

# Scientific Program

## Wednesday, 24<sup>th</sup> May

17:00-17.15	<b>L. Dei</b>	Greetings from The Rector of Università degli Studi di Firenze
17:15-17:45	<b>C.T. Supuran</b>	Welcome and opening lecture: A tribute to Andrea Scozzafava's career and scientific achievements
17:45-18:15	<b>S. Parkkila</b>	Update on CA research, 2015-2017
19:30		Welcome drink and dinner

## Thursday, 25<sup>th</sup> May

### SESSION I

#### Comparative aspects of new CA families, isozymes and their structural investigations

Chairman: *C.T. Supuran*

9:00-9:30	<b>M. Barboiu</b>	Dynamic constitutional screening of CA Inhibitors and activators
9:30-9:45	<b>R. Mckenna</b>	Structural insight towards CA isoform specific Inhibitors: cautions and hopes
9:45-10:00	<b>T.S. Peat</b>	The structural side of different Carbonic Anhydrases
10:00-10:30	<b>G. De Simone</b>	Interaction of Carbonic Anhydrase IX with CAND1: structural and functional features
10:30-11:00	<i>Coffee Break</i>	

Chairman: *A. Scozzafava*

11:00-11:30	<b>A. Akdemir</b>	Molecular modelling studies of CAIs: understanding binding and suggesting new ligands
11:30-11:45	<b>M. Krasavin</b>	Direct Sulfochlorination of heterocycles as a speedy entry into isoform-selective Carbonic Anhydrase Inhibitors
11:45-12:00	<b>P. Guglielmi</b>	New strategies for Carbonic Anhydrases inhibition: probenecid-amino acid derivatives as atypical and selective Inhibitors of hCA tumor-related isoforms IX and XII
12:00-12:30	<b>R. Cimaz</b>	Pathogenesis of juvenile idiopathic arthritis
12:30-13:30	<i>Lunch</i>	

## SESSION II

### Regulation/expression of CA isoforms in cancer

Chairman: *S. Pastorekova*

15:00-15:30	<b>R.J. Gillies</b>	CA IX and Warburg's Paradox
15:30-16:00	<b>S. Fais</b>	Association between the proton pump inhibitor lansoprazole and Carbonic Anhydrase IX Inhibitors a future combined therapy against cancer
16:00-16:30	<i>Coffee break</i>	
16:30-17:00	<b>S. Dedhar</b>	The Interactome of metabolic enzyme Carbonic Anhydrase IX reveals novel roles in tumor cell migration and invadopodia/MMP-14-mediated invasion

Chairman: *S. Parkkila*

17:00-17:30	<b>S. Pastorekova</b>	CA IX regulates metabolic responses of cancer cells to tumor microenvironment
17:30-17:45	<b>S.C. Frost</b>	Does Carbonic Anhydrase IX expression drive metastatic disease?
17:45-18:00	<b>H.M. Said</b>	Modulation of Carbonic Anhydrase 9 expression by the regulative effect of hypoxia and cytokines in human hepatocellular carcinoma disease
18:00-19:30	<i>Poster Session</i>	
19:30	<i>Dinner</i>	
20:30-21:45	<i>Poster Session</i>	

## Friday 26<sup>th</sup> May

## SESSION III

### CAs as drug and diagnostic targets

Chairman: *D. Vullo*

9:00-9:30	<b>J.Y. Winum</b>	Multivalent Carbonic Anhydrase Inhibitors
9:30-10:00	<b>F. Carta</b>	Carbonic Anhydrase Inhibitors: discovery of new chemical entities and novel applications for the inhibitors for the management of

neuropathic pain, cerebral ischemia and arthritis

10:00-10:15	<b>S. Thibaudau</b>	Superacid chemistry for Carbonic Anhydrases Inhibitors discovery
10:15-10:45	<i>Coffee Break</i>	
		<i>Chairman: F. Carta</i>
10:45-11:00	<b>M. Mori</b>	Computationally-driven design of CA Inhibitors
11:00-11:30	<b>W.A. Donald</b>	Rapid, ultrasensitive protein structure determination by mass spectrometry
11:30-11:45	<b>S. Akocak</b>	Synthesis and biological evaluation of aromatic and heterocyclic Bis-Sulfonamide Schiff bases as Carbonic Anhydrase I, II, VII and IX Inhibitors
11:45-12:10	<b>D. Vullo</b>	Carbonic Anhydrase Activators: Mechanism of action, possible applications in the therapy of Alzheimer's Disease and implications on CAs in bacteria
12:10-12:30	<b>Z. Fisher</b>	Neutron crystallographic studies of cancer-related human Carbonic Anhydrase IX reveal details of water displacement and hydrogen bonding in inhibitor binding
12:30-12:45	<b>S.M. Monti</b>	Insights into the proteoglycan-like domain of Carbonic Anhydrase IX
12:45-13:00	<b>G.J. Atkins</b>	Novel roles for carbonic anhydrases in osteocyte-regulated bone homeostasis
13:00-14:00	<i>Lunch</i>	

#### *SESSION IV*

#### **Roles of CAs in human diseases**

*Chairman: C. Capasso*

15:00-15:30	<b>M.A. Illies</b>	Theranostic CA IX Inhibitors engineered from a delivery perspective
15:30-15:45	<b>R. Gitto</b>	Selective inhibitors of hCA VII based on isoquinoline scaffold for the treatment of CNS pathologies
15:45-16:00	<b>L. Di Cesare Mannelli</b>	Pain relieving effects of new Non Steroidal Anti-Inflammatory Drugs and Carbonic Anhydrase Inhibitors hybrids (NSAIDs-CAIs): systemic and intrarticular treatments against rheumatoid arthritis
16:00-16:30	<i>Coffee Break</i>	

*Chairman: G. De Simone*

16:30-16:45	<b>E. Masini/L. Lucarini</b>	CA IX/COX-2 inhibitors as a new class of anti-inflammatory drugs
16:45-17:00	<b>M. Ferraroni</b>	X-RAY structure of a tetrameric type II $\beta$ -Carbonic Anhydrase from the pathogenic bacterium vibrio cholera
17:00-18:30		Journal of Enzyme Inhibition and Medicinal Chemistry Editorial Board meeting
17:00-19:00	<i>Poster Session</i>	<b>(Parallel sessions)</b>
20:00-23:00	<i>Banquet</i>	<i>Stabilimento Termale Tettuccio, Viale Verdi 71-Montecatini Terme</i>

## **Saturday, 27<sup>th</sup> May**

### *SESSION V*

#### **CAs in microorganisms**

*Chairman: S. Carradori*

9:00-9:30	<b>G. Costantino</b>	Computer-Aided identification of potential Anti-infective compounds as selective Carbonic Anhydrase Inhibitors
9:30-9:45	<b>C. Capasso</b>	New light on bacterial Carbonic Anhydrases
9:45-10:00	<b>A.B. Vermelho</b>	Carbonic Anhydrases from Trypanosoma and Leishmania as anti-protozoan drug targets
10:00-10:15	<b>A. Karioti</b>	New natural product Carbonic Anhydrase Inhibitors incorporating phenol moieties
10:15-10:30	<b>B.V. Alvarez</b>	Carbonic Anhydrase Inhibitors in chronic and acute myocardial infarction
10:30-11:00	<i>Coffee Break</i>	

### *SESSION VI*

#### **Young researchers**

*Chairman: G. Costantino*

11:00-11:15	<b>M. Bozdag</b>	Novel tumor associated Carbonic Anhydrase Inhibitors: derivatives of SLC-0111
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11:15-11:30	<b>A. Angeli</b>	Intramolecular oxidative deselenization of acylselenoureas: a facile synthesis of benzoxazole amides and Carbonic Anhydrase Inhibitors
11:30-11:45	<b>S. Del Prete</b>	Inhibition studies of Carbonic Anhydrases from pathogenic microorganisms
11:45-12:00	<b>A. Nocentini</b>	Design, synthesis and spectroscopic evaluation of novel fluorescent styryl pyridinium Carbonic Anhydrase Inhibitors
12:00	A. Scozzafava, S. Parkkila, C.T. Supuran: Closing remarks: Announcements regarding the next International CA conference, Bucharest, Romania (24-27 June 2018)	