

Sunday September 1, 2019

09:00 Excursions - Tour 1

14:00 Excursions - Tour 2

15:30 Registration

17:30 **Opening**

Prof. Varinder K. AGGARWAL (UNIVERSITY OF BRISTOL, Bristol, United Kingdom)

Dr Spiros LIRAS (APPLE TREE PARTNERS, New York, United States)

Dr Yves P. AUBERSON (NOVARTIS & EFMC, Basel, Switzerland)

Dr Gene VAISBERG (CHEMBRIDGE CORPORATION, San Diego, United States)

Prof. Emmanuel MIKROS (UNIVERSITY OF ATHENS, Athens, Greece)

18:00 **Opening Lecture**

The Art and Science of Total Synthesis and its Impact on Biology and Medicine: From the Fundamentals to the Translational (T01)

Prof. K.C. NICOLAOU

(RICE UNIVERSITY, Houston, United States)

19:00 **Welcome Reception**

20:00 **End of the Day**

Monday September 2, 2019

08:00 Registration

Session Chair

Prof. Varinder K. AGGARWAL
(UNIVERSITY OF BRISTOL, Bristol, United Kingdom)

08:30 Nature's Medicine Chest: Opportunities for Synthesis and Drug Discovery (T02)

Prof. Margaret Anne BRIMBLE
(THE UNIVERSITY OF AUCKLAND, Auckland, New Zealand)

09:15 Drug Discovery in Academia (T03)

Prof. Oliver PLETTENBURG
(LEIBNIZ UNIVERSITY HANNOVER, Hannover, Germany)

10:00 Practical and Asymmetric Gilman-Speeter Synthesis of B-Lactams (OC01)

Prof. Plato MAGRIOTIS
(UNIVERSITY OF PATRAS, Patras, Greece)

10:15 Coffee Break and Exhibition

10:45 Discovery of First in Class, Orally Bioavailable p300/CBP HAT Domain Inhibitors (T04)

Dr Michael MICHAELIDES
(ABBVIE, North Chicago, United States)

11:30 Novel Bacterial Topoisomerase Inhibitors (NBTI) with Potent Gram-Negative Activity (T05)

Dr Cornelia ZUMBRUNN
(IDORSIA PHARMACEUTICALS, Allschwil, Switzerland)

12:15 Rapid Exploration of Synthetically Tractable Chemical Space and Lead Optimization Using a Combination of Reaction-Based Enumeration, Active Learning, and Free Energy Calculations (OC02)

Dr Tatjana BRAUN
(SCHRÖDINGER, Mannheim, Germany)

12:30 Lunch and Exhibition

13:00 Schrödinger Workshop: Using LiveDesign for Collaborative and Data Driven Drug Design

Session Chair

Dr Malin LEMURELL
(ASTRAZENECA, Gothenburg, Sweden)

14:00 Catalytic Chirality Generation: New Strategies for Organic Synthesis (T06)

Prof. John BOWER
(UNIVERSITY OF BRISTOL, Bristol, United Kingdom)

14:45 Nucleophilic Boron for the Synthesis of Functionalized Small Rings (T07)

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

15:30 A Radical Approach for the Late-Stage Functionalization of Phosphinic Peptides (OC03)

Programme

Mr Angelos LELIS
(UNIVERSITY OF ATHENS, Athens, Greece)

15:45 Coffee Break and Exhibition

**16:15 EFMC Prize Winner EFMC-YMCS 2018
Development of Release-And-Report Kinase Inhibitors as Molecular Tools for Investigating
Neurodegenerative Disorders (OC04)**

Dr Cassandra LEE FLEMING
(UNIVERSITY OF GOTHENBURG, Gothenburg, Sweden)

16:30 Photoinduced Assembly of C–N Bonds (T08)

Prof. Daniele LEONORI
(UNIVERSITY OF MANCHESTER, Aachen, Germany)

17:15 Practical Heteroatom- and Group-Transfer Reactions (T09)

Dr Laszlo KURTI
(RICE UNIVERSITY, Houston, United States)

18:00 Closing of the Day

Tuesday September 3, 2019

Session Chair

Prof. Emmanuel MIKROS
(UNIVERSITY OF ATHENS, Athens, Greece)

08:30 Design and Synthesis of Chemical Probes for Bromodomains (T10)

Prof. Stuart CONWAY
(UNIVERSITY OF OXFORD, Oxford, United Kingdom)

09:15 A Medicinal Chemist's Perspective on Solute Carriers: Avoiding or Targeting them (T11)

Dr Kim HUARD
(GENENTECH, San Francisco, United States)

10:00 Stabilizing Inactive Conformations of MALT1 AS an Effective Strategy to Inhibit its Protease Activity (OC05)

Dr Jean-Baptiste LANGLOIS
(NOVARTIS INSTITUTES FOR BIOMEDICAL RESEARCH, Basel, Switzerland)

10:15 Coffee Break and Exhibition

10:45 A Chemical Approach to Map Protein Interactions at the Cell Surface (T12)

Dr Erik HETT
(MERCK EXPLORATORY SCIENCE CENTER, Boston, United States)

11:30 From Fragments to Antibody Drug Conjugates in Emerging Oncology Targeted Therapies (T13)

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

12:15 Macrocyclic Modalities for Modulation of Protein-Protein Interactions (OC06)

Dr Stéphanie GUERET
(ASTRAZENECA MPI SATELLITE UNIT, Mölndal, Sweden)

12:30 Lunch and Exhibition

13:30 Poster Session 1 (odd numbers)

Session Chair

Dr Gene VAISBERG
(CHEMBRIDGE CORPORATION, San Diego, United States)

14:30 Awareness of PAINS (Pan Assay Interference Compounds) can Accelerate the Drug Discovery Process (T14)

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

15:15 Artificial Intelligence in ADMET Modeling and Compound Profiling (T15)

Dr Karl-Heinz BARINGHAUS
(SANOFI, Frankfurt, Germany)

16:00 Antimicrobial Activity of Curcumin Analog PGV-6, HGV-6 and GVT-6 (OC07)

Dr Leni RITMALENI
(GADJAH MADA UNIVERSITY, Yogyakarta, Indonesia)

16:15 Coffee Break and Exhibition

Programme

- 16:45** **Sustainable by Design Anti-Trypanosomatid Small Molecules: an Aspirational Goal for Medicinal Chemistry (T16) - ChemMedChem Lecture**
Prof. Maria Laura BOLOGNESI
(UNIVERSITY OF BOLOGNA, Bologna, Italy)
- 17:30** **Artificial Intelligence in de Novo Molecular Design (T17)**
Dr Ola ENKVIST
(ASTRAZENECA, Mölndal, Sweden)
- 18:15** **Closing of the Day**

Wednesday September 4, 2019

Session Chair

Dr Yves P. AUBERSON
(NOVARTIS & EFMC, Basel, Switzerland)

- 08:30 Amides and Chemical Education as Vehicles for Innovation (T18)**
Prof. Neil GARG
(UNIVERSITY OF CALIFORNIA, Los Angeles, United States)
- 09:15 Discovery of AZD5718, a Novel 5-lipoxygenase Activating Protein (FLAP) Inhibitor (T19)**
Dr Malin LEMURELL
(ASTRAZENECA, Gothenburg, Sweden)
- 10:00 Discovery of GSK701, a Novel Orally Effective Preclinical Drug Candidate for the Treatment of Malaria (OC08)**
Dr Jose Ignacio MARTIN
(GSK, Tres Cantos, Spain)
- 10:15 Coffee Break and Exhibition**
- 10:45 Design and Implementation of de Novo Biosynthetic Cascades (T20)**
Prof. Sabine FLITSCH
(UNIVERSITY OF MANCHESTER, Manchester, United Kingdom)
- 11:30 Catalysis for Total Synthesis (T21)**
Prof. Alois FÜRSTNER
(MAX PLANCK INSTITUT FÜR KOHLENFORSCHUNG, Muelheim an der Ruhr, Germany)
- 12:15 Developing a 'Reverse-Biomimetic' Synthesis of Aroenate and its Analogues (OC09)**
Ms Louise EAGLING
(UNIVERSITY OF BRISTOL, Bristol, United Kingdom)
- 12:30 Lunch and Exhibition**
- 13:30 Poster Session 2 (even numbers)**

Session Chair

Prof. Christoforos KOKOTOS
(UNIVERSITY OF ATHENS, Athens, Greece)

- 14:30 Development and Application in Flow of Sustainable Synthetic Methodologies that Use Singlet Oxygen as Green Oxidant and Cascade Reaction Facilitator (T22)**
Prof. Georgios VASSILIKOGIANNAKIS
(UNIVERSITY OF CRETE, Heraklion, Greece)
- 15:15 Prize Ceremony**
Dr Yves P. AUBERSON
(NOVARTIS & EFMC, Basel, Switzerland)
- 15:20 EFMC Prize for a Young Medicinal Chemist in Academia
From the Elucidation of the Mechanism of Vitamin E to the Design of Innovative Drugs that Limit Inflammation and Enhance Resolution (OC10)**

Programme

Dr Andreas KOEBERLE
(UNIVERSITY OF JENA, Jena, Germany)

**15:35 EFMC Prize for a Young Medicinal Chemist in Industry
Cipargamin-Biocatalysis in the Discovery and Development of an Antimalarial Drug (OC11)**

Dr Radka SNAJDROVA
(NOVARTIS PHARMA AG, Basel, Switzerland)

15:50 Coffee Break and Exhibition

16:20 Flow Chemistry and Photochemistry as a Tool for Drug Discovery (T23)

Dr Jesus ALCAZAR
(JANSSEN RESEARCH & DEVELOPMENT, Toledo, Spain)

17:05 Closing of the Day

20:00 Symposium Banquet

Thursday September 5, 2019

Session Chair

Dr Spiros LIRAS
(APPLE TREE PARTNERS, New York, United States)

- 08:30 Start Selective and Rigidify: The Discovery Path Towards the Next Generation of EGFR Tyrosine Kinase Inhibitors (T24)**
Dr Harald ENGELHARDT
(BOEHRINGER-INGELHEIM, Vienna, Austria)
- 09:15 RNA Therapeutics: New Chemical Modalities Becoming a Therapeutic Reality (T25)**
Dr Konrad BLEICHER
(F.HOFFMANN-LA ROCHE LTD, Basel, Switzerland)
- 10:00 Removable Directing Groups for Late-Stage Functionalisation (OC12)**
Dr Miriam O'DUILL
(NATIONAL UNIVERSITY OF IRELAND, Galway, Ireland)
- 10:15 Coffee Break and Exhibition**
- 10:45 TLR7/8 Antagonists: from Screening to in vivo Potency (T26)**
Dr Claudia BETSCHART
(NOVARTIS INSTITUTES FOR BIOMEDICAL RESEARCH, Basel, Switzerland)
- 11:30 Allosteric Activation of a Master Metabolic Regulator AMPK: Drug Discovery Opportunities and Challenges (T27)**
Dr Kimberly CAMERON
(PFIZER, Cambridge, United States)
- 12:15 Closing Remarks & Prize Ceremony**
- 12:30 End of the Symposium**