EFMC-ISMC 2016

Confirmed Speakers

Award & Prize Lectures

NAUTA AWARD FOR PHARMACOCHEMISTRY
Molecular Recognition Studies with Chemical and Biological Systems: A Multi-Dimensional Approach to Support Structure-Based Drug Design



Prof. François DIEDERICH
(ETH ZURICH, Zürich, Switzerland)

UCB-EHRLICH AWARD FOR EXCELLENCE IN MEDICINAL CHEMISTRY
Traversing the Valley of Death in Anticancer Drug Discovery



Prof. Paul J. HERGENROTHER
(UNIVERSITY OF ILLINOIS, Urbana, United States)

IUPAC-RICHTER PRIZE
The Discovery of Sofosbuvir: A Breakthrough Curative Therapy for Hepatitis C



Dr Michael SOFIA
(ARBUTUS BIOPHARMA, Doylestown, United States)

PROUS INSTITUTE-OVERTON AND MEYER AWARD FOR NEW TECHNOLOGIES IN DRUG DISCOVERY
Nanobody-Enabled HTS for the Discovery of GPCR Agonists



Prof. Jan STEYAERT
(VUB, Brussels, Belgium)

Plenary Lectures

The European Research Council (ERC) and its Support for Medicinal Chemistry



Prof. Klaus BOCK
(UNIVERSITY OF COPENHAGEN , Copenhagen, Denmark)

Cross-Coupling Approaches to Saturated N-Heterocycles



Prof. Jeffrey BODE
(ETH ZURICH, Zürich, Switzerland)

Science, Art and Drug Discovery, a Personal Perspective



Sir Simon CAMPBELL
(SCIENTIFIC CONSULTANT, Poole, United Kingdom)

Robotics, Artificial Intelligence, and Medicinal Chemistry: A Look Into the Future

Confirmed Speakers



Dr Derek LOWE
(VERTEX PHARMACEUTICALS, Cambridge, United States)

DNA-Encoded Chemical Libraries



Prof. Dario NERI
(ETH ZÜRICH, Zürich, Switzerland)

Late-Stage Fluorination



Prof. Tobias RITTER
(MAX-PLANCK-INSTITUT FÜR KOHLENFORSCHUNG, Mulheim, Germany)

Heterocycles and Medicinal Chemistry: The Importance of Innovative Synthesis



Dr Anthony WOOD
(PFIZER, Stevenage, Herts, SG1 2NY, United Kingdom)

Invited Speakers

Peptide Drugs to Target GPCR - State of the Art and Innovative Applications

Challenges in the Discovery of Sigma-1 Receptor Antagonists for the Treatment of Pain



Dr Carmen ALMANSA
(ESTEVE, Barcelone, Spain)

Histone Acetyltransferase Inhibitors, from Screening to Optimization - a Tricky Track



Prof. Jonathan BAELL
(MONASH UNIVERSITY, Parkville, Australia)

Direct and Synergistic Inhibition of The HCV NS5A Protein



Dr Makonen BELEMA
(BRISTOL-MYERS SQUIBB, Wallingford, United States)

RSC Prize Lecture:
Chemical Pharmacology of Protein Conjugates and Natural Products (2016 Chem Soc Rev Emerging Investigator Lectureship)



Prof. Gonçalo BERNARDES
(INSTITUTO DE MEDICINA MOLECULAR, PORTUGAL & UNIVERSITY OF CAMBRIDGE, Cambridge, United Kingdom)

The Painful Reality of Drug Discovery and Development

Confirmed Speakers

Dr Paul BESWICK
(UNIVERSITY OF SUSSEX, Brighton, United Kingdom)

Tackling Neurodegenerative Diseases Through Multi-Target and Theranostic Small Molecules



Prof. Maria Laura BOLOGNESI
(UNIVERSITY OF BOLOGNA, Bologna, Italy)

Towards a More Generalized and Automated Approach for Small Molecule Synthesis



Prof. Martin D. BURKE
(UNIVERSITY OF ILLINOIS, Urbana, United States)

Regorafenib Eye Drops for Wet AMD – Challenges in Translatability of Preclinical Data Into Clinical Efficacy



Dr Michael BÖTTGER
(BAYER PHARMA, Wuppertal, Germany)

The Need of Implementing Intramolecular Hydrogen Bonding (IMHB) Considerations in Drug Discovery and How to do it



Prof. Giulia CARON
(UNIVERSITY OF TORINO, Torino, Italy)

RSC Prize Lecture:
Advanced Chemical Genetics for Epigenetics: Bump and Hole and PROTACs (2016 MedChemComm Emerging Investigator Lectureship)



Prof. Alessio CIULLI
(UNIVERSITY OF DUNDEE, Dundee, United Kingdom)

Identification of Allosteric Inhibitors of GPCRs Using SBDD



Dr Miles CONGREVE
(HEPTARES, Welwyn Garden City, United Kingdom)

Pharmacological Reversion of Antibiotic Resistance in Mycobacterium Tuberculosis : Design of SMART Trojan Molecules to Reprogram The Bacteria



Prof. Benoit DEPREZ
(INSTITUT PASTEUR OF LILLE, Lille, France)

New Antibacterial Agents in the Pipeline



Dr Eric DESARBRE
(BASILEA PHARMACEUTICA, Basel, Switzerland)

Confirmed Speakers

Expanding the Macrocycle Chemical Space



Prof. Alexander DÖMLING
(UNIVERSITY OF GRONINGEN, Groningen, The Netherlands)

Exploiting Linked Open Data - Transporter Profiling and Beyond



Prof. Gerhard ECKER
(UNIVERSITY OF VIENNA, Vienna, Austria)

Releasing the Brake on Apoptosis. Discovery of Bcl-2 Family Protein Inhibitors



Dr Steven ELMORE
(ABBVIE, North Chicago, United States)

New Pseudokinase Drug Targets in the Human Kinome



Prof. Patrick EYERS
(UNIVERSITY OF LIVERPOOL, Liverpool, United Kingdom)

Switch Control Inhibitors: an Advance in Type II Kinase Inhibition



Dr Daniel FLYNN
(DECIPHERA PHARMACEUTICALS, Lawrence, United States)

Intramolecular Hydrogen Bond Expectations in Medicinal Chemistry



Dr Fabrizio GIORDANETTO
(D.E. SHAW RESEARCH LLC, New York, United States)

Research, Development & Innovation at Aché Laboratórios Farmacêuticos



Dr Cristiano GUIMARAES
(ACHÉ PHARMACEUTICAL, Brazil)

Discovery and Development of the Highly Potent, Highly Selective Cathepsin S Inhibitor RG7625 for the Treatment of Autoimmune Diseases



Dr Wolfgang HAAP
(F. HOFFMANN-LA ROCHE, Basel, Switzerland)

Phage-Encoded Combinatorial Chemical Libraries Based on Bicyclic Peptides



Prof. Christian HEINIS
(ECOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE (EPFL), Lausanne, Switzerland)

Confirmed Speakers

The Design and Evaluation of URAT1 Inhibitors for the Treatment of Hyperuricemia and Gout

Dr David HEPWORTH
(PFIZER MEDICINES DESIGN, Cambridge, United States)

Discovery of AZD3241 is a Potent and Selective Myeloperoxidase Inhibitor for the Treatment of Neurodegenerative Disorders



Dr Jörg HOLENZ
(ASTRAZENECA NEUROSCIENCE, Collegeville, United States)

The Development of Pyrrolobenzodiazepine in Antibody Drug Conjugates



Dr Philip HOWARD
(SPIROGEN LTD, London, United Kingdom)

Utilization of Novel Benzoxaboroles as Drug Candidates to Treat Neglected Tropical Diseases



Dr Robert T. JACOBS
(ANACOR PHARMACEUTICALS, California, United States)

Inhibition of Prenylated KRAS: Tools to Discover and Characterize RAS Ligands



Dr Johanna JANSEN
(NOVARTIS, Emeryville, United States)

The Identification of GSK2879552, a Mechanism Based Irreversible Inhibitor of the Histone Lysine Demethylase LSD1



Dr Neil W. JOHNSON
(GLAXOSMITHKLINE, Collegeville, United States)

Possibilities and Pitfalls: Disease Modifying Drugs for Alzheimer's Disease



Dr Eric KARRAN
(FOUNDATIONAL NEUROSCIENCE CENTER, ABBVIE, Cambridge, United States)

The Cellular Uptake of Pharmaceutical Drugs is Transporter-Mediated - A Problem not of Biophysics but of Systems Biology



Prof. Douglas KELL
(UNIVERSITY OF MANCHESTER, Manchester, United Kingdom)

Peptides and Peptidomimetics: Overcoming Problems of Activity, Selectivity and Bioavailability of Integrin Ligands



Dr Horst KESSLER
(TECHNISCHE UNIVERSITÄT MÜNCHEN, Garching, Germany)

Confirmed Speakers

Robot Scientists, the Replication Crisis, and Cancer



Prof. Ross KING
(UNIVERSITY OF MANCHESTER, Manchester, United Kingdom)

Validating New Epigenetic Targets by Selective Protein Interaction Inhibitors of Bromodomains



Prof. Stefan KNAPP
(GOETHE UNIVERSITY FRANKFURT, Frankfurt am Main, Germany)

Discovery of the HCV NS5A Inhibitor MK-8408 (RUZASVIR)



Dr Joe KOZLOWSKI
(MERCK, SHARP & DOHME, Rahway, United States)

Intramolecular Hydrogen Bonding as a Design Element in Medicinal Chemistry



Dr Bernd KUHN
(F. HOFFMANN-LA ROCHE, Basel, Switzerland)

DNA-Encoded Chemical Library for Protein-Protein Interactions



Dr Jin LI
(HITGEN LTD , Chengdu, Sichuan, China)

First Time Disclosure of a Development Candidate to Treat Severe Acute Pancreatitis through a Drug Discovery Partnership Between GSK and the University of Edinburgh



Dr John LIDDLE
(GLAXOSMITHKLINE, Mölndal, Sweden)

Ligand-Targeted Therapeutic and Imaging Agents for Multiple Human Diseases



Prof. Philip S. LOW
(PURDUE UNIVERSITY, West Lafayette, United States)

Targeting the Janus-Faced Nature of IDO1 in Immuno-Oncology



Prof. Antonio MACCHIARULO
(UNIVERSITY OF PERUGIA, Perugia, Italy)

Enterobactin-Dependent Iron Uptake Pathway as a Gate for Antibiotic Trojan Horse Strategies Against Pseudomonas Aeruginosa



Dr Gaëtan MISLIN
(UNIVERSITY OF STRASBOURG, Illkirch-Graffenstaden, France)

Confirmed Speakers

The Back of The Eye: Treatment Challenges and Opportunities



Dr Muneto MOGI
(NOVARTIS INSTITUTES FOR BIOMEDICAL RESEARCH, Cambridge, United States)

Molecular Design, Synthesis and Trypanocidal Activity of Dipeptidyl Nitriles as Cruzain Inhibitors



Prof. Carlos MONTANARI
(UNIVERSITY OF SAO PAULO, Sao Paulo, Brazil)

Medicinal Chemistry of Purinergic Signalling: Targets and Drugs for the Immunotherapy of Cancer



Prof. Christa MÜLLER
(UNIVERSITY OF BONN, Bonn, Germany)

Potent and Highly Selective Bromodomain Ligands… a Platform for Reaction Discovery



Prof. Cristina NEVADO
(UNIVERSITY OF ZURICH, Zurich, Switzerland)

Small Molecule Approaches to Immune-Modulation in Cancer



Dr Ronan O'HAGAN
(MERCK, SHARP & DOHME, Boston, United States)

Molecular Pharmacodynamics of Visual Cycle Modulators in Protection Against Retinal Degeneration



Prof. Krzysztof PALCZEWSKI
(CASE WESTERN RESERVE UNIVERSITY, Cleveland, United States)

Targeted Covalent Inhibitors of Bruton's Tyrosine Kinases - Design, Evaluation and Follow-up



Prof. Zhengying PAN
(PEKING UNIVERSITY, Shenzhen, China)

Discovery of AG-120 – A First-in-class Inhibitor of IDH1 Mutant Enzymes for the Treatment of Cancers Harboring IDH1 Mutations



Dr Janeta POPOVICI-MULLER
(AGIOS PHARMACEUTICALS, United States)

Discovery of a First-in-Class PAR4 Antagonist as a Novel Antithrombotic



Dr Scott PRIESTLEY
(BRISTOL-MYERS SQUIBB, Hopewell, United States)

Confirmed Speakers

Antibody Imaging and Therapy Using in Vivo Click and Click-to-Release Strategies



Dr Marc ROBILLARD
(TAGWORKS PHARMACEUTICALS, Eindhoven, The Netherlands)

Discovery of Clinical Candidate Ribuvaptan, a Dual Acting Vasopressin V1a/V2 Receptor Antagonist for the Treatment of Heart Failure



Dr Carsten SCHMECK
(BAYER, Wuppertal, Germany)

Big Dada in Medicinal Chemistry?



Prof. Gisbert SCHNEIDER
(ETH ZÜRICH, Zürich, Switzerland)

Mechanistic and Inhibition Studies on Metallo-Beta-Lactamases



Prof. Christopher J. SCHOFIELD
(UNIVERSITY OF OXFORD, Oxford, United Kingdom)

Solute Carriers, Metabolism and Drug Response: a Magic Triangle



Prof. Giulio SUPERTI-FURGA
(RESEARCH CENTER FOR MOLECULAR MEDICINE (CEMM), Vienna, Austria)

Discovery of Novel LPA1 Antagonist: Design and SAR Studies



Dr Masahiko TERAKADO
(ONO PHARMACEUTICAL, Osaka, Japan)

Discovery & Optimzation of Clips-Constrained Bicyclic Peptides (2clips) Using Pepscan Peptide Arrays



Prof. Peter TIMMERMAN
(PEPSCAN THERAPEUTICS, Lelystad, The Netherlands)

Nucleophilic Boron for the Preparation of Highly Functionalized Small Rings



Prof. Mariola TORTOSA
(AUTONOMOUS UNIVERSITY OF MADRID, Madrid, Spain)

Targeting Long-Chain Fatty Acid Receptors FFA1 and FFA4 for Treatment of Metabolic Diseases



Prof. Trond ULVEN
(UNIVERSITY OF SOUTHERN DENMARK, København Ø, Denmark)

Confirmed Speakers

Broad Multiparametric Profiling of Kinase Inhibitors



Dr Herman VAN VLIJMEN
(JANSSEN, Beerse, Belgium)

The Discovery and Development of Novel Macrofilaricidal Agents for the Treatment of Onchocerciasis and Lymphatic Filariasis



Dr Thomas VON GELDERN
(ABBVIE, Chicago, United States)

Chemical Biological Modulation of KRas-Signaling



Prof. Herbert WALDMANN
(MAX PLANCK INSTITUTE OF MOLECULAR PHYSIOLOGY, Dortmund, Germany)

Small Molecule Binding Sites on the RAS: SOS Complex Can Be Exploited for Inhibition of RAS Activation



Dr. Jon WINTER-HOLT
(ASTRAZENECA, Macclesfield, United Kingdom)

Studying Ciliary Trafficking and How it Leads to RAS Drug Candidates



Prof. Alfred WITTINGHOFER
(MAX PLANCK INSTITUTE OF MOLECULAR PHYSIOLOGY, Dortmund, Germany)

Advances in the Development of Covalent EGFR Inhibitors: from Early Hits to Osimertinib



Dr Gail WRIGLEY
(ASTRAZENECA, Cambridge, United Kingdom)

Discovery of Brain-Penetrable LpPLA2 Inhibitor for Alzheimer's Disease



Dr Xiaomin ZHANG
(GLAXOSMITHKLINE, Shanghai, China)

Chemical Biology Efforts in Cancer Drug Discovery



Prof. Huchen ZHOU
(SHANGHAI JIAO TONG UNIVERSITY, Shanghai, China)

Oral Communication

Anti-Wolbachia (A·WOL) Drug Discovery: Novel Hit Finding Via Ligand Based Virtual Screening Combined With HTS

Confirmed Speakers



Dr Neil G BERRY
(UNIVERSITY OF LIVERPOOL, Liverpool, United Kingdom)

EFMC Prize for a Young Medicinal Chemist in Academia
Sigma Hole Bonding in Kinase Drug Discovery



Prof. Frank BÖCKLER
(EBERHARD-KARLS UNIVERSITY TUEBINGEN, Tübingen, Germany)

Intramolecular Hydrogen Bonds in the Design of CREBBP Bromodomain Ligands



Prof. Stuart CONWAY
(UNIVERSITY OF OXFORD, Los Angeles, United States)

Discovery of PF-06840003, a Novel IDO1 Inhibitor for Cancer Immunotherapy



Dr Stefano CROSIGNANI
(ITEOS THERAPEUTICS SA, Gosselies, Belgium)

Mining Structural Protein-Ligand Interactions to Navigate Medicinal Chemistry Space



Dr Chris DE GRAAF
(VU UNIVERSITY AMSTERDAM, Cambridge, United Kingdom)

Drug Targets in the Solute Carrier Classification (SLC)



Dr Daniela DIGLES
(UNIVERSITY OF VIENNA, Vienna, Austria)

Antiplatelet and Antithrombotic Activity of 1,2,5-Oxadiazole-2-N-Oxide Derivatives



Mr Luiz Antonio DUTRA
(STATE UNIVERSITY OF SAO PAULO - UNESP, Araraquara, Brazil)

Discovery of Ubrogepant (MK-1602): a Potent, Selective and Orally Bioavailable CGRP Receptor Antagonist for the Acute Treatment of Migraine



Dr Mark FRALEY
(MERCK, SHARP & DOHME, West Point, United States)

The evoSpace - A Synthesis-Driven Environment that Finds Accessible, Well-Behaved Compounds by Design



Dr Marcus GASTREICH
(BIOSOLVEIT, St. Augustin, Germany)

Confirmed Speakers

Atypical Bile Acids as Chemical Probes for Diagnosis and Therapy Monitoring of Progressive Cholestatic Liver Disease in HSD3B7 Patients



Prof. Antimo GIOIELLO
(UNIVERSITY OF PERUGIA, Perugia, Italy)

Photoisomerisable Allosteric Modulators Allow a Fine Control of mGlu Receptors with Light in Vivo (EFMC-YMCS Presentation Prize)



Mr Xavier GÓMEZ-SANTACANA
(VRIJE UNIVERSITEIT AMSTERDAM, Amsterdam, The Netherlands)

Optimising Membrane Interactions to Achieve Duration of Action for Inhaled Drug Candidates



Dr Mark HEALY
(NOVARTIS INSTITUTES FOR BIOMEDICAL RESEARCH, Cambridge, United States)

Towards Low-Risk Painkillers: Human Dipeptidyl Peptidase III (hDPPIII) as a Novel Target for Therapeutic Pain Intervention



Ms Shalinee JHA
(GRAZ UNIVERSITY OF TECHNOLOGY, Graz, Austria)

Delivering First-in-Class In Vitro Chemical Probes Against Poly (ADP Ribose) Glycohydrolase (PARG)



Dr Allan JORDAN
(CANCER RESEARCH UK MANCHESTER INSTITUTE, Manchester, United Kingdom)

Rapid Discovery of Potent and Selective Covalent Inhibitors via Covalent Docking



Dr Nir LONDON
(THE WEIZMANN INSTITUTE OF SCIENCE, Rehovot, Israel)

Attempts at Oral Delivery of a Series of Short Unnatural Peptides: Still Like Pushing a Camel Through the Eye of a Needle?



Dr Claudio MAPELLI
(BRISTOL-MYERS SQUIBB, United States)

Systemic Administration of an Allosteric GSK-3 Inhibitor Delays Photoreceptor Cell Death and Preserves Visual Function in a Retinitis Pigmentosa Mouse Model



Prof. Ana MARTINEZ
(CSIC, Madrid, Spain)

Exploring Hit-Identification Strategies for Energy-Coupling Factor Transporters, a Novel Target for the Development of Antibiotics

Confirmed Speakers



Ms Leticia MONJAS GOMEZ
(UNIVERSITY OF GRONINGEN, Groningen, The Netherlands)

Classification of Adamts Binding Sites: the First Step Toward Selective ADAMTS7 Inhibitors



Mrs Michaela MÜLLER
(UNIVERSITÄT ZU LÜBECK, Lübeck, Germany)

Functionally Irreversible Non-Covalent Inhibitors of FAAH: a Safer Approach?



Dr Philippe NANTERMET
(MERCK & CO. INC (MSD), West Point, United States)

From Fragment to in vivo Activity for a Challenging PPI Target: the Discovery of Potent Inhibitors of the KEAP1-NRF2 Interaction



Dr David NORTON
(ASTEX PHARMACEUTICALS, Cambridge, United Kingdom)

Phenotypic Screening for the Discovery of Novel Molecules for Therapeutic Heart Regeneration



Dr Alleyn T. PLOWRIGHT
(ASTRAZENECA, Cambridge, United Kingdom)

EFMC Prize for a Young Medicinal Chemist in Industry
Inhibition of the COP9 Signalosome as a Novel Approach to Treat Cancer”



Dr Jean QUANCARD
(NOVARTIS, Basel, Switzerland)

How can Advances in Cryo-Electron Microscopy Revolutionize Medicinal Chemistry?



Dr Neil RANSON
(UNIVERSITY OF LEEDS, Leeds, United Kingdom)

Identifying Synthetic Opportunities Using Chemplanner - How Computers Assist Chemists in Covering a Greater Synthetic Space



Dr Orr RAVITZ
(WILEY, Chichester, United Kingdom)

Modulation of RS67,333: from a 5-HT4R Partial Agonist to the Identification of Several Promising Multi-Target Directed Ligands for Alzheimer's Disease

Confirmed Speakers



Prof. Christophe ROCHAIS
(UNIVERSITY OF CAEN, Caen, France)

Novel Antibody-Tetrazine Conjugate for Breast Cancer Imaging



Mr Eduardo RUIVO
(UNIVERSITY OF ANTWERP, Antwerp, Belgium)

Driving Tumors into Mitotic Catastrophe - Lead Generation of MPS1 Inhibitors Leading to Two Clinical Candidates BAY 1161909 and BAY 1217389



Dr Volker K. SCHULZE
(BAYER PHARMA AG, Berlin, Germany)

Effects of Novel Acylhydrazones Derived From 4-Quinolone on the Acetylcholinesterase Activity and A?42 Peptide Fibrils Formation



Mrs Gisele SILVESTRE DA SILVA
(UNICAMP, São Paulo, Brazil)

Non Coding RNA as a Small Molecule Druggable Target



Dr Graham SMITH
(MERCK, SHARP & DOHME, Boston, United States)

First Disclosure of CDZ173 - Discovery of a New Generation of Potent and Selective PI3K Delta Inhibitors for Autoimmune and Inflammatory Diseases



Dr Nicolas SOLDERMANN
(NOVARTIS, Basel, Switzerland)

The Development of DDD853651; a Potential Candidate for the Treatment of Visceral Leishmaniasis



Dr Michael THOMAS
(UNIVERSITY OF DUNDEE, Dundee, United Kingdom)

Interaction of 4,5,6,7-Tetrahydrobenzo[1,2-D]Thiazoles with the Cellular Chaperone HSP90 as a Potential Pathway to Inhibit Hepatitis C Virus Replication



Prof. Tihomir TOMASIC
(UNIVERSITY OF LJUBLJANA, Ljubljana, Slovenia)

Rapid Composition of Tricyclic Spiranoid Lactones: Access to Natural Frames and Application in Selective Silencing of the Pain Receptor TRPV1

Confirmed Speakers



Prof. Dmitry TSVELIKHOVSKY
(THE HEBREW UNIVERSITY OF JERUSALEM, Jerusalem, Israel)

Discovery of In Vivo Active and Selective Diacylglycerol Lipase-Alpha Inhibitors



Prof. Mario VAN DER STELT
(LEIDEN UNIVERSITY, Leiden, The Netherlands)