

Programme

Sunday September 4, 2022

13:30 Registration

AGORA HALL

16:00 Opening Ceremony

Dr Luc VAN HIJFTE (SYMERES, Nijmegen, The Netherlands)
Prof. Rebecca DEPRez-POULAIN (INSERM - UNIVERSITÉ DE LILLE / INSTITUT PASTEUR OF LILLE, Lille, France)
Prof. Rui MOREIRA (UNIVERSITY OF LISBON, Lisbon, Portugal)
ATHENA AUDITORIUM

16:20 EFMC Fellows Ceremony

Prof. Rui MOREIRA
(UNIVERSITY OF LISBON, Lisbon, Portugal)

16:35 Opening Lecture - Patient Testimonial

Chair

Dr Tatjana ROSS
(MERCK HEALTHCARE KGAA, Darmstadt, Germany)

16:50 Musical Interlude

17:00 EFMC Awards Ceremony

Prof. Rui MOREIRA
(UNIVERSITY OF LISBON, Lisbon, Portugal)

**17:20 NAUTA PHARMACOCHEMISTRY AWARD FOR MEDICINAL CHEMISTRY AND CHEMICAL BIOLOGY
AL001 - Pseudo Natural Products – Chemical Evolution of Natural Product Structure**

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

Chairs

Prof. Henk TIMMERMAN (VU UNIVERSITY AMSTERDAM, Oegstgeest, The Netherlands)
Dr Anede NAUTA (PROF. DR. W. TH NAUTA STICHTING, The Netherlands)

18:05 GDCh - Klaus Grohe Prize Ceremony

Laudatio

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

Prize Ceremony

Dr Rolf ALBACH
(GDCH & COVESTRO, Cologne, Germany)

Programme

- 18:15** **KLAUS GROHE PRIZE**
PR001 - Discovery of a Druggable Copper-signaling Pathway that Drives Cell Plasticity and Inflammation
Dr Raphaël RODRIGUEZ
(INSTITUT CURIE, Paris, France)
- 19:00** **Welcome Reception sponsored by WuXi AppTec**

RHODES HALL
- 20:00** **End of the Day**

Programme

Monday September 5, 2022

08:00 **Registration**

AGORA HALL

08:30 **UCB EHRLICH AWARD FOR EXCELLENCE IN MEDICINAL CHEMISTRY**
AL002 - Small Molecule Drugs and where to find them - Approaches to Hit Generation and Lead Optimisation

Prof. Mike WARING
(NEWCASTLE UNIVERSITY, Newcastle upon Tyne, United Kingdom)

ATHENA AUDITORIUM

Chair

Dr Adrian HALL
(UCB BIOPHARMA SRL, Braine-l'Alleud, Belgium)

09:15 **PL001 - Boosting « Chance and Necessity » with Experience and Molecular Creativity**

Prof. Benoit DEPRez
(INSTITUT PASTEUR DE LILLE, Lille, France)

Chair

Dr Luc VAN HIJFTE
(SYMERES, Nijmegen, The Netherlands)

10:00 **Exhibition & Coffee**

RHODES HALL

Session Session 1 'Chemical Biology'

Beyond PROTACS, Monovalent and Glues Degraders

RHODES12 AUDITORIUM

10:30 **Session Chair**

Dr Laura M. LUH
(BAYER, Wuppertal, Germany)

10:35 **LE001 - Strategies to Discover Molecular Glue Degraders at Scale**

Dr Cristina MAYOR-RUIZ
(IRB BARCELONA, Barcelona, Spain)

11:15 **LE002 - Haven't Got a Glue: Protein Surface Variation for the Design of Molecular Glue Degraders**

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

11:35 **LE003 - Antibody-Protac Conjugates: an Approach for Targeted Selective BRD4 Degradation in HER2+ Phenotypes**

Dr Maria MANEIRO
(UNIVERSIDADE DE SANTIAGO DE COMPOSTELA, Santiago de Compostela, Spain)

11:55 **LE004 - Discovery And Profiling of AZ'6421: an Oral ER α -Protac with an in vitro-in vivo Disconnect**

Dr Thomas HAYHOW
(ASTRAZENECA, Cambridge, United Kingdom)

Session Session 2 'Drug Discovery'

Renaissance of Natural-Product Inspired Drug Discovery in the 21st Century

ATHENA AUDITORIUM

10:30 **Session Chair**

Dr Boris VAUZEILLES
(INSTITUT DE CHIMIE DES SUBSTANCES NATURELLES, Gif-sur-Yvette, France)

Programme

- 10:35 LE005 - Big Data Analyses for the Discovery of Lead Structures from Nature**
Prof. Judith ROLLINGER
(UNIVERSITY OF VIENNA, Vienna, Austria)
- 11:15 LE006 - Design of Naturally Inspired Anti-Cancer Compounds that Modulate Cholesterol Homeostasis**
Dr Fanny ROUSSE
(ICSN - CNRS, Gif sur Yvette, France)
- 11:35 LE007 - Reduce to the Max: Functionally Optimized Natural Products via Chemical Synthesis**
Prof. Karl GADEMANN
(UNIVERSITY OF ZÜRICH, Zürich, Switzerland)
- 11:55 LE008 - Tuning the Reactivity of the Natural Product Andrographolide: Towards Targeted Covalent Inhibitors for the Treatment of Inflammation**
Prof. Christina CHAI
(NATIONAL UNIVERSITY OF SINGAPORE, Singapore, Singapore)

Session Session 3 'Technologies'

Methods for Late-Stage Functionalization

HERMES AUDITORIUM

10:30

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

10:35 LE009 - New Synthetic Chemistry to Probe the Biology of Modified Nucleic Acids

Prof. Matthew GAUNT
(UNIVERSITY OF CAMBRIDGE, Cambridge, United Kingdom)

11:15 LE010 - Tritiation of Pharmaceuticals Via Late Stage C-H Functionalization

Dr Dieter MURI
(ROCHE · PHARMA RESEARCH AND EARLY DEVELOPMENT (PRED), Basel, Switzerland)

11:35 LE011 - Late-Stage Functionalizations

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

11:55 LE012 - Chemical Modification of Wild-type Proteins

Dr Bauke ALBADA
(WUR, Wageningen, The Netherlands)

12:15 Exhibition & Lunch

RHODES HALL

12:15 Schrödinger workshop
Digital Chemistry in Action: Combining physics-based modelling, AI/ML and experimental data in collaborative decision making

ROOM RISSO 8

12:15 Mestrelab Research workshop
Automate your analytical workflows with Mnova Gears: Relieve your teams from long and tedious tasks!

ROOM RISSO 6

Session Flash Poster Session 1

FP01 to FP10

Opportunity for 10 young scientists to present a summary of their poster

Discover the presenters [here](#)

RHODES12 AUDITORIUM

RHODES12 AUDITORIUM

Programme

Session Flash Poster Session 2

FP11 to FP20

Opportunity for 10 young scientists to present a summary of their poster

Discover the presenters [here](#)

ATHENA AUDITORIUM

ATHENA AUDITORIUM

Session Flash Poster Session 3

FP21 to FP30

Opportunity for 10 young scientists to present a summary of their poster

Discover the presenters [here](#)

HERMES AUDITORIUM

HERMES AUDITORIUM

Session Session 4 'Chemical Biology'

Targeting Epigenetic Modifications in Cancer Therapy / ICBS Session

RHODES12 AUDITORIUM

13:45 Session Chair

Prof. Zaneta NIKOLOVSKA-COLESKA
(UNIVERSITY OF MICHIGAN, Ann Arbor, United States)

13:50 LE013 - Disrupting hDot1L and MLL Oncofusion Protein Interactions as a Novel Therapeutic Strategy

Prof. Zaneta NIKOLOVSKA-COLESKA
(UNIVERSITY OF MICHIGAN, Ann Arbor, United States)

14:30 LE014 - New Opportunities for Studying the Function of the Nucleosome Remodeling Factor, NURF, Through Inhibition and Degradation

Prof. William POMERANTZ
(UNIVERSITY OF MINNESOTA, Minneapolis, United States)

14:50 LE015 - New Generation of EZH2 Inhibitors for Cancer Therapy: A Computer-Aided Drug Design Approach in Epigenetics

Dr Filipa RAMILO-GOMES
(UNIVERSITY OF LISBON, Lisboa, Portugal)

15:10 EFMC-YMCS Prize 2021

LE016 - A Mating Mechanism to Generate Diversity for the Darwinian Selection of DNA-encoded Synthetic Molecules

Mr Lluç FARRERA SOLER
(UNIVERSITY OF GENEVA, Geneva, Switzerland)

Session Session 5 'Drug Discovery'

Drugging the Undruggable : Targeting Transcription Factors / ACSMEDI Session

ATHENA AUDITORIUM

13:45 Session Chair

Dr Anthony ROMERO
(ORIC PHARMACEUTICALS, South San Francisco, United States)

13:50 LE017 - Chemical Probe Discovery for Recalcitrant Targets *Virtual Presentation*

Prof. Angela KOEHLER
(MIT KOCH INSTITUTE FOR INTEGRATIVE CANCER RESEARCH, Cambridge, United States)

14:30 LE018 - Transcription Factors as Drug-Discovery Targets

Prof. Fraydoon RASTINEJAD
(UNIVERSITY OF OXFORD, Oxford, United Kingdom)

14:50 LE019 - Discovery of KB-0742, a Potent, Selective, Orally Bioavailable Small Molecule Inhibitor of CDK9/Cyclin T1 for MYC-Dependent Cancers

Dr David FREEMAN
(KRONOS BIO, INC. , Massachussetts, United States)

Programme

15:10 LE020 - Inhibiting the MYC Oncogene through Cell Active Max-E47 (ME-47)

Dr Amy BITTNER MCCracken
(MSD, New Jersey, United States)

Session Session 6 'Technologies'

Hit Discovery with DNA-Encoded Libraries

HERMES AUDITORIUM

13:45 Session Chair

Dr Andreas BRUNSCHWEIGER
(TU DORTMUND, Dortmund, Germany)

13:50 LE021 - Innovating DNA-encoded Chemical Library Technology for Better Ligand Discovery

Dr Jörg SCHEUERMANN
(ETH ZÜRICH, Zürich, Switzerland)

14:30 LE022 - A DNA Barcode with Enhanced Chemical Stability for DNA-encoded Library Design

Dr Andreas BRUNSCHWEIGER
(TU DORTMUND, Dortmund, Germany)

14:50 LE023 - Exploiting DNA-encoded Library Technology for the Discovery of Novel Antibody Recruiting Molecules Against LOX-1

Ms Katherine MACFARLANE
(UNIVERSITY OF STRATHCLYDE, London, United Kingdom)

15:10 LE024 - Photoactivated Covalent Capture of DNA-encoded Fragments to Identify Ligands for Challenging Targets

Prof. Roderick HUBBARD
(VERNALIS, Cambridge, United Kingdom)

15:30 Exhibition & Coffee

RHODES HALL

Session SCT (Société de Chimie thérapeutique) Prize Session

ATHENA AUDITORIUM

16:00 Ceremony for the 2022 Galapagos Award for Drug Discovery Chemistry (in partnership with Société de Chimie thérapeutique)

Chairs

Prof. Rebecca DEPRez-POULAIN (INSERM - UNIVERSITÉ DE LILLE / INSTITUT PASTEUR OF LILLE, Lille, France)

Dr Alexis DENIS (GALAPAGOS, Ile de France, France)

**16:10 GALAPAGOS AWARD LECTURE (Award-winning Team: Bioversys/University of Lille/GSK)
LE025 - Rejuvenating Ethionamide for Treatment of Tuberculosis - TRICKy, but Possible**

Dr Modesto REMUINAN
(GSK, Tres Cantos (Madrid), Spain)

Session Session 7

First Time Disclosures - Part 1

ATHENA AUDITORIUM

16:30 Session Chair

Dr Pilar MANZANO-CHINCHON
(GLAXOSMITHKLINE, Tres Cantos (Madrid), Spain)

16:35 LE026 - First-time Disclosure of M1069, a Highly Selective Dual Inhibitor of Adenosine A_{2a}/A_{2b} Receptors With Improved Therapeutic Activity Compared to A_{2a} Receptor Selective Antagonists

Dr Kai SCHIEMANN
(MERCK HEALTHCARE KGAA, Darmstadt, Germany)

17:05 LE027 - Discovery of BI 456906, a Novel Long-acting GCG/GLP-1 Receptor Dual Agonist for the Treatment of Patients With Obesity

Programme

Dr Peter HAEBEL
(BOEHRINGER INGELHEIM PHARMA GMBH & CO. KG, Biberach Riss, Germany)

17:35 LE028 - Discovery of AZD5462, an Oral Agonist of the Relaxin Family Peptide Receptor 1 (RXFP1) for the Treatment of Cardiorenal Disease

Dr Kenneth GRANBERG
(ASTRAZENECA, Mölndal, Sweden)

18:05 Poster Session 1 & Networking

AGORA HALL

19:35 End of the Day

Programme

Tuesday September 6, 2022

**08:30 PROUS INSTITUTE - OVERTON AND MEYER AWARD FOR NEW TECHNOLOGIES IN DRUG DISCOVERY
AL003 - How PROTACs Work: Molecular Recognition and Design Principles**
Prof. Alessio CIULLI
(UNIVERSITY OF DUNDEE, Dundee, United Kingdom)
ATHENA AUDITORIUM

08:30 Chair
Dr Josep Jr. PROUS
(PROUS INSTITUTE FOR BIOMEDICAL RESEARCH, Barcelona, Spain)

09:15 PL002 - The Shape and Modification of RNA in Health and Disease
Prof. Eric MISKA
(UNIVERSITY OF CAMBRIDGE, Cambridge, United Kingdom)

09:15 Chair
Dr Maria DUCA
(UNIVERSITY OF CÔTE D'AZUR, Nice, France)

10:00 Exhibition & Coffee

RHODES HALL

Session Session 8 'Chemical Biology'

Addressing Cooperative Ligand Binding in Drug Discovery / EUCHEMS Session

RHODES12 AUDITORIUM

- 10:30 Session Chair**
Prof. Luc BRUNSVELD
(EINDHOVEN UNIVERSITY OF TECHNOLOGY, Eindhoven, The Netherlands)
- 10:35 LE029 - Fragment-Based Approaches to Stabilize Protein-Protein Interactions**
Prof. Michelle ARKIN
(UNIVERSITY OF CALIFORNIA, San Francisco, CA, United States)
- 11:15 LE030 - Development of Bisubstrate Inhibitors to Tackle Epigenetics**
Dr Paola B. ARIMONDO
(INSTITUT PASTEUR - CNRS, Paris, France)
- 11:35 LE031 - Identification and Structure-activity Relationship Profiling of Positive Allosteric Modulators Targeting Muscarinic Acetylcholine Receptors**
Dr Manuela JORG
(MONASH UNIVERSITY, Parkville, Australia)
- 11:55 LE032 - Molecular Glues for the 14-3-3 Interactome**
Dr Richard DOVESTON
(UNIVERSITY OF LEICESTER, Leicester, United Kingdom)

Session Session 9 'Drug Discovery'

Time to Act Against Antimicrobial Resistance

ATHENA AUDITORIUM

- 10:30 Session Chair**
Prof. Maria-Jesus PÉREZ-PÉREZ
(INSTITUTO DE QUÍMICA MÉDICA, Madrid, Spain)
- 10:35 LE033 - The Global Antibiotic R&D Partnership: Helping to Advance the Discovery & Development of New Treatments for Bacterial Infections**
Dr Benjamin BLASCO
(THE GLOBAL ANTIBIOTIC RESEARCH & DEVELOPMENT PARTNERSHIP (GARDP) , Geneva, Switzerland)

Programme

- 11:15 LE034 - Novel Tetrazole Inhibitor of Mycobacterium Tuberculosis Tryptophan Synthase**
Dr Lourdes ENCINAS
(GLAXOSMITHKLINE, Madrid, Spain)
- 11:35 LE035 - Discovery and Preclinical Development of ANT3310, a Broad-Spectrum β -Lactamase Inhibitor which Potentiates Meropenem Against Carbapenem-Resistant Bacteria**
Dr David DAVIES
(ANTABIO SAS, Labège, France)
- 11:55 LE036 - Discovery of Pseudomonas Aeruginosa Elastase LasB Inhibitors by in Situ Click Chemistry**
Dr Virgyl CAMBERLEIN
(HIPS - HELMHOLTZ-INSTITUT FÜR PHARMAZEUTISCHE FORSCHUNG SAARLAND, Saarbrücken, Germany)

Session Session 10 'Technologies'

New Screening Technologies : Affinity Selection - Mass Spectrometry

HERMES AUDITORIUM

- 10:30 Session Chair**
Dr Didier ROCHE
(EDELIRIS, Lyon, France)
- 10:35 LE037 - Adapting the Affinity MS Technology to GPCR Ligand Discovery *Virtual Presentation***
Prof. Wenqing SHUI
(SHANGHAITECH UNIVERSITY, Shanghai, China)
- 11:15 LE038 - EDELIRIS Keychemical Space™ and GPCR : Identification of Allosteric Binders by AS-MS**
Dr Renaud PRUDENT
(EDELIRIS, Lyon, France)
- 11:35 LE039 - High Throughput Affinity Screening for Rapid Hit Discovery and Prosecuting Intractable Targets**
Dr Jarrod WALSH
(ASTRAZENECA, Macclesfield, United Kingdom)
- 11:55 LE040 - Accelerating Drug Discovery with the Integration of Affinity Selection Mass Spectrometry (ALIS)**
Mr Bryan CHOI
(RELAY THERAPEUTICS, Cambridge, United States)

12:15 Exhibition & Lunch

RHODES HALL

- 12:15 WuXi AppTec workshop**
Introduction to Self-Service DNA-Encoded libraries (DELs)

ROOM RISSO 6

- 12:15 Chemical Computing Group workshop**
De Novo Design of Novel Compounds to Meet Multiple Property Constraints

ROOM RISSO 8

Session Flash Poster Session 4

FP31 to FP40

Opportunity for 10 young scientists to present a summary of their poster

Discover the presenters [here](#)

RHODES12 AUDITORIUM

RHODES12 AUDITORIUM

Programme

Session Flash Poster Session 5

FP41 to FP50

Opportunity for 10 young scientists to present a summary of their poster

Discover the presenters [here](#)

ATHENA AUDITORIUM

ATHENA AUDITORIUM

Session Flash Poster Session 6

FP51 to FP60

Opportunity for 10 young scientists to present a summary of their poster

Discover the presenters [here](#)

HERMES AUDITORIUM

HERMES AUDITORIUM

Session Session 11 'Chemical Biology'

Targeting Self-Associating Proteins & Biomolecular Condensates in Drug Discovery

RHODES12 AUDITORIUM

13:45 Session Chair

Prof. Raphaël FREDERICK
(UCLOUVAIN, Brussels-Woluwe, Belgium)

13:50 LE041 - Targeting Protein-Protein Interactions of Receptor Complexes

Prof. Kristian STROMGAARD
(UNIVERSITY OF COPENHAGEN, Copenhagen, Denmark)

14:30 LE042 - Leveraging Biomolecular Condensates for Drug Discovery

Dr Marta FRIGOLE-VIVAS
(DEWPOINT THERAPEUTICS GMBH, Dresden, Germany)

14:50 LE043 - Polarity-sensitive Fluorescent Probes for Cellular Organelles: from Chemical to Genetically Encoded Targeting

Dr Andrey KLYMCHENKO
(UNIVERSITÉ DE STRASBOURG, Illkirch, France)

15:10 LE044 - Interrogating Lactate Dehydrogenases Oligomeric Interfaces Using (Stapled) Peptides And Small Molecules

Dr Léopold THABAULT
(INSTITUTE OF CANCER RESEARCH, London, United Kingdom)

Session Session 12 'Drug Discovery'

Covalent Drugs

ATHENA AUDITORIUM

13:45 Session Chair

Dr Samir JEGHAM
(SANOFI R&D, Montpellier, France)

13:50 LE045 - Inhibiting KRAS: Strategies, Structures, and Lessons Learned in the Invention of Sotorasib

Dr Brian LANMAN
(AMGEN, Thousand Oaks, CA, United States)

14:30 LE046 - Covalent Fragment Approaches in Drug Discovery

Prof. György KESERU
(HUNGARIAN ACADEMY OF SCIENCES, Budapest, Hungary)

14:50 LE047 - Discovery of Covalent Protein Kinase Inhibitors Targeting Cysteines in the Hinge Region

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

15:10 LE048 - Discovery of Novel Covalent, EGFR WT Sparing, HER2 Selective Inhibitors for the Treatment of Her2 Exon 20 Insertion Driven Tumours

Programme

Dr Birgit WILDING
(BOEHRINGER INGELHEIM, Vienna, Austria)

Session Session 13 'Technologies'

Next Generation Medicinal Chemistry - an EFMC² Session

HERMES AUDITORIUM

- 13:45 Session Chair**
Dr Clara CHRIST
(BAYER, Berlin, Germany)
- 13:50 Introduction to EFMC²**
Dr Richard LEWIS (NOVARTIS PHARMACEUTICALS, Basel, Switzerland)
Dr Franz VON NUSSBAUM (NUVISAN, Berlin, Germany)
- 14:00 LE049 - Driving Lead Optimization with BRADSHAW**
Dr Darren GREEN
(GSK, Stevenage, United Kingdom)
- 14:30 LE050 - A Perspective on AI and Automation for the Medicinal Chemistry Lab *Virtual Presentation***
Prof. Connor COLEY
(MIT, Cambridge, United States)
- 14:50 LE051 - The Power and Pitfalls of Machine Learning in Early Stage Drug Discovery**
Prof. Charlotte DEANE
(UNIVERSITY OF OXFORD, Oxford, United Kingdom)
- 15:10 LE052 - Using AI to Derive Valuable Insights from Drug Discovery Data**
Dr Matthew SEGALL
(OPTIBRIUM, Cambridge, United Kingdom)
- 15:30 Exhibition & Coffee**

RHODES HALL

Session Session 14

First Time Disclosures -Part 2

ATHENA AUDITORIUM

- 16:00 Session Chair**
Dr Leena OTSOMAA
(ORION PHARMA, Espoo, Finland)
- 16:05 LE053 - mPGES1 Inhibitors: First Time Disclosure of Clinical Candidate BI01029539 / GS-248**
Dr Roland PFAU
(BOEHRINGER INGELHEIM PHARMA GMBH&CO. KG, Ingelheim am Rhein, Germany)
- 16:35 LE054 - First Disclosure of Cannabinoid Receptor Type 2 Agonist Rg7774 – An Innovative Oral Treatment for Diabetic Retinopathy**
Dr Uwe GREETHER
(F. HOFFMANN-LA ROCHE, Basel, Switzerland)
- 17:05 LE055 - Discovery and Optimisation of Potent, Slow-dissociating Inhaled PI4KB Inhibitors**
Dr Sophie BERTRAND
(GSK, Stevenage, United Kingdom)
- 17:35 LE103 - Discovery of a Selective Oral CCR4 Antagonist RPT193 for Treatment of Atopic Dermatitis and other Allergic Disorders**
Dr Mikhail ZIBINSKY
(RAPT THERAPEUTICS, INC., South San Francisco, United States)
- 18:05 Poster Session 2 & Networking**

AGORA HALL

- 19:35 End of the Day**

Programme

Programme

Wednesday September 7, 2022

- 08:30 PL003 - Necessity is the Mother of Invention: Natural Products and the Chemistry They Inspire**
Prof. Sarah E. REISMAN
(CALIFORNIA INSTITUTE OF TECHNOLOGY, Pasadena, United States)
ATHENA AUDITORIUM
- Chair**
Prof. Karl-Heinz ALTMANN
(ETH ZÜRICH, Zürich, Switzerland)
- 09:15 EFMC Prizes for Young Medicinal Chemist or Chemical Biologist in Academia and in Industry Ceremony & Lectures**
- Chair**
Prof. Rui MOREIRA
(UNIVERSITY OF LISBON, Lisbon, Portugal)
- 09:20 EFMC PRIZE FOR A YOUNG MEDICINAL CHEMIST OR CHEMICAL BIOLOGIST IN INDUSTRY PR002 - Chemical Biology Strategies Applied to Phenotypic Screening and Targeted Protein Degradation Discovery Programs**
Dr Marie-Helene LARRAUFIE
(ALMIRALL, Barcelona, Spain)
- 09:40 EFMC PRIZE FOR A YOUNG MEDICINAL CHEMIST OR CHEMICAL BIOLOGIST IN ACADEMIA PR003 - Chemical Biology Tools for Enlightening Drug Discovery**
Prof. Olalla VÁZQUEZ
(PHILIPPS-UNIVERSITÄT MARBURG, Marburg, Germany)
- 10:00 Exhibition & Coffee**

RHODES HALL

Session Session 15 'Chemical Biology'

In vivo Chemistry to Study Biological Mechanisms and to Develop Innovative Tools for Therapy and Diagnosis

RHODES12 AUDITORIUM

- 10:30 Session Chair**
Dr Frédéric TARAN
(CEA/SACLAY, Gif-sur-Yvette, France)
- 10:35 LE056 - Chemically-Triggered Payload Release in-vivo**
Dr Marc ROBILLARD
(TAGWORKS PHARMACEUTICALS, Eindhoven, The Netherlands)
- 11:15 LE057 - Tumor Activated Therapy**
Prof. Sebastien PAPOT
(UNIVERSITY OF POITIERS, Poitiers, France)
- 11:35 LE058 - Investigating and Controlling mRNAs Via Chemo-enzymatic Modification**
Prof. Andrea RENTMEISTER
(UNIVERSITY OF MÜNSTER, Münster, Germany)
- 11:55 LE059 - Fast Detection and Imaging of Hydrogen Peroxide with New Borinic Probes**
Dr Boris VAUZEILLES
(INSTITUT DE CHIMIE DES SUBSTANCES NATURELLES, Gif-sur-Yvette, France)

Programme

Session Session 16 'Drug Discovery'

Rising Horizons of Small Molecule Immunotherapies and Beyond

ATHENA AUDITORIUM

10:30 Session Chair

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

10:35 LE060 - Tipping the Balance: MALT1 Inhibitors with Paradoxical Effects on the Immune System

Dr Jean QUANCARD
(NOVARTIS, Basel, Switzerland)

11:15 LE061 - The discovery of the Clinical Candidate AZD0284, a Orally Bioavailable Inverse Agonist of RORγ for the Treatment of Psoriasis

Dr Frank NARJES
(ASTRAZENECA, Gothenburg, Sweden)

11:35 LE062 - Macrolide Inspired Macrocycles as Effective Disruptors of the IL-17A/IL-17RA Interaction

Dr Dijana PESIC
(SELVITA, Zagreb, Croatia)

11:55 LE063 - NR2F6 Antagonists: in Vitro Pharmacology and Preclinical Data of a Potential Next Generation Immuno-oncology Therapy

Dr Francesco GRECO
(TES PHARMA SRL, Corciano, Italy)

Session Session 17 'Technologies'

Innovative Synthetic Technologies for Drug Discovery

HERMES AUDITORIUM

10:30 Session Chair

Dr Cara BROCKLEHURST
(NOVARTIS, Basel, Switzerland)

10:35 LE064 - Molecular Vending Machines for the On-Demand Synthesis of Drug-Like Molecules

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

11:15 LE065 - Photocatalysis in Drug Discovery

Dr Lisa CANDISH
(BAYER, Wuppertal, Germany)

11:35 LE066 - Visible-light Photocatalysis: a Powerful Tool in the Pursuit of New Pharmaceuticals

Dr Giulia BERGONZINI
(ASTRAZENECA, Gothenburg, Sweden)

11:55 LE067 - Iridium-catalyzed C-H Activation Methods for Late-stage Functionalization of Pharmaceuticals

Dr Erik WEIS
(ASTRAZENECA, Mölndal, Sweden)

12:15 Exhibition & Lunch

RHODES HALL

Session Session 18

Highlights in Medicinal Chemistry Part 1

RHODES12 AUDITORIUM

13:15 Session Chair

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

13:20 LE068 - Formulation Strategies for Compounds with Challenging Physicochemical Properties

Programme

Prof. Guy VAN DEN MOOTER
(KULEUVEN, Leuven, Belgium)

14:00 LE069 - Dual Inhibition of P53-MDM2/4 Interactions With Spiropyrazoline Oxindoles

Ms Elizabeth A. LOPES
(UNIVERSITY OF LISBON, Lisboa, Portugal)

14:20 LE070 - Optimization of TEAD P-Site Binding Fragment Hit into In Vivo Active Lead MSC-4106

Dr Timo HEINRICH
(MERCK, DARMSTADT, Germany)

14:40 LE071 - A New Dual Mode of Action to Treat Pain - From Scratch to Pre-Clinical Candidate

Dr Anita WEGERT
(SYMERES, Nijmegen, The Netherlands)

Session Session 19 'Drug Discovery'

Targeting RNA by Small Molecules
Session Sponsored by Sanofi

ATHENA AUDITORIUM

13:15 Session Chair

Dr Hasane RATNI
(SKYHAWK THERAPEUTICS, Basel , Switzerland)

13:20 LE072 - Enabling Technologies for Revealing Druggable Paths in RNA Biology

Dr Amanda GARNER
(UNIVERSITY OF MICHIGAN, Ann Arbor, United States)

14:00 LE073 - Targeting RNA with Small Molecules, A New Therapeutic Strategy

Dr Yann FORICHER
(SANOFI, Vitry-sur-Seine, France)

14:20 LE074 - Fundamental Basis for SMN2 Specific Splicing Correction by Small Molecules and Bulge Repair Mechanism

Dr Sébastien CAMPAGNE
(INSERM BORDEAUX, BORDEAUX, France)

14:40 LE075 - Bis-3-chloropiperidines Targeting TAR RNA as a Novel Strategy to Impair the HIV-1 Nucleocapsid Protein

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

Session Session 20 'Technologies'

AI in Drug Discovery / CPA Session

HERMES AUDITORIUM

13:15 Session Chair

Prof. Mingyue ZHENG
(SHANGHAI INSTITUTE OF MATERIA MEDICA, Shanghai, China)

13:20 LE076 - Uncertainty Quantification: Considering the Reliability of Artificial Intelligence in Drug Design *Virtual Presentation*

Dr Dingyan WANG
(SHANGHAI INSTITUTE OF MATERIA MEDICA, Shanghai, China)

14:00 LE077 - Innovative Therapeutic Target Discovery based on OMIC Technology and Machine Learning *Virtual Presentation*

Prof. Feng ZHU
(ZHEJIANG UNIVERSITY, Hangzhou, China)

14:20 LE078 - Opportunity and Challenge of Artificial Intelligence (AI) in Drug Delivery *Virtual Presentation*

Prof. Defang OUYANG
(MACAU UNIVERSITY, Macau, China)

14:40 LE079 - In Silico Prediction of Brain Penetration - High Accuracy Achieved

Dr Herve GENESTE
(ABBVIE, Ludwigshafen, Germany)

Programme

15:00 **End of the Day**

15:45 **Excursions**

20:00 **Banquet**

Programme

Thursday September 8, 2022

Session Session 21 'Chemical Biology'

Mining the Phosphosignaling Networks

RHODES12 AUDITORIUM

08:30 Session Chair

Dr Nadia AHMAD
(CHARLES RIVER LABORATORIES, Harlow, United Kingdom)

08:35 LE080 - The Phosphatase Family: a Widely Neglected Target Space for Small-Molecule Drug Discovery

Dr Gerhard MÜLLER
(ANAVO THERAPEUTICS, Leiden, The Netherlands)

09:15 LE081 - A Novel Fragment-Based Ligand Design Tool : Application to Kinase Research

Prof. Pascal BONNET
(UNIVERSITY OF ORLÉANS, Orléans, France)

09:35 LE082 - Protein Phosphatase 2A, a Druggable Tumor Suppressor for Cancer Therapy

Prof. Jukka WESTERMARCK
(UNIVERSITY OF TURKU, Turku, Finland)

09:55 LE083 - Mining the Leishmania Kinome

Dr Exequiel PORTA
(DURHAM UNIVERSITY, Durham, United Kingdom)

Session Session 22 'Drug Discovery'

New Treatments for Current and Future Pandemics

ATHENA AUDITORIUM

08:30 Session Chair

Prof. Ana MARTINEZ
(CSIC, Madrid, Spain)

08:35 LE084 - Searching for Drugs against Pandemic Viruses

Dr Carmen GIL
(CENTRO DE INVESTIGACIONES BIOLÓGICAS (CSIC), Madrid, Spain)

09:15 LE085 - Addressing Current Challenges in Antiviral Therapies Against Emerging RNA Viruses

Dr Karine ALVAREZ
(AIX-MARSEILLE UNIVERSITY, Marseille, France)

09:35 LE086 - Embrace Complexity: in Silico Polypharmacological Profiling to Repurpose Medicines and Design New Drugs

Dr Andrea BECCARI
(DOMPÉ PHARMA, L'Aquila, Italy)

09:55 LE087 - Human Dihydroorotate Dehydrogenase Inhibitor MEDS443: a Magic Bullet Against Coronaviruses

Dr Stefano SAINAS
(UNIVERSITY OF TORINO, Torino, Italy)

Session Session 23

Highlights in Medicinal Chemistry Part 2

HERMES AUDITORIUM

08:30 Session Chair

Prof. Roberto DI SANTO (SAPIENZA UNIVERSITY OF ROME, Rome, Italy)
(SANOFI-AVENTIS DEUTSCHLAND GMBH)

08:35 IUPAC-RICHTER PRIZE 2022

PR004 - Drug Discovery in Academia: A Drug For Glioblastoma Multiforme

Prof. Michael E. JUNG
(UCLA CHEMISTRY & BIOCHEMISTRY, Los Angeles, United States)

Programme

- 09:15 LE088 - Discovery of Clinical Candidate CHF-6366: a Super-soft Heterobifunctional Muscarinic Antagonist and α 2-adrenoceptor Agonist (MABA) for the Inhaled Treatment of Respiratory Diseases**
Dr Laura CARZANIGA
(CHIESI FARMACEUTICI SPA, PARMA, Italy)
- 09:35 LE089 - Discovery of JNJ-1245, a Novel and Potent Fluoroallylamide Mcl-1 Inhibitor for the Treatment of Hematologic Malignancies**
Dr Soufyan JERHAOU
(JANSSEN PHARMACEUTICA NV, Beerse, Belgium)
- 09:55 LE090 - Structure-Guided Design of Foldamer-Based Inhibitors of Protein-Protein Interactions**
Dr Gilles GUICHARD
(UNIVERSITY OF BORDEAUX, CBMN, Bordeaux, France)

10:15 Exhibition & Coffee

RHODES HALL

Session Session 24 'Chemical Biology'

Chemical Probes for Target Identification & Validation / EUFEPS Session

RHODES12 AUDITORIUM

- 10:45 Session Chair**
Dr Joanna REDMOND
(FRANCIS CRICK INSTITUTE, London, United Kingdom)
- 10:50 LE091 - Chemical Probes and How to Find Them**
Dr Alex PAUTSCH
(BOEHRINGER INGELHEIM PHARMA GMBH & CO. KG, Biberach, Germany)
- 11:30 LE092 - De Novo Cyclic Peptides as Chemical Tools to Explore Epigenetic Regulation**
(SANOFI-AVENTIS DEUTSCHLAND GMBH)
Dr Louise WALPORT (THE FRANCIS CRICK INSTITUTE, London, United Kingdom)
- 11:50 LE093 - Chemical Probes for Targets in Lipid Signalling**
Prof. Eugen PROSCHAK
(GOETHE UNIVERSITY OF FRANKFURT, Frankfurt/Main, Germany)
- 12:10 LE094 - First Selective Nanomolar Inhibitors of ERAP2 for Modulation of the Antigen Presentation**
Prof. Rebecca DEPREZ-POULAIN
(INSERM - UNIVERSITÉ DE LILLE / INSTITUT PASTEUR OF LILLE, Lille, France)

Session Session 25 'Drug Discovery'

Drug Discovery in Targeting Neurodegenerative Disorders / ACSMEDI Session

ATHENA AUDITORIUM

- 10:45 Session Chair**
Prof. Rong HUANG
(PURDUE UNIVERSITY, West Lafayette, IN, United States)
- 10:50 LE095 - Beyond Amyloid and Tau: Exploring Alternative Therapeutic Targets Using an Integrative Approach**
Prof. Daniel WATTERSON
(NORTHWESTERN UNIVERSITY, Chicago, United States)
- 11:30 LE096 - Discovery of Selective NKCC1 Inhibitors for the Treatment of Core Symptoms in Autism, Down Syndrome, and Brain Disorders with Defective NKCC1/KCC2 Ratio**
Dr Marco BORGOGNO
(IAMA THERAPEUTICS SRL, Genoa, Italy)
- 11:50 LE097 - Selective Butyrylcholinesterase Inhibitors for Alleviating Symptoms of Dementia**
Dr Urban KOSAK
(UNIVERSITY OF LJUBLJANA, Ljubljana, Slovenia)
- 12:10 LE098 - Modulation of TDP-43-pathway by Brain Penetrant Protein Kinase Inhibitors, a New Hope for ALS and Related Disorders**
Prof. Ana MARTINEZ
(CENTRO DE INVESTIGACIONES BIOLÓGICAS-CSIC, Madrid, Spain)

Programme

Session Session 26 'Technologies'

Radiochemistry / AFMC Session

HERMES AUDITORIUM

- 10:45 Session Chair**
Prof. Sun CHOI
(EWHHA WOMANS UNIVERSITY, Seoul, Korea, South)
- 10:50 LE099 - Radiotheragnostics from Bench-to-Bedside *Virtual Presentation***
Prof. Roger SCHIBLI
(ETH ZURICH, Zürich, Switzerland)
- 11:30 LE100 - Evaluation of Cancer Immunity and Development of Novel Radiolabeling Method with Astatin-211 *Virtual Presentation***
Dr Mikako OGAWA
(HOKKAIDO UNIVERSITY, Sapporo, Japan)
- 11:50 LE101 - Medicinal Chemistry in the Development of Molecular Imaging Probes Targeting Prostate-Specific Membrane Antigen**
Prof. Youngjoo BYUN
(KOREA UNIVERSITY, Sejong, Korea, South)
- 12:10 LE102 - Development of First PET Tracers for the Imaging of CD73 Expression in Triple-negative Breast Cancer**
Dr Anna JUNKER
(EUROPEAN INSTITUTE FOR MOLECULAR IMAGING, Muenster, Germany)
- 12:30 Closing Lecture**

ATHENA AUDITORIUM

PL004 - Drivers of Innovation in Drug Discovery

Prof. Outi VAARALA
(ORION CORPORATION, Espoo, Finland)

Chair

Prof. Gianluca SBARDELLA
(UNIVERSITY OF SALERNO, Fisciano, Italy)

13:15 Closing Remarks, EFMC-YSN PhD Prizes, Poster Prizes & Welcome to EFMC-ISMIC 2024

Dr Maria DUCA (UNIVERSITY OF CÔTE D'AZUR, Nice, France)
Prof. Rui MOREIRA (UNIVERSITY OF LISBON, Lisbon, Portugal)
Prof. Roberto DI SANTO (SAPIENZA UNIVERSITY OF ROME, Rome, Italy)