



Programme

Sunday, May 20th

17:00 – 19:30: Registration and posters' billsticking

19:45 – 21:00: Dinner

Sala Bracci – Certosa di Pontignano

21:00: **Welcome: Prof. Maurizio Botta – University of Siena, Italy**

21:10 – 22:00: **Dr. Rino Rappuoli – GSK Vaccines (Italy): Vaccines 2018**

22:00: Cantucci&Vinsanto

Monday, May 21st

Sala Bracci – Certosa di Pontignano

Chairman: Prof. Peter Wipf

09:00 – 09:45: **Prof. Dennis Liotta – Emory University (USA): Novel Therapeutics for Treating Viral Diseases, Cancers and Inflammatory Disorders**

09:55 – 10:40: **Dr. Vincenzo Summa – IRBM Science Park (Italy): The discovery of Grazoprevir a pangenotype HCV protease inhibitor approved for the cure of HCV infected patients**

10:50 – 11:10: Coffee Break

Chairman: Prof. Filippo Minutolo

11:10 – 11:55: **Prof. Rob Leurs – Vrije Universiteit Amsterdam (Netherlands): Target and phenotypic-based drug discovery for Neglected Tropical Diseases**

12:05 – 12:50: **Prof. Andrew D. Westwell – Cardiff University (UK): Designing Drugs to Treat Resistant and Metastatic Cancers**

13:00 – 14:30: Lunch

Sala Bracci – Certosa di Pontignano

Unavir Session

14:45 – 14:55: **Dr. Laura Maccari – Lead Discovery Siena (Italy): Overview of the Project UNAVIR**

14:55 – 15:15: **Dr. Annalaura Brai – Lead Discovery Siena (Italy): DDX3 Inhibitors: the Human Response to the Emerging Arboviral Threat**

15:20 – 15:40: **Prof. Mauro Pistello – University of Pisa (Italy): Assessment of the Antiviral Potency of DDX3 Helicase Inhibitors against Cocksackie B Virus**

15:45 – 16:05: **Prof. Maurizio Zazzi – University of Siena (Italy): Targeting Human DDX3 Protein to Inhibit Dengue Virus**

16:10 – 16:30: **Dr. Giulio Poli – University of Siena (Italy): Multifaceted Approach to Discover New Inhibitors of Zika Virus**

16:35 – 16:55: Coffee Break

Chairman: Prof. William Jorgensen

16:55 – 17:40: **Prof. Stephen Neidle – University College London (UK): Tackling Complex Human Diseases with Small Molecules that Target Quadruplex Nucleic Acids: Progress and Challenges**

17:50 – 18:35: **Prof. Bruce Maryanoff – Scripps Research Institute (retired) (USA): Novel Mimetics of Apolipoprotein A-I as Antiatherosclerosis Agents**

19:45 – 21:00: Dinner



21:00: Wine Tasting

Tuesday, May 22nd

Sala Bracci – Certosa di Pontignano

Chairman: Prof. Rob Leurs

09:00 – 09:45: **Prof. William Jorgensen – Yale University (USA):** *Computer-Aided Discovery of Enzyme Inhibitors*

09:55 – 10:40: **Prof. Gabriele Cruciani – University of Perugia (Italy):** *A New Procedure for Fast and Automatic Metabolite Identification of Complex Therapeutic Peptides*

10:50 – 11:10: Coffee Break

Chairman: Prof. Daniel Rauh

11:10 – 11:55: **Prof. Thierry Langer – University of Vienna (Austria):** *Pharmacophore-based Analysis of MD Trajectories: Towards Understanding KD of Protein Ligands*

12:05 – 12:50: **Prof. Karl-Heinz Altmann – ETH Zürich (Switzerland):** *Total Synthesis and SAR Investigation of Selected Bioactive Natural Products*

13:00 – 14:30: Lunch

Sala Bracci – Certosa di Pontignano

Chairman: Prof. Marco Lolli

14:45 – 15:30: **Prof. Laszlo Kurti – Rice University (USA):** *Practical Heteroatom-Transfer Reagents and Reactions*

15:40 – 16:25: **Prof. Michel Baltas – Paul Sabatier University Toulouse III (France):** *Use of Mechanochemistry and Classical Synthesis to Elaborate Active/Potentially Active Nitrogen Contained Heterocyclic Scaffolds*

16:35 – 16:55: Coffee Break

Chairman: Prof. Gian Cesare Tron

16:55 – 17:40: **Prof. Paolo Melchiorre – Institute of Chemical Research of Catalonia (Spain):** *Synthetic Chemistry in the Excited State*

17:50 – 18:35: **Prof. Katherine L. Seley-Radtke – University of Maryland, Baltimore (USA):** *Rational (and sometimes Irrational!) Strategies in Nucleoside Drug Design*

19:30: Bus departure from Certosa di Pontignano to Piazza Gramsci (Siena)

20:00 – 22.45: Social Dinner

Wednesday, May 23rd

Sala Bracci – Certosa di Pontignano

Chairman: Prof. Stephen Neidle

09:00 – 09:45: **Prof. Peter Wipf – University of Pittsburgh (USA):** *Chemical Regulation of Calcium Flux for the Treatment of Catastrophic Neurological Events*

09:55 – 10:25: **Dr. Sharon Bryant – Inte:Ligand (Austria):** *Innovative Molecular Design with LigandScout*

Young researchers' session

10:35 – 10:45: **Dr. Carlotta Granchi – University of Pisa (Italy):** *Discovery and Optimization of Benzoylpiperidine Derivatives as New Reversible, Potent and Selective MAGL Inhibitors*



10:50 – 11:10: Coffee Break

11:10 – 11:20: **Dr. Stefano Sainas – University of Turin (Italy):** Development of Potent Human Dihydroorotate Dehydrogenase Inhibitors able to Induces Myeloid Differentiation

11:25 – 11:35: **Dr. Giulio Goti – Institute of Chemical Research of Catalonia (Spain):** Photochemical Organocatalysis for the Enantioselective β -Acylation of Enals

11:40 – 11:50: **Dr. Bertrand Schweitzer-Chaput – Institute of Chemical Research of Catalonia (Spain):** Dithiocarbamate Anion Catalysis: Beyond Single Electron Transfers in Photomediated Radical Generation

11:55 – 12:05: **Nicole Bozza – University of Parma (Italy):** 2-Substituted Acetamide EGFR Inhibitors to Overcome Acquired T790M Resistance and Mitigate Side Effects

12:10 – 12:20: **Francesco Bavo – University of Milan (Italy):** Novel $\alpha 7$ Antagonists as Potential Anticancer Agents

12:25 – 12:35: **Massimiliano Runfola – University of Pisa (Italy):** Optimization of 3-iodothyronamine Synthetic Analogue as Novel Therapeutic Option for Neurological Disorders

12:40 – 12:50: **Daniela Tomaselli – Sapienza University of Rome (Italy):** Dual G9A Methyltransferase/LSD1 Demethylase or Selective LSD1 Inhibitors: Our Structural Manipulation of the Quinazoline Scaffold

13:00 – 14:30: Lunch

Sala Bracci – Certosa di Pontignano

14:30 – 14:45: Sci Young Award

Chairman: Prof. Thierry Langer

14:45 – 15:30: **Prof. A. Ganesan – University of East Anglia (UK):** Fifty Years of Epigenetic Therapy

15:40 – 16:25: **Prof. Alan Kozikowski – President and CEO of StarWise Therapeutics (USA):** Urea-Based Prostate Specific Membrane Antigen (PSMA) Ligands for the Diagnosis and Therapy (THERANOSTIC) of Prostate Cancer

16:35 – 16:55: Coffee Break

Chairman: Prof. Hugo Kubinyi

16:55 – 17:40: **Prof. Dieter Schinzer – University of Magdeburg (Germany):** Chemistry and Biology of Sorangicins

17:50 – 18:10: **Dr. Lucia Tamborini – University of Milan (Italy):** In-Flow Biocatalytic Preparation of Nucleoside Analogues of Pharmaceutical Interest

18:15 – 19:15: Poster Session

19:45 – 21:00: Dinner

21:00: Wine Tasting

Thursday, May 24th

Sala Bracci – Certosa di Pontignano

Chairman: Prof. Katherine L. Seley-Radtke

09:00 – 09:45: **Prof. Daniel Rauh – Technical University of Dortmund (Germany):** Lesson to Be Learned: The Molecular Basis of Kinase-Targeted Therapies and Drug Resistance in Cancer



09:55 – 10:40: **Prof. Hugo Kubinyi** – BASF SE and University of Heidelberg (retired) (Germany):

ADME/Tox Problems? Rescue Your Drug

10:50 – 11:10: Coffee Break

Chairman: Prof. Antimo Gioiello

11:10 – 11:55: **Prof. Ian Baxendale** – Durham University (UK): *Working towards larger scales using flow approaches in multi-step synthesis*

12:05 – 12:25: **Dr. Gilles Berger** – Université Libre de Bruxelles (Belgium): *Modern computational tools in catalysis, drug synthesis and design*

12:30 – 13:00: Best Poster Award and Closing Remarks

13:00 – 14:30: Farewell Lunch