identify new innovative drugs and drug targets. However, it remains a challenge for research scientists to quickly and easily obtain information and use it to make informed decisions. Our Competitive intelligence workbench is aimed to provide a self-services platform to enable scientists to access the latest information from both internal and external sources and make decisions with strong supporting data. In this project, we integrated multiple sources using big data approach and built various reusable components and services to find associations among compounds, target and clinical phenotypes, which is useful for novel repurposing opportunities, MOA elucidation, etc. We also developed project dashboards that provide comprehensive knowledge overview on projects in an easy to navigate interface. Scientists were able to access the most recent advances in their chosen fields to support decision-making. More important, the change of information access methods will decrease the data bottleneck for new medicine innovation and ever change landscape of Research.</p> <p><b>Huijun Wang, Associate Principle Scientist, Merck</b></p>
<b>12.00 – 12.30</b>	<p><b>Understanding Bias In Library Design: Is It Time To Break-off Our Love Affair With p-CIPh, Suzuki Chemistry And Amide Bonds?</b></p> <p>We have determined that both the selection of reagents and reactions used in library synthesis heavily favor certain functional groups (e.g. p-CIPh) and reaction types (e.g. Amide, Suzuki, S<sub>N</sub>Ar). The justification for this bias does not seem to be scientific, but rather driven by historical reasons of synthetic ease. The continued accumulation of these types of compounds reinforces a misleading bias that these are privileged fragments and reactions types, and thus propagates further investment in these areas. Furthermore, these types of reactions result in very narrow population of chemical shape space towards linear and rod-shaped compounds. Uptake of diverse reaction types and reagents are likely needed to expand chemical diversity for the new generation of drug discovery target classes.</p> <p><b>Dean Brown, Director of External Chemistry, AstraZeneca Pharmaceuticals</b></p>	<p><b>Challenges And Opportunities For Translational CNS Drug Discovery</b></p> <p>Neurological and psychiatric diseases impact millions of patients and their families, and the need for new therapeutics remains a significant unmet medical need. This presentation will discuss specific research strategies for optimizing CNS drug discovery and development, including target selection and validation, development of translational biomarkers, establishment of robust PK/PD relationships and optimization of early clinical studies to enable rapid POC. A range of recent examples will be presented and discussed.</p> <p><b>Christopher Winrow, Director, Neurology &amp; Insomnia, Merck Research Laboratories</b></p>
<b>12.30 – 13.30</b>	<b>Lunch and One to One Meetings x3- Cortez Ballroom</b>	
<b>13.30 – 14.00</b>	<p><b>Panel Discussion: Role Of Medicinal Chemistry</b></p> <ul style="list-style-type: none"> <li>The R&amp;D ecosystem and the role of medicinal chemistry in small molecule discovery</li> <li>Novel approaches in medicinal chemistry</li> </ul> <p><b>Panellists:</b>  <b>Dean Brown, Director of External Chemistry, AstraZeneca Pharmaceuticals</b></p> <p><b>Jennifer Riggs-Sauthier, Vice-President, Chemistry, Nektar Therapeutics</b></p> <p><b>Paul Greenspan, Senior Director of Oncology Chemistry, Takeda</b></p>	<p><b>Bioinformatics Approaches To MicroRNA Drug Discovery</b></p> <ul style="list-style-type: none"> <li>LIMS system for oligonucleotide compounds</li> <li>Mining of published microRNA targets</li> <li>Tissue-Disease-Gene networks</li> </ul> <p><b>Adam Pavlicek, Senior Director, Discovery Technologies and Orphan Diseases, Regulus Therapeutics</b></p>

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For more information please contact [marketing@oxfordglobal.co.uk](mailto:marketing@oxfordglobal.co.uk)

	Conference Room: North Park 1	Conference Room: Hillcrest 1
	<b>Stream 1: Discovery Chemistry &amp; Drug Design</b>	<b>Stream 2: Supporting Innovation with Informatics Tools</b>
14.00 – 14.30	<p><b>Inhibition Of E1 Enzymes: Leveraging A Single Pharmacophore Toward Selective Inhibitors Of Multiple Targets</b></p> <ul style="list-style-type: none"> <li>E1 enzymes catalyze the first step of the process that appends ubiquitin and related peptides (Nedd8, SUMO, etc.) to lysine sidechains of substrate proteins</li> <li>A series of adenosine analogues, in which the 5'-hydroxy group is substituted with a sulfamate moiety, were found to be potent and selective inhibitors of the Nedd8-activating enzyme</li> <li>The high potency of this class of molecules is driven by the NAE-catalyzed formation of a covalent bond between the C-terminus of NEDD8 and the sulfamate nitrogen, resulting in a peptide-inhibitor adduct which has very high affinity for NAE</li> <li>Using this principle, potent and selective inhibitors of other members of this enzyme class have also been identified</li> </ul> <p><b>Paul Greenspan, Senior Director of Oncology Chemistry, Takeda</b></p>	<p><b>Implementing Bioinformatics Tools In The Immunology Therapeutic Area</b></p> <ul style="list-style-type: none"> <li>Discovering novel therapeutic approaches that satisfy unmet medical needs and bring us to better disease understanding requires understanding of molecular and physiological processes and mechanisms in both healthy and diseased tissues</li> <li>Representing relationships between entities such as gene expressions or human clinical measurements as networks reveals their global structure and at the same time allows for focusing onto sub-components of particular relevance to the questions being considered.</li> <li>We have developed a web-based platform for data integration and visualization that is accessible to anyone with a Johnson &amp; Johnson network account. Through an easy-to-use interface, it gives users the ability to retrieve hundreds of molecular networks stored in an internal repository, display them in a visualizer using annotation-driven styles, extract sub-networks containing genes of interest and access internal tools and external resources</li> </ul> <p><b>Radu Dobrin, Associate Director, Johnson &amp; Johnson</b></p>
	<b>Conference Room: North Park 1</b>	
14.30 – 15.00	<p><b>Innovative Strategies For Peptide Drug Discovery</b></p> <ul style="list-style-type: none"> <li>Case study of degarelix, a self-depotting GnRH antagonist for prostate cancer</li> <li>Engineering the physicochemical properties of peptides</li> <li>Human PK/PD of long duration of action degarelix/FIRMAGON</li> </ul> <p><b>Adeela Kamal, Senior Director, Therapeutic Area Head for Urology and Translational Research, Ferring Pharmaceuticals</b></p>	
15.00 – 15.30	<b>Exhibition Room: Cortez Ballroom</b> <b>Afternoon Refreshments</b>	
15.30 – 16.00	<p><b>Fragment-based Discovery Of A Novel MAP4K4 <i>in Vivo</i> Tool Compound G-495</b></p> <ul style="list-style-type: none"> <li>MAP4K4 is a serine/threonine protein kinase implicated in the regulation of many key biological processes such as metabolism, inflammation, angiogenesis, and cancer</li> <li>Identification of potent and selective MAP4K4 inhibitors is critical for studying its function in various disease contexts</li> <li>Fragment-based screening led to the discovery of two fragments which evolved into two medchem series</li> <li>One of the series demonstrated excellent potency and selectivity through binding to an unusual protein conformation, and yielded a novel biological tool compound (GNE-495) with efficacy in retinal angiogenesis model</li> </ul> <p><b>Huifen Chen, Senior Scientist, Computational Drug Design, Genentech</b></p>	
16.00 – 16.30	<p><b>Targeted Delivery Of Therapeutic Oligonucleotides Enhances Potency 10-60 Fold In The Liver</b></p> <ul style="list-style-type: none"> <li>Oligonucleotide therapeutics represent the third distinct platform for drug discovery with 3 FDA approved therapies and &gt;100 drugs currently in development</li> <li>Hepatocytes in the liver synthesize and secrete apolipoproteins, hormones, and coagulation factors and represent an important cell-type for oligonucleotide therapeutics</li> <li>Chemically modified oligonucleotides can be efficiently delivered to hepatocytes by targeting the Asialoglycoprotein receptor using tri-antennary GalNAc conjugates</li> </ul> <p><b>Thazha P. Prakash, Director, Medicinal Chemistry, Ionis Pharmaceuticals, Inc</b></p>	
16.30	<b>End of Conference</b>	