

# 8<sup>th</sup> Indo-Italian Workshop on Chemistry and Biology of Antioxidants

*Organized by*

Department of Physiology and  
Pharmacology  
"Vittorio Erspamer"  
Sapienza University of Rome



Institute for  
Biomolecular  
Chemistry of  
CNR



*November 29<sup>th</sup> - December 2<sup>nd</sup> 2010*

## Venues

*Room A, Department of Biochemical Sciences  
Room D, "Plesso Tecce"  
Sapienza University  
P.le Aldo Moro 5, Rome*

# THEORETICAL APPROACHES FOR INVESTIGATION OF MOLECULAR PROPERTIES OF ORGANIC MOLECULES AND CHEMICAL REACTIONS

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Modern quantum-chemical methods allow us to estimate the energetics of chemical reactions and to determine the structure of different molecules with precision comparable with that obtained from experiment.

Tautomerism is one of the most important processes involved in chemical reactions as well as in living systems. Tautomeric equilibria have been studied for a long time and a large number of methods have been applied for investigation of tautomeric conversions. We review our work that we have been doing in the field of keto-enol and amino-imino equilibria in aqueous solutions, especially for 5-fluorouracil, its anions and 2-amino-4-oxo-thiazoline. The solvent can control the dynamics of a proton transfer reaction via two distinct types of solute-solvent interactions. The first are long-range solvent polarization interactions and the second – specific short-range hydrogen bonding interactions. In the latter case an explicit interaction with a limited number of solvent molecules could influence the whole reaction path by lowering the energy barrier due to the direct participation of solvent molecules in the proton transfer. The solvent effects are considered in the framework of three different solvation models: a continuum only description, a discrete description in terms of solute-solvent clusters, and a discrete/continuum description in terms of clusters embedded in a continuum. The basis set and electron correlation effects on the energy barriers of tautomerization and the energy differences between tautomers are also analyzed.

Basing on the results of *ab initio* calculations at high level of theory, the relative energies of the structures participating in isomeric, tautomeric or rotameric equilibria can be inferred. Combination of theoretical calculations and NMR spectroscopy is promising for investigation of such equilibria. The comparison of calculated and experimentally determined chemical shifts can be used to find the most stable form of the studied compound. Combination of theoretical calculations and IR or/and UV-vis spectroscopy is also promising. Rare cases of solid state tautomerism are considered.

We presented mechanism of excited state proton transfer (ESIPT) reaction in 2-acetyl-1,3-indandione (2AID). This reaction was studied by quantum-chemical methods and UV-vis and fluorescence spectroscopy. The spectral properties and photostability of 2AID allow us to propose it as a new promising sunscreen agent.

The possibility to create quantum-chemical models of a series of natural antioxidants and their radicals is considered.



	<p>3. <i>Fulvio Ursini</i>. REDEFINITION OF ANTIOXIDANT PARADIGM: FROM FREE RADICAL SCAVENGING TO HORMESIS</p> <p>4. <i>Tiziana Parasassi</i>. REDOX MODULATION OF SIGNAL TRANSDUCTION IN PROLIFERATION/DIFFERENTIATION SWITCH: FROM CELLS IN VITRO TO THE CLINIC.</p> <p>5. <i>Mauro Serafini</i>. DIETARY MODULATION OF OXIDATIVE STRESS IN HUMANS: PHYSIOLOGICAL MEANING AND VALUE OF THE NON ENZYMATIC ANTIOXIDANT CAPACITY (NEAC).</p> <p>6. <i>Antonio Speciale, Joselita Chirafisi, Elisabetta Ricciardi, Sirajudheen Anwar, Antonella Saija, Francesco Cimino</i>. CYANIDIN-3-O-GLUCOSIDE MODULATES ENDOTHELIAL ADAPTIVE RESPONSE BY REGULATING NRF2 TRANSCRIPTION FACTOR: A SPECIFIC ROLE BEYOND ANTIOXIDANT ACTIVITY.</p>
16:00-16:30	Coffee break
16:30-18:30	SESSION III Chaipersons: Anna Giovanetti and Jens Pedersen
	<p>1. <i>Marina Borro, Giovanna Gentile, Luana Lionetto e Maurizio Simmaco</i>. AN INTEGRATED PLATFORM FOR EVALUATION OF THE INDIVIDUAL PROFILE OF DEFENCE AGAINST OXIDATIVE STRESS</p> <p>2. <i>Emiliano Basso, Stefano Leone, Fabio Polticelli, Tommaso Cornetta and Renata Cozzi</i>. THE MULTIPLE ROLES OF RESVERATROL IN CANCER CELLS: CELL CYCLE DELAY, GAP JUNCTIONS MODULATION AND INHIBITION OF TOPOISOMERASE II ACTIVITY.</p> <p>3. <i>Eugenio Luigi Iorio</i>. THE EVALUATION OF OXIDATIVE STRESS IN CLINICAL PRACTICE. SEARCHING FOR THE IDEAL BIOMARKER</p> <p>4. <i>Zeenat Jahan, Tommaso Cornetta, Alessandro Desideri, Akhilesh Datt Pandey, Stefano Rufini, Anna Giovanetti, Silvia Castelli</i> USE OF SACCHAROMYCES CEREVISIAE AS SYSTEM MODEL TO STUDY HUMAN TOPOISOMERASE IB ROLE IN DNA DAMAGE INDUCED BY LOW DOSES IONIZING RADIATION</p> <p>5. <i>Raffaele Fabrini, Alessio Bocedi, Valentina Pallottini, Lorena Canuti, Michele De Canio, Andrea Urbani, Valeria Marzano, Tommaso Cornetta, Pasquale Stano, Anna Giovanetti, Lorenzo Stella, Antonella Canini, Giorgio Federici, and Giorgio Ricci</i>. NUCLEAR SHIELD: A MULTI-ENZYME TASK-FORCE FOR NUCLEUS PROTECTION</p> <p>6. <i>M. Fioramonti, Sandra. Incerpi, Caterina. Tanzarella e Antonio Antoccia</i>. IS THERE A LINK BETWEEN DSB-REPAIR AND ROS-DETOXIFICATION IN THE DNA DAMAGE RESPONSE? THE LESSON FROM CHROMOSOMAL INSTABILITY SYNDROMES</p>
20:00	Dinner
	<p style="text-align: center;"><b>December 1<sup>st</sup> 2010</b></p> <p style="text-align: center;"><b>Room D, "Plesso Tecce"</b> <b>Sapienza University of Rome</b></p>
9:00-11:00	SESSION IV Chaipersons: Irena Kostova and Paolo Sarti
	<p>1. <i>Gurmeet Singh</i>. TRIPHENYL PHOSPHONIUM DERIVATIVES - POTENTIAL ANTIOXIDANTS FOR THE CORROSION INHIBITION</p> <p>2. <i>Venelin Enchev, Silvia Angelova, Nadezhda Markova</i>. THEORETICAL APPROACHES FOR INVESTIGATION OF MOLECULAR PROPERTIES OF ORGANIC MOLECULES AND CHEMICAL REACTIONS</p> <p>3. <i>Petko Aloy, Ivanka Tsakovska, Ilza Pajeva</i>. HYBRID</p>