Joint Euromar 2010 and 17th ISMAR Conference: A WorldWide Magnetic Resonance Conference
Florence, July 4-9, 2010

1) Summary

Some 1250 scientists from over 50 countries gathered in Florence from July 4th to July 9th to discuss about the latest developments in the field of magnetic resonance and improve communication and cooperation for fruitful research developments. The annual EUROMAR conference was held in conjunction with the triennial ISMAR conference, giving rise to a new format congress.
Housed at the Congress Center in Florence, the conference saw an ambitious and wide ranging lecture programme. The Chairman Ivano Bertini, together with the Program Committee composed by representatives of the two societies and other experts had assembled a tightly packed programme consisting of 8 plenaries, a pre-conference lecture, a closing session with 3 lectures on "Highlights of the Conference", some awards lectures, about 200 session talks organized in 6/7 parallel sessions and 3 poster sessions – all in about 110 hours of science.
Satellite events were the Bruker and Varian Users' meetings (on July 4th) as well as the GIDRM/GIRM (i.e., Italian Magnetic Resonance Discussion Group/Interdivisional Group of Magnetic Resonance of the Italian Chemical Society) annual meeting (on July 10th). Science related topics as research funding, scientific societies' management, networking activities were discussed during lunch and dinner times. A commercial exhibition was held with the participation of about 25 companies as the ideal forum to show their latest products and to meet with all interested participants.

2) Description of the scientific content and discussion at the event

Preconference lecture.
Ray Freeman (Cambridge, UK) presented the first highlights on NMR with a lecture entitled "Speed", discussing the several ways for speeding up NMR measurements through the concept of hyperdimensional spectroscopy.

The plenary lectures: from in vivo to art.
Lyndon Emsley (Université de Lyon, F) presented ultrafast NMR solid state NMR methods for the characterization of organometallic systems to be used in heterogeneous catalysis. The potentiality of static and magic angle spinning solid state NMR to learn about antimicrobial and amyloid peptides in membranes was shown by Frances Separovic (University of Melbourne, AU).
Innovations in MRI was the topic of three talks: Daniel Rugar (IBM Almaden Research Center, CA) introduced the basic principles of nanoscale magnetic resonance force microscopy, a technique that achieves a 100 million-fold improvement in sensitivity over conventional MRI and resolution better than 10 nm; Sarah Nelson (UCSF, CA) presented advancements in MR for *in vivo* studies integrating anatomic with physiological and metabolic imaging; applicability and limitations of NMR and MRI in art were critically discussed by the Nobel Prize laureate Richard Ernst (ETH Zürich, CH).
The application of solution NMR in structural biology was described in the talks by Christian Griesinger (Max Planck Institute for Biophysical Chemistry, Göttingen, D), who focused on the possibility to explore dynamics and learn from it about protein recognition, folding and refolding upon aggregation in infection biology and neurodegeneration, and by Charalampos Kalodimos (Rutgers State University, NJ), who described the characterization of supramolecular protein systems to determine the functional mechanisms of molecular machineries.

Hitoshi Ohta (Kobe University, JP) presented developments and applications of multi-extreme THz ESR Systems.
The lectures were superb and encountered the greatest satisfaction of the audience.

Awards.
Clare P. Grey from the University of Cambridge (UK), was awarded the Ampere Prize and gave a lecture bringing energy storage and conversion into play. She described the application of new NMR approaches to correlate structure and dynamics with function in lithium-ion batteries and solid oxide fuel cells, showing the potentiality of *in situ* NMR experiments to examine the local structure, the location of the vacancies and how these factors affect protonic/oxygen ion motion.
Robert Griffin from MIT (Cambridge, MA), recipient of the ISMAR Prize, focused on the developing field of DNP as an approach to significantly increase sensistivity in MAS and solution NMR, sweeping from the advances in instrumentation, new polarization agents and applications in structural studies of amyloid and membrane proteins.
The talk of the Andrew Prize Lecturer, Benjamin Wylie (University of Columbia, New York, NY), dealt with the use of solid state magic angle spinning NMR methods to measure structurally dependent anisotropic properties in proteins.
On Monday, the scientific sessions ended with the ceremony for the PhD degree *honoris causa* in Structural Biology issued by the University of Florence to Tony W. Keller (Bruker), who gave the *lectio magistralis* "50 Years Of Innovation" .
The ISMAR young investigator, recipient of the award sponsored by Magritek, was Andi Mainz (FMP, Berlin, Germany) for its presentation "The bigger the better: Large protein complexes investigated in solution by MAS NMR". He was the winner of the contest among four finalists, all selected from poster submissions.
The three winners of the Wiley Prize Contest, open to investigators under the age of 40, were: Mathilde Giffard (CEA Grenoble, France) with the presentation "Effect of RF phase shift on the Third Spin Assisted Recoupling in Solid-state NMR, Meike Roth (Max Planck Institute for Polymer Research, Germany) with the presentation "Constant ^{1}H and ^{13}C signal enhancement in NMR using hollow fiber membranes and parahydrogen", and Alexej Jerschow (New York University, NY, USA) with the presentation "Cutoff-free Traveling Wave NMR".
The awards lectures further pointed out the advancements in the various areas.

Sessions and special sessions
The main body of the scientific programme was composed by 6 to 7 parallel sessions which featured 200 session lectures lasting 25' and 38 short (15') oral presentations promoted from the submitted posters. Ten-minutes discussion was allowed after each talk.
The sessions focused on the following topics (listed in alphabetical order):
Alternative detection methods
Bio EPR
Catalysis
Chemical engineering
Computational Classical Mechanics
Computational Quantum Mechanics
Diffusion
DNP
EPR
Fibrils
Food
Force Microscopy

High Pressure
Hybrid Systems
Hyperpolarization
Imaging
Instrument developing
In vivo
Liquid crystals
Liquid State NMR
Low-field NMR
Magnetic materials
Mechanistic systems biology
Membranes
Metabolomics
Metalloproteins
Methods for electrons and nuclei
Methods in structural biology
Molecular imaging
Nanomicroscopy and spectroscopy
NMR and Art
NMR and geophysics
Nuclear and electron relaxation
Pharma
Physics and magnetic resonance of electrons and nuclei
Porous media
Protein dynamics
Quadrupolar nuclei
Quantum computing
Quantum dots and semiconductors
Small molecules liquid NMR
Solid state NMR
Solid state bioNMR
Spin dynamics
Spin labeling
Strongly correlated systems
Structural Biology
Theory

A special session named CASD-NMR was organized. CASD_NMR (Critical Assessment of Automated Structure Determination of Proteins from NMR data) is a rolling community-wide experiment in the frame of the e-NMR Computational Infrastructure, involving developers of software tools / protocols for the automated calculation of protein structures from NMR data. The goal of CASD-NMR is to help advance the relevant methodology in order to reach the level of quality and reliability required for direct structure deposition in the PDB. CASD-NMR will also produce extensive data sets that will be useful to develop better methods for NMR structure validation. State of the art of this project was set by the five lecturers Andrea Cavalli, Peter Güntert, Torsten Hermann, Michael Nigels and Geerten Vuister.
Berhard Blümich, Donatella Capitani, Eleonora Del Federico, Paola Fantazzini, Federica Presciutti and Antonio Scamellotti lectured in the special session on NMR and Cultural Heritage dedicated to the memory of Anna Laura Segre.

The round table “Excerpts from bioNMR in Europe” was chaired by Harald Schwalbe (Frankfurt) and Claudio Luchinat (Florence) with the participation of eight speakers from leading European Institutions who touched key subjects in solid state and solution bio-NMR and discussed perspectives in terms of European collaboration and new European institutions.
The session was followed by a round table on “Strategies for bioNMR in Europe” where the European projects EU-NMR, East-NMR and the currently under negotiation project Bio-NMR were presented to the international audience.

Posters.
More than 730 posters were on display throughout the whole conference, with three official poster sessions with high attendance and intense discussion. Multiple poster areas were organized according to the following thematic areas: Biological Systems (276 contributions), *In vivo*/Imaging (47 contributions), Solid State and Materials/Quadrupolar Nuclei (101 contributions), Small Molecules/Pharma & Metabolomics (112 contributions), Theory & Methods (162 contributions) and 26 poster from the hosting institution (CERM).
Space for late abstracts, which do not enter in the above statistics, was also available in each area.
Some of the posters were selected by the program committee for oral presentations.

Highlights of the conference.
On Friday the closing ceremony was preceded by three speakers who, at the plenary level, summarized the main achievements of the conference in their field of expertise: Silvio Aime presented “Advances in Bioimaging”, Malcom H. Levitt “Advances in Methods and Spectroscopy” and Brian D. Sykes “Advances in BioNMR”.

3) Assessment of the results and impact of the event on future direction of the field
The conference was extremely successful in terms of participation: combining ISMAR and EUROMAR meetings in the touristically and culturally attractive location of Florence was the proper recipe to approximately double the number of participants with respect to the already successful previous EUROMAR meetings.
The conference brought together scientists from industry and academia across Europe and from around the world. Ample participation from young scientist, in particular graduate students and post-doctoral fellows, was achieved thanks to a number of sponsorships and mainly through the ESF contribution. It represented an unique opportunity for them to learn about trends and perspectives in magnetic resonance and for networking and creating new contacts and cooperations.
Enterprises interest was testified by the vendor exhibition, which included leading companies in magnetic resonance, showing their latest innovations in magnetic resonance and related fields. The exhibition was also selected by some research institutions as a means to present their ongoing scientific projects.
The conference was an occasion for Bruker to celebrated its 50 years of innovation activities, while Agilent Technologies Inc. announced in a vendor seminar its acquisition of scientific-equipment maker Varian, Inc. .
Companies and scientific societies supported the congress organization thus gaining in their visibility within the worldwide magnetic resonance community.
The Round Table on bioNMR was an occasion to discuss the interplay and synergism between scientists and manufacturer and about deeper involvement of research SMEs in European initiatives.

The presentations of the “Highlights” speakers formed the cornerstone for the evaluation of the scientific value and impact of the conference.
As introduced by Malcom Levitt, advances in magnetic resonance impact on improved methodology and new contexts and applications. The former can be subdivided in three main lines i.e., experimental methodology, theoretical methodology and simulation methodology. While theory is focused on calculations of spin interactions and spin dynamics, the experimental methodology deals with improved signal polarization and detection and data processing. Improving experimental methodology is closely linked to industrial development and production of high-performance scientific instruments. The emerging contexts were identified as quantum information, solid-state physics and materials, surface science, structural biology, metabolomics and cultural heritage.
From Silvio Aime advancements in bioimaging presented at the conference deal with hyperpolarization, image acquisition systems, contrast enhancements and molecular and cellular imaging.
Brian Sykes recollected the main results in bioNMR, that registered and increasing interest in the dynamics features of biomacromolecules, and in the obtainment of structural information on systems of increasing size and complexity like membrane proteins and protein assemblies.

4) Final programme of the meeting

Sunday, July 4

9:00 am - 4:00 pm	REGISTRATION VARIAN Users' Meeting (Sala onice) 12:00 - 4:00 pm BRUKER Luncheon Symposium (Lecture Hall B) 1:00 - 4:00 pm
4:00 - 4:30 pm	Conference Opening: WELCOME (Lecture Hall A)
4:30 - 5:10 pm	Hans W. Spiess presents: AMPERE PRIZE Winner, ISMAR PRIZE Winner and
5:10 - 5:40 pm	ANDREW PRIZE LECTURE - **Benjamin J. Wylie** Solid-state Magic-angle Spinning NMR Methods for Tensor Measurements and Protein Structure Refinement Using Chemical Shift Tensors (Lecture Hall A)
5:40 - 6:30 pm	Lucia Banci presents: PRECONFERENCE LECTURE - **Ray Freeman** - Speed (Lecture Hall A)
6:30 - 9:30 pm	WELCOMING RECEPTION

Monday, July 5 - Morning Program

9:00-9:50 am	Chair: Z. Luz, Plenary lecture (Sacconi Medal): **Lyndon Emsley** - NMR on Surfaces (Lecture Hall A)					
Lecture Hall	A	B	C	D	E	F
Chair	F.C.L. Almeida	L.L. Cheng	R. Deslauriers	K. Pervushin	T. Fujiwara	E. Goovaerts
10:00-10:25 am	**A. Bax** The Sticky Fingers of Influenza Visualized by Modern Solution NMR	**G.A. Morris** New DOSY and Pure Shift NMR Tools for the Chemist	**M. Neeman** Imaging Angiogenesis: Microenvironmental Control of Vascular Remodeling	**M. Kainosho** Exploring the Missing NMR Information by Selective Isotope Labeling Methods	**T. Meersmann** Hyperpolarized Krypton-83 Magnetic Resonance	**M.K. Bowman** High-Resolution Pulsed EPR: Separating and Connecting Peaks
10:25-10:35 am	Discussion					
10:35-10:50 am	**D.M. Korzhnev** Atomic Resolution NMR Structure of a Transient and Low Populated Protein Folding Intermediate	**I.F. Duarte** Metabolic Signatures of Lung Cancer in Biofluids: an NMR-Metabonomics Study	**F. Mitsumori** Towards Understanding Transverse Relaxation Mechanisms of Tissue Water in Human Brain	**J.D. van Beek** The Haupt Effect under Static and Magic-Angle Spinning Conditions	**E. Markhasin** Balanced Triple Resonance Probe for Cryogenic MAS NMR and Dynamic Nuclear Polarization at 700 MHz	**I. Kaminker** Simultaneous Acquisition of Pulse EPR Orientation Selective Spectra
10:50-11:00 am	Discussion					
11:00-11:25 am	**M. Ubbink** Transient Protein-Protein Interactions Studied by NMR	**B. Jiménez** ^{1}H NMR Based Metabolomics for Early Disease Diagnosis	**M. Rudin** Adaptive Changes in Brain Function in Response to Pathological and Physiological Challenges: fMRI in Rodents to Assess Plasticity in the CNS	**B. Brutscher** Novel NMR Tools for the Study of Folded and Unfolded Proteins	**T.F. Prisner** High Field Dynamic Nuclear Polarization in Aqueous Solutions	**J. Granwehr** Comparing Longitudinal and Transverse Detection of EPR
11:25-11:35 am	Discussion					
11:35-11:50 am	**P. Neudecker** High-Resolution Structure Determination of a Low-Populated Folding Intermediate from NMR Relaxation Dispersion Experiments	**J. Farjon** SERF-filtered Experiments: New Enantio-selective Tools for Deciphering Complex Spectra of Racemic Mixtures Dissolved in Chiral Oriented Media	**G.L. Chadzynski** Region Specific Frequency Differences Between Water and Metabolite Resonances within the Human Brain	**J. Herzfeld** Rapid 3D MAS NMR at Critical Sensitivity	**K.V. Kovtunov** Parahydrogen-Induced Polarization in Heterogeneous Hydrogenation: an Aqueous Phase, MOF and SILP Catalysts	**D.M. Sheppard** Measurements of Quadrupolar Coupling Constants in Deuterium Labelled Ubiquitin
11:50-12:00 am	Discussion					
12:00-12:25 pm	**D. Cowburn** NMR Studies of Protein-Protein Interactions	**E. Holmes** Statistical Spectroscopy: Tools for Metabolic Profiling	**B.K. Rutt** Controlled Self-Assembly of Nanoparticles: A General Template for Developing "Smart" MRI Contrast Agents	**J.H. Freed** Pulse Dipolar ESR and Protein Superstructures: Signaling Apparatus in Bacterial Chemotaxis and Varying Structures of alpha-Synuclein	**W. Köckenberger** Dissolution Dynamic Nuclear Polarisation NMR spectroscopy with a Dedicated Spectrometer	**A. Blank** Measurement of Complex Diffusion in the Micro-sec Time Scale and 10 nm Length Scale by Electron Spin Resonance
12:25-12:35 pm	Discussion					
12:35-12:50 pm	**A.M.S. Duarte** Analysis of the ATPase Cycle of a 200 kDa Molecular Chaperone by NMR	**C. Hilty** Unraveling Multi-step Reactions by Real-time DNP-NMR	**O. Reynaud** A Robust Protocol for Diffusion-Weighted Functional MRI on Rodents at 7 Tesla	**Y. Nishiyama** ^{1}H-^{14}N 2D Solid-State NMR under Very Fast MAS: A Few Minutes Observation for a Sample Less Than 1 mg	**V. Mugnaini** *Ex-situ* DNP and Water Soluble Perchlorinated Trityl Radicals: A Flourishing Match	**D.G. Gadian** Lanthanide Chelates as Relaxation Switches for Brute Force Polarisation
12:50-1:00 pm	Discussion					

Monday, July 5 - Afternoon Program

1:00-3:00 pm	LUNCH BREAK			EUROMAR BOARD OF TRUSTEES (Sala onice)		
3:00-4:45 pm	**POSTER SESSION (posters 3n-2)**					
Lecture Hall	A	B	C	D	E	F
Chair	G.A. Spyroulias	K. Zangger	R. Mulder	A. Lecroisey	S.-I. Tate	B. Guigliarelli
4:45-5:10 pm	**T.-h. Huang** Molecular Interaction between SUMO and the Death-Associated Protein-6 (Daxx)	**M. Kaupp** Quantum-Chemical Computation of Magnetic Resonance Parameters: From EPR of Metalloenzymes to NMR of Paramagnetic Systems	**R.T. Branca** Detection of Brown Adipose Tissue Using Intermolecular Zero Quantum Coherences	**L.M. Gierasch** Insights into Allostery: The Hsp70 Molecular Chaperone	**M. Roth** *(Magnetic Resonance in Chemistry Award for Young Scientists Prize Winner)* Constant ^{1}H and ^{13}C Signal Enhancement in NMR Using Hollow Fiber Membranes and Parahydrogen	**N.J. Turro** Trapping and Magnetic Manipulation of the Spin Isomers of $H_2@C_{60}$
5:10-5:20 pm	Discussion					
5:20-5:45 pm	**M. Delepierre** Molecular Basis of Viral Pathogenicity	**M. Jaszuński** NMR Shielding Constants and Nuclear Magnetic Moments - *ab initio* Methods of Quantum Chemistry and Experiment	**J. Frahm** Magnetic Resonance Imaging in Real Time	**H. Molinari** Structural Bile-ology	**M. Bennati** Studies of Dynamic Nuclear Polarization (DNP) in Liquids: Understanding the Overhauser Mechanism for New Experimental Designs	**A.J. Sederman** Sparse and Bayesian Magnetic Resonance Techniques: Application to Transient and Flowing Systems
5:45-5:55 pm	Discussion					
6:00-6:50 pm	Chair: G. Parigi, Plenary lecture: **Christian Griesinger** - Molecular Dynamics and Neurodegeneration as Seen by NMR Spectroscopy (Lecture Hall A)					
6:50-6:55 pm	Chair: M.H. Levitt, Our thanks to Hans Förster on the occasion of his retirement					
6:55 - 10:00 pm	PhD degree *honoris causa* to Tony W. Keller - Lectio magistralis: 50 Years Of Innovation (Lecture Hall A)					
	ISMAR EXECUTIVE COMMITTEE			BRUKER EVENING		

Tuesday, July 6 - Morning Program

9:00 - 9:50 am	Chair: E.D. Becker, Plenary lecture: **Sarah J. Nelson** - In Vivo Applications of MR Physiological and Metabolic Imaging (Lecture Hall A)						
Lecture Hall	A	B	C	D	E	F	G
Chair	X. Salvatella	J. Harmer	D.E. Warschawski	V.A. Atsarkin	M. Caffrey	K.-P. Dinse	A. Rosato
							Critical assessment of Automatic Structure Determination by NMR (CASD-NMR)
10:00 - 10:25 am	**S. Grzesiek** Characterization of Unfolded and Folded Protein States by Novel NMR Methods	**P.J. Hore** Animal-Detected EPR: Cryptochromes as Magnetic Sensors	**M. Hong** Structure and Dynamics of the Influenza M2 Proton Channel by Solid-State NMR	**D. Loss** Spin Electric Effects in Molecular Antiferromagnets	**A.P. Valente** Portrayal of Complex Dynamic Properties of Defensins by NMR: Multiple Motions Associated with Membrane Interaction	**F. Deng** Spatial Proximity of Acid Sites in Microporous Zeolites as Studied by ^{1}H and ^{27}Al DQ MAS Solid-state NMR Spectroscopy	**M. Nilges** ARIA, Bayesian Structure Calculation and CASD
10:25 - 10:35 am	Discussion						
10:35 - 11:00 am	**H.J. Dyson** Folded-Globule States of Proteins Detected by NMR	**G. Jeschke** Modeling of Protein Structural Transitions from EPR Constraints-Scope and Caveats	**G. Veglia** Characterization Ground and Excited States of Membrane Proteins by Hybrid Solution and Solid-State NMR Methods	**J. van Slageren** Frequency Domain Magnetic Resonance in Molecular Magnetism	**C. Arrowsmith** Structural Genomics of Chromatin Interacting Proteins	**P. Sozzani** Nanoporous Solids: Gas storage, Host-Guest Interactions and Dynamics	**P. Güntert** Blind-Test Evaluation of Automated Protein Structure Determination by NMR and New Developments in CYANA
11:00 - 11:10 am	Discussion						
11:10 - 11:35 am	**Y. Shi** A Large Intrinsically Disordered Region in SKIP and its Disorder-Order Transition Induced by PPIL1 Binding Revealed by NMR	**R.O. Louro** Mind the Gap: Paramagnetic NMR Studies of the Trans-Periplasmic Bioenergetic Chains Linked to Extracellular Metallic Ores	**I.D. Campbell** Intracellular Activation of Integrin Membrane Receptors	**D. Gatteschi** EMR of Iron Molecular Nanomagnets	**I. Shimada** Structural Basis of the Interaction between Chemokines and Their G-protein-coupled Receptors	**M. Brustolon** Electron Paramagnetic Resonance and the Graphite World	**T. Herrmann** CASD-NMR and Liquid- and Solid-State NMR Experiment-Driven Modeling of Macromolecular Systems with UNIO
11:35 - 11:45 am	Discussion						
11:45 - 12:10 pm	**A. Gräslund** The Amyloid β Peptide Involved in Alzheimer's Disease: Molecular Interactions, Secondary Structure Conversions and Aggregation	**S. Un** High-Field EPR Studies of Mn(II) Binding in Biological Systems	**A.S. Arseniev** Structure and Dynamics of Bitopic and Politopic Membrane Helical Proteins	**A. Lascialfari** NMR and Muon Spin Relaxation in Molecular Nanomagnets	**R.A. Byrd** Multi-component Protein:Protein Complexes: The Impact of Long-range Restraints Derived from PRE, PCS, RDCs, Intermolecular NOE, and SAXS Data	**N. Müller** Nuclear Spin Noise - Fundamental Insights and Applications	**A. Cavalli** Protein Structure Determination from NMR Chemical Shifts
12:10 - 12:20 pm	Discussion						
12:20 - 12:45 pm	**J.C.C. Chan** Solid-State NMR Study of the Formation of Steric Zipper in Amyloid Fibrils		**S.J. Opella** Development of NMR Methods for Studying Membrane Proteins	**P.G. Baranov** Magnetic Resonance in Semiconductor Nanostructures: EPR, ESE, ENDOR and ODMR Studies	**R. Riek** The Relationship between the 3D Structures and Properties of Amyloids	**C.J. Pickard** Exploring Structure Space – Theory and Experiment Combined	**G.W. Vuister** New Tools for NMR Structure Validation. Application to the CASD-NMR Structures
12:45 - 12:55 pm	Discussion						

Tuesday, July 6 - Afternoon Program

1:00 - 3:00 pm	LUNCH BREAK	AMPERE BUREAU MEETING (Sala onice)
3:00 - 4:45 pm	**POSTER SESSION (posters 3n - 1)**	
4:45 - 6:00 pm	Chair: A. Bax, ISMAR YOUNG INVESTIGATOR AWARD FINALISTS (Sponsored by Magritek): **E. Y. Chekmenev**: Automated Parahydrogen-Induced Polarizer (PHIP) Employing Low Field NMR Spectrometer, Tunable RF Circuit and *in situ* Detection **D. Delli Castelli**: Magnetically Oriented Nanovesicles as MRI CEST Agents **C. Lendel**: Structure Based Drug Design for Intrinsically Unstructured Proteins **A. Mainz**: The Bigger the Better: Large Protein Complexes Investigated in Solution by MAS NMR (Lecture Hall A)	
6:00 - 6:50 pm	Chair: T. I. Smirnova, Plenary lecture: **Hitoshi Ohta** - Developments and Applications of Multi-Extreme THz ESR System (Lecture Hall A)	
6:50 - 10:00 pm	Kevin Meldrum, Marketing Director of Research Products at Agilent Technologies Welcome to Agilent: A Continued Commitment to NMR (Lecture Hall A)	
	ISMAR FULL COUNCIL MEETING	AGILENT/VARIAN EVENING

Wednesday, July 7 - Morning Program

9:00-9:50 am	Chair: P.W. Kuchel, AMPERE PRIZE LECTURE: **Clare P. Grey** - Energy Storage and Conversion: Using Local Structural Probes to Understand and Optimise the Functioning of Battery and Fuel Cell Materials (Lecture Hall A)					
Lecture Hall	A	B	C	D	E	F
Chair	C. Luchinat, H. Schwalbe	G. Batta	P. Hoefer	R.W. Martin	L.D. Spicer	J.-P. Korb
	Excerpts from bioNMR in Europe					
10:00-10:25 am	**H. Schwalbe** Riboswitch-RNAs in Transcriptional Regulation and RNA Thermometers in Translational Regulation Studied by NMR Spectroscopy	**A. Ciulli** Biophysical and Structural Approaches in Fragment-Based Screening: Probing Molecular Recognition for Chemical Biology and Drug Discovery	**J. Reimer** Optical Nuclear Hyperpolarization in Semiconductors	**A. Samoson** Introducing New Variables to MAS NMR	**F. Arnesano** Interaction of Cisplatin with Transport Proteins: Solution and In-Cell NMR Studies	**D. Goldfarb** Nanometer Scale Distance Measurements in Proteins Using Gd^{3+} Spin Labeling
10:25-10:35 am	Discussion					
10:35-11:00 am	**I.C. Felli** Progress in ^{13}C Direct Detection for Biomolecular NMR	**M. Pellecchia** NMR Based Drug Discovery: Screening and Design of Novel Chemical Probes	**V.S. Bajaj** Remotely Detected Magnetic Resonance Imaging and Velocimetry	**E.R. deAzevedo** NMR Approaches for Studying Intermediate Dynamics in Organic Solids and Their Applications in the Study of Electroluminescent Polymers	**M. Shirakawa** Structures, Functions and Stability of Proteins in Mammalian Cells Investigated by In-Cell NMR Spectroscopy	**B.J. Gaffney** Mapping Inhibitor Binding Sites on a Large Enzyme by Electron Spin-Spin Derived Distances
11:00-11:10 am	Discussion					
11:10-11:35 am	**R. Boelens** Dynamics of Ubiquitination Complexes	**T. Carlomagno** Mechanisms of Intermolecular Recognition and Drug Design by INPHARMA: Theory and Applications	**L. Frydman** Payback Time: Spatially Encoded NMR as a Novel MR Imaging Modality - Principles and Prospects	**S.P. Brown** High-Resolution Solid-State NMR Methods for the Structural Characterisation of Organic Solids	**R.S. Norton** Structure and Interactions of Malaria Surface Proteins	**S. Appelt** New Developments in Low Field Nuclear Magnetic Resonance
11:35-11:45 am	Discussion					
11:45-12:10 pm	**V. Sklenár** High-Dimensionality Experiments and Assignment Strategies for Partially Disordered Proteins with Highly Repetitive Sequences	**C. Dalvit** Fluorophilic Protein Environments Probed with ^{19}F NMR-Based Fragment Screening	**R. Gruetter** Ultra-High Field Imaging and Spectroscopy at 14 Tesla	**N.C. Nielsen** New Twists to Dipolar Recoupling in Biological Solid-State NMR: Optimal Control, Multiple-Field Oscillation, Recoupling without Decoupling, and Resolution Enhancement	**G. Varani** RNA-Binding Peptidomimetics Repress HIV Viral Replication by Specifically Inhibiting Transcriptional Activation	**R.G. Bryant** Biological Interface Dynamics from Magnetic Relaxation Dispersion
12:10-12:20 pm	Discussion					
12:20-12:45 pm	**M. Pons** Multiple Signal Integration by the Intrinsically Disordered Unique Domain of Human c-Src: An NMR View	**P. Selenko** Cells, Drugs and NMR	**H.H. Segnorile** Quasi-Equilibrium in Liquid Crystal ^1H Spins Via Eigen-Selective Decoherence (12:20-12:35)	**H.J.M. de Groot** Self-Assembling Natural and Artificial Light-Harvesters	**J. Feigon** New Insights into Structure and Dynamics of Riboswitch and Telomerase RNAs	**J. Kowalewski** Joint Analysis of NMRD and EPR Data by Slow-Motion Theory: Two Medium-Sized Gd(III) Complexes as an Example
12:45-12:55 pm	Discussion					

Wednesday, July 7 - Afternoon Program

1:00 - 3:00 pm	LUNCH BREAK			AMPERE COMMITTEE MEETING (Sala Onice)		
Lecture Hall	A	B	C	D	E	F
Chair	C. Luchinat, H. Schwalbe	B. Blümich	J.P. Yesinowski	R. Blinc	B. Kieffer	H.-J. Steinhoff
	Excerpts from bioNMR in Europe	*NMR and Cultural Heritage (dedicated to Anna Laura Segre)*				
3:00 - 3:25 pm	**B.H. Meier** Protein Structures by Solid-State NMR: Recent Progress	**A. Sgamellotti** Portable NMR in Cultural Heritage: the Contribution of Annalaura Segre **F. Presciutti** Characterization of Binders in Ancient and Modern Paintings by NMR-MOUSE	**W.S. Warren** Extending T_1 and T_2 Relaxation Times to Improve Contrast and Sensitivity	**F. Haarmann** Shielding and Quadrupole Coupling Parameter of Intermetallic Compounds: NMR Experiment and Quantum Mechanical Calculations	**R. Bittl** EPR/ENDOR on Complex Metal Centers in Enzymes – From Single Crystals to Whole Cells	**W. Lubitz** Intermediates in Hydrogenase Catalysis Studied by Advanced EPR Techniques
3:25 - 3:35 pm	Discussion					
3:35 - 4:00 pm	**A. Böckmann** Structural Studies of Prion Fibrils by Solid-State NMR Spectroscopy	**E. Del Federico** Unilateral NMR as a Tool to Characterize Deterioration Processes and Follow Up Conservation Treatments in Works of Art	**M. Botta** Optimizing the Relaxivity of Macromolecular MRI Contrast Agents	**N.J. Curro** Probing Novel Electronic States in Strongly Correlated Electron Materials Using NMR and NQR	**G.M. Smith** Very High Sensitivity, Orientation Dependent, Long-Range Distance Measurements in Biomolecules Using PELDOR at 94 GHz	**G.R. Hanson** Insights into Metal Ion Mutagenesis and Catalysis of Dinuclear Mn Metallohydrolases Utilising EPR Spectroscopy
4:00 - 4:10 pm	Discussion					
4:10 - 4:35 pm	**C. Redfield** Control of Periplasmic Interdomain Thiol:Disulfide Exchange in the Transmembrane Oxidoreductase DsbD	**P. Fantazzini** Advantages and Pitfalls of Magnetic Resonance for Fluids in Porous Media Applied to Cultural Heritage	**T.J. Meade** The Coordination Chemistry of Signal Amplification and Targeting for MR Probe Development	**M. Horvatić** High-Field NMR as a Powerful Tool to Study "Exotic" Phases in Quantum Spin Systems	**A.J. Vila** Invisible States in Paramagnetic Copper Proteins	**J.J.G. Moura** NMR and DOCKING Studies on Electron Tranfer Complexes
4:35 - 4:45 pm	Discussion					
4:45 - 5:10 pm	ROUND TABLE Strategies for bioNMR in Europe	**D. Capitani** Nuclear Magnetic Resonance in Cultural Heritage	**R.E. Lenkinski** The Development of a Gadolinium Based MR Contrast Agent for the Visualization of Malignant Micro-calcification in Human Breast Cancer	**M. Edén** New Methods for Solid-State NMR Simulations and Studies of Bio-mimetic Apatite-Formation from Mesoporous Bioactive Glasses	**G.M. Clore** Hybrid Structure Determination Methods, Paramagnetic Relaxation and Differential Relaxation	**S. Van Doorslaer** A Combined EPR and DFT Approach to Tackle Chiral Catalysis
5:10 - 5:20 pm		Discussion				
5:20 - 5:45 pm		**B. Blümich** Mobile NMR and Cultural Heritage	**I. Furó** Wood NMR and MRI: Molecules, Interactions, and Motion	**P.K. Madhu** Recoupling and Sensitivity Enhancement in Half-Integer Spin Quadrupolar Nuclei	**O. Schiemann** PELDOR on DNA: Orientations, Dynamics, Bending, Non-Covalent Labelling and Protein Binding	**I.V. Koptyug** A Closer Look at Heterogeneous Catalysis: Applications of and Novel Hypersensitive Tools for the NMR/MRI Toolkit
5:45 - 5:55 pm	Discussion					
6:00 - 6:50 pm	Chair: J.W. Emsley, Plenary lecture: **Richard R. Ernst** - Why NMR and MRI, As Useful As They Are for Analyzing Art, Are Sometimes Outperformed by Other Techniques, Such As RAMAN (Lecture Hall A)					
6:50 - 7:15 pm	AMPERE GENERAL ASSEMBLY (Lecture Hall A)			JEOL EVENING		
7:15 - 11:00 pm						

Thursday, July 8 - Morning Program

9:00-9:50 am	Chair: F. M. Poulsen, Plenary lecture: **Frances Separovic** - Resolving Antimicrobial and Amyloid Peptides in Membranes (Lecture Hall A)					
Lecture Hall	A	B	C	D	E	F
Chair	A. Goldbourt	M. Ernst	J. Bargon	L. Mueller	B. G. Karlsson	R. Pierattelli
10:00-10:25 am	**R.E. Wasylishen** Progress in Interrogating Quadrupolar Nuclei via Solid-State NMR Spectroscopy	**A.P.M. Kentgens** Developing NMR Tools to Study Nanoliter Solids and Liquids Samples	**J.H. Ardenkjaer-Larsen** New Developments in Dissolution-DNP for in Vivo Imaging	**M.H. Levitt** Singlets, Triplets and Multipoles: Spin Rotational Symmetries in Solids and Liquids	**K.V.R. Chary** Structure, Dynamics and Ca^{2+}-Binding Properties of Intrinsically Unfolded And Folded βγ-Crystallins	**A.G. Palmer III** Joint Analysis of Conformational Dynamics in Ribonuclease H using NMR Spectroscopy and Molecular Dynamics Simulations
10:25-10:35 am	Discussion					
10:35-10:50 am	**V. Vitzthum** Solid-State Nitrogen-14 Nuclear Magnetic Resonance Enhanced by Dynamic Nuclear Polarization Using a Gyrotron	**R.M. Fratila** Multinuclear Nanoliter NMR Spectroscopy in a Microfluidic Chip	**P. Berthault** Toward Molecular Imaging Using ^{129}Xe NMR-based Biosensors	**I. Kuprov** Analytical Derivatives of Spin Dynamics Simulations	**J. Angulo** Ligand–Receptor Binding Affinities from Saturation Transfer Difference (STD) NMR Spectroscopy: The Binding Isotherm of STD Initial Growth Rates	**S. Haber-Pohlmeier** Water Flow from Soil to Roots Investigated by MRI
10:50-11:00 am	Discussion					
11:00-11:25 am	**A. Watts** Differential Dynamics of Bound Ligands in Membrane Targets	**R.M. Wiesendanger** Atomic-Resolution Spin Mapping and Magnetometry at the Atomic Level	**B. Driehuys** Recent Progress in Clinical Hyperpolarized ^{129}Xe MRI	**T. Takui** A Few Steps towards the Implementation of Molecular Spin Quantum Computers: Pulse-Based Electron Magnetic Resonance Spin Technology	**S.J. Glaser** Optimal Control of Spins Systems: Robust Pulses, Coherence Transfer and Decoupling	**C.W.M. Kay** From Biology to Business: Combining EPR with Thin Films to Create a Sensor?
11:25-11:35 am	Discussion					
11:35-11:50 am	**A. Lesage** Surface Enhanced NMR Spectroscopy by Dynamic Nuclear Polarisation	**M. Fellenberg** Characterization of Picomole Amounts of Oligosaccharides from Glycoproteins by ^{1}H NMR Spectroscopy	**T.K. Meldrum** A Xenon-based Molecular Sensor Assembled on an MS2 Viral Capsid Scaffold	**B.E. Bode** Does Radical Pair Recombination Act as a Quantum Measurement?	**Y. Elias** Heat-Bath Cooling of Spins in Amino Acids	**N. Cox** A Tyrosyl-Dimanganese Coupled Spin System in Ribonucleotide Reductase of *C. ammoniagenes*: A Multifrequency EPR and X-ray Crystallography Study
11:50-12:00 pm	Discussion					
12:00-12:25 pm	**H. Oschkinat** The Structure of Human αB-Crystallin by Solid-State NMR and Small-Angle X-ray-Scattering, and Some Exciting Adventures with DNP	**M. Takigawa** Probing Novel Order and Dynamics in Strongly Correlated Electron Systems by NMR	**K. Golman** Hyperpolarization: Possibilities and Impossibilities	**S. Gambarelli** Pulsed EPR Studies of Decoherence in Rare Earth Ions and Coupled Systems	**M.C.D. Tayler** Relaxometry of Singlet Nuclear Spin States (12:00-12:15)	**F.A. Walker** Protein Structure and Dynamics of the Nitrophorins from a New World Blood-Sucking Insect
12:25-12:35 pm	Discussion					
12:35-12:50 pm	**B. Bechinger** Solid-State NMR Spectroscopy of Oriented Membrane Polypeptides at 100 K with Signal Enhancement by Dynamic Nuclear Polarization	**J. Boisbouvier** Towards Real-Time NMR Studies of Biological NanoMachines	**V.V. Zhivonitko** Microfluidic Gas-Flow Profiling Using Combined Parahydrogen-Induced Polarization and Remote Detection MRI Techniques	**G. Mitrikas** Solid-State Quantum Gates based on Hybrid Electron-Nuclear Spin Systems		**E. Duchardt-Ferner** Anatomy of a Minimalistic Riboswitch: Highly Modular Structure and Ligand Binding by Conformational Capture by the 27nt Neomycin Sensing Regulatory RNA Element
12:50-1:00 pm	Discussion					

Thursday, July 8 - Afternoon Program

1:00 - 3:00 pm	LUNCH BREAK		INTERNATIONAL EPR/ESR SOCIETY - Highlights of AGM2010 and presentation of Silver Medal (Lecture Hall F)		EMAR-ESF steering committee meeting (Sala onice)	
3:00 - 4:45 pm	**POSTER SESSION (posters 3n)**					
Lecture Hall	A	B	C	D	E	F
Chair	K. Jackowski	J. Schraml	N. Nestle	K.E. Kövér	J. Led	Y. Sanakis
4:45 - 5:10 pm	**M. Baldus** Selective Membrane Transport Systems Investigated by Solid-State NMR Spectroscopy	**K.R. Koch** Isotope Effects in ^{195}Pt High-Resolution NMR: Unambiguous Assignment Method of all $[PtX_{6-n}(H_2O)_n]^{n-2}$ (X = $^{35/37}$Cl/$^{79/81}$Br, n = 0-5) Complexes in Aqueous Solution	**M. Garwood** Frequency-Swept MRI: No Sound or Echoes	**P.R. Vasos** In Search of Line Narrowing, Extended Spin Memory, and Enhanced Polarisation: Through the Looking Glass of NMR	**G. Otting** Lanthanide Tagging for Protein Structure Determination	**E.J.L. McInnes** Probing the Physics of Antiferromagnetic Rings by EPR Spectroscopy
5:10 - 5:20 pm	Discussion					
5:20 - 5:45 pm	**H. Akutsu** Solid-State NMR Analysis of H^+-ATP Synthase Subunit c-Ring in Membranes	**M. van Gastel** Triplet state EPR Spectroscopy of Bioluminescent Proteins	**K. Nicolay** The Challenges and Opportunities of Molecular Imaging with MRI	**D. Budker** Detection of Nuclear Magnetization with Optical Magnetometers: From Remote-Detection Imaging to Measuring J-Couplings at Zero Field	**A.M. Gronenborn** Synergy between NMR and cryo-EM - Novel Findings for HIV Capsid Function	**A.-L. Barra** HF-EPR Study of Magnetic Anisotropy in Tetrairon(III) Single-Molecule Magnets
5:45 - 5:55 pm	Discussion					
6:00 - 6:50 pm	Chair: R. Kaptein, ISMAR PRIZE LECTURE sponsored by CIL - **Robert G. Griffin** - High Field Dynamic Nuclear Polarization - The Renaissance (Lecture Hall A)					
6:50 - 7:15 pm	ISMAR GENERAL ASSEMBLY (Lecture Hall A)					
7:30 - 10:00 pm	ROMANTIC SUNSET RECEPTION AT BOBOLI GARDEN					

Friday, July 9 - Morning Program

9:00 - 9:50 am	Chair A. Kumar: Plenary lecture: **Daniel Rugar** - Force-Detected Nanoscale MRI: Recent Progress and Challenges Ahead (Lecture Hall A)						
Lecture Hall	A	B	C	D	E	F	G
Chair	M. Piccioli	A. Spisni	D. Fiat	V.Y. Orekhov	G. Melacini	H. Van As	J. Vervoort
10:00 - 10:25 am	**R. Fattorusso** From Eukaryotes to Prokaryotes (or Vice Versa?): Single Classical Zinc Fingers as DNA Binding Domains	**D.S. Cafiso** Conformational Exchange and Dynamics in Membrane Transporters Determined by Site-Directed Spin Labeling	**H. Desvaux** Non Linear Spin-Dynamics of Dissolved Hyperpolarized Xenon	**J. Jokisaari** NMR of Atomic and Small Molecular Probes in Anisotropic Liquids	**R. Brüschweiler** Protein Dynamics, NMR, and Force Fields	**H. Maeda** Towards an NMR Spectrometer Operating beyond 1 GHz: Operation of a 500 MHz High Temperature Superconducting NMR	**L. Mannina** NMR Methodology in Food Analysis
10:25 - 10:35 am	Discussion						
10:35 - 11:00 am	**L. Ragona** Structural and Dynamic Determinants of the Multistep Bile Salt Binding to Lipid Binding Proteins	**G.J. Gerfen** Structure/Function of Radical Enzymes	**S.B. Duckett** Transfer of *Para* hydrogen Derived Spin Order Sensitizes MRI and NMR Measurements by Three Orders of Magnitude	**J.H. Prestegard** Long-Range and Orientational Constraints for Membrane Associated Complexes	**E. Bordignon** Maltose and Vitamin B12 Importers: Modeling the Conformational Changes during Transport with Interspin Distance Restraints	**S. Xu** Magnetic Resonance Imaging and Magnetic Molecular Imaging with Atomic Magnetometers	**M. Spraul** Integration of Nontargeted and Targeted Screening by NMR
11:00 - 11:10 am	Discussion						
11:10 - 11:35 am	**S. Grimaldi** Probing Semiquinone Binding to Nitrate Reductase A by Pulsed EPR Spectroscopy	**D. Nietlispach** Solution-NMR Structure Determination of the Seven-Helical Transmembrane Protein Sensory Rhodopsin	**L. Schröder** Encapsulated Xenon as an NMR Sensor for Biomedical Applications	**C.M. Thiele** Residual Dipolar Couplings (RDCs) as Restraints in Organic Structure Determination	**D. Kern** Choreographing an Enzyme's Dance –Surprises Exposed by NMR, Crystallography and Computation	**D. Sakellariou** Rotating Micro-coils for High-Resolution Spectroscopy and MRI Microscopy	**U. Günther** Cancer Metabolomics: From Diagnostics to Drug Discovery
11:35 - 11:45 am	Discussion						
11:45 - 12:10 pm	**J. Plavec** DNA G-Quadruplex Structures and Cation Interactions	**F.M. Marassi** NMR Structural Studies of Bacterial Virulence Factor Membrane Proteins	**K.M. Brindle** Detecting Tumour Responses to Treatment Using Hyperpolarized ^{13}C Magnetic Resonance Spectroscopic Imaging	**B.F. Chmelka** ^{29}Si-^{29}Si Scalar and Dipolar Couplings as Constraints for Determining Complicated Silicate Structures	**D. Fushman** Insights into Structure, Dynamics, and Interactions in Multidomain Systems	**M.S. Sherwin** Free-Electron Laser-Based Pulsed EPR at 240 GHz and Beyond	**A.S. Edison** The Merging of Metabolomics and Natural Products: Applications in Chemical Communication of Nematodes
12:10 - 12:20 pm	Discussion						
12:20 - 12:45 pm	**T. Madl** (Solvent) PRE-Assisted Structural Analysis of Large Protein Complexes (12:20-12:35)	**T.A. Cross** Sorting Structural Reality from Among the Artifacts: The M2 Proton Channel	**R.R. Rizi** Assessment of Lung Function with Polarized MRI		**M. Vendruscolo** Advances in the Characterization of Free Energy Landscapes of Proteins by NMR Spectroscopy	**A. Jerschow** *(Magnetic Resonance in Chemistry Award for Young Scientists Prize Winner)* Cutoff-free Traveling Wave NMR	**Y. Wang** Metabonomics our Wormy World
12:45 - 12:55 pm	Discussion						

Friday, July 9 - Afternoon Program

1:00 - 3:00 pm	LUNCH BREAK			JOINT EUROMAR 2011/EFEPR 2011 SCIENTIFIC COMMITTEE MEETING (Sala Onice)			
Lecture Hall	A	B	C	D	E	F	G
Chair	L. Zidek	S.M.C. Menezes	I.C.P. Smith	F. Toma	D.C. Ailion	P.J.M. van Bentum	I. Moura
3:00 - 3:25 pm	**W. Koźmiński** Multidimensional NMR beyond Resolution Limitations	**J. Wrachtrup** Generating Complex Spin Quantum States from Single Electrons and Nuclear Spins	**A. Heerschap** In Vivo Multi-Nuclear Magnetic Resonance	**S. Mammi** Possible Role of Structural Modifications of DJ-1 under Oxidative Stress in Parkinson Disease	**S.E. Ashbrook** Investigating Disorder in Ceramics: Multinuclear Solid-State NMR and First-Principles Calculations	**M. Giffard** *(Magnetic Resonance in Chemistry Award for Young Scientists Prize Winner)* Effect of RF Phase Shift on the Third Spin Assisted Recoupling in Solid-state NMR	**D.J. Craik** Structure-Activity Studies of Cyclotides: Ultrastable Plant Proteins with Applications in Drug Design
3:25 - 3:35 pm	Discussion						
3:35 - 4:00 pm	**M. Billeter** Principles and Practice of Projection-Decomposition Tools for Resonance Assignments and Protein Structure	**D. Suter** Spin-Qubits for Quantum Information Processing	**K. Ugurbil** Human Imaging with Ever Increasing Magnetic Fields and Strange RF Behavior	**C.L. Khetrapal** NMR in Neurological, Gastrointestinal and Liver Diseases, Infection and Open Heart Surgery	**D. Massiot** Sorting Out Chemical and Geometrical Contributions in Disordered Materials	**P. Grandinetti** Pathway Symmetries in Magnetic Resonance	**A.W. Rutherford** EPR studies of the Quinone-Iron Complex Photosystem II
4:00 - 4:10 pm	Discussion						
4:10 - 5:00 pm	Chair: H. Rueterjans, Plenary lecture: **Charalampos G. Kalodimos -** Structural and Dynamic Basis for the Assembly of Protein Machineries by NMR (Lecture Hall A)						
5:00 - 5:30 pm	Chair: I. Bertini (Lecture Hall A) **Silvio Aime** - Advances in Bioimaging						
5:30 - 6:00 pm	**Malcom H. Levitt** - Advances in Methods and Spectroscopy						
6:00 - 6:30 pm	**Brian D. Sykes** - Advances in BioNMR						
6:30 pm	CLOSURE						
8:00 pm to the following day	CONFERENCE BANQUET						