

Programma Scientifico Divisione di Chimica Farmaceutica

MERCOLEDÌ 15 SETTEMBRE 2021	
<i>Sessione comune</i>	
<i>Chairpersons: Gianluca Sbardella</i>	
9:30-10:00	<i>FAR KN001 – Giuseppe Campiani, University of Siena, IT</i> Old but Gold: Tracking the New Guise of Histone Deacetylases as Biomarkers and Therapeutic Targets in Rare Diseases. The role of Isoform 6
10:00-10:30	<i>FAR KN002 – György Keserű, Research Center for Natural Sciences, HU</i> The role of the secondary binding pocket in GPCR pharmacology
<i>Sessione parallela 1</i>	
<i>Chairpersons: Stefano Moro</i>	
10:30-10:45	<i>FAR OR001 – Agnese Pippione, University of Turin, IT</i> Targeting prostate cancer with multiple-targeting ligands: Activity on both AKR1C3 enzyme and androgen receptor
10:45-11:00	<i>FAR OR002 – Andrea Spinaci, University of Camerino, IT</i> Synthesis and Characterization of New A3 Adenosine Receptors Ligands as Potential Anti-Cancer Agent
<i>Sessione parallela 2</i>	
<i>Chairpersons: Patrizia Diana</i>	
10:30-10:45	<i>FAR OR003 – Francesca Musumeci, University of Genoa, IT</i> Design, synthesis, and biological evaluation of a new series of pyrazolo[3,4-d]pyrimidines active as SGK1 inhibitors. A lead optimization study
10:45-11:00	<i>FAR OR004 – Giuseppe La Regina, Sapienza University of Rome, IT</i> New Pyrroles Derivatives as Anti-Glioblastoma and Anti-Chronic Myeloid Leukemia Agents
11:00-11:15	Coffee Break
<i>Sessione comune</i>	
<i>Chairpersons: Gianluca Sbardella</i>	
11:15-11:45	<i>FAR KN003 – Tracey Pirali, University of Eastern Piedmont, IT</i> The Power of Multi-Component Reactions in Drug Discovery: Soft Drugs, PROTACs and more
<i>Sessione parallela 1</i>	
<i>Chairpersons: Stefano Alcaro</i>	
11:45-12:00	<i>FAR OR005 – Simona Musella, European Biomedical Research Institute, IT</i> Identification and characterization of a potent TRPM8 antagonists with in vivo analgesic properties
12:00-12:15	<i>FAR OR006 – Letizia Crocetti, University of Florence, IT</i> Synthesis of pyrazolo[1,5-a]quinazolines as ligand of $\alpha 1\beta 3\gamma 2$-GABAA receptor subtype and molecular modelling studies
12:15-12:30	<i>FAR OR007 – Carmine Ostacolo, University of Naples “Federico II”, IT</i> Discovery of CP86, a potent neuronal Kv7 channel activator with in vivo anticonvulsant effects
<i>Sessione parallela 2</i>	
<i>Chairpersons: Marco Mor</i>	
11:45-12:00	<i>FAR OR008 – Laura Scalvini, University of Parma, IT</i> N-Acylethanolamine acid amidase (NAAA): mechanism of palmitoylethanolamide hydrolysis revealed by mechanistic simulations

12:00-12:15	<i>FAR OR009 – Leonardo Brunetti, University of Bari “Aldo Moro”, IT</i> Multiple causes, multiple targets: FAAH as a centerpiece for therapy of multifactorial pathologies
12:15-12:30	<i>FAR OR010 – Rita Turnaturi, University of Catania, IT</i> Influence of the N-substituent of (–)-cis-N-Normetazocine in the modulation of the functional profile at MOR, DOR and KOR: from agonist to antagonist through multitarget ligands
	<i>Sessione comune</i>
	<i>Chairpersons: Gianluca Sbardella</i>
12:30-13:00	<i>FAR KN004 – Marco Radi, University of Parma, IT</i> Navigating the antiviral drug discovery space: exploring different routes toward new broad-spectrum agents
13:00-14:00	Intervallo Pranzo – Lunch Break
	<i>Epouser session</i>
14:00-15:00	<i>Epouser session 1 (FAR PO001 – FAR PO020)</i>
	<i>Sessione comune</i>
	<i>Chairpersons: Gianluca Sbardella, Gabriele Costantino</i>
15:00-15:45	<i>FAR MD001 - Kenneth A. Jacobson, National Institutes of Health, USA</i> Pratesi Medal Lecture - Design and Therapeutic Potential of Adenosine and P2Y Receptor Ligands
15:45-16:00	<i>FAR PZ001 – Ciro Milite, University of Salerno</i> DCF Prize - Modulators of Coactivator-Associated Arginine Methyltransferase 1 (CARM-1): There and Back Again
16:00-16:15	<i>FAR PZ002 – Mariateresa Giustiniano, University of Naples “Federico II”</i> DCF Prize - Isocyanide Chemistry from the Ground (state) to the Star(s):
16:15-17:00	<i>FAR MD002 –Antonello Mai, Sapienza University of Rome</i> Giacomello Medal Lecture - Lecture for the receipt of the “Giordano Giacomello” medal by the Medicinal Chemistry Division of the Italian Chemical Society
17:00-17:15	Coffee Break
	<i>Sessione parallela 1</i>
	<i>Chairpersons: Violetta Cecchetti, Gabriele Costantino</i>
17:15-17:30	<i>FAR OR011 – Marilia Barreca, University of Palermo, IT</i> Inhibition of non-Hodgkin lymphoma cell growth by pyrrolo[1,2]oxazole derivatives
17:30-17:45	<i>FAR OR012 – Laura Braconi, University of Florence, IT</i> A new strategy to overcome multidrug resistance (MDR) in cancer cells: P-gp and hCAXII multitarget inhibitors
17:45-18:00	<i>FAR OR013 – Daniela Carbone, University of Palermo, IT</i> Synthesis and preclinical evaluation of a new generation of 1,2,4-triazine-based PDK modulators: a novel therapeutic approach to halt cancer growth.
18:00-18:15	<i>FAR OR014 – Arianna Gelain, University of Milan, IT</i> Unraveling the interaction mechanism of a benzothiadiazole-2,2-dioxide derivative with STAT3: towards novel direct inhibitors
	<i>Sessione parallela 2</i>
	<i>Chairpersons: Vincenza Andrisano, Giancarlo Aldini</i>
17:15-17:30	<i>FAR OR015 – Lucia Tamborini, University of Milan, IT</i> Flow-based redox biotransformations for food and pharma applications
17:30-17:45	<i>FAR OR016 – Federica Ianni, University of Perugia, IT</i> Stability of chlorogenic acid as model system after household microwave treatment
17:45-18:00	<i>FAR OR017 – Ilaria Frosi, University of Pavia, IT</i> Comparison of different extraction methods to recover bioactive compounds from corn waste (<i>Zea mays</i> L.)
18:00-18:15	<i>FAR OR018 – Maria Contente, University of Milan, IT</i> Valorization of food wastes and residues through glycosidases

VENERDÌ 17 SETTEMBRE 2021	
<i>Sessione comune</i>	
<i>Chairpersons: Gianluca Sbardella</i>	
9:30-10:00	<i>FAR KN005 – Yimon Aye, EPFL, CH</i> Leveraging precision electrophile signaling toward drug discovery
10:00-10:30	<i>FAR KN006 – Antimo Gioiello, University of Perugia, IT</i> Enabling synthesis and technologies to develop bile acid-inspired lead compounds
<i>Sessione parallela 1</i>	
<i>Chairpersons: Antimo Gioiello</i>	
10:30-10:45	<i>FAR OR019 – Francesca Ferlenghi, University of Parma, IT</i> A sulfonyl fluoride derivative selectively inhibits EGFR L858R/T790M/C797S by covalent modification of the catalytic lysine
10:45-11:00	<i>FAR OR020 – Angelica Artasensi, University of Milan, IT</i> Novel potential DPP IV/ CA II inhibitors for the treatment of Type 2 Diabetes
<i>Sessione parallela 2</i>	
<i>Chairpersons: Tracey Pirali</i>	
10:30-10:45	<i>FAR OR021 – Maria Dichiara, University of Catania, IT</i> Design, synthesis and pharmacological evaluation of 4-carbamothioylphenyl sigma-1 receptor antagonists for pain treatment
10:45-11:00	<i>FAR OR022 – Giacomo Rossino, University of Pavia, IT</i> Identification of novel Sigma 1 Receptor antagonists based on arylalkanolamine scaffold for the treatment of neuropathic pain
<i>Sessione comune</i>	
<i>Chairpersons: Gianluca Sbardella</i>	
11:00-11:30	<i>FAR KN007 – Andrea Stevenazzi, Italfarmaco, IT</i> The Selective Inhibition of Histone Deacetylase 6 (HDAC6)
<i>Sessione parallela 1</i>	
<i>Chairpersons: Maria Laura Bolognesi, Michele Mari</i>	
11:30-11:45	<i>FAR OR023 – Giannamaria Annunziato, University of Parma, IT</i> Investigational Studies on Cyclopropane– Carboxylic Acid Derivatives Targeting O-Acetylserine Sulphydrylase as Colistin Adjuvants
11:45-12:00	<i>FAR OR024 – Simone Lucarini, University of Urbino, IT</i> Phenotype screening of a bisindole chemical library identifies URB1483 as a new antileishmanial agent with topoisomerase IB as molecular target
12:00-12:15	<i>FAR OR025 – Santo Previti, University of Messina, IT</i> Development of peptidyl Michael acceptors for S3 pocket investigation of rhodesain, cysteine protease of Trypanosoma brucei rhodesiense
12:15-12:30	<i>FAR OR026 – Valentina Straniero, University of Milan, IT</i> Development of benzodioxane-benzamides inhibitors of FtsZ as potent broad-spectrum antimicrobial agents
<i>Sessione parallela 2</i>	
<i>Chairpersons: Tiziano Bandiera, Isabella Romeo</i>	
11:30-11:45	<i>FAR OR027 – Marilena Muraglia, University of Bari “Aldo Moro”, IT</i> To042: prospective lead compound for the treatment of myotonic syndromes
11:45-12:00	<i>FAR OR028 – Sebastiano Intagliata, University of Catania, IT</i> Development of Mutual Prodrugs of 5-Fluorouracil and Heme Oxygenase 1 Inhibitor as Anticancer Agents
12:00-12:15	<i>FAR OR029 – Luca Pinzi, University of Modena and Reggio Emilia, IT</i> LigAdvisor: a web server to perform in silico explorations on crystallographic ligands and known drugs for polypharmacology and drug repurposing
12:15-12:30	<i>FAR OR030 – Lucilla Turco, Aptuit-Evotec, IT</i> NMR contributions to process chemistry sustainability in the pharmaceutical research area

<i>Sessione comune</i>	
<i>Chairpersons: Gianluca Sbardella</i>	
12:30-13:00	<i>FAR KN008 – Anna K.H. Hirsch, Helmholtz Institute for Pharmaceutical Research Saarland, DE</i> Addressing underexplored anti-infective targets
13:00-14:00	Intervallo Pranzo – Lunch Break
<i>Eposter session</i>	
14:00-15:00	<i>Eposter session 1 (FAR PO021 – FAR PO042)</i>

MARTEDÌ 21 SETTEMBRE 2021	
<i>Sessione comune</i>	
<i>Chairpersons: Gianluca Sbardella</i>	
9:30-10:00	<i>FAR KN009 – Anders Bach, University of Copenhagen, DK</i> Targeting Protein-Protein Interactions Involved in Oxidative Stress using Fragment-Based Drug Discovery
10:00-10:30	<i>FAR KN010 – Giancarlo Aldini, University of Milan, IT</i> Chemical and molecular mechanisms of cellular and extra-cellular antioxidants
<i>Sessione parallela 1</i>	
<i>Chairpersons: Alberto Massarotti</i>	
10:30-10:45	<i>FAR OR031 – Marco Catto, University of Bari “Aldo Moro”, IT</i> A second life for MAO inhibitors: from CNS diseases to cancer
10:45-11:00	<i>FAR OR032 – Stefano Sainas, University of Turin, IT</i> Apoptotic and differentiating therapy for AML using potent human dihydroorotate dehydrogenase inhibitor
<i>Sessione parallela 2</i>	
<i>Chairpersons: Fabrizio Micheli</i>	
10:30-10:45	<i>FAR OR033 – Claudia Sorbi, University of Modena and Reggio Emilia, IT</i> Constrained 1,4-Dialkylpiperazines as Dopamine Transporter (DAT) Inhibitors to Fight Psychosis and Cocaine Addiction
10:45-11:00	<i>FAR OR034 – Elisa Uliassi, University of Bologna, IT</i> Psychotropic-based bifunctional compounds for neurodegenerative diseases
<i>Sessione comune</i>	
<i>Chairpersons: Gianluca Sbardella</i>	
11:00-11:30	<i>FAR KN011 – Tiziano Bandiera, IIT, IT</i> Discovery of a picomolar potency corrector of F508del-CFTR chloride channel
<i>Sessione parallela 1</i>	
<i>Chairpersons: Roberto Di Santo, Paola Conti</i>	
11:30-11:45	<i>FAR OR035 – Francesca Spyraakis, University of Turin, IT</i> Identification of carbapenemase broad-spectrum inhibitors through in silico methodologies
11:45-12:00	<i>FAR OR036 – Serena Massari, University of Perugia, IT</i> 1,2,4-Triazolo[1,5-a]pyrimidines: Efficient One-step Synthesis and Functionalization as Antiviral Agents
12:00-12:15	<i>FAR OR037 – Alessandra Altomare, University of Milan, IT</i> An integrated metabolomic and proteomic approach for the identification of covalent inhibitors of the main protease (Mpro) of SARS-COV-2 from crude natural extracts
12:15-12:30	<i>FAR OR038 – Antonella Messori, Sapienza University of Rome, IT</i> Discovery of non-DKA Derivatives endowed of Selective Activity against Ribonuclease H Function of the HIV-1 Reverse Transcriptase
<i>Sessione parallela 2</i>	
<i>Chairpersons: Giannamaria Annunziato, Giulio Vistoli</i>	
11:30-11:45	<i>FAR OR039 – Salvatore Di Maro, University of Campania “L. Vanvitelli”, IT</i> Peptides from Bench to Clinical Studies: our experience with CXCR4

11:45-12:00	<i>FAR OR040 – Azzurra Stefanucci, University of Chieti-Pescara “G. D’Annunzio”, IT</i> A novel β-hairpin peptide derived from the ARC repressor selectively interacts with the major groove of B-DNA
12:00-12:15	<i>FAR OR041 – Stefano Tomassi, University of Naples “Federico II”, IT</i> Shading the activity of a CXCR4-interacting peptide by 1,4- and 1,5-disubstituted [1,2,3]-triazole-based cyclization
12:15-12:30	<i>FAR OR042 – Rosa Bellavita, University of Naples “Federico II”, IT</i> Grafting Temporin L Peptides: Old Tactics for New Antimicrobial Weapons
	<i>Sessione comune</i>
	<i>Chairpersons: Gianluca Sbardella</i>
12:30-13:00	<i>FAR KN012 – Pedro Gois, University of Lisbon, PT</i> Exploring B-Complexes as likers for Targeting drug conjugates
13:00-14:00	Intervallo Pranzo – Lunch Break
	<i>Eposter session</i>
14:00-15:00	<i>Eposter session 1 (FAR PO043 – FAR PO064)</i>