

# XLI NATIONAL CONGRESS ON MAGNETIC RESONANCE



PISA  
17-19 SETTEMBRE 2012

*dedicated to Ivano Bertini*

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## SCIENTIFIC PROGRAM



UNDER THE AUSPICES OF



Società Chimica Italiana



UNIVERSITA' DI PISA



Consiglio Nazionale  
delle Ricerche

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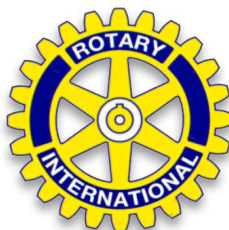
FONDAZIONE

ANTONIO  
DE MARCO

**JEOL**



**RIVOIRA**



**STELAR**

**VPnMr**  
Vanni Piccinotti

## MONDAY September 17<sup>th</sup>

14.00-14.15

Opening

**Chair: H. Molinari**

14.15-15.00 Commemoration of Ivano Bertini: **C. Luchinat**, CERM, Università di Firenze, *40 years of NMR with Ivano... "outside the box"*

**Chair: M. Cremonini**

15.00-16.00 GIDRM/GIRM Gold medal award: **M. Paci**, Università di Roma Tor Vergata, *NMR spectroscopy of molecules, polymers, peptides, proteins*

**Chair: M. Geppi**

16.00-16.20 2011 Segre Fellowship: **C. Facchin**, Università di Padova, *Characterization of unifloral honey markers identified through an NMR-based fingerprinting approach*

16.20-16.40 2011 Segre Fellowship: **C. Di Meo**, Università di Roma La Sapienza, *Anomalous enhanced water diffusion in polysaccharide hydrogels studied by PGSE NMR*

16.40-17.50

*Coffee break* + Poster Session

**Chair: M. Geppi**

17.50-18.35 **M.H. Levitt**, University of Southampton  
*Singlet NMR*

**Parallel sessions**

**DYNAMICS**

**METABOLOMICS**

**Chair: M. Botta**

**Chair: L. Mannina**

18.35-19.05 **S. Borsacchi**, Università di Pisa,  
*Dynamics from solid-state NMR: three approaches for three different stories*

**J.M. Garcia-Manteiga**, Istituto San Raffaele Milano, *Metabolomics of plasma cells. From cell lines to multiple myeloma patients*

19.05-19.25 **L. Fusaro**, Université Libre de Bruxelles,  
*Insight into the dynamics of carboxylate groups as revealed by <sup>17</sup>O dynamics*

**A.P. Sobolev**, IMC-CNR Roma, *Leaf metabolomics and water status as seen by NMR*

19.25-19.45 **M. Mauri**, Università di Milano-Bicocca,  
*Time domain NMR for nanoparticle size measurement and surface characterization*

**M. Vezzoso**, Innovative Solutions Bari, *Metabolomic profiling of table grapes during pre- and post-harvest periods*

## TUESDAY September 18<sup>th</sup>

### Morning

#### The scientific legacy of Ivano Bertini - Chair: H. Molinari

- 8.45-9.15 **L. Banci**, CERM, Università di Firenze, *NMR in mechanistic systems biology: from structures to function*
- 9.15-9.35 **M. Piccioli**, CERM, Università di Firenze, *NMR experiments for paramagnetic molecules*
- 9.35-9.55 **P. Turano**, CERM, Università di Firenze, *Iron proteins: new sites and functions*
- 9.55-10.15 **R. Pierattelli**, CERM, Università di Firenze, *Direct <sup>13</sup>C detection NMR to characterize intrinsic disorder in proteins*
- 10.15-10.35 **F. Cantini**, CERM, Università di Firenze, *Latest news on SOD1*
- 10.35-10.55 **G. Parigi**, CERM, Università di Firenze, *Monitoring the conformational heterogeneity of multidomain proteins*
- 10.55-11.15 **E. Luchinat**, CERM, Università di Firenze, *Monitoring protein maturation steps in living cells with atomic resolution by NMR*
- 11.15-11.40 *Coffee break*

#### Chair: R. Fattorusso

- 11.40-12.00 Bruker Biospin: **S. Wegner**, *New developments in solid-state NMR*
- 12.00-12.45 **D.I. Svergun**, EMBL Hamburg, *Small-Angle X-Ray Scattering and its joint use with NMR to study the structure of biological macromolecules in solution*
- 12.45-13.00 Stelar: **S. Bubici**, *Fast field cycling relaxometry: applications in materials science*
- 13.00-14.15 *Lunch*

## TUESDAY September 18<sup>th</sup>

### Afternoon

**Chair: V. Barone**

**14.25-15.00** **A. Pastore**, NIMR-MRC London, *Kaleidoscopic protein self-assembly: the AXH domain of ATAXIN-1 undergoes a complex multiple equilibrium of species in solution*

#### Parallel sessions

#### BIOMOLECULES

#### SMALL MOLECULES

**Chair: F. Arnesano**

**Chair: D.O. Cicero**

**15.00-15.30** **D. Picone**, Università di Napoli Federico II, *The mechanism of 3D domain swapping in BS-RNASE: when two is better than one*

**S. Provera**, Aptuit Verona, *NMR applied in measurement of physical properties of drugs: the critical micelle concentration*

**15.30-15.50** **C. Zucchelli**, Istituto San Raffaele Milano, *Human Sp140 PHD finger has an unusual fold recognized by PIN1*

**M.R. Chierotti**, Università di Torino, *<sup>1</sup>H DQ CRAMPS solid-state NMR experiments for probing hydrogen-bond networks in Ru(II) building blocks*

**15.50-16.10** **M. Bellanda**, Università di Padova, *Structural insights on 1-C-GRX1 and 1C-GRX3 from Trypanosoma Brucei, two novel potential drug targets against the pathogenic parasite*

**V. Gallo**, Politecnico di Bari, *Solution and solid-state NMR study on metal-coordinated white phosphorus*

**16.10-17.30**

*Coffee Break* + Poster Session

**17.30-19.25**

GIDRM/GIRM assembly

**19.25-19.30**

Announcement of poster competition winners

**21.00**

*Social Dinner at Santa Croce in Fossabanda*

## WEDNESDAY September 19<sup>th</sup>

### Morning

#### Chair: M. Geppi

8.45-9.35 **C.A. Veracini**, Università di Pisa, *Magnetic resonance in Pisa from the sixties to present days* - Special lecture in occasion of his 70<sup>th</sup> birthday

9.35-9.55 Agilent Technologies: **M.A. Cremonini**, *Adventures with qEstimate*

#### Chair: H. Molinari

9.55-10.50 Oral presentations of poster competition winners

10.50-11.20 *Coffee break*

#### Parallel sessions

#### BIOMOLECULES

#### METHODOLOGY

##### Chair: S. Mammi

##### Chair: M. Piccioli

11.20-11.40 **F. Munari**, Max Planck Institute Göttingen, *NMR studies of HP1-histone<sup>3</sup> interaction in the high molecular weight nucleosome system*

**G. Palazzo**, Università di Bari, *Detailed structure of microemulsions: a pulsed gradient spin-Echo NMR approach*

11.40-12.00 **F. Camponeschi**, Università di Siena, *Exploring the interaction of copper with membrane-bound  $\alpha$ -synuclein*

12.00-12.20 **C. Smal**, Fundación Instituto Leloir Buenos Aires, *Discovering function from protein structure: the BA42 protein from the antarctic bacteria *B. argentinensis* is a novel phosphatase*

**D. Lalli**, CERM, Università di Firenze, *Investigation of ferritin by solid-state NMR*

12.20-12.40 **M. D'Onofrio**, Università di Verona, *Exploring the ligand binding capability of human liver fatty acid binding protein*

**M.K. Dibbanti**, Università di Milano-Bicocca, *Forensic differentiation of latex gloves and polyurethane foams by TD-NMR*

12.40-13.00 **G. Malgieri**, Seconda Università degli Studi di Napoli, *How the structural metal ion influences the mechanism of folding of the prokaryotic zinc finger domain*

**S. Colombo Serra**, Bracco Imaging Torino, *Electronic and nuclear spin dynamics in the thermal mixing model of dynamic nuclear polarization*

13.00-14.15 *Lunch*

## WEDNESDAY September 19<sup>th</sup>

### Afternoon

#### Parallel sessions

#### MATERIALS

#### MRI AND BIOMEDICINE

**Chair: C. Forte**

**Chair: E. Terreno**

**14.15-14.45** **D. Capitani**, IMC CNR-Roma, *Nuclear magnetic resonance in the study of materials*

**P. Marzola**, Università di Verona, *Nanoparticles as cell labeling tools in magnetic resonance imaging*

**14.45-15.15** **S. Spera**, Istituto G. Donegani, ENI Novara, *Solid state NMR as a useful approach towards the comprehension of how morphology influences BHJ solar cells performance*

**E. Gianolio**, Università di Torino, *Imaging cell decision*

**15.15-15.35** **E. Callone**, Università di Trento, *Sol-gel derived montmorillonite/silica hybrid coatings on steel for corrosion protection: a solid state NMR analysis*

**G. Digilio**, Università del Piemonte Orientale, *Novel Gd(III)-based MRI probes for the molecular imaging MMPs*

**Chair: G. Valensin**

**15.35-15.50** Euriso-Top: **E. Baltazar-Lépine**, *A short presentation of Euriso-Top company*

**15.50-16.35** **F. Capozzi**, Università di Bologna, *Foodomics and nuclear magnetic resonance spectroscopy, an inseparable combination for the dynamic study of food quality*

**16.35**

*Closure*