

3rd Meeting of the Paul Ehrlich MedChem Euro-PhD Network Program:

27 th September 2013	
14:00	Registration, Placement of Posters
15:00	Opening Ceremony Elias Maccioni and Danijel Kikelj
	Session 1- Chairperson: Danijel Kikelj
16:00	OL-1 Opening Lecture Micaela Morelli - University of Cagliari: "The story of adenosine A2A antagonists in Parkinson's disease: from their synthesis to clinical trials"
16:45	Coffee Break and poster presentation
17:15	Paul Ehrlich MedChem Euro-PhD Label Award Elias Maccioni and Danijel Kikelj
PE AW 1	Rita Meleddu - University of Cagliari: "Synthesis and biological activity evaluation of new dual-inhibitors of both associated functions of HIV-1 RT"
PE AW 2	Matjaz Brvar - National Institute of Chemistry of Ljubljana: "Structure-based design of novel DNA gyrase B inhibitors"
18:15	Oral Communications
O-1	Davide Deodato – University of Siena: "Synthesis, molecular modeling and biological evaluation of novel benzofurazane derivatives active against Influenza A Virus"
O -2	Ivana Defrenza - University of Bari: "1,3-benzothiazole derivatives: design, synthesis and evaluation of their antimicrobial activity"
19:30	Welcome Reception
28 th September 2013	
	Session 2- Chairperson: Fernanda Borges
9:15	OL-2 Opening Lecture Stefano Alcaro - Magna Graecia University of Catanzaro: "Suggestions for PhD students to invest into Computational Methods for Drug Discovery purposes"
10:00	Oral Communications
O-3	Alexandra Gaspar - University of Porto: "Discovery of dual-target agents based on chromone scaffold for Parkinson´s disease"
O-4	Maria Chatzopoulou - Aristotle University of Thessaloniki: "Minimizing acidity in a series of aldose reductase inhibitors: the case of 2-fluoro-4-(1H-pyrrol-1-yl)phenol as a scaffold"
O-5	Ziga Hodnik - University of Ljubljana: "Mimetics of solomonsterols as novel pregnane X receptor antagonists"
10:45	Coffee Break and Poster Session
	Session 3- Chairperson: Athina Geronikaki
11:15	Oral Communications
O-6	Jiri Mikusek – Charles University of Prague: "Novel biologically active quinazolines"
O-7	Cristina Ciancimino - University of Palermo: "Isoindolo[1,5]benzoxazepine

	as potential antitumor and/or antiviral agents"
O-8	Federica Moraca - Magna Graecia University of Catanzaro: "Reconstructing the Berberine binding free energy through funnel-metadynamics simulations"
O-9	Andrew Anighoro - University of Modena and Reggio Emilia: "A computational polypharmacology protocol within the Hsp90 interactome"
O-10	Lena Huck - Complutense University of Madrid: "Synthesis of potential anti-tubercular agents from arilmethylene-2,5-diketopiperazines"
13:00	Lunch
	Session 4- Chairperson: Katarzyna Kiec-Kononowicz
15:00	OL-3 Opening Lecture Enzo Tramontano – University of Cagliari: "Strategies for the development of HIV-1 Ribonuclease H inhibitors: a still under exploration target"
15:45	Oral Communications
O-11	Daniele Giallombardo - University of Palermo: "Synthesis and biological evaluation of cycloheptapyrrolo systems"
O-12	Thomas Nagel - University of Vienna: "Synthesis and antiproliferative activity of new cytotoxic tri- and tetraazabenz[3,2-a]11yridine-5,6-dione derivatives"
O-13	Roberta Fazi - University of Siena: "Design of human DDX3 inhibitors as antiviral agents"
16:30	Coffee Break and poster presentation
	Session 5- Chairperson: Stefano Alcaro
17:00	Oral Communications
O-14	Barbora Servusová - Charles University of Prague: "Pyrazinamide: Insight into antimycobacterial activity of selected 6-alkylamino derivatives"
O-15	Silvia Alvarez Perez - CEU San Pablo University of Madrid: "[2+2+2] Cyclotrimerization of alkynes and isocyanates/isothiocyanates catalyzed by Ruthenium Carbenes"
O-16	Sangyong Lee - University of Bonn: "Search for nucleotide pyrophosphatase/phosphodiesterase 1 (NPP1) inhibitors: potential novel drugs"
17:45	Fausto Chiapparini - Biotage: "Flash chromatography instrument presentation"
18:30	Paul Ehrlich Network Meeting
20:00	Paul Ehrlich Network Dinner
29th September 2013	
	Session 6- Chairperson: Norbert Haider
9:15	OL-4 Opening Lecture Michele Parrinello - Swiss Federal Institute of Technology Zurich: "Simulating milliseconds processes without special-purpose computers"
10:00	Oral Communications
O-17	Giulia Bianchini - Complutense University of Madrid: "A biology-oriented synthesis of a promising multi-target ligand against Trypanosomatid Diseases"
O-18	Nicola Anzani - University of Cagliari: "N-alkylamides from Otanthus maritimus: structure elucidation, binding affinity for cannabinoid receptors"

	and computational study"
O-19	Tiago Silva - University of Porto: "Towards the development of multi-target directed drugs for neurodegenerative disorders based on the cinnamic acid scaffold"
10:45	Coffee Break and Poster Session
	Session 7- Chairperson: Beatriz de Pascual-Teresa
11:15	OL-5 Opening Lecture Danijel Kikelj - University Of Ljubljana: "Adventures in antibacterial drug discovery: From inhibitors of intracellular steps of peptidoglycan biosynthesis to gyrase B inhibitors"
12:00	Oral Communications
O-20	Efres Belmonte Reche - CEU San Pablo University of Madrid: "Hydroxy chalcogenide Morita-Baylis-Hillman-alkylation reaction: New intermolecular applications with cyclic enones as substrates and alkyl or allyl halides as electrophiles"
O-21	Sotirios Katsamakas - University of Ljubljana: "Towards novel potential antibacterial drugs through DNA gyrase B inhibition"
O-22	Thalia Liargkova - Aristotle University of Thessaloniki: "Design, synthesis and biological evaluation of chalcones and aurones with possible anti-inflammatory and insect antifeedant activities"
13:00	Closing Remarks
13:30	Lunch