

Programme

Plenary Lectures

STRATEGIES FOR THE DISCOVERY OF INNOVATIVE THERAPEUTICS

Prof Magid ABOU-GHARBIA
(TEMPLE UNIVERSITY, Philadelphia, United States)

Life on the Edge: The Nature and Origins of Protein Misfolding Diseases

Prof. Chris DOBSON
(UNIVERSITY OF CAMBRIDGE, Cambridge, United Kingdom)

Drug Discovery for Neglected Diseases

Prof. Paul HERRLING
(NOVARTIS INTERNATIONAL, Basel, Switzerland)

Chemical Tools for the Study of Complex Biological Systems

Prof. Barbara IMPERIALI
(MASSACHUSETTS INSTITUTE OF TECHNOLOGY, Cambridge, United States)

The Nauta Award for Pharmacochemistry (EFMC)
Changing Paradigms in Drug Discovery

Prof. Hugo KUBINYI
(UNIVERSITY OF HEIDELBERG, Weisenheim am Sand, Germany)

The UCB-Ehrlich Award for Excellence in Medicinal Chemistry (EFMC)
Automated Oligosaccharide Synthesis as Platform for Vaccine Development

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

GlaxoSmithKline Award for Outstanding Achievement in the Field of Chemical Biology
Exploring Chemical Space with Aptamers

Dr. Michael FAMULOK
(UNIVERSITY OF BONN, Bonn, Germany)

**The Prous Institute-Overton and Meyer Award for New Technologies in Drug Discovery (EFMC)
New Tools for Molecule Makers: Emerging Technologies**

Prof. Steven V. LEY
(UNIVERSITY OF CAMBRIDGE, Cambridge, United Kingdom)

Session 1. Novel Lead Finding Approaches

Session Chair

Prof. Hans Ulrich STILZ
(SANOFI-AVENTIS, Cambridge, United States)

Integration of Fragment Derived Structure-Based Design into the Discovery and Development of Selective Kinase Inhibitors for Treatment of Human Cancers

Dr. Gavin HIRST
(SGX PHARMACEUTICALS, San Diego, United States)

Fragment Based Lead Discovery

Prof. Roderick E. HUBBARD
(UNIVERSITY OF YORK / VERNALIS, York, United Kingdom)

Search for Taxoid Mimics Using Dynamic Combinatorial Chemistry Targeting Tubulin

Ms Claire LE MANACH
(ICMMO, Orsay, France)

Session 2. Chemistry Strategies to Reduce Attrition in Drug Discovery

Session Chair

Dr Geoffrey STEMP
(GLAXOSMITHKLINE, Harlow, United Kingdom)

From Fragment to Clinic

Dr David REES
(ASTEX THERAPEUTICS, Cambridge, United Kingdom)

Chemical Strategies for Successful Clinical Development

Dr. Christopher N. JOHNSON
(GLAXOSMITHKLINE, Harlow, United Kingdom)

Recent Strategies Around Predicting Oral Absorption

Dr DAVID MILLAN
(PFIZER, Sandwich, United Kingdom)

Session 3. Emerging Drugs

Session Chair

Dr Bernd RIEDL
(BAYER PHARMA, Wuppertal, Germany)

The Discovery and Development of Rivaroxaban

Dr. Susanne ROEHRIG
(BAYER SCHERING PHARMA, Wuppertal, Germany)

Identification and development of PI3K inhibitors - Path to the clinic

Dr. Carlos GARCIA-ECHEVERRIA
(NOVARTIS PHARMA, Basel, Switzerland)

Discovery of TMC278: a Next Generation NNRTI Drug, Highly Active against Human Immunodeficiency Virus Type-1

Dr Jérôme GUILLEMONT
(TIBOTEC, Val de Reuil, France)

Session 4. Kinase Selectivity-Is it Necessary? (ACS)

Session Chair

Prof. David ROTELLA
(WYETH, MONTCLAIR, United States)

Kinase Selectivity in Drug Discovery - the Challenges and Opportunities

Dr. Dennis POWELL
(WYETH RESEARCH, Pearl River, United States)

Development of Dibenzosuberones as Potent and Highly Selective p38 MAPK Inhibitors

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

CDK Inhibition - Selectivity Issues in Principle and in Practice

Dr. Andrew THOMAS
(ASTRAZENECA R&D, Macclesfield, United Kingdom)

Session 5. Predictive ADME/Tox Methods: What to Apply When?

Session Chair

Dr Scott BOYER
(ASTRAZENECA, Barcelona, Spain)

Predictive ADME: Examples from the Real World

Dr. Andrew Mark DAVIS
(ASTRAZENECA R&D, Loughborough, United Kingdom)

Virtual Methods for Predicting Off-Target Pharmacology

Prof. Jordi MESTRES
(IMIM AND UNIVERSITY POMPEU FABRA, Girona, Spain)

Predicting Brain to Blood Drug Partitioning: Progress and Limitations

Prof. Gabriele CRUCIANI
(UNIVERSITY OF PERUGIA, Perugia, Italy)

Session 6. Macromolecular and Polymeric Drugs

Session Chair

Prof. Abraham J. DOMB
(HEBREW UNIVERSITY OF JERUSALEM, Jerusalem, Israel)

PEG Conjugation in Drug Development and Discovery

Prof. Francesco M. VERONESE
(UNIVERSITY OF PADOVA, Padova, Italy)

Multivalency of Polymer Therapeutics Used for the Integration of Anti-angiogenic Therapy with Chemotherapy

Dr. Ronit SATCHI-FAIRANO
(TEL AVIV UNIVERSITY, Tel Aviv, Israel)

5'-Phosphate Mimics within Altritol-Modified siRNAs and Inhibition of MDR1 Expression

Dr Arthur VAN AERSCHOT
(KULEUVEN, LEUVEN, Belgium)

Session 7. Fragment-Based Drug Discovery (ACS)

Session Chair

Dr. Jeffrey ALBERT
(ASTRAZENECA, Wilmington, United States)

EVolution: Design and Implementation of a Fragment Discovery Platform

Dr. John BARKER
(EVOTEC, OXON, United Kingdom)

Fragment-Based Discovery: What Has it Achieved so far?

Dr. Alexander ALEX
(PFIZER, Sandwich, United Kingdom)

Fragment-Based Methods and the Discovery of BACE-1 Inhibitors for Alzheimer's

Dr. Jeffrey ALBERT
(ASTRAZENECA, Wilmington, United States)

Session 8. Imaging Ligands and Biomarkers (EUFEPS)

Session Chair

Prof. Pia VUORELA
(ÅBO AKADEMI UNIVERSITY, Turku, Finland)

Fluorometry and FRET in Measuring Biomarkers and Monitoring Cell Signaling Cascade

Dr. Ilkka HEMMILA
(PERKINELMER LIFE SCIENCES, Turku, Finland)

Mass Sensitive Ligands Useful for Biomarker Discovery and Validation

Dr. Rainer VOEGELI
(PROTEOME SCIENCES, Cobham, United Kingdom)

Design of Spin-Labeled Sulfonamides as Carbonic Anhydrase Inhibitors

Dr Alessandro CECCHI
(UNIVERSITY OF FLORENCE, Sesto Fiorentino, Italy)

Session 9. Natural Products as Starting Points in Drug Discovery

Session Chair

Dr. Erden BANOGLU
(GAZI UNIVERSITY, Ankara, Turkey)

Biodiverse Natural Products in Drug Discovery

Prof. Douglas KINGHORN
(OHIO STATE UNIVERSITY, Columbus, United States)

How to Use The Structural Diversity of Natural Products for Drug Discovery

Dr. Philipp KRASTEL
(NOVARTIS INSTITUTES FOR BIOMEDICAL RESEARCH, Basel, Switzerland)

Selectivity in the Antibacterial Activity of Minor Groove Binders, Derivatives of the Natural Product, Distamycin

Prof Colin SUCKLING
(UNIVERSITY OF STRATHCLYDE, Glasgow, Scotland, United Kingdom)

Session 10. Neurodegenerative Diseases

Session Chair

Prof Magid ABOU-GHARBIA
(TEMPLE UNIVERSITY, Philadelphia, United States)

Protein Misfolding and Self-assembly in Neurodegenerative Diseases: From Mechanistic Studies to Therapeutic Strategies

Prof. Hilal A. LASHUEL
(EPFL, Lausanne, Switzerland)

Approaches to the Treatment of Cognitive Dysfunction and Alzheimer's Disease

Dr AI ROBICHAUD
(SAGE, Princeton, United States)

Halomethylketones (Hmks): Gsk-3 Inhibitors with Disease-Modifying Properties for Alzheimer's Disease Therapy

Prof. Ana MARTINEZ
(INSTITUTO DE QUIMICA MEDICA-CSIC, Madrid, Spain)

Session 11. Type 2 Diabetes

Session Chair

Prof. Koen AUGUSTYNS
(UNIVERSITY OF ANTWERP, Antwerp, Belgium)

DPP-4 Inhibitors: Galvus® / Vildagliptin and Following Generations

Dr. Daniel BAESCHLIN
(NOVARTIS INSTITUTES FOR BIOMEDICAL RESEARCH, Basel, Switzerland)

Peptidic and Nonpeptidic Glucagon-Like Peptide 1 Receptor Agonists

Dr Jesper LAU
(NOVO NORDISK, Maaloev, Denmark)

Irreversible Inhibition of DPP 8/9 by Dipeptide derived Diaryl Phosphonates

Dr Pieter VAN DER VEKEN
(UNIVERSITY OF ANTWERP, Antwerpen, Belgium)

Session 12. Progress in COPD and Asthma Therapy

Session Chair

Dr. Matthias GRAUERT
(BOEHRINGER INGELHEIM, Biberach, Germany)

Recent Developments in CCR3 Antagonists

Dr. George V. DE LUCCA
(BRISTOL-MYERS SQUIBB, Princeton, United States)

PI3Kgamma Inhibitors: Aspirin of the 21st Century?

Dr. Thomas RÜCKLE
(MERCK SERONO, Geneva, Switzerland)

4-Oxo-Beta-Lactams (Azetidine-2,4-diones) Based Novel Potent Inhibitors of Elastase

Dr JALMIRA MULCHANDE
(LISBON UNIVERSITY, Lisbon, Portugal)

Session 13. Allosteric Modulation and GPCR Drug Discovery

Session Chair

Prof. Rob LEURS
(VU UNIVERSITY AMSTERDAM, Amsterdam, The Netherlands)

The Potential of Allosteric Modulation for GPCR Drug Discovery

Prof. Arthur CHRISTOPOULOS
(MONASH UNIVERSITY, Parkville, Australia)

Therapeutic Opportunities for Small Molecule Modulators of Chemokine Receptors

Dr. Thomas J. SCHALL
(CHEMOCENTRYX, Mountain View, United States)

High-Throughput Screening of Potential Drug Candidates For Gpr-17 Receptor by Fac-MS: Development and Application of a New Gpr17 Stationary Phase

Prof. Gabriella MASSOLINI
(UNIVERSITY OF PAVIA, Pavia, Italy)

Session 14. Oncology

Session Chair

Dr Jeremy DAVIS
(UCB, Slough, United Kingdom)

Eg5 Inhibitors

Dr Paul COLEMAN
(MERCK RESEARCH LABORATORIES, Collegeville, United States)

Allosteric Akt Inhibitors

Dr. George HARTMANN
(MERCK RESEARCH LABORATORIES, West-Point, United States)

PLK1 Inhibitor (BI-2536)

Dr. Matthias HOFFMANN
(BOEHRINGER INGELHEIM, Biberach, Germany)

Session 15. Immunology & Immunomodulation

Session Chair

Dr Katerina LEFTHERIS
(VITAE PHARMACEUTICALS, SF Bay Area, CA, United States)

Current Aspects and Future Trends in Immunomodulation

Dr. Qihong ZHAO
(BRISTOL-MYERS SQUIBB, Princeton, United States)

Advances in Targeting Glucocorticoids

Dr. Markus BERGER
(BAYER SCHERING PHARMA, Berlin, Germany)

Target Validation and Lead Identification of Selective Cb2 Receptor Agonists for the Treatment of Inflammation and Pain

Dr Doris RIETHER
(BOEHRINGER-INGELHEIM, Biberach an der Riss, Germany)

Session 16. Antipsychotic Targets

Session Chair

Prof Klaus P BOGESO
(H. LUNDBECK A/S, Valby, Denmark)

NK3 Receptors

Dr Klaus Baek SIMONSEN
(LUNDBECK, San Diego, United States)

PDE10 Inhibitors

Dr Spiros LIRAS
(PFIZER GLOBAL RESEARCH, New York, United States)

Dopamine System Stabilizers

Prof. György DOMANY
(GEDEON RICHTER PLC, Budapest, Hungary)

Session 17. Antivirals

Session Chair

Dr Maria Jose CAMARASA
(CSIC, Madrid, Spain)

Targetting the Glycans on the Viral Envelope, A Novel Therapeutic Concept

Dr. Jan BALZARINI
(REGA INSTITUTE FOR MEDICAL RESEARCH, Leuven, Belgium)

Lethal Mutagenesis as a New Antiviral Strategy

Prof. Esteban DOMINGO
(UNIVERSIDAD AUTONOMA DE MADRID, Madrid, Spain)

'New Developments in NNRTIs of HIV; from TIBO to Rilpivirine

Dr. JAN HEERES
(, Vosselaar, Belgium)

Session 18. Pain

Session Chair

Dr Erin DIMAURO
(AMGEN, Cambridge, United States)

Emerging Treatments for Chronic Pain: Prospects and Challenges.

Dr. Stefan MCDONOUGH
(AMGEN, Cambridge, United States)

Discovery of a Selective TRPV1 Antagonist, AMG 517: A Clinical Candidate for the Treatment of Pain

Mr Mark NORMAN
(AMGEN, Thousand Oaks, United States)

Novel alpha2delta Ligands for the Treatment of Neuropathic Pain

Dr. Graham N. MAW
(PFIZER, Sandwich, United Kingdom)

Session 19. Exploring the Chemical Space

Session Chair

Profs. Herbert WALDMANN & STEFAN WETZEL
(MAX PLANCK INSTITUTE OF MOLECULAR PHYSIOLOGY, Dortmund, Germany)

Computer-Assisted Molecular Design: Voyages to the (un)known

Prof. Gisbert SCHNEIDER
(JOHANN WOLFGANG GOETHE UNIVERSITY, Zürich, Switzerland)

The Quest for Bioisosterism in the “Other Side” of Chemical Space

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

Exploration of Chemical Space for Drug Discovery by Database Generation

Prof. Jean-Louis REYMOND
(UNIVERSITY OF BERN, Bern, Switzerland)

Scaffold Hunter: Charting and Exploring Chemical Space

Dr. Stefan WETZEL
(MAX PLANCK INSTITUTE OF MOLECULAR PHYSIOLOGY, Dortmund, Germany)

Session 20. Chemokines

Session Chair

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

CXCR4 Antagonists: Relevance to Cancer Chemotherapy

Prof. Nobutaka FUJII
(KYOTO UNIVERSITY, Kyoto, Japan)

Selective Dual CCR2/5 Antagonists

Dr. Wolfgang MILTZ
(NOVARTIS PHARMA, Basel, Switzerland)

Biological Profiling of Anti-HIV Agents using in Silico Techniques: Insights into CCR5 Ligands Binding Through Homology Buildings, 3D-QSAR, Docking and Shape Matching Virtual Screening

Mr Antonio CARRIERI
(DDIPARTIMENTO FARMACO-CHIMICO, Bari, Italy)

Session 21. Systems Level Research Informs Drug Target Identification and Therapy Design

Session Chair

Prof. Harel WEINSTEIN
(CORNELL UNIVERSITY, New York, United States)

Drug Discovery, Drug Delivery and Therapeutic Monitoring by Molecular, Cellular and Functional Imaging of Atherothrombosis

Dr. Zahi A. FAYAD
(MOUNT SINAI SCHOOL OF MEDICINE, New York, United States)

Understanding Drug Mechanisms and Designing Therapy at the Systems Level of the Functional Human Interactome

Prof. Gianni CESARENI
(UNIVERSITY OF ROME 'TOR VERGATA', Rome, Italy)

Special Structural, Dynamic and Functional Characteristics of Membrane Proteins and their Signaling Partners that Determine the Mode and Putative Success of Therapy Design Targeting Cellular Signaling Systems.

Prof. Harel WEINSTEIN
(CORNELL UNIVERSITY, New York, United States)

Session 22. New Computational Approaches Supporting Drug Design

Session Chair

Prof. Jordi MESTRES
(IMIM AND UNIVERSITY POMPEU FABRA, Girona, Spain)

Overview on New Computational Tools Supporting Drug Design

Prof. Tudor I. OPREA
(UNIVERSITY OF NEW MEXICO, San Diego, CA, United States)

Novel Tools for Data Gathering

Dr. Muthukumarasamy KARTHIKEYAN
(NATIONAL CHEMICAL LABORATORY, Pune, India)

Novel Tools for Data Classification

Dr Ansgar SCHUFFENHAUER
(NOVARTIS INSTITUTES FOR BIOMEDICAL RESEARCH, Basel, Switzerland)

Novel Tools for Data Exploitation

Dr. Elisabet GREGORI-PUIGJANE
(CHEMOTARGETS, Barcelona, Spain)

Session 23. Druggability of Protein-Protein Interactions

Session Chair

Mr Peter NUSSBAUMER
(LEAD DISCOVERY CENTER, DORTMUND, Germany)

Mapping the Binding Site of Substrate Targeting Gamma-secretase Modulators. Phase III Candidates for Alzheimer's Disease Utilize a Novel Protein-protein Interaction

Prof. Boris SCHMIDT
(TU DARMSTADT, Darmstadt, Germany)

Rational Design of Cytotoxic Peptides from the Analysis of Protein-Protein Interactions in Microtubules

Dr pieraccini STEFANO
(UNIVERSITY OF MILANO, Milano, Italy)

Peptidomimetic Inhibitors of the PSD-95/NMDA Receptor Interaction

Mr Anders BACH
(UNIVERSITY OF COPENHAGEN, Copenhagen, Denmark)

Dynamic Ligation Screening: A Method for the Site-Directed Discovery of Inhibitory Fragments

Prof Jörg RADEMANN
(UNIVERSITÄT LEIPZIG, Leipzig, Germany)

Session 24. Systems Biology and Medicinal Chemistry

Session Chair

Prof Christian NOE
(UNIVERSITY OF VIENNA, Vienna, Austria)

Network Based Drug Discovery

Prof. Hans WESTERHOFF
(VU UNIVERSITY AMSTERDAM, Amsterdam, The Netherlands)

Systems Biology – What Does it Mean for Pharmaceutical Science?

Prof Christian NOE
(UNIVERSITY OF VIENNA, Vienna, Austria)

Integrated Approach for the Multireceptorial Design of Antipsychotic Agents

Dr Jana SELENT
(UNIVERSITAT POMPEU FABRA, Barcelona, Spain)

Session 25. Structure Based Drug Design (AFMC)

Session Chair

Prof. Esin AKI-SENER
(ANKARA UNIVERSITY, Ankara, Turkey)

Quantum Chemical Calculation of Protein-Ligand Interaction

Prof. Isao NAKANISHI
(KYOTO UNIVERSITY, Higashi-osaka, Japan)

Inhibiting ROS Toxicity in Alzheimer's Disease: Structural Studies of Amyloid-Beta and Metal Ion Complexes

Dr. Jose VARGHESE
(CSIRO, Parkville, Australia)

Access and Binding of Local Anesthetics in the Closed Sodium Channel

Ms Iva BRUHOVA
(MCMaster UNIVERSITY, Hamilton, Canada)

Session 26. Modulators of Adenosine and P2Y Receptors

Session Chair

Prof. Kenneth A. JACOBSON
(NIDDK, Bethesda, United States)

Engineering of Purine Receptors and Their Ligands

Prof. Kenneth A. JACOBSON
(NIDDK, Bethesda, United States)

New modulators of A3 and A2B adenosine receptors

Prof. Pier Giovanni BARALDI
(UNIVERSITY OF FERRARA, Ferrara, Italy)

Allosteric Modulation of Purine Receptors

Prof. Ad P. IJZERMAN
(LEIDEN UNIVERSITY, Leiden, The Netherlands)

Session 27. Addressing Therapeutic Complexity in Oncology with Med. Chem.

Session Chair

Dr Janet ROBERTSON
(TES PHARMA, Corciano , Italy)

Alternatives to Kinase Inhibitors for Cancer Therapies

Prof. Giovanni GAVIRAGHI
(SIENA BIOTECH, Siena, Italy)

Endothelin Converting Enzyme Inhibitors as Anticancer Agents for Human Glioblastoma. A Comparison with Endothelin Receptor Antagonists

Dr. Lucienne JUIILLERAT
(CENTRE HOSPITALIER UNIVERSITAIRE VAUDOIS, Lausanne, Switzerland)

Structure-Activity Relationships and Cancer-Selective Toxicity of Novel Inhibitors of Gli1 Transcription

Dr Naoaki FUJII
(ST.JUDE CHILDREN'S RESEARCH HOSPITAL, Memphis, United States)

FORUM DISCUSSION

A.Golinowska3 [LINK TO FORUM DISCUSSION PARTICIPANTS](#)

How to close the gap between academic training in medicinal chemistry and industrial reality?

Moderator

Prof. Péter MÁTYUS
(SEMMEIWEIS UNIVERSITY, Budapest, Hungary)

WORKSHOPS

[ACCELRY'S NIKEM LINK TO WORKSHOPS DESCRIPTION](#)

ACCELRY'S

A.Golinowska COOL TOOLS FROM ACCELRY'S: HELPING TO AUTOMATE MEDICINAL CHEMISTRY EVERYDAY TASKS
(BIOVIA, Belgium)

NIKEM RESEARCH

A.Golinowska2 FROM IDEAS TO PRECLINICAL CANDIDATES: MEDCHEM-DRIVEN DRUG DISCOVERY AT NIKEM