OXFORD GLOBAL

16th Annual Drug Discovery Summit

8 - 9 June 2015, Berlin, Germany

Drug Discovery Streams

Key Discovery Strategies: Target Based Discovery and Phenotypic Screening
Evaluating the utility of target based discovery; does it actually hinder R&D productivity?
Atypical therapeutic modalities for drug discovery
Multi-parameter lead optimization
Discovery case studies: antibody therapeutics
The impact of target-based approaches on drug discovery

Screening and Assays: Enabling Technologies
Exploring the resurgence of phenotypic screening through key case studies
Facilitating screening of combined libraries
The search for physiologically relevant screen models: iPSC and primary cells
Using gene-expression profiling to inform lead selection

Preclinical Biomarkers and Translational Medicine
Developing clinically relevant preclinical models for cancer immunotherapy
Investigating disease pathways early in drug discovery to improve clinical attrition
Preclinical biomarkers in CNS drug discovery
Leveraging data to support translational medicine
Validating biomarkers

Supporting innovation: Data and Information Management
Managing complex discovery portfolios
Addressing the challenges of open innovation
Making the most of discovery data
Enabling disease stratification and biomarker discovery with novel informatics platforms
Automated druggability assessment
Overcoming the challenges of translational research IT

Discovery Chemistry Streams

Discovery Chemistry: Latest Case Studies
The use of enabling chemistry technologies to accelerate the drug discovery and development process
A new pharmacophore modeling approach
Key learnings from ligand binding studies
Current perspectives in fragment and structure based discovery
Analysing structure-activity relationships
A novel virtual screening approach

Drug Design: Novel Approaches
Novel computational tools for drug design
Lead optimisation: considering solubility, druggability and potency
Designing multi-target drugs
The importance of binding site water molecules/networks in drug design
New perspectives from computational approaches on druggability, selectivity and kinetics

Benefits to Attending

✓ **Hear from and meet with the people shaping the pharmaceutical landscape**. Attendees include: VP's and Directors from Bristol-Myers Squibb, AstraZeneca, MedImmune, GlaxoSmithKline, Pfizer, Janssen, Novartis, AbbVie, Biogen Idec, Shire, Sanofi, Boehringer Ingelheim, Roche and UCB

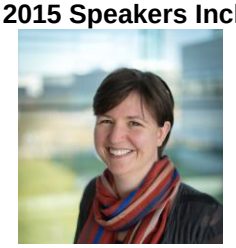
✓ **Discuss the latest innovations in drug discovery** including atypical therapeutic modalities for drug discovery, novel screening tools using iPSC and primary cells, gene expression profiling and new IT tools to support R&D pipelines

✓ **Discover collaborative solutions to discovery chemistry challenges** by considering key lead optimisation considerations for solubility, drugability and potency, more effective PPI targeted drug design, and how to make best use of computational tools for drug design

✓ **Unparalleled networking opportunities**. The two-day congress format combines dedicated networking breaks, pre-organised 1-2-1 meetings and our popular drinks reception. The exhibition hall and poster presentation spaces offer a relaxed and professional environment for discussion

✓ **The 16th Annual Drug Discovery Summit brings together over 250 industry leaders** working in drug discovery, discovery chemistry and drug design

2015 Speakers Include



Donna Finch
MedImmune

Christoph Weissner
Asceneuron

Araz Raoof
Janssen

Meet Senior Decision Makers
250 VPs, Directors & Senior Managers from leading pharmaceutical organisations, biotech companies and academic institutions will attend the event. Delegate job titles include:

Drug Discovery	Discovery Chemistry
Target Based Discovery	Medicinal Chemistry
Drug Design	Lead optimisation
Affinity Screening	R&D informatics

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	Library Optimisation
Fragment Based Drug Discovery	Predictive Biomarkers
Computational Chemistry	Screening Technology

Venue: The Summit will be held at the Hotel Palace Berlin in Germany
www.drugdiscovery-summit1.com
www.discoverychemistry-congress1.com

Confirmed Speakers 2015:

- Litao Zhang, VP, Leads Discovery & Optimization, Bristol-Myers Squibb
- Araz Raoof, Scientific Affairs & Analysis, Janssen Pharmaceutica
- Axel Vater, VP Drug Discovery and Preclinical Research, NOXXON Pharma AG
- Jörg Eder, Executive Director, Novartis Institutes for Biomedical Research
- Stevan Djuric, Senior Director, Discovery Chemistry and Technologies, AbbVie
- Hank Wu, Director, R&D IT, Biogen Idec
- Steve England, Director, Head of Future Therapeutics & Technologies, AbbVie
- Silvia Guionaud, Senior Pathologist, MedImmune
- Armin Bauer, Director, External Cooperations, Sanofi
- Juan-Miguel Jimenez, Senior Director, Head of Chemistry UK, Vertex Pharmaceuticals Europe
- Malin Lemurell, Director of Medicinal Chemistry, AstraZeneca
- Jinghai James Xu, Executive Director of Corporate Development, Merck & Co.
- Andrew Stamford, Executive Director, Discovery Chemistry, Merck
- Bernard Barlam, Associate Director of Medicinal Chemistry, AstraZeneca Oncology Innovative Medicines
- Donna Finch, Principal Scientist, MedImmune
- Stefan Schunk, Head of Exploratory Chemistry, Grünenthal GmbH
- Peter Clements, Director of Pathology at GlaxoSmithKline
- Bill Cairns, Director, Target Sciences, GlaxoSmithKline
- Philip M Arlen, President and CEO, Precision Biologics
- Philip Groth, IT Business Partner, Bayer Pharma AG
- Friedrich Rippmann, Director, Global Computational Chemistry, Merck
- Nicolas Fischer, Head of Research, NovImmune SA
- Matthias Frech, Director, Merck KGaA
- Johannes Grosse, Head of Cardiovascular Inflammatory and Metabolic Disease Group, Takeda Cambridge
- Christoph Weissner, COO, Asceneuron
- Xavier Leroy, Associate Director Drug Discovery, Actelion Pharmaceuticals Ltd
- Laurent Schio, Head Medicinal Chemistry France, Sanofi
- Ingo Mügge, Senior Research Fellow, Boehringer Ingelheim Pharmaceuticals, Inc.
- Matti Lepistö, Associate Principal Scientist, AstraZeneca
- Martin Hemmerling, Principal Scientist, AstraZeneca R&D Mölndal
- Ivan Efremov, Senior Principal Scientist, Worldwide Medicinal Chemistry, Pfizer Inc
- David Drake, UK Regional Architect Lead, AstraZeneca
- David Henderson, Liaison Manager, Bayer Pharma AG
- Luc Van Rompaey, VP Translational Medicine, arGEN-X
- Jonathan Mason, Senior Research Fellow / Head CADD, Heptares
- Sara Colombetti, Group Leader Immunopharmacology, Roche Innovation Center Zürich
- Jutta Heim, Senior Consultant, Evolva SA
- Rod Hubbard, Professor and Senior Fellow, University of York and Vernalis Research
- Eugen Proschak, Professor, Goethe University of Frankfurt
- Chas Bountra, Professor of Translational Medicine, CSO, SGC, University of Oxford
- Michele Parrinello, Professor in Computational Sciences, ETH Zürich and Università Della Svizzera Italiana
- Simon Ward, Professor of Medicinal Chemistry & Director of Translational Drug Discovery, University of Sussex
- Matthias Rarey, Professor, University of Hamburg
- Ulla-Carin Tornberg, Principal Scientist, BioInvent International AB
- Willis Read-Button, Director of Operations, Genometry
- Matt Tudor, Principal Scientist, Screening & Protein Sciences, Merck Sharpe & Dohme
- Pieter Peeters, Senior Director Computational Sciences and Systems Biology, Janssen Research & Development
- Francois Sautel, Head of Natural Substances Chemistry Unit, Pierre Fabre
- Andrew Payne, Senior Group Leader, UCB
- Michael-Friedrich Boettcher Global Clinical Project Lead, Bayer
- Steven Rust, Senior Scientist, MedImmune
- Tomasz Rzymski, Principal Investigator, Selvita S.A.

If you're on Twitter, make sure to follow us @drugdiscovery1 and join the Congress conversation on #DDSummit15

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16th Annual Drug Discovery Leaders Summit and 3rd Annual Discovery Chemistry and Drug Design Congress
Day 1 – Monday 8th June

07.30 – 08.20	**Registration: Burgund Foyer**		
	Conference Room: Burgund III		
08.20 – 08.25	**Oxford Global Welcome Address**		
08.25 – 08.30	**Stream Chair Welcome Address: Andreas Scheel, EVP In Vitro Biology, Evotec (UK) Ltd**		
08.30 – 09.00	**Keynote Presentation:** **The Evolving Nature Of Therapeutics; Challenges For Our Industry** • Will small molecules and biologics remain the mainstay of future therapeutics? • Some of the potential disruptors on the horizon • How industry needs to innovate to embrace the changing therapeutic landscape **Steve England, Director, Head of Future Therapeutics & Technologies, AbbVie**		
	Drug Discovery Leaders Summit		**Discovery Chemistry & Drug Design Congress**
	Key Discovery Strategies: Target Based Discovery and Phenotypic Screening		**Discovery Chemistry: Latest Case Studies**
	Conference Room: Burgund III		**Conference Room: Burgund I**
	Stream Chair: Andreas Scheel, EVP In Vitro Biology, Evotec (UK) Ltd		**Stream Chair: Stevan Djuric, Senior Director, Discovery Chemistry and Technologies, AbbVie**
09.00 – 09.30	**The Changing Face Of Technology Innovation In Drug Discovery: High Throughput Screening Paradigm Shift From Genotype To Phenotype** • Discuss technology transformation to meet novel science and diverse discovery portfolio • Transition screening technology options from traditional one target per screen to multiple target in parallel • Implement phenotypic screen capability across discovery processes • Provide technology innovation case studies • Project the paradigm shift of high throughput screening from genotype to phenotype **Litao Zhang, VP, Leads Discovery & Optimization, Bristol-Myers Squibb**		**Use Of Enabling Chemistry Technologies To Accelerate The Drug Discovery And Development Process** The talk will focus on advancements in the area of high throughput chemistry and reaction development. Also covered will be applications in the analytical chemistry area using MS based technologies to support PK studies and product protection activities **Stevan Djuric, Senior Director, Discovery Chemistry and Technologies, AbbVie**
	Key Discovery Strategies: Target Based Discovery and Phenotypic Screening	**Screening & Assays: Enabling Technologies**	**Discovery Chemistry: Latest Case Studies**
	Conference Room: Burgund III	**Conference Room: Burgund II**	**Conference Room: Burgund I**
	Stream Chair: Andreas Scheel, EVP In Vitro Biology, Evotec (UK) Ltd	**Stream Chair: John Unitt, Director of Bioscience, Sygnature Discovery**	**Stream Chair: Stevan Djuric, Senior Director, Discovery Chemistry and Technologies, AbbVie**
09.30 – 10.00	**Novel Disease-Relevant Screening Paradigms For Phenotypic Drug Discovery** • Novel assay systems with complex and disease-relevant read-outs will be presented • Multiple case studies will be discussed illustrating opportunities and pitfalls of phenotypic drug discovery • Target deconvolution strategies will be presented **Andreas Scheel, EVP In Vitro Biology, Evotec (UK) Ltd** 	**A New Future For HTS: Facilitating Screening Of Combined Libraries** • Combining pharma libraries broadens the chemical space you can access in HTS • IP Models are supported by independent "honest data broker" • State-of-the-art facilities support efficient screening of larger and/or combined libraries **Steven van Helden, Business Development and HTS Lead, European Lead Factory, Pivot Park Screening Centre** 	**The Application Of Extended Hückel Theory For Pharmacophore Modeling** • A new pharmacophore modeling approach based on a semi-empirical method using Extended Hückel Theory (EHT) • An automated chemically aware model for generating pharmacophore features which encode interaction energies • EHT based pharmacophore models account for ligand resonance and electron withdrawing effect **Markus Kossner, Scientific Services Manager, Chemical Computing Group** 

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10.00 – 11.00	Bordeaux Suite and Foyer: Morning Refreshments: Exhibition & Poster Presentation Session: One To One Meetings x 3		
	Conference Room: Burgund III	**Conference Room: Burgund II**	**Conference Room: Burgund I**
11.00 – 11.30	**Target Safety Assessment: Planning For Success** Safety issues in drug development can be compound based or target based. Avoiding targets with intrinsic high risk to patients is an important step towards success. Methods of target safety assessment and examples for targets dropped on safety grounds will be discussed. **Silvia Guionaud, Senior Pathologist, MedImmune**	**Real-Time Pharmacology - In-Vitro And In-Vivo** • Partial and biased agonists • Kinetics • Koff • Residence time • Target engagement in-vivo **Xavier Leroy, Associate Director Drug Discovery, Actelion Pharmaceuticals Ltd**	**Isoform Selective PI3K Inhibitors - Discovery Of Two Clinical Candidates:** • AZD8186, a Potent and Selective Inhibitor of PI3Kb and PI3Kd inhibitor for the treatment of PTEN deficient tumours, and • AZD8835, a Potent and Selective Inhibitor of PI3Ka and PI3Kd for the treatment of PIK3CA-dependent cancers. • Chromen-4-one 6-carboxamides as PI3Kb/d inhibitors: structure activity relationships, optimisation of potency and physical properties • 2-amino pyridines / pyrazines as PI3Ka inhibitors: improving general kinase selectivity; optimisation of potency and physical properties. **Bernard Barlam, Associate Director of Medicinal Chemistry, AstraZeneca Oncology Innovative Medicines**
11.30 – 12.00	**TruBind™ BSI Analysis Facilitates Target – Small Molecule Binding Research In CNS, GPCR, Kinase, And Allosteric Studies** TruBind BSI technology uniquely provides free-solution, label-free, and conformation sensitive detection of target engagement and Kd determination for small molecule drug candidates. This presentation opens with a brief description of TruBind technology and then proceeds to review its application in the analysis of CNS aggregate - storage disease (Alzheimer's, Lewy Body); Class A, B, and C GPCR targets; and type I, II, and III inhibitors of Bcr-Abl kinase. A particular focus upon allosteric studies will be presented. **Scot Weinberger, EVP R&D, Co-Founder & Director, Molecular Sensing** 	**Natural Products As Library Blue Prints - Structure And Function** Natural products are evidently an outstanding resource for drug discovery. Advancing a natural product hit into the clinic is nevertheless a challenging task. One of many hurdles to overcome is the access and tractability of natural product scaffolds. Many programs in the past addressed the chemical enablement of natural product core structures. Classical natural product total synthesis often does not allow wider variations in scaffold and exit vector diversity. Semi-synthesis sometimes lacks variability in scaffold stereochemistry and functionality. Several more general programs addressing the synthetic access of natural product scaffolds have been started in the past. Establishing biological meaningful diversity complemented by rationally designed biological focused libraries seems therefore a rewarding task. Reliable synthetic access and flexibility in terms of regio- and stereochemistry allows addressing natural product pharmacophores in a tractable and efficient way. Starting from a wide range of synthetic and pure natural product libraries AnalytiCon established a set of Fragments from Nature, a platform of highly scaffold diverse macrocycles and a natural product pharmacophore centered program. **Lars Ole Haustedt, Director Projects & Innovation, AnalytiCon Discovery GmbH** 	**Inhaled Drug Discovery- Case Histories And Strategies** • Introduction to inhaled drug discovery, specific requirements for inhaled drugs • Inhalation by design: optimisation of physicochemical properties, PK and target residence time • Case histories from LAMA, MABA and enzyme inhibitor projects **Robert Heald, Director of Medicinal Chemistry, Argenta, a Charles River Company** 

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Day 1 – Monday 8th June

	Conference Room: Burgund III	Conference Room: Burgund II	Conference Room: Burgund I
12.00 – 12.30	**Impact Of Target-Based Approaches On The Discovery Of 1st In Class Drugs** • Relative contributions of target- and systems-based approaches for 1st in class drugs approved between 1999 and 2014 • Examples of successful target-based drug discovery projects in the field of proteases **Jörg Eder, Executive Director, Novartis Institutes for Biomedical Research**	**Virtual Screening Of Large Accessible Combinatorial Chemistry Spaces** In silico screening has been an accepted hit finding approach in drug discovery for many years. Accessibility of virtual screening hits is often limited to compounds already synthesized. To increase the size of accessible chemical spaces that can be practically explored with virtual screening techniques we have developed software and workflows that combine the powers of primary 3D virtual screening approaches with those of combinatorial chemistry (Methods 2015, 71:14). Following a virtual screen, a number of libraries for lead identification may be synthesized and tested. Here we present a 3D shape and pharmacophore based virtual screening approach that is capable of in silico searching through tens of trillions of virtual compounds from tens of thousands of combinatorial libraries. An example will be presented of applying the workflow to identifying a novel RORC inverse agonist exhibiting a novel binding mode confirmed by X-ray crystallography. **Ingo Mügge, Senior Research Fellow, Boehringer Ingelheim Pharmaceuticals, Inc.**	**Optimization Of Natural Products Leads For The Therapy Of Tuberculosis** • Re-investigation of a "forgotten" antibiotic • Lead optimization and establishment of structure-activity relationships by a total synthesis approach • Discovery of a pre-clinical candidate with outstanding combination effects in a TB in vivo model **Armin Bauer, Director External Cooperations, Sanofi**
12.30 – 13.00	**Discovery And Development Of A Monoclonal Antibody Against A Novel Target For The Treatment Of Colorectal Cancer** • Discovery of Novel target specific agent, Identification of Target, • Preclinical Studies demonstrating function of antibody • Phase 2 Colorectal Cancer Study and Results **Philip M Arlen, President and CEO, Precision Biologics**	**Therapeutic Antibodies To Difficult Target Classes: A Novel Human MAb To The Class A G-protein Coupled Receptor Formyl-Peptide Receptor 1** • At MedImmune we have been pushing the limits of what is tractable to antibody therapies • We present a case study where we identified and engineered an antibody to a Class A GPCR for potency, species cross-reactivity while maintaining specificity • The unusual structure of the final antibody and what it means for discovery of antibodies to similar challenging target classes • What we have learned about FPR-1 involvement in human disease as a consequence of identifying a highly specific, high potency antibody **Donna Finch, Principal Scientist, MedImmune**	**Biophysical Methods In Drug Discovery: Their Applications And Integration** • Efficient use biophysical methods in the early drug discovery process • Integrated use of different methods • Examples in fragment based lead discovery • Impact on compound selection • Initiatives to further advance the biophysical methods in drug discovery **Matthias Frech, Director, Merck KGaA**
13.00 – 14.00	**Bordeaux Suite and Foyer: Lunch: One to One Meetings x 2**		
14.00 – 14.30	**Centre For Therapeutic Target Validation: A Pioneering Public-Private Research Initiative** • Generation of evidence on the validity of therapeutic drug targets based on genome-scale experiments and analysis. • Creation of an R&D framework that applies to a wide range of human diseases; committed to sharing data openly with the scientific community. • Integration of genomics, proteomics and chemistry data with disease biology knowledge to address drug discovery attrition. **Bill Cairns, Director, Target Sciences, GlaxoSmithKline**	**The Use Of Disease-Relevant Cellular Systems In Screening Cascades For Small And Large Molecule Drug Discovery** • The establishment of screening cascades based on cell biology relevant to disease • Case studies of small molecule and antibody projects • Translation of assay biology into disease settings **Andrew Payne, Senior Group Leader, UCB**	**Current Perspectives In Fragment-Based Discovery** • Choosing and using fragments in lead discovery • Turning enzymes on with fragments • 3D fragments – getting beyond the hype **Rod Hubbard, Professor and Senior Fellow, University of York and Vernalis Research**

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	Conference Room: Burgund III	Conference Room: Burgund II	Conference Room: Burgund I
14.30– 15.00	**Selective CDK8 Inhibitor SEL120-34A Alters Expression Of Interferon-Related DNA Damage Resistance Signature Genes In Solid Tumors** • SEL120-34A is a novel selective inhibitor of CDK8 • CDK8 is activated in response to stromal-cancer cells interactions and regulates transcriptional activity of STATs • SEL120-34A is a potent inhibitor of interferon-related DNA damage resistance signature in cancer cells in vitro and in vivo **Tomasz Rzymski, Principal Investigator, Selvita S.A.** Selvita	**One Hour Workshop: Library-Scale Gene-Expression Profiling: Technology and Applications** • L1000™ Expression Profiling produces gene-expression profiles from crude cell lysates in 384-well plate format at a rate of thousands a day and at only a fraction of the cost of conventional methods • the availability of a high-throughput gene-expression profiling method enables a range of pharmaceutical discovery and development applications • case studies illustrate the use of L1000 for primary screening, library characterization, and hit prioritization **Case Studies:** **1) L1000™ Expression Profiling** • L1000™ Expression Profiling produces gene-expression profiles from crude cell lysates in 384-well plate format at a rate of thousands a day and at only a fraction of the cost of conventional methods • direct measurement of one thousand specially selected landmark genes and inference of the levels of the remainder using an algorithm trained on tens of thousands of historical gene-expression profiles • uniquely enables applications ranging from primary screening, library characterization, hit prioritization, target deconvolution, indication discovery, and direct and seamless integration with public L1000 data from the LINCS Program **Willis Read-Button, Director of Operations, Genometry** **2) Applications And Analyses Of L1000 Profiling In Pharmaceutical Early Discovery** • Phenotypic screening hit triage and mode-of-action hypothesis generation • Evolving approaches to analysis of compound transcriptomic data **Matt Tudor, Principal Scientist, Screening & Protein Sciences, Merck Sharpe & Dohme** **3) How Gene-Expression Profiling Informs Lead Selection At Janssen R&D** • Gene-expression profiles provide information that can be used for decision making when choosing which chemotypes to advance • High-dimensional data from gene-expression profiles and bioactivity-based target predictions aid in hit triaging, compound characterization and target deconvolution • Utilization of specific distance measures for various high-dimensional biological data can improve compound characterization **Pieter Peeters, Senior Director Computational Sciences and Systems Biology, Janssen Research & Development** genometry	**High-Throughput Strategies To Boost The Discovery And Development Of Drugs** • An introduction to the unlocking power of automation followed by a selection of case studies • Step change in solid compound management • Solid-phase and liquid-phase library synthesis in disposable vials / reactors • Crystallisation, polymorph, salt and solubility screening • Formulation screening (e.g. SMEEDs, hot melt extrusion) **Rolf Gueller, Chief Executive Officer, Chemspeed Technologies AG** CHEMSPEED® TECHNOLOGIES

15.00 – 15.30	**Everything Old Is New Again: Revolutionizing Drug Discovery With Human Biology And Diversity**
	Recent advances in human-based disease models and screening technology are reinvigorating phenotypic-based drug discovery efforts. This presentation will discuss some of these advances, specifically through;
	• Explaining how induced pluripotent stem cell (iPSC) technology brings human biology and diversity into the laboratory.
	• Demonstrating that relevant in-vitro human biology enables effective phenotypic screens for both discovery efforts and early toxicity studies.
	• Providing case studies that confirm the utility and implementation of iPSC-based genetic and environmental disease models and phenotypic screens across defined models and from clinical populations.
	
	Blake Anson, Product Manager, Cellular Dynamics International
	
	Cellular Dynamics international
			Modern Process Screening And Characterization Technology For Meeting Today And Future Drug Design Challenges
			Modern drug development organizations face many challenges, like meeting regulatory requirements for process and product knowledge, increasing the speed of development, and de-risking manufacturing processes to reduce Out Of Spec (OOS) lots. Automation can help in two key ways:
			• Design experiments that inform scientific decisions and move development programs forward
			  ○ By coupling the Freeslate automation systems with LEA and DOE techniques, you can get to the better scientific answers faster and with less material consumed
			• Save time and money by having more detailed knowledge about your processes earlier in your drug development cycle
			  ○ Nothing costs more money than OOS manufacturing lots - these lots are unsellable and cost organizations millions of dollars
			  ○ A QbD development approach combined with the power of automation can dramatically improve process and product knowledge, de-risking submissions and ultimately the manufacturing process
			  ○ Freeslate has technologies that enable companies to develop robust processes that minimize the project risk as it moves through development and out to the plant
			
			John S. Senaldi, President & CEO, Freeslate
			
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	Conference Room: Burgund III	Conference Room: Burgund II	Conference Room: Burgund I
15.30 – 16.00	**Seamless Transition From Mono- To Multi-Specific Therapeutic Antibody Formats** • Simultaneous targeting of several pathways can lead to superior efficacy and enable novel modes of actions that cannot be achieved with monoclonal antibodies. • Antibody combinations or multi-specific formats can mediate multiple targeting, but also lead to different downstream biological effects. • We have developed an antibody generation platform that facilitates the transition between different formats while maintaining a human IgG structure, thus enabling evaluation and selection of the best modality for further development. **Nicolas Fischer, Head of Research, NovImmune SA**	**Improving Drug Discovery Decision-Making Through Natural Substances Network Innovation** With the largest private collection of herbal extracts and 50 years of expertise in the plant area, PIERRE FABRE LABORATORIES possesses a great source of innovation. To foster the potential of Natural Products in Life Science industries, we decided to launch an Open Innovation initiative based on our collection. We propose to share HTS-formatted samples from our collection with R&D laboratories and to assist them with our phytochemistry expertise. Our goal is to build collaborations that will lead to innovative discoveries in various fields such as Pharma, Consumer Care, Animal Health or Agrochemistry **Francois Sautel, Head of Natural Substances Chemistry Unit, Pierre Fabre**	**Utility of Synthetic Biology in Discovering Novel Chemical Structures** Synthetic biology has been heralded as a new bioengineering platform for the production of bulk and specialty chemicals, drugs, and fuels. Here, we report on the isolation of approx. 100 novel pharmaceutical compounds produced using a combinatorial genetics approach with artificial chromosomes in baker's yeast. Of the molecules found, >75% have not been described previously; 20% of the compounds exhibit novel scaffolds. Their structural and physicochemical properties comply with established rules of drug- and fragment-likeness and exhibit increased structural complexities compared to synthetically produced fragments. In summary, the synthetic biology approach described here represents a completely new, complementary strategy for hit and early lead identification that can be easily integrated into the existing drug discovery process. **Jutta Heim, Senior Consultant, Evolva SA**
16.00 – 16.40	**Bordeaux Suite and Foyer: Afternoon Refreshments, Exhibition & Poster Presentation Session and One To One Meetings x 2**		
16.40 – 17.10	**Working 'Openly' Together To Transform Target Discovery** • Pre-competitive network comprising several pharmas, SMEs, academics and patient groups • Crowd source science on novel targets • Focus on genetically/ clinically identified targets and functional in vitro patient assays **Chas Bountra, Professor of Translational Medicine, CSO, SGC, University of Oxford**	**Discovery Of Clinically Relevant Targets And Antibodies By Phenotypic Screening** • Discovery of novel, disease-related targets • Isolation of antibodies specific for up-regulated targets without prior knowledge of target identity • Phenotypic screening using primary patient material **Ulla-Carin Tornberg, Principal Scientist, BioInvent International AB**	**Cebranopadol, A Novel Potent Analgesic - Its Discovery From A Medchem Perspective** This talk will cover the discovery of the first spirocyclic lead and its subsequent optimization into Cebranopadol. **Stefan Schunk, Head of Exploratory Chemistry, Grünenthal GmbH**
17.10 – 17.40	**The Spiegelmer Discovery Platform: From In Vitro Evolution Of L-Aptamers To Clinical Proof Of Concept** • Aptamers are highly specific target-binding chemical entities that can be generated by an evolutionary in vitro selection process. • Spiegelmers are mirror-image aptamers that are stable in plasma and can be used as therapeutics. • Recent data from the Spiegelmer pipeline will be presented. **Axel Vater, VP Drug Discovery and Preclinical Research, NOXXON Pharma AG**	**Cellular Imaging: A Key Phenotypic Screening Strategy For Predictive Toxicology** • Incorporate phenotypic screening as a key strategy will increase confidence in the predictivity of any discovery toxicology paradigm • Cellular imaging serves as the "phenotypic anchor" to identify same toxicologic pathology that encompasses an array of underlying mechanisms • Case studies: hepatotoxicity, cardiotoxicity, genetic (including mutagenic, aneugenic or clastogenic) toxicity **Jinghai James Xu, Executive Director of Corporate Development, Merck & Co**.	**Discovery Of MK-8931: A BACE Inhibitor In Phase 3 Clinical Development For Alzheimer's Disease** This presentation will discuss: • Alzheimer's disease, the amyloid hypothesis, and b-secretase (BACE1) • Fragment-based approach to BACE1 active site-directed ligands and their evolution to leads with CNS drug-like properties • Multi-parameter lead optimization culminating in the discovery of MK-8931 and its preclinical and Phase 1 PK/PD profile **Andrew Stamford, Executive Director, Discovery Chemistry, Merck**

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	Conference Room: Burgund III	Conference Room: Burgund II	Conference Room: Burgund I
17.40– 18.10	**Phenotypic Screening For Therapeutic Antibodies** • Target-agnostic, or 'phenotypic' screening is an increasingly popular and effective approach for both small molecule and biologics drug discovery • For antibody drug discovery, phenotypic selection is a potential growth area and exciting new targets are emerging from this strategy • An antibody phenotypic selection strategy has been employed at MedImmune to find novel targets and infectious disease and oncology examples will be discussed **Steven Rust, Senior Scientist, MedImmune**	**Appetite Regulation By Insl5 – An Orexigenic Enteroendocrine Hormone** • Enteroendocrine hormones are the main signals of the gut-brain axis responsible for the efficacy of bariatric surgery, and consequently 'hot spots' for pharmacological intervention • Insl5 is a hormone secreted by L-cells of the colon upon fasting • Administration stimulates food intake establishing its orexigenic function • Inhibition of its cognate receptor is a new opportunity for drug discovery aiming at reducing appetite **Johannes Grosse, Director Metabolic Diseases, Takeda Cambridge**	**Drug Discovery – A Structured Approach To Building A Discovery Portfolio** • Integration of structural biology into ion channel and enzyme inhibitor projects • Challenges of establishing and managing a portfolio of projects in an academic environment **Simon Ward, Professor of Medicinal Chemistry & Director of Translational Drug Discovery, University of Sussex**
18.10	**End Of Day One** **Bordeaux Suite: Networking Drinks**		

16th Annual Drug Discovery Leaders Summit and 3rd Annual Discovery Chemistry and Drug Design Congress
Day 2 – Tuesday 9th June

	Conference Room: Burgund III
	Stream Chair: Sylviane Boucharens, Co-founder, COO and CSO, BioAscent Discovery Ltd.
08.30 – 09.00	**Keynote Presentation** **How To Improve Attrition In Clinical Drug Development Already In Discovery** • There is urgent need to investigate disease pathways early in drug discovery to improve clinical attrition • We propose a new discovery model focused on biomedical research principles • A fundamental change is required in the linear R&D model currently used **Araz Raoof, Scientific Affairs & Analysis, Janssen Pharmaceutica**

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Day 2 – Tuesday 9th June

	Drug Discovery Leaders Summit	Discovery Chemistry & Drug Design Congress
	Supporting Innovation: Data & Information Management	**Drug Design: Novel Approaches**
	Conference Room: Burgund III	**Conference Room: Burgund I**
	Stream Chair: Sylviane Boucharens, co-founder, COO and CSO, BioAscent Discovery Ltd.	**Stream Chair: Markus Kossner, Scientific Services Manager, Chemical Computing Group**
09.00 – 09.30	**Perspectives And Challenges Of Translational Research IT** • Translational Medicine IT faces many challenges, e.g. IT infrastructure, proliferation of platforms and data and the need for new ways of (interdisciplinary) working • I will show our approach to tackle these challenges and give an outlook on our path forward **Philip Groth, IT Business Partner, Bayer Pharma AG**	**Discovery And Characterization Of ATR Inhibitors For The Treatment of Cancer** DNA damaging agents, such as cisplatin, or ionising radiation (IR), represent the cornerstone for the treatment of cancer. However, for the majority of patients they provide only modest benefit. One reason for this is the presence of highly effective cellular processes that detect and repair damaged DNA. ATR kinase is a key mediator for one such cellular repair process that responds to replication stress, a potentially lethal form of DNA damage that arises when cells attempt to replicate damaged DNA. **Juan-Miguel Jimenez, Senior Director, Head of Chemistry UK, Vertex Pharmaceuticals Europe**
	Supporting Innovation: Data & Information Management	**Drug Design: Novel Approaches**
09.30 – 10.00	**The Importance Of An Integrated Informatics Solutions To Support The New Life Sciences Research Paradigms** • Maximizing efficiency of research with integrated informatics workflows • Common support for biologics and small molecule research • Support for collaborative networked research **Robert Brown, VP of Global Informatics, Dotmatics Ltd** 	**Data-Driven Drug Design: Deriving And Applying Actionable Information** This talk will outline trends and opportunities in pharma for organizing and analyzing data across the research landscape to better design drugs. Examples will highlight successes and identify best practices **Tim Hoctor, Vice President, Life Science Solutions Services, Elsevier** 
10.00 – 10.30	**Compound Passport - Addressing The Challenges Of Asset Rights Management In The World Of Open Innovation** The trend towards Open Innovation presents new challenges for the management of an organisation's compound assets. It is important to ensure that any compound subject to a 3rd party agreement is managed and used in accordance with the contractual obligations. This talk will describe the journey from concept to implementation of a Compound Passport Service (CPS). CPS allows collaboration assets to be controlled in a proactive way and provides information on their permitted usage to other systems, in order to facilitate approval tracking and compliance. **David Drake, UK Regional Architect Lead, AstraZeneca**	**Inhibitors Of The Inducible Nitric Oxide Synthase (iNOS) Dimer Complex Developed Using Fragment Assisted Lead Generation, Structure Based Design And Metabolism Identification** iNOS (Inducible Nitric Oxide Synthase) has long been considered to be a promising anti-inflammatory drug target. We will here disclose how structure based design was used to guide scaffold hopping and the identification and development of a novel series of dimer inhibitors of iNOS showing good selectivity towards eNOS and nNOS. Fragment screening was use to assist lead identification and scaffold changes to mitigate metabolic instability and formation of reactive metabolites in the bicyclic core of the compounds. The structure activity relationship, metabolism and pharmacokinetic profiles will be discussed with a special emphasis on the Medicinal Chemistry design approaches taken to mitigate the risks identified and how the series was developed to give compounds with low nM cellular IC50s and lead-like properties. **Malin Lemurell, Director of Medicinal Chemistry, AstraZeneca**
10.30 – 12.10	**Bordeaux Suite and Foyer: Morning Refreshments: Exhibition & Poster Presentation Session: One To One Meetings x 5**	
12.10 – 13.10	**Bordeaux Suite and Foyer: Lunch: One To One Meetings x 2**	

16th Annual Drug Discovery Leaders Summit and 3rd Annual Discovery Chemistry and Drug Design Congress
Day 2 – Tuesday 9th June

	Supporting Innovation: Data & Information Management	**Drug Design: Novel Approaches**
	Conference Room: Burgund III	**Conference Room: Burgund I**
	Stream Chair: Sylviane Boucharens, co-founder, COO and CSO, BioAscent Discovery Ltd.	**Stream Chair: Markus Kossner, Scientific Services Manager, Chemical Computing Group**
13.10 – 13.40	**Accelerating Biotech To The Speed Of Patient Lives** Transforming IT and Informatics at Biogen is at the heart of the company's strategic commitment to use technology, data and analytics to inform the drug discovery process, unlock new insights, improve patient care and drive innovation. This presentation shares work in progress and lessons learned at Biogen. • Biogen's compelling case for precision medicine • Using wearables, apps and sensors to monitor real world evidence • Deploying the new gold standard of Cloud computing for NextGen Sequencing and large scale partnerships • Conducting experiments in technology innovation **Hank Wu, Director, R&D IT, Biogen Idec**	**High End GPCR Candidate Design: Full Structure-Based Drug Design Including Water Network Energetics For Potency, Selectivity And Kinetics** • Full 'high end' SBDD for GPCRs • The importance of binding site water molecules/networks & their energetics in drug design • New perspectives from computational approaches on druggability, selectivity and kinetics **Jonathan Mason, Senior Research Fellow / Head CADD, Heptares**
13.40 – 14.10	**Automated Druggability Assessment For Target Prioritization** • Automatic detection of pockets and subpockets is now feasible. • We have developed quantitative approaches for the estimation of (small molecule) druggability. • The simulation of *transient* pockets allows for the identification of novel intervention sites (on known proteins). • A prioritisation of the kinome for drug discovery will be presented **Friedrich Rippmann, Director, Global Computational Chemistry, Merck**	**Design And Rationale For Exquisite Selectivity Of Preclinical And Clinical Kinase Inhibitors.** The development of the targeted therapy concept in Oncology as well as the clinical demand for much better tolerated treatments have conducted research programs in pharmaceutical companies towards the discovery of selective kinase inhibitors in particular. We will review some key aspects of the kinase activation processes via conserved motives and conformational changes and how the pioneering kinase drugs have interfered with them. We will then present the drug design strategies that have been pursued in Sanofi in several kinase related discovery projects and a rationale for achieving high selectivity (and potency) in preclinical and clinical kinase inhibitors. **Laurent Schio, Head Medicinal Chemistry France, Sanofi**
14.10 – 14.40	**eTRIKS: European Translational Information And Knowledge Management Services** Enabling disease stratification and biomarker discovery by… • Driving the adoption of a common open source platform, based on the tranSMART software • Promoting multi-study data harmonisation • Developing best practice guidelines and resources for the re-use of research data • Providing advice and support for translational research projects • eTRIKS is a consortium supported by the Innovative Medicines Initiative **David Henderson, Liaison Manager, Bayer Pharma AG**	**Structure-Guided Discovery Of Novel Non-Steroidal Selective Glucocorticoid Receptor Modulators (SGRMs) And Optimization To Clinical Candidates For Inhalation Administration** 1. Structure and biophysics guided discovery of novel SGRM lead (Matti Lepistö) • Identification of key structural triggers for *in vitro* functionality of Glucocorticoid receptor (GR) modulators • Ligand-induced differentials of co-regulator recruitment • Hybrid lead from different SGRM series enabling step change in potency 2. Inhalation design principles applied leading to clinical candidates (Martin Hemmerling) • Soft drug design for minimized systemic exposure of active principles • Optimized solid state properties for increased lung retention along with 24h duration of effect in an airway inflammation model **Matti Lepistö, Associate Principal Scientist, AstraZeneca and Martin Hemmerling, Principal Scientist, AstraZeneca R&D Mölndal**
14.40 – 15.00	**Afternoon Refreshments**	

For more information please contact marketing@oxfordglobal.co.uk

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Day 2 – Tuesday 9th June

	Preclinical Biomarkers and Translational Medicine	Drug Design: Novel Approaches
	Conference Room: Burgund III	**Conference Room: Burgund I**
	Stream Chair:	**Stream Chair: Markus Kossner, Scientific Services Manager, Chemical Computing Group**
15.00 – 15.30	**ARGX-110 Immunotherapy For Malignancies: A Biomarker Approach** • CD70, a TNF family member modulating immune response via interaction with CD27, is highly expressed by multiple tumor types • ARGX-110 antibody, targeting CD70, provides a multi-pronged approach to tackle tumors and their microenvironment • Biomarker strategy developed to measure target-mediated efficacy and disease modification for ARGX-110 oncology trials **Luc Van Rompaey, VP Translational Medicine, arGEN-X**	**Design Of Multitarget Drugs** • polypharmacology: an introduction • recognition of polypharmacological drug action • multitarget drugs: design concepts • case studies of multitarget drugs **Eugen Proschak, Junior Professor, Goethe University of Frankfurt**
15.30 – 16.00	**Preclinical Biomarkers In CNS Drug Discovery** • Early integration of biomarker validation and development in drug discovery projects to increase efficacy of CNS drug development • The importance of target engagement biomarkers with clinical translatability • The stony road towards biomarkers for CNS disease progression **Christoph Weissner, Chief Operating Officer, Asceneuron SA**	**Kinetics Of Protein-Ligand Unbinding: Predicting Pathways, Rates, And Rate-Limiting Steps** A crucial factor for drug efficacy is not just the binding affinity, but also the mean residence time in the binding pocket, usually quantified by its inverse, k_{off}.This is an important parameter that regulates the time during which the drug is active. Whereas the calculation of the binding affinity is by now routine, the calculation of k_{off} has proven more challenging because the timescales involved far exceed the limits of standard molecular dynamics simulation. We propose a metadynamics-based strategy that allows reaching timescales of seconds, and estimate k_{off} along with unbinding pathways and associated dynamical bottlenecks. A few practical examples are worked out. This work is a step towards a more effective computer-based drug design. **Michele Parrinello, Professor in Computational Sciences, ETH Zürich and Università Della Svizzera Italiana**
16.00 – 16.30	**Developing Clinically Relevant Preclinical Models For Cancer Immunotherapy: A Complex Task** • Cancer immunotherapy: what's missing in most common preclinical tumour models for drug development • Moving towards "high bar" preclinical tumour models - from xenografts to immuno-competent to humanized models; from cell lines to GEMMs to PDX • In vivo profiling of cancer immuno-therapies in clinically relevant preclinical tumor models **Sara Colombetti, Group Leader Immunopharmacology, Roche Innovation Center Zürich**	**Molecular Design: Examples For An Interactive Approach** • Interactive software tools allow medicinal chemists to insert their knowledge and intuition in an optimal way • In library design, interactivity can replace rigid workflows for compound selection allowing to customize focussed screening collections • In lead optimization, structure-based design can be coupled with efficient scoring systems to create an interactive protein-sensitive editor for leads. **Matthias Rarey, Professor, University of Hamburg**
16.30	**End of Conference**	