

Scientific Program

MONDAY 26/4

Chair: *Claudiu Supuran*

14.30-14.50 Opening ceremony

Luigi Dei (Rector of the University of Florence)

Patrizio Blandina Former Director of Neurofarba and of the Faculty of Pharmacy

Gianluca Sbardella President of the Medicinal Chemistry Division

Claudiu T Supuran - Co-chair of the Organizing Committee

14.50-15.40 Opening lecture

Dario Neri

(ETH Zürich, Switzerland)

FROM ENCODED LIBRARIES TO CLINICAL-STAGE TARGETED THERAPEUTICS

15.40-16.10 KeyNote1

Rita Petracca

(Imperial College London, UK)

RAPID SELECTION OF NOVEL MACROCYCLIC PEPTIDES AS MODULATORS OF RAB27A-EFFECTOR INTERACTIONS

16.10-16.30 Break

Chair: *Francesco Di Leva*

16.30-17.00 KeyNote2

Marco Pieroni

(University of Parma, Italy)

LIGAND BASED DRUG DESIGN TO EXPAND THE ANTITUBERCULAR ARSENAL

Session A Chair: <i>Francesco Di Leva</i>	Session B Chair: <i>Isabella Romeo</i>
17.00-17.20 OC1	17.00-17.20 OC5
<i>Eleonora Gianquinto</i> (University of Torino, Italy) VIRTUAL SCREENING IDENTIFIES CROSS-CLASS INHIBITORS OF CLINICALLY RELEVANT SERINE- AND METALLO-BETA-LACTAMASES	<i>Tommaso Felicetti</i> (University of Perugia, Italy) EFFICIENT ONE-STEP SYNTHESIS OF DIFFERENTLY FUNCTIONALIZED 1,2,4-TRIAZOLO[1,5-a]PYRIMIDINES
17.20-17.40 OC2	17.20-17.40 OC6
<i>Maria Laura Pavone</i> (University of Parma, Italy) NOVEL ADJUVANT STRATEGIES TO OVERCOME ANTIMICROBIAL RESISTANCE	<i>Maria Chiara Pismataro</i> (University of Perugia, Italy) HYBRID SMALL MOLECULES TARGETING THE PA-PB1 INTERFACE OF INFLUENZA A VIRUS POLYMERASE
17.40-18.00 OC3	17.40-18.00 OC7
<i>Laura Mourot</i> (University of Strasbourg, France) OPTIMIZATION OF A NOVEL FAST ACTING TRANSMISSION BLOCKING ANTIMALARIAL AGENT	<i>Michela Puxeddu</i> (University of Roma "la Sapienza", Italy) INHIBITION OF ZIKA VIRUS REPLICATION BY NOVEL INHIBITORS OF NS2B/NS3 COMPLEX
18.00-18.20 OC4	18.00-18.20 OC8
<i>Pasquale Linciano</i> (University of Pavia, Italy) PHENOTYPIC AND MACHINE LEARNING APPROACHES FOR HIT TO LEAD OPTIMIZATION OF BROAD SPECTRUM NON-TOXIC ANTIPARASITIC AGENTS	<i>Irina Stefanelli</i> (University of Napoli, Italy) INTEGRATING ARTIFICIAL INTELLIGENCE AND CHEMICAL SYNTHESIS TO DISCOVER NEW POTENT ANTIFLAVIVIRUS AGENTS

Tuesday 27/4

Chair: Rita Petracca

14.30-15.00 KeyNote3

Azzurra Stefanucci

(University of Chieti-Pescara "G. D'Annunzio" - Winner of the DCF2020 Award)

POTENT, EFFICACIOUS, AND STABLE CYCLIC OPIOID PEPTIDES WITH LONG LASTING ANTINOCICEPTIVE EFFECT AFTER PERIPHERAL ADMINISTRATION

Session A Chair: Rita Petracca	Session B Chair: Alberto Massarotti
15.00-15.20 OC9	15.00-15.20 OC13
<u>Claudia Albertini</u> (University of Bologna, Italy) TURNING CROMOLYN-IBUPROFEN DRUG COMBINATION INTO SINGLE-MOLECULE CONJUGATES POLYPHARMACOLOGICAL APPROACH FOR ALZHEIMER'S DISEASE	<u>Rebecca Appiani</u> (University of Milano, Italy) BEHAVIOURAL AND PHARMACOLOGICAL PROFILES OF ZEBRAFISH ADMINISTERED HIGH AFFINITY $\alpha 4\beta 2$ NICOTINIC ACETYLCHOLINE RECEPTOR LIGANDS
15.20-15.40 OC10	15.20-15.40 OC14
<u>Eleonora Cescon</u> (University of Trieste, Italy) SCAFFOLD REPURPOSING OF AN IN-HOUSE CHEMICAL LIBRARY: IDENTIFICATION OF NEW CK1δ INHIBITORS	<u>Davia Prischich</u> (IBEC, Barcellona, Spain) IN VIVO PHOTOPHARMACOLOGY OF ADRENERGIC RECEPTORS
15.40-16.00 OC11	15.40-16.00 OC15
<u>Gabriele Carullo</u> (University of Siena, Italy) HARNESSING AN EPIGENETIC APPROACH TO TREAT INHERITED RETINAL DISEASES: SYNTHESIS OF NEW HDAC INHIBITORS ACTIVE IN ZEBRAFISH MODEL OF RETINAL BLINDNESS	<u>Costanza Ceni</u> (University of Pisa, Italy) NOVEL POTENT AGONISTS OF THE GPR55 RECEPTOR BASED ON THE 3-BENZYLQUINOLIN-2(1H)-ONE SCAFFOLD
16.00-16.20 OC12	16.00-16.20 OC16
<u>Samuele Maramai</u> (University of Siena, Italy) SUBTYPE SELECTIVE γ-AMINO BUTYRIC ACID TYPE A RECEPTORS (GABAAR) MODULATORS ACTING AT THE BENZODIAZEPINE BINDING SITE	<u>Gianmarco Elisi</u> (University of Parma, Italy) MOLECULAR DYNAMICS CHARACTERIZATION OF A LIPOPHILIC PATHWAY FOR THE UNBINDING OF MELATONIN RECEPTOR LIGANDS

16.20-16.40 Coffee break

Chair: Marco Pieroni

16.40-17.10 KeyNote4

Stella Cascioferro (Università di Palermo)

ANTIBIOFILM STRATEGY IN THE FIGHT AGAINST ANTIBIOTIC RESISTANCE

Session A Chair: Marco Pieroni	Session B Chair: Paolo Rovero
17.10-17.30 OC17	17.10-17.30 OC20
<u>Giulio Poli</u> (University of Pisa, Italy) NEW NONCOVALENT MONOACYLGLYCEROL LIPASE (MAGL) INHIBITORS IDENTIFIED THROUGH PHARMACOPHORE-DRIVEN VIRTUAL SCREENING STUDY	<u>Irene Brusa</u> (University of Bologna, Italy) HIT OPTIMIZATION FOR THE DISCOVERY OF NOVEL RNFS INHIBITORS AS CORRECTORS OF THE MUTANT CFTR CHLORIDE CHANNEL IN CYSTIC FIBROSIS
17.30-17.50 OC18	17.30-17.50 OC21

<i>Nicola Gambacorta</i> (University of Bari, Italy) ARTIFICIAL INTELLIGENCE AND MULTIOBJECTIVE OPTIMIZATION FOR THE DE NOVO DESIGN OF TARGETED CHEMICAL LIBRARIES	<i>Emma Baglini</i> (University of Pisa, Italy) NOVEL POSITIVE ALLOSTERIC MODULATORS OF A2B ADENOSINE RECEPTOR ACTING AS BONE MINERALIZATION PROMOTERS
17.50-18.10OC19	17.50-18.10OC22
<i>Giorgio Amendola</i> (University of Campania Luigi Vanvitelli, Italy) PYRMD: USING ARTIFICIAL INTELLIGENCE TO ACCELERATE LIGAND-BASED VIRTUAL SCREENING	<i>Alessandra Cipriano</i> (Winner of the "2021 Best PhD thesis" award, University of Salerno, Italy) RATIONAL DESIGN, SYNTHESIS, AND IN VITRO EVALUATION OF CELL ACTIVE CHEMICAL PROBES FOR BROMODOMAIN-CONTAINING PROTEINS

Wednesday 28/4

Chair: *Stella Cascioferro*

14.30-15.00 [KeyNote5](#)

Paolo Rovero

(University of Firenze)

PERSPECTIVES IN PEPTIDE-BASED SARS-COV-2 VACCINATION STRATEGIES

Session A Chair: <i>Stella Cascioferro</i>	Session B Chair: <i>Giannamaria Annunziato</i>
15.00-15.20OC23	15.00-15.20OC27
<i>Sara Tengattini</i> (University of Pavia, Italy) CHEMICAL GLYCOSYLATION OF RECOMBINANT AG85 ANTIGENS: ON THE WAY TO A NOVEL TUBERCULOSIS VACCINE	<i>Giovanna Baron</i> (University of Milano, Italy) METABOLOMIC, PROTEOMIC AND COMPUTATIONAL STUDIES TO EVALUATE THE LIPID-LOWERING AND ANTI-STEATOTIC EFFECTS OF POLYPHENOLS FROM BERGAMOT LEAVES
15.20-15.40OC24	15.20-15.40OC28
<i>Fosca Errante</i> (University of Firenze, Italy) DESIGN AND SYNTHESIS OF SARS-COV-2 ANTIGENS FOR DIAGNOSTICS AND VACCINOLOGY	<i>Doretta Cuffaro</i> (University of Pisa, Italy) EXOSITE INHIBITION OF ADAMTS-5 BY A GLYCOCONJUGATED ARYL SULFONAMIDE
15.40-16.00OC25	15.40-16.00OC29
<i>Rosa Bellavita</i> (University of Napoli, Italy) SELF-ASSEMBLED ANTIMICROBIAL PEPTIDES TO CHALLENGE RESISTANT BACTERIA	<i>Carlo Matera</i> (University of Milano, Italy) DESIGN, SYNTHESIS AND PHARMACOLOGICAL CHARACTERIZATION OF A PHOTOSWITCHABLE INHIBITOR OF FOLATE METABOLISM
16.00-16.20OC26	16.00-16.20OC30
<i>Lara Davani</i> (University of Bologna, Italy) INVESTIGATION OF Aβ PEPTIDE EFFECTS ON SH-SY5Y CELLS: A LIPIDOMIC APPROACH FOR ALZHEIMER'S DISEASE DRUG DISCOVERY	<i>Niamh O'Mahoney</i> (University College Cork, Ireland) CHARACTERISATION OF PHARMACEUTICAL FORMULATIONS USING BROADBAND ACOUSTIC RESONANCE DISSOLUTION SPECTROSCOPY (BARDS).

16.20-17.00 Coffee break

Chair: **Gabriele Costantino**

Round Table: **COVID19 VACCINES IN ITALY: CHALLENGES AND OPPORTUNITIES**

Roberto Burioni, Università Vita-Salute San Raffaele (Milano, Italy),

Bruno Alfonsi, Director Market Access, BioNet-Asia

Duccio Mattii, Quality Director, GSK

Ruggero Bettini, University of Parma (Italy)

Thursday 29/4

Chair: *Azzurra Stefanucci*

14.30-15.00 KeyNote6

Francesco Di Leva

University of Napoli "Federico II" – Winner of the DCF2020 Award

MULTIFUNCTIONAL $\alpha\beta6$ INTEGRIN-TARGETING RGD PEPTIDES: FROM COMPUTER-AIDED DESIGN TO BIOMEDICAL APPLICATIONS

Session A Chair: <i>Azzurra Stefanucci</i>	Session B Chair: <i>Michele Mari</i>
15.00-15.20OC31	15.00-15.20OC34
<i>Daniela Carbone</i> (University of Palermo, Italy) THIAZOLE NORTOPSENTIN ANALOGS TARGETING CANCER STEM CELLS: TOWARD THE DEVELOPMENT OF NEW ANTI-COLORECTAL CANCER AGENTS	<i>Marta Serafini</i> (Winner of the "2021 Best PhD thesis" award, University of Piemonte Orientale, Italy) TARGETING THE KYNURENINE PATHWAY WITH NEW MODALITIES: FROM A VIRTUAL SCREENING TO THE IDENTIFICATION OF TWO NOVEL IDO1 INHIBITORS
15.20-15.40OC32	15.20-15.40OC35
<i>Caterina Carraro</i> (University of Padova, Italy) DRUG DISCOVERY MEETS OMICS: THE CASE STUDY OF 3-CHLOROPIPERIDINES	<i>Stefano Sainas</i> (University of Torino, Italy) THE INHIBITION OF HUMAN DHODH BY M433 LEADS TO DIFFERENTIATION AND APOPTOSIS IN ACUTE MYELOID LEUKEMIA
15.40-16.00OC33	15.40-16.00OC36
<i>Fábio Pedroso de Lima</i> (University of Minho, Portugal) 3H-CHROMENO[2,3-d]PYRIMIDIN-4(5H)-ONES - SYNTHESIS AND BIOLOGICAL EVALUATION AS ANTICANCER AGENTS	<i>Alessandra Feoli</i> (University of Salerno, Italy) DEVELOPMENT OF A MICROSCALE THERMOPHORESIS-BASED METHOD FOR SCREENING INHIBITORS OF THE METHYL-LYSINE READER PROTEIN MRG15

16.00-16.30 Coffee break

Chair: *Maria Novella Romanelli*

16.30-16.40 **Marco Macchia**

(Director of the European School of Medicinal Chemistry)

Presentation of ESMEC 2021

16.40-17.30 Closing lecture

Antonello Mai

University of Roma "La Sapienza"

TOGETHER IS BETTER: EPIGENETIC POLYPHARMACOLOGY

17.30 Gianluca Sbardella, Maria Novella Romanelli

Prizes & Closing remarks