



XLII National Congress, Bari, 22-24 September 2014

## Program

### Monday September 22<sup>nd</sup>

10:00-13:00	<b>Registration</b>	
11:00-12:00	<b>Innovative solutions</b>	
12:00-13:00	<b>Bruker users meeting</b>	<b>Agilent users meeting</b>
13:00-14:00	<b>Lunch</b>	
14:00-14:30	<b>Opening</b>	
14:30-15:30	<b>GIDRM/GIRM gold medal award. Chair: M. Cremonini</b> N. Niccolai: My long way from 90 MHz ..... to few THz	
15:30-15:50	<b>Annalaura Segre fellowship 2013. Chair: H. Molinari</b> S. Zanzoni :Set-up and optimization of electroporation protocols to achieve high cell viability and eukaryotic intracellular uptake of isotope-labeled proteins for in-cell NMR	
15:50-16:35	<b>Plenary Lecture. Chair: V. Gallo</b> P. Mastroianni: Application of heteronuclear NMR spectroscopy for mechanistic and structural studies on platinum complexes	
16:35-17:40	<b>Coffee break + Poster session</b>	
	<b>Parallel session A. Chair: L. Mannina</b>	<b>Parallel session B. Chair: A. Spisni</b>
17:40-18:10	F. Cesare Marincola: From breast milk to cheese: some NMR-based metabolomics applications	F. Rastrelli: NMR of monolayer-protected nanoparticles
18:10-18:30	N. Proietti: Portable NMR as a non invasive tool for monitoring the water status of fruits	R. Luisi: Nitrogen stereodynamics as key factor in the reactivity of small heterocycles
18:30-18:50	G. Praticò: NMR-based metabolomics of breast milk to evaluate the effect of phenotype, lactation period and dietary intervention	C. Airoidi: Identification of new anti-neurodegenerative compounds through the NMR screening of natural extracts
18:50-19:10	A. Rizzuti: NMR based statistical hetero-spectroscopy for knowledge transfer in vine leaves quality assessment	C. R. Girelli: Sterical and electronic effects in $[PtCl_2(\eta^2-CH_2=CH_2)(N^{\wedge}N)]$ complexes assessed by NMR
19:10-19:30	A. Ventrella: Characterization of table grape quality by nuclear magnetic resonance coupled with chemometrics	P. Mazzei : Quantitative evaluation of non covalent interactions between glyphosate and dissolved humic substances by NMR spectroscopy
19.30-20.00	<b>GIRM Assembly</b>	

### Tuesday September 23<sup>rd</sup>

9:00-9:45	<b>Plenary Lecture. Chair: P. Turano</b> M. Zweckstetter: NMR spectroscopy in neurodegeneration: Tau and TSPO
9:45-10:05	<b>Bruker Sponsor Lecture. Chair: P. Turano</b> B. Perrone: When the speed matter(s): from very fast MAS to static solid state NMR
10:05-11:20	<b>Coffee break + Poster session</b>

	<b>Parallel session A. Chair: F. Arnesano</b>	<b>Parallel session B. Chair: M. Chierotti</b>
11:20-11:50	<b>L. Ragona:</b> Design of new anti-angiogenic agents targeting fibroblast growth factor-2 interactions with tyrosine-kinase receptor and heparan sulphate proteoglycans	<b>G. Mollica:</b> Residual Dipolar Couplings: a tool for NMR crystallography
11:50-12:10	<b>F. Favretto:</b> Characterization of bile salt binding to recombinant human liver fatty acid binding protein	<b>F. Martini:</b> Crystallographic properties of zirconium phosphonates by means of $^{19}\text{F}$ and $^1\text{H}$ solid-state NMR
12:10-12:30	<b>A. Lasorsa:</b> Cisplatin handover from the copper transporter ATOX1 to ATP7A (MBD1) in near physiological conditions	<b>S. Todisco:</b> Application of solid state NMR spectroscopy to investigate on chemical shift anisotropy in dinuclear platinum complexes
12:30-13:00	<b>D. O. Cicero:</b> The interaction of BA42, a new phosphatase from the antartict, with divalent metals ions	<b>A. Bagno:</b> Predicting the NMR spectra of paramagnetic iron complexes by DFT

13:00-14:30 **Lunch**

	<b>Parallel session A. Chair: L. Calucci</b>	<b>Parallel session B. Chair: N. Niccolai</b>
14:30-15:00	<b>G. Pileio:</b> Long-lived localisation in MRI	<b>G. Colafemmina:</b> NMR studies of internuclear interactions in micellar systems
15:00-15:20	<b>A. Pagoto:</b> Lipid-based nanosystems targeting the activated endothelium for the in vivo visualization by MRI of localized inflammation	<b>V. Di Tullio:</b> Single-sided NMR to study transport of water in agar gels used as cleaning tool in conservation of cultural heritage
15:20-15:40	<b>M. Muñoz Ubeda:</b> Novel nanocarriers based on lipophilic mono- and disaccharides/DPPE encapsulating Gd(III) complexes as efficient MRI probes	<b>C. Corsaro:</b> $^1\text{H}$ HR-MAS NMR investigation on the molecular degradation of ancient documents
15:40-16:25	<b>Plenary Lecture. Chair: V. Gallo</b> <b>A. Macchioni:</b> NMR as an essential tool for investigating molecular transition metal catalysts	

16:25-17:30 **Coffee break + Poster session**

17:30-18:15	<b>Plenary Lecture. Chair: M. Gussoni</b> <b>D. Delli Castelli:</b> Ln(III)HPDO3A complexes as paramagnetic MRI-CEST agents	
18:15-18:35	<b>Agilent Sponsor Lecture. Chair: M. Gussoni</b> <b>M. Cremonini:</b> NUS for everyone: not uniform sampling made easy	
18:35-20:00	<b>GIDRM assembly + announcement of poster competition winners</b>	

20:30 **Social dinner**

**Wednesday September 24<sup>th</sup>**

8:45-9:30	<b>Plenary Lecture. Chair: M. Geppi</b> <b>S. Ashbrook:</b> Investigating disorder in the solid state using NMR spectroscopy	
9:30-10:15	<b>Lectures of poster competition winners. Chair: H. Molinari</b>	
	<b>Parallel session A. Chair: M. Geppi</b>	<b>Parallel session B. Chair: S. Mammi</b>
10:15-10:45	<b>S. Bracco:</b> Modulation of rotor dynamics and recognition of host-guest interactions in highly porous materials	<b>M. Veronesi:</b> $^{19}\text{F}$ NMR for functional screening and fragment based approach
10:45-11:05	<b>F. Grifasi:</b> Solid-state characterization of coordination polymers for electroluminescent applications	<b>A. Mucci:</b> Assessment of freezing effects and diagnostic potential of biobank healthy and neoplastic breast tissues through HR-MAS NMR spectroscopy
11:05-11:25	<b>G. Paul:</b> Zeolites for decontamination of polluted water: a combined solid-state NMR and FTIR study	<b>M. Gussoni:</b> Perfusates and tissue analysis by NMR and EPR spectroscopy: a potential predictive tool for kidney graft outcome

11:25-11:45 **Coffee break**

	<b>Parallel session A. Chair: D. Cicero</b>	<b>Parallel session B. Chair: G. Musco</b>
11:45-12:15	<b>S. Ciofi Baffoni:</b> Copper and Fe/S cluster trafficking: two sides of the same coin	<b>M. Tessari:</b> SABRE hyperpolarization and quantitative analysis of complex mixtures: application to coffee extracts
12:15-12:35	<b>M. Gallo:</b> The N-terminal region of human frataxin	<b>L. Del Coco:</b> Intercultivar and intracultivar variations of Apulian EVOOs studied by $^1\text{H}$ NMR metabolic profiling
12:35-12:55	<b>C. Zucchelli:</b> NMR and Sp140 PHD finger: structure, phosphorylation and PIN1 interaction	<b>A. Sobolev:</b> Metabolic identity and variability of endive and escarole cultivars grown in Lazio and Puglia
12:55-13:40	<b>Plenary Lecture. Chair: P. Turano</b> <b>I.F. Duarte:</b> NMR metabolomics: developments and applications in cancer profiling and toxicological studies	

13:40-15:00 **Closure and lunch**