

# Programme

**Sunday, May 15<sup>th</sup>**

## **Sala Affresco – Certosa di Pontignano**

17.00 - 19.00: Registration and posters billsticking

20.00: Dinner

## **Sala Bracci – Certosa di Pontignano**

21.00 – 21.10: Welcome: **Prof. Maurizio Botta – University of Siena (Italy)**

21.10 – 22.00: **Prof. Dennis Liotta – Emory University (USA):** Is academic drug development an oxymoron?

22.00: Cantucci e Vinsanto

**Monday, May 16<sup>th</sup>**

## **Sala Bracci – Certosa di Pontignano**

Chairman: Prof. Dennis Liotta

09.00 – 09.45: **Prof. Stephen Hanessian – University of Montreal (Canada) and University of California, Irvine (USA):** Total synthesis and biological relevance of norditerpenoid natural products

09.55 – 10.40: **Prof. Maria José Camarasa - Consejo Superior de Investigaciones Científicas (Spain):** DPPiV/CD-26 enzyme mediated activation of amide prodrugs

10.50 – 11.10: Coffee Break

Chairman: Prof. Markus Kalesse

11.15 – 12.00: **Prof. Paolo Melchiorre - Institute of Chemical Research of Catalonia (Spain):** Enantioselective photo-organocatalysis - making chiral molecules with light

12.10 – 12.55: **Prof. Katherine L. Seley-Radtke - University of Maryland, Baltimore Co. (USA):** Flex-nucleosides – a strategic approach to antiviral therapeutics for neglected diseases

13.00 – 14.30: Lunch

## **Sala Bracci – Certosa di Pontignano**

Chairman: Prof. Stephen Hanessian

15.00 – 15.45: **Prof. Stephen Neidle - University College, London (UK):** The discovery of ridinilazole (SMT19969), a new antibiotic to treat *Clostridium difficile*, a neglected hospital- and community-based infective disease

15.55 – 16.40: **Prof. Markus Kalesse - Leibniz Universität Hannover (Germany):** The synthesis of the anti-viral natural products Aetheramide A and Haprolid

16.45 – 17.05: Coffee Break

## SHORT PRESENTATIONS

Chairman: Prof. Maria José Camarasa

17.10 – 17.40: **Prof. Marco Lolli – University of Torino (Italy):** How to reach high quality druggable chemical space: the application of an in house hydroxyazoles bioisosteric tool to design innovative AKR1C3 inhibitors

17.45 – 18.15: **Prof. Subhabrata Sen - Shiv Nadar University (India):** Novel multicomponent reactions in the synthesis of bioactive heterocycles

## FLASH COMMUNICATIONS

18.20 – 18.35: **Dr Eoin Gould – St.Andrews University:** Novel Trypanosomatid inhibitors inspired by nature

18.35 – 18.50: **Prof Fernanda Roversi – Unicamp, Campinas, São Paulo, Brasil :** Selective HCK inhibitor acts only in leukemia cells by activating cell death and modulating oncogenic pathway

18.50 – 19.05: **Chiara Borsari – University of Modena – Reggio Emilia:** Synthesis of novel ether phospholipids derivatives bearing 5-membered heteroaromatic rings

20.00: Dinner and Wine Tasting

**Tuesday, May 17<sup>th</sup>**

### Sala Bracci – Certosa di Pontignano

Chairman: Prof. Gabriele Cruciani

09.00 – 09.45: **Prof. William Jorgensen - Yale University (USA):** Design and synthesis of inhibitors of HIV-1 Reverse Transcriptase and MIF

09.55 – 10.40: **Prof. Helena Danielson - Uppsala University (Sweden):** Supporting design of antiviral drugs using interaction kinetic analysis

10.50 – 11.10: Coffee Break

Chairman: Prof. Thierry Langer

11.15 – 12.00: **Prof. Gabriele Cruciani - Università di Perugia (Italy):** Late stage functionalization chemistries in drug discovery

12.10 – 12.55: **Prof. Hugo Kubinyi - BASF SE and University of Heidelberg (retired) (Germany):** Implementing drug metabolism into lead structure optimization

13.00 – 14.30: Lunch

### Sala Bracci – Certosa di Pontignano

Chairman: Prof. Hugo Kubinyi

15.00 – 15.45: **Prof. Thierry Langer - University of Vienna (Austria):** Chemical feature-based 3D pharmacophores: from a static concept to a dynamic one

15.55 – 16.40: **Prof. Christian Ottmann - Eindhoven University of Technology (Netherlands)**: Small-molecule stabilization of 14-3-3 protein-protein interactions

16.45 – 17.05: Coffee Break

### SHORT PRESENTATIONS

Chairman: Prof. Katherine L. Seley-Radtke

17.10 – 17.40: **Dr. Franco Lombardo - Biogen (USA)**: In silico ADME: some ideas and direction from a group of industrial scientists

17.45 – 18.15: **Prof. Stefano Alcaro – University of Catanzaro (Italy)**: The drug discovery approach based on the multi-targeting paradigm

18.15 – 19.00: Poster Session

### Ristorante Spadaforte, Piazza del Campo, Siena

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

20.30: Networking Dinner

### Wednesday, May 18<sup>th</sup>

#### Sala Bracci – Certosa di Pontignano

Chairman: Prof. Dieter Schinzer

09.00 – 09.45: **Prof. Alan Kozikowski - University of Illinois, Chicago (USA)**: Some adventures at the interface of chemistry and medicine – drug discovery for neglected and orphan diseases

09.55 – 10.40: **Prof. Matteo Zanda - University of Aberdeen (UK)**: Fluorinated bile acid derivatives as PET tracers to study hepatic transporters in vivo

10.50 – 11.10: Coffee Break

Chairman: Prof. Alan Kozikowski

11.15 – 12.00: **Prof. Karl-Heinz Altmann – ETH Zürich (Switzerland)**: Synthetic and biological studies of macrocyclic natural products

12.10 – 12.55: **Dr. Leen Delang - KU Leuven (Belgium)**: Antivirals, a lot achieved, yet a long way to go

13.00 – 14.30: Lunch

#### Sala Bracci – Certosa di Pontignano

Chairman: Prof. Matteo Zanda

15.00 – 15.45: **Prof. Kevin Burgess - Texas A & M University (USA)**: Using EKO to sample conformational sweet-spots in peptidomimetic design

15.55 – 16.40: **Prof. Dieter Schinzer - University of Magdeburg (Germany)**: Drug synthesis: translating organic synthesis into therapeutic products

16.45 – 17.05: Coffee Break

Chairman: Prof. Christian Ottmann

17.10 – 17.55: **Prof. Ulrike Holzgrabe - University of Würzburg (Germany):** Concepts to simultaneously optimize activity, solubility, bioavailability and toxicity

### FLASH COMMUNICATIONS

18.00 – 18.15: **Margarita Puente – GSK, Spain:** Improving efficiency in the discovery of novel antimalarial agents: successful advances towards candidate selection

18.15 – 18.30: **Dr Stephen Ojo – St.Andrews University, UK:** Design and synthesis of an anti-HIV drug: application of yeast three hybrid approach for identification of drug-protein interaction

18.30 – 18-45: **Catarina Garcia – Universidade Lusófona de Humanidades e Tecnologias, Portugal:** 6,7-dehydroroyleanone as a scaffold for the development of novel anti-cancer agent

18.45 – 19.00: **Dr Gaetano Fiorillo – Naxospharma, Italy:** Recent advances in antitumor berberines

20.00: Dinner and Wine Tasting

**Thursday, May 19<sup>th</sup>**

### Sala Bracci – Certosa di Pontignano

Chairman: Prof. Yves Mely

09.00 – 09.45: **Prof. Dario Neri - ETH Zürich (Switzerland):** DNA-encoded chemical libraries

### THINPAD SESSION

09.55 – 10.20: **Dr. Mattia Mori – University of Siena and IIT, CLNS@Sapienza (Italy):** THINPAD: Targeting the HIV-1 nucleocapsid protein to fight antiretroviral drug resistance

10.25 – 10.50: Coffee Break

Chairman: Prof. Stephen Neidle

10.55 – 11.40: **Dr. Vincenzo Summa - IRBM (Italy):** From hit to drug: the discovery of Isentress<sup>TM</sup>, the first in class HIV-Integrase inhibitor

11.45 – 12.30: **Prof. Yves Mely - University of Strasbourg (France):** Development and application of screening assays to disclose molecules targeting HIV-1 reverse transcriptase and nucleocapsid protein

12.30 – 13.00: **Prof. Romano Silvestri - Sapienza University of Roma (Italy):** Twenty years of sulfone non-nucleoside HIV-1 reverse transcriptase inhibitors

13.00-13.30: Best Poster Award (By ACS MedChemLetters) and Closing Remarks

13.30: Farewell Lunch