

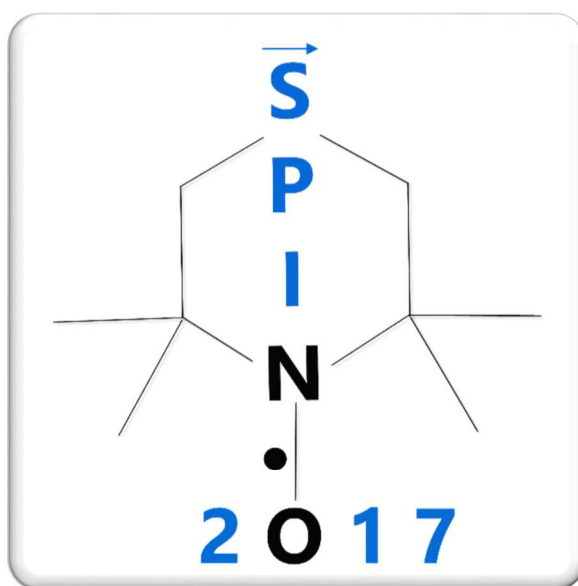


Spin-2017

The 8th Conference on Nitroxide Radicals

Padova - Italy
September 10 -14, 2017

Book of Abstracts



2017

Welcome to SPIN-2017

Dear Colleague,

On behalf of the Organizing Committee, it's my pleasure to give you a warm welcome at the SPIN-2017 Conference on Nitroxides.

I'm proud to announce that 25 countries are represented in this Conference, whose aim is the advance in the knowledge of nitroxides, the inspiration of new ideas and the dissemination of the results obtained in this field. The scientific contributions collected in this Book of Abstracts proof that nitroxides still deserve the attention of the scientific community.

This is the 8-th edition of this Conference, initiated in Hungary in 1979 and chaired by Prof. Dr. Kálmán Hideg. In Padova nitroxides have been used since the 60's in the group of prof. G. Giacometti, and since then the molecules have been studied theoretically (prof. P. L. Nordio) for the development of new spin relaxation theories, and experimentally by EPR spectroscopy (prof. C. Corvaja and prof. M. Brustolon) for the characterization of their physicochemical properties. More recently also organic groups started to take advantage of these molecules for the syntheses of new compounds (prof. C. Toniolo). I'm convinced that Padova is an appropriate location for this Conference, and I hope you will enjoy your staying here for the scientific level offered by the contributors to this Conference, and for the opportunities offered by this historical city founded more than 2500 years ago.

The exchange of information during the oral and the poster sessions, and the activation of new collaborations during the free time used in most scientific Congresses, and also in this one, underlie the concept that, for scientists, the advance of the knowledge is better reached by a cooperative system than a competitive system. Possibly it works not only in science.

I invite you to walk around the city, looking for the frescos, the painting and the masterpieces of Giotto, Giusto de' Menabuoi, Donatello and others, to look at the Galileo's Cattedra or to simply enjoy the shadow under the ancient trees of the most ancient botanic garden in the world. I wish that all these activities, done with other colleagues, can be the catalyst for the formation of new links!

See you under the Goethe's Palm and enjoy the Conference!

Antonio Barbon

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List of Posters

1	Agostini Alessandro	Mainz Germany	Application of Dynamic Electron Polarization to the study of the accessibility of protein-bound chlorophylls
2	Akita Takuya	Osaka Japan	Liquid Crystalline Chiral Nitroxide Radicals as Novel Magneto-Optical Soft Materials
3	Anjos Jorge L. V.	Catalão Brazil	Study of interactions between formulations lipids with lipids in the stratum corneum by Electron Paramagnetic Resonance
4	Assafa Tufa	Bochum Germany	Interaction of pro-apoptotic spin-labelled BIM BH3 peptides with solvents and Bcl-2 proteins
5	Bagryanskaya Elena	Novosibirsk Russia	C—ON Bond Homolysis of Alkoxyamines Triggered by Paramagnetic Copper(II) and Zinc(II) Salts: NMR and Kinetic Investigations and NMP
6	Bernada Florian	Marseille France	Design and synthesis of stable free radicals as polarizing agents for Dynamic Nuclear Polarization Magic-Angle Spinning (MAS) solid-state NMR at high frequency
7	Biondi Barbara	Padova Italy	Synthesis, Conformational Analysis, and Membrane Interaction Mechanism of Spin-Labeled, Medium-Length Peptaibiotics
8	Bortolus Marco	Padova Italy	New lipo-nitroxides as antioxidant agents targeting lipid peroxidation
9	Elas Martyna	Krakow Poland	Oxidative stress imaging in invasive murine breast cancer tumors
10	Filippov Sergey	Prague Czech Republic	Synthesis and solution properties of PHPMA based copolymers containing stable nitroxyl radicals: nanoparticles with excellent EPR imaging properties and their interactions with blood plasma proteins
11	Formaggio Fernando	Padova Italy	The first blue-colored bis-nitronyl nitroxide peptides
12	Franchi Paola	Bologna Italy	E-cigarettes induce toxicological effects that can raise the cancer risk. The contribute of EPR radical probe technique
13	Galazzo Laura	Padova Italy	Investigating myosin alterations in atrophic and hypertrophic muscles from mice by means of CW-EPR
14	Gallo Salvatore	Milano Italy	Spin trapping as tool for investigating radiation induced free radicals in biologically active molecules
15	Godt Adelheid	Bielefeld Germany	Combining nitroxide labels with Gd(III)-based labels in model compounds for the investigation of EPR-based distance determination techniques

16	Golysheva Elena A.	Novosibirsk Russia	Dynamical Transition in Protein Lysozyme Observed by Pulsed EPR of Spin Probes and Labels
17	Klose Daniel	Zurich Switzerland	Calculation of Rotamer Libraries for novel Spin Labels and application to Tyrosines
18	Lecourt Constance	Lyon France	Multifunctional Layered Two-Dimension Manganese (II) – Radical Frameworks: Switchable Spintronic Materials
19	Lobysheva Irina	Louvain Belgium	Clinical Application of the EPR Spectroscopy: characterization of reduced thiols and oxidative stress in the vasculature.
20	Matveeva Anna G.	Novosibirsk Russia	Multi-Gaussian Monte Carlo DEER analysis as applied to biradicals and spin-labeled DNA
21	Mezzina Elisabetta	Bologna Italy	Structural changes of a doubly spin-labelled chemically driven molecular shuttle probed by PELDOR spectroscopy
22	Morris Jason	Marseille France	Photosensitive Alkoxyamines: Mechanistic Insights
23	Peggion Cristina	Padova Italy	The power of EPR in investigating functionalization and penetration into fibers of cotton-bound antimicrobial peptides
24	Pertici Vincent	Marseille France	Synthesis of a degradable block copolymer from a macro-alkoxyamine for spinal cord repair in rat
25	Pliss Evgenii	Yaroslav Russia	Kinetic and Quantum-Chemical Analysis of Cyclic Mechanisms of Reactions of Nitroxyl and Peroxyl Radicals in Oxidizing Unsaturated Compounds
26	Pliss Roman	Yaroslav Russia	Role of Nitroxyl Radicals in Establishing the Mechanism of Process Oxidation of Methyl Linoleate in Solutions and Micelles
27	Polienko Yuliya	Novosibirsk Russia	Mitochondria-Targeted Sterically Shielded Nitroxides
28	Poryvaev Artem	Novosibirsk Russia	EPR spin probe approach for MOF investigation
29	Preoteasa Eugen A.	Bucharest Romania	Tempo-hydrazone may form H-bond association biradicals? A new effect with potential for nitroxide labeling of hydrogels
30	Rogozhnikova Olga	Novosibirsk Russia	Recent progress in chemistry and applications of persistent triarylmethyls
31	Sameach Hila	Ramat Gan Israel	Structural and dynamics characterization of the MerR family metalloregulator CueR in its repression and activation states

32	Sen' Vasily	Chernogolovka Russia	Low molecular chitosan–(poly)nitroxides: Synthesis and evaluation as antioxidants on free radical-induced erythrocyte hemolysis
33	Shilova Irina	Chernogolovka Russia	Molecular mobility of nanocellulose gels
34	Sjakste Nikolajs	Riga Latvia	Association of nitrite concentration in biological fluids with lifestyle and blood biochemical parameters
35	Steinhoff Heinz-Jürgen	Osnabrück Germany	Bioorthogonal spin labeling of proteins in living E.coli cells using click chemistry
36	Sultani Haider	Halle Germany	Spin-labelled diketopiperazines and peptide–peptoid chimera by Ugi-multi-component-reactions
37	Sukhanov Andrey A.	Kazan Russia	Time-resolved EPR study of TEMPO-Bodipy triad
38	Švajdlenková Helena	Bratislava Slovak Republic	Spin probe dynamics in relation to free volume and relaxation dynamics: cis-1,4-(poly)isoprene
39	Syryamina Victoria	Novosibirsk Russia	Small concentrations of alamethicin induce self-assembling and capturing effect in membranes
40	Timofeev Vladimir P.	Moscow Russia	Influence of Synthetic Steroids on Membrane Dynamical Structure Revealed by Lipid Spin Label
41	Toffoletti Antonio	Padova Italy	Enhanced ISC for the modulation of molecular excited state lifetimes and processes in nitroxide-BODIPY dyads and for TTA upconversion
42	Trukhin Dmitry	Novosibirsk Russia	Facile and Convenient Syntheses of Monofunctional TAM Radicals, TAM Spin Labels, and TAM Multispin Systems
43	Valora Gabriele	Göttingen Germany	Long-range distance measurements in TEMPO-labelled RNAs with pulse EPR spectroscopy
44	Yamazaki Taira	Osaka Japan	Synthesis and Magnetic Properties of Nitroxide Biradical Liquid Crystal
45	Zaripov Ruslan	Kazan Russia	ENDOR study of ¹³ C enriched nitroxide radicals and biradicals
46	Zerbetto Mirco	Padova Italy	An integrated computational approach to the Electron Paramagnetic Resonance characterization of rigid ³ ₁₀ -helical peptides with TOAC nitroxide spin labels
47	Zurlo Enrico	Leiden The Netherlands	Rigid Spin Labels for Improved Distance and Dynamics in Intrinsically Disordered Proteins and Peptides

Poster 14

Spin trapping as tool for investigating radiation induced free radicals in biologically active molecules

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Since from the second half of the last century the spin trapping has found wide applications in chemistry, biology and medicine [1]. Of particular interest are the studied of the free radicals induced in biologically active molecules, such as DNA and proteins, when they are exposed to ionizing radiation. Their characterization allows to investigate the radiation-induced primary processes inside living cells. Indeed, ionizing radiations produce many kinds of free radicals through direct action; radicals can be formed also by indirect actions. However, the direct detection of these radicals is hard to obtain as they have a too short lifetime and this makes difficult to record them by conventional electron spin resonance (ESR) technique. This limitation can be overcome by means of spin-trapping method wherein these short-lived free radicals are converted using a diamagnetic scavenger (the spin trap) to longer-lived radicals (the spin adducts), which can be conveniently investigated by means of ESR.

Here, we review a combined method of ESR and spin trapping to identify free radicals induced by direct ionization as well as OH-radical reactions in nucleic-acid related and protein-related compounds. ESR combined with spin trapping remains a useful method for clarifying these processes in a living organism.

[1] Janzen, E.G. Spin-trapping. *Acc Chem Res* **1971**,4, 31–40

[2] Kuwabara, M.; Hiraoka, W; Osamu, I; Applications of the Spin-Trapping Method in Radiation Biology, Chapter in “Applications of EPR in Radiation Research” Springer, 2014, 353-384

[3] Fattibene, P.; Paulicelli, E.; Palma, V.; Patrono, C.; Testa, A.; Pietraforte, D.; *Proceedings of EPRBIODOSE Conference 2015*