### **Award & Prize Lectures**

PROUS INSTITUTE-OVERTON AND MEYER AWARD FOR NEW TECHNOLOGIES IN DRUG DISCOVERY Activity-Based Proteomics - Protein and Ligand Discovery on a Global Scale



Prof. Benjamin CRAVATT (THE SCRIPPS RESEARCH INSTITUTE, La Jolla, United States)

# NAUTA AWARD FOR PHARMACOCHEMISTRY Tools and Drugs for Purine Targets - Important Players in Inflammation and Cancer



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

# UCB-EHRLICH AWARD FOR EXCELLENCE IN MEDICINAL CHEMISTRY How Best to Discover Bioactive Small Molecules?



Prof. Adam NELSON (UNIVERSITY OF LEEDS, Leeds, United Kingdom)

## **Plenary Lectures**

# The Therapeutic Challenge of the New Era: Developing and Making Available Life Changing Treatment to Patients with Rare Diseases



Dr Diego ARDIGO (CHIESI GROUP, PARMA, Italy)

## Zika Virus: An Old Virus with a New Face



Prof. Tatjana AVSIC-ZUPANC (UNIVERSITY OF LJUBLJANA, Ljubljana, Slovenia)

## Sugars & Proteins: Glycomimetics to Target Infectious Disease



Prof. Benjamin DAVIS (OXFORD UNIVERSITY, Oxford, United Kingdom)

## It's a Small-Molecule World: Medicinal Chemistry Challenges and Opportunities for the Next Decade



Dr Bayard HUCK (MERCK BIOPHARMA, Darmstadt, Germany)

**Smart Chemical Probes: from Bromodomain Ligands to Natural Products** 

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

Development of Non-Nucleosidic Compounds against DNA Viruses of the Herpes Group. The Era After Nucleosides: Letermovir and Pritelivir



Dr Helga RÜBSAMEN-SCHAEFF (AICURIS GMBH & CO. KG, Wuppertal, Germany)

## Synthetic Glycoconjugate Vaccines against Bacterial Infections



Prof. Peter H. SEEBERGER (MAX PLANCK INSTITUTE OF COLLOIDS AND INTERFACES, Berlin, Germany)

## **Invited Speakers**

## Intracellular DNA Sensing in Health and Disease



Prof. Andrea ABLASSER (EPFL, Lausanne, Switzerland)

# Beyond Single-Target Activities: Using Polypharmacology and Systems Readouts for Compound Selection and Mode-of-Action Analysis



Prof. Andreas BENDER (UNIVERSITY OF CAMBRIDGE, United Kingdom)

### Stuck in a Rut with Old Chemistry



Dr Jonas BOSTRÖM (ASTRAZENECA, Mölndal, Sweden)

# In silico Polypolpharmacology



Dr Giovanni BOTTEGONI (HEPTARES THERAPEUTICS, Welwyn Garden City, United Kingdom)

# Use of Cyclic Dinucleotides (CDNs) to Induce Stimulator of Interferon Genes (STING)-Dependent Antitumor Immunity



Dr Cedric BOULARAN (INVIVOGEN, Toulouse, France)

Towards the Development of Novel Inhibitors for Chikungunya Virus Infection: Approaches in Structure-Activity-Metabolism Relationship (SAMR) Studies



Prof. Christina CHAI (NATIONAL UNIVERSITY OF SINGAPORE, Singapore, Singapore)

# Targeting 'Undruggable' Transcription and Translation Factors for Degradation with Low Molecular Weight Cereblon Modulators



Dr Philip CHAMBERLAIN (CELGENE, San Diego, United States)

### "Micro-Pharmacokinetics": How Local Drug Concentration Influences Observed Binding Kinetics



Prof. Steven CHARLTON (UNIVERSITY OF NOTTINGHAM, Nottingham, United Kingdom)

# Asymmetric Synthesis of Statin API as the Hypolipidemic Agents: The Evolution from the Chemical Kinetic Resolution to the Asymmetric Catalytic Technology (An Odessy)



Prof. Fener CHEN (FUDAN UNIVERSITY, Shanghai Shi, China)

# Modification of Cyclic Dinucleotides to Enhance Modulation of the Innate Immune Response



Dr Diane COE (GLAXOSMITHKLINE, Stevenage, United Kingdom)

### Target Binding Kinetics and its Relevance in the in vivo Context



Dr Liesbeth DE LANGE (UNIVERSITY OF LEIDEN, Leiden, The Netherlands)

# Unravelling the Mysteries of the Sphinx: Novel Targets and Small-Molecule Therapeutics from the Sphingolipid Synthesis and Signaling Pathway



Prof. Bernard FLYNN (MONASH UNIVERSITY, Parkville, Australia)

# Capturing Biological Activity in Natural Product Fragments by Chemical Synthesis



Prof. Karl GADEMANN (UNIVERSITY OF ZÜRICH, Zürich, Switzerland)

## PET Molecular Imaging - an Overview



Prof. Antony GEE (KING'S COLLEGE LONDON, London, United Kingdom)

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### First Time Disclosure of BI 409306, a First in Class PDE9 Inhibitor for the Treatment of CNS Diseases



Dr Riccardo GIOVANNINI (BOEHRINGER INGELHEIM, Biberach, Germany)

## Nonpeptidic Selective Inhibitors of Immunoproteasome



Prof. Stanislav GOBEC (UNIVERSITY OF LJUBLJANA, Ljubljana, Slovenia)

### **Novel Hybrid Macrocyclic Modalities for Structure-Based Protein Mimetics**



Dr Stéphanie GUERET (ASTRAZENECA-MAX PLANCK INSTITUTE SATELLITE UNIT, Mölndal, Sweden)

## Discovery of a Novel Oral NO- and Heme-Independent sGC Activator BAY 1101042



Dr Michael G. HAHN (BAYER HEALTHCARE, Wuppertal, Germany)

# Allosteric Modulation of the mGlu2 Receptor: from Structure-Kinetic Relationships to in vivo Efficacy (2017 MedChemComm Emerging Investigator Lectureship)



Prof. Laura HEITMAN (UNIVERSITY OF LEIDEN, Leiden, The Netherlands)

#### Breaking the Limits in Analyzing Carbohydrate Recognition by NMR



Dr Jesus JIMENEZ-BARBERO (CIC BIOGUNE, Derio, Spain)

### Tankyrase Inhibitor Development: Evidence for Potential in Cancer Immune Therapy

Prof. Stefan KRAUSS (UNIVERSITY OF OSLO, Oslo, Norway)

### The Discovery of Semaglutide - A Journey from Ala Scan to Structural Design of GLP-1 Analogues



Dr Jesper LAU (NOVO NORDISK, Maaloev, Denmark)

# EGFR Triple Mutant L858R\_T790M\_ C797S Recent Set-Backs and New Hope in Fighting Mutant Non-Small Cell Lung Cancer



Prof. Stefan LAUFER (UNIVERSITY OF TÜBINGEN, Tübingen, Germany)

### Artificial Intelligence. Not Just Another Name for in Silico Design



Dr David E. LEAHY (THE DISCOVERY BUS LTD, Macclesfield, United Kingdom)

# Multi-Functional Treatments for Multi-Factorial Neurodegenerative Disorders: the Challenge of Alzheimer's Disease



Dr Mark J. MILLAN (INSTITUT DE RECHERCHES SERVIER, Croissy-sur-Seine, France)

# A Multidisciplinary Strategy to Synthetic Carbohydrate-Based Conjugates for Vaccination against Shigella: from Concept to First-in-Human Study



Dr Laurence MULARD (PASTEUR INSTITUTE, Paris, France)

# Recent Advances in Bifunctional Degrader Molecules (e.g. SNIPER) for Targeted Protein Degradation via the Ubiquitin Proteasome System; Status and Outlook



Dr Mikihiko NAITO (NATIONAL INSTITUTE OF HEALTH SCIENCES, Tokyo, Japan)

### Activity-Based Glycosidase Profiling in Biomedicine and Biotechnology



Prof. Hermen OVERKLEEFT (LEIDEN UNIVERSITY, Leiden, The Netherlands)

#### Obeticholic Acid, Leading in the NASH Race. History and Perspectives



Prof. Roberto PELLICCIARI (TES PHARMA SRL, Corciano, Italy)

#### Discovery of LOU064, a Covalent BTK Inhibitor with Best in Class Selectivity



Dr Robert PULZ (NOVARTIS PHARMA, Basel, Switzerland)

# Synthesis and Fungicidal Activity of a New Family of Oxysterol Binding Protein Inhibitors



Dr Laura QUARANTA (SYNGENTA AG, Basel, Switzerland)

## **Small Molecule Immune Checkpoint Antagonists for Cancer Therapy**



Dr Murali RAMACHANDRA (AURIGENE DISCOVERY TECHNOLOGIES LTD, Bangalore, India)

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## Discovery of RG7916, a Selective SMN2 Splicing Modifier for the Treatment of Spinal Muscular Atrophy



Dr Hasane RATNI (F. HOFFMANN-LA ROCHE LTD, Basel, Switzerland)

# Natural Products as Leads in Agrochemistry



Dr Joachim RHEINHEIMER (BASF, Ludwigshafen am Rhein, Germany)

#### An Iron Hand over Cancer Stem Cells



Dr Raphaël RODRIGUEZ (INSTITUT CURIE, Paris, France)

## Controlling Sphingosine-1-Phosphate Levels as a Therapeutic Strategy



Dr Webster L. SANTOS (VIRGINIA TECH, Blacksburg, United States)

### Design and Rationale for Exquisite Selectivity of Preclinical and Clinical Kinase Inhibitors



Dr Laurent SCHIO (SANOFI, Vitry sur Seine, France)

## PET in Neuroscience Drug Discovery and Development



Dr Magnus SCHOU (KAROLINSKA INSTITUTE, Stockholm, Sweden)

## **Computer-Aided Synthesis Planning**



Dr Marwin SEGLER (BENEVOLENTAI, Cambridge, United Kingdom)

## C-Natruiretic Peptide Agonists for Cardiovascular Disease



Prof. David SELWOOD (UNIVERSITY COLLEGE LONDON, London, United Kingdom)

# Design and Synthesis of Congerners of Cyclic ADP-Ribose, a Ca2+-Mobilizing Second Messenger, Toward Identification of the Target Protein



Prof. Satoshi SHUTO (HOKKAIDO UNIVERSITY, Sapporo, Japan)

# Design, Synthesis, and Mechanism of ?-Glucocerebrosidase Activators for Gaucher's and Parkinson's Diseases



Prof. Richard B. SILVERMAN (NORTHWESTERN UNIVERSITY, Evanston, IL, United States)

### **New Chemical Libraries in Exploration of Chemical Space**



Prof. Jurij SVETE (UNIVERSITY OF LJUBLJANA, Ljubljana, Slovenia)

### Cell Permeability with Beyond 'Rule of 5' Modalities – Do We Understand How This Works?



Dr Nick TERRETT (MERCK SHARP & DOHME RESEARCH GMBH (MSD), Kriens, Switzerland)

#### In vivo Anti-Viral and -Tumor Effect Of 3'3'-cAIMP STING Activation



Dr Martin K. THOMSEN (AARHUS UNIVERSITY, Aarhus C, Denmark)

#### The Zinc-Degrome



Dr Nicolas THOMÄ (FRIEDRICH MIESCHER INSTITUTE FOR BIOMEDICAL RESEARCH, Basel, Switzerland)

# Discovery of JNJ-64619178 as a Potent and Selective PRMT5 Inhibitor for the Treatment of Lung and Hematologic Cancers



Dr Jan Willem THURING (JANSSEN PHARMACEUTICA NV, Beerse, Belgium)

## **Tricyclic Peptides via Templated Tandem CLIPS/CUAAC Cyclizations**



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

## All Bugs are Shallow: Open Source Drug Discovery



Prof. Matthew TODD (UNIVERSITY COLLEGE LONDON, London, United Kingdom)

Targeting the Monomeric Intrinsically Disordered Structural State of Tau and Alpha-Synuclein by Small Molecules as a Potential Therapeutic Strategy for Alzheimer's and Parkinson's Disease



Dr Gergely TOTH (CANTABIO PHARMACEUTICALS INC., Palo Alto, United States)

## Cyclic Dinucleotide STING Agonists as Anti-Tumor Agents



Dr Wes TROTTER (MSD, Boston, United States)

# Discovery of LJN452 (Tropifexor), a Highly Potent, Non-Bile Acid FXR Agonist for the Treatment of Cholestatic Liver Diseases and NASH



Dr David TULLY (NOVARTIS, Emeryville, United States)

## Positive Allosteric Modulators of the GABA-B Receptor



Dr Sean C. TURNER (ABBVIE, Ludwigshafen am Rhein, Germany)

# The Value of Orthogonal Techniques for Elucidating Binding Site(s) of GPCR Allosteric Modulators: a Case Study With Positive Allosteric Modulators of Dopamine Receptors



Dr Anne VALADE (UCB, Braine-l'Alleud, Belgium)

# **New Modalities for Complex and Unprecedented Biological Targets**



Dr Eric VALEUR (ASTRAZENECA, IMED BIOTECH UNIT, Cambridge, United States)

## **Re-Energising Small Molecule Drug Discovery**



Dr Willem VAN HOORN (EXSCIENTIA, Dundee, United Kingdom)

## Synthesis of MedChem-Relevant Gem-Difluorocycloalkane Building Blocks



Prof. Dmytro VOLOCHNYUK (ENAMINE LTD, Kyiv, Ukraine)

## A New Target in Fungal Protein Biosynthesis: Shared Learnings for AgChem and MedChem



Dr Franz VON NUSSBAUM (BAYER AG, Berlin, Germany)

# **Targeting of Cancer Specific Glycopeptide Epitopes**



Prof. Hans WANDALL (UNIVERSITY OF COPENHAGEN, Copenhagen, Denmark)

### Active Site Inhibitors of Sphingosine 1-Phosphate Lyase - Exploring Novel Biology with Tool Compounds



Dr Sven WEILER (BASILEA PHARMACEUTICA INTERNATIONAL LTD., Basel, Switzerland)

## **PET for Oncology Drug Discovery and Development**



Prof. Bert WINDHORST (VU UNIVERSITY MEDICAL CENTER, Amsterdam, The Netherlands)

## Discovery of Peptidomimetics Targeting Protein-Protein Interactions of Alpha-Synuclein



Dr Wolfgang WRASIDLO (UNIVERSITY OF CALIFORNIA SAN DIEGO, La Jolla, United States)

### Small Molecule Immunomodulators that Target Toll-Like Receptors



Prof. Hang YIN (TSINGHUA UNIVERSITY, Beijing, China)

## **Practical Asymmetric Hydrogenation**



Prof. Xumu ZHANG (SOUTHERN UNIVERSITY OF SCIENCE AND TECHNOLOGY, Guangdong, China)

## Understanding Aggregation Inhibition of Alpha-Synuclein and Tau by Small Molecules



Prof. Markus ZWECKSTETTER (MAX PLANCK INSTITUTE FOR BIOPHYSICAL CHEMISTRY, Göttingen, Germany)

### **Oral Communications**

# Discovery and Clinical Evaluation of MK-8150, a Novel Nitric Oxide Donor with a Unique Mechanism of Nitric Oxide Release



Dr Amjad ALI (MERCK & CO. INC., Kenilworth, United States)

### Brain-Penetrant Autophagy Modulators for Treating Neurodegenerative Diseases

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Dr Steve ANDREWS (UNIVERSITY OF CAMBRIDGE, Cambridge, United Kingdom)

Discovery of AZD4573, a Potent and Selective Inhibitor of CDK9 that Enables Transient Target Engagement for the Treatment of Haematological Malignancies



Dr Bernard BARLAAM (ASTRAZENECA, Cambridge, United Kingdom)

First Disclosure of the Clinical Candidate BAY-840, a Potent And Selective hBradykinin B1 Antagonist for the Treatment of Chronic Inflammatory Diseases, Generated within the Bayer-Evotec Strategic Alliance



Dr Stefan BÄURLE (BAYER AG, Berlin, Germany)

Metabotropic Glutamate Receptor Type 2 Positive Allosteric Modulators (mGlu2 Receptor PAMS) as a Transformational Epilepsy Treatment



Dr Jose CID (JANSSEN R&D, Toledo, Spain)

Targeting Non Essential Bacterial Targets as a Novel Route to Counteract Bacterial Resistance



Prof. Gabriele COSTANTINO (UNIVERSITY OF PARMA, Parma, Italy)

EFMC Prize for a Young Medicinal Chemist in Industry
The Challenges of Restoring Programmed Cell Death Through MCL1 Inhibition



Dr Marton CSEKEI (SERVIER RESEARCH INSTITUTE OF MEDICINAL CHEMISTRY, Budapest, Hungary)

Discovery of Candidates for PET Molecular Imaging of Pathological TDP-43 Aggregates in Frontotemporal Dementia and Amyotrophic Lateral Sclerosis Patients



Dr Vincent DARMENCY (AC IMMUNE SA, Lausanne, Switzerland)

New Small-Molecule Immune Checkpoint Inhibitors: A Step Forward in Cancer Immunotherapy



Ms Ana Rita DE CARVALHO ACURCIO (UNIVERSITY OF LISBON, Lisbon, Portugal)

Potency and Patents, New Arenas for Matched Molecular Pair Analysis in the Al World

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Dr Al DOSSETTER (MEDCHEMICA LIMITED, Macclesfield, United Kingdom)

### Synthetic Small-Molecule RNA Ligands: Scope and Therapeutic Applications



Dr Maria DUCA (UNIVERSITÉ CÔTE D'AZUR, Nice, France)

#### **Chemical Probes for New Therapeutic Concept Discovery**



Dr Peter ETTMAYER (BOEHRINGER-INGELHEIM, Vienna, Austria)

# Identification of New Antimalarial GSK607: An Example of Adaptive and Differentiated Early Drug Development



Dr Esther FERNANDEZ (GLAXOSMITHKLINE, Tres Cantos, Spain)

# Development of Potent, Selective, CNS Penetrant Small Molecule Inhibitors of Notum to Potentiate Wnt Signaling for the Maintainance of Synaptic Function in Alzheimer's Disease



Prof. Paul FISH (ARUK UCL DRUG DISCOVERY INSTITUTE, London, United Kingdom)

## Drugging the Fbw7 E3 Ligase with a Combined Computational and Biophysical Approach



Dr Carles GALDEANO (UNIVERSITY OF BARCELONA, Barcelona, Spain)

# Buruli Ulcer and the mTOR Pathway: Total Synthesis, Structure-Activity and Target Elucidation Studies of Mycolactones



Prof. Matthias GEHRINGER (UNIVERSITY OF TUEBINGEN, Tuebingen, Germany)

# Large-Scale Analysis of Kinase Inhibitors' Target Binding Kinetics and its Implications for Drug Discovery



Ms Victoria GEORGI (BAYER AG, Berlin, Germany)

Discovery of the TYK2 Selective Inhibitor PF-6826647 for the Treatment of Crohn's Disease, and Other Autoimmune Conditions

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Dr Brian GERSTENBERGER (PFIZER, Cambridge, United States)

# Integrated System for the Expedited Generation and Characterization of Drug-Like Libraries for Hit-to-Lead Explorations



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

# IUPAC-Richter Prize Lecture Discovery of CFTR Modulators For The Treatment of Cystic Fibrosis



Dr Peter GROOTENHUIS (VERTEX PHARMACEUTICALS, San Diego, United States)

## ASTX660, the First Fragment-Derived IAP Antagonist in the Clinic



Dr Steven HOWARD (ASTEX THERAPEUTICS, Cambridge, United Kingdom)

# Glycoside Antagonists of Bacterial Lectins: New Treatment Options for Recurrent and Antibiotic Resistant



Prof. James JANETKA (WASHINGTON UNIVERSITY IN SAINT LOUIS, Saint Louis, United States)

#### Discovery of First-in Class, Selective and Noncovalent Small Molecule Inhibitors of DNMT1



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

### Discovery of GDC-0077: A Highly Selective Inhibitor and Degrader of Mutant PI3K-Alpha



Dr Jamie KNIGHT (CHARLES RIVER, Harlow, United Kingdom)

## The Discovery of CNP520, an Amino-1,4-Oxazine BACE Inhibitor in Prevention Studies



Dr Rainer MACHAUER (NOVARTIS PHARMA AG, Basel, Switzerland)

A Dual Modulator of Farnesoid X Receptor and Soluble Epoxide Hydrolase to Treat Non-Alcoholic Steatohepatitis (EFMC-YMCS Presentation Prize)

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Dr Daniel MERK (ETH ZÜRICH, Zürich, Switzerland)

### Development of Small-Molecule Inhibitors of Adipose Triglyceride Lipase (ATGL)



Ms Anna MIGGLAUTSCH (TU GRAZ, Graz, Austria)

#### Development of Novel Sialyltransferase Inhibitors via Computer Aided Drug Design



Mr Andrew MONTGOMERY (UNIVERSITY OF WOLLONGONG, Wollongong, Australia)

# Small-Molecule Stabilization of Protein-Protein Interactions by Natural Products, Supramolecular Ligands, Fragments and Macrocycles



Dr Christian OTTMANN (EINDHOVEN UNIVERSITY OF TECHNOLOGY, Eindhoven, The Netherlands)

### AMPA Receptor Positive Allosteric Modulators Based on New Scaffolds: Design, Synthesis, and Studies



Dr Vladimir A. PALYULIN (LOMONOSOV MOSCOW STATE UNIVERSITY, Moscow, Russia)

# Charting the Structure-Resistance Landscape of Novel Antibiotics



Mr Tamas REVESZ (BIOLOGICAL RESEARCH CENTRE, HUNGARIAN ACADEMY OF SCIENCES, Szeged, Hungary)

## Small Molecules Inhibiting PD1-PDL1 Immune Checkpoint



Dr Shabnam SHAABANI (UNIVERSITY OF GRONINGEN, Groningen, The Netherlands)

## Anti-HBV Drug Discovery Enabled by Structure-Based Drug Design and Phenotypic Screening



Dr Hong SHEN (ROCHE INNOVATION CENTER, Shanghai, China)

## Mechanisms of HIV-1 Nucleocapsid Protein Inhibition by Small Molecules Targeting RNA



Dr Alice SOSIC (UNIVERSITY OF PADOVA, Padova, Italy)

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Discovery and Optimization of Non-Covalent, Selective, and Bioavailable Small Molecule Inhibitors of the KEAP1-Nrf2 Pathway



Dr Hauke SZILLAT (SANOFI, Frankfurt, Germany)

EFMC Prize for a Young Medicinal Chemist in Academia Carbohydrate-binding Proteins as Targets for Anti-Infectives and Diagnostics: ESKAPE pathogen Pseudomonas aeruginosa and its Lectins



Dr Alexander TITZ (HELMHOLTZ INSTITUTE FOR PHARMACEUTICAL SCIENCES, Saarbrücken, Germany)

Discovery of SPL-707: A Potent, Selective, and Orally Bioavailable SPPL2a Inhibitor



Dr Juraj VELCICKY (NOVARTIS INSTITUTES FOR BIOMEDICAL RESEARCH, Basel, Switzerland)

The First Class of Orally Available Mono-Saccharide Galectin-3 Inhibitors for Treatment of Fibrosis (NASH) and Cancer



Dr Fredrik ZETTERBERG (GALECTO BIOTECH, Gothenburg, Sweden)

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