



DETAILED PROGRAM

Sunday, 2 July 2017

from 12.00	Registration opens
13.00-16.00	Bruker Symposium (Baltic Ballroom, 3rd floor) 12:00 Lunch and registration 13:00 Welcome & Update on Bruker / Werner Maas 13:20 New Multi-receive Capabilities with the AVANCE NEO and TopSpin News / Rainer Kuemmerle 13:50 TBA, Gaël De Paëpe, INAC (CEA – Grenoble Alpes University), France 14:20 Quantitative Magnetic Resonance Techniques / Sylwia Kacprzak/Rainer Kerssebaum 14:45 Coffee break 15:05 Probe news – iProbe, CrP / Aitor Moreno 15:30 Pharma: InsightMR and Fragment Based Screening / Matteo Pennestri 16:00 End of the session
16.00-16.30	Welcome coffee
16.30-19.00	Opening and Prize Session chair: Lucio Frydman, Wiktor Koźmiński 16.30 Welcome by Bernhard Blümich on behalf of Ampere 16.35 Welcome by Lucio Frydman on behalf of Euromar 16.40 Welcome and information, Wiktor Koźmiński 16.50 Raymond Andrew prize introduction Beat Meier 16.55 Raymond Andrew prize lecture 17.15 Varian Young Investigator Award prize introduction Lucio Frydman 17.20 Varian Young Investigator Award prize lecture 17.50 Presentation of the Ernst Prize Lucia Banci 18.05 Ernst Prize lecture
19.00-21.00	Welcome Mixer



Monday, 3 July 2017

08.45-10.05 Plenary Session 1 (Grand Ballroom) chair: Kevin Brindle			
08.45	<i>Hyperpolarised ¹²⁹Xe MRI - methods and applications</i> Jim Wild (UK)		
09.25	<i>Applications of magnetic resonance to study fluid flows and transport in porous media: Exploiting undersampling in magnetic resonance</i> Lynn Gladden (UK)		
10.05-10.30 Coffee break			
10.30-12.30	S01 New hardware, new tricks (Grand Ballroom ABC) chair: Dimitrios Sakellariou	S02 Structural EPR 1 (Grand Ballroom DEF) chair: Marina Bennati	S03 Methods in biosolids (Congress Hall) chair: Beat Meier
10.30	<i>Using Quasioptics and EPR to Optimize mm-wave fields in DNP NMR probes</i> Kurt Zilm, USA	<i>Dipolar spectroscopy with broadband pulses</i> Thomas Prisner, Germany	<i>Optimized and selective (hyper)polarization usage</i> Manuel Etzkorn, Germany
11.00	<i>Universal quantum control with zero-field Nuclear Magnetic Resonance</i> Teng Wu, Germany	<i>Local electrostatics and dielectric constants by side-directed spin-labeling EPR of ionizable nitroxides</i> Alex Smirnov, USA	<i>Indirect ¹⁴N detection methods for structural analysis of proteins in solid-state NMR</i> Maria Concistre, UK
11.20	<i>B₀ field instability, T₁-noise and means to suppress it</i> Maxim Mayzel, Sweden	<i>smFRET and DEER distance measurements as applied to disordered and structured proteins</i> Tatyana Smirnova, USA	<i>MAS solid-state NMR: Asynchronous recoupling, decoupling and multiple data acquisition</i> Kshama Sharma, India
11.40	<i>Extension of nuclear spin T₁ by precipitation and dissolution</i> James Eills, UK	<i>Structure of the proton:fumarate symporter SLC26Dg in lipid environment studied with EPR spectroscopy</i> Eva Jaumann, Germany	<i>Access to side-chain protons with >100 kHz MAS</i> Jan Stanek, France
12.00	<i>DNP in rotating solids sans depolarization</i> Gaël De Paëpe, France	<i>Structure-reactivity relationships in heterogeneous catalysis revealed by advanced EPR techniques</i> Mario Chiesa, Italy	<i>Conformational plasticity in the NaK channel revealed by solid-state NMR</i> Adam Lange, Germany
12.30-13.30 Lunch			
12.30-13.30	Jeol Lunch Symposium (Congress Hall) <i>What's new in JEOL's NMR?</i> Dr. Jun Ashida (JEOL)		
13.30-15.30 P01 Poster Session / odd numbers			



(Baltic Ballroom)

15.30-17.30	S04 Materials NMR (Grand Ballroom ABC) chair: Marek Potrzebowski	S05 MRI and MRS (Grand Ballroom DEF) chair: Lynn Gladden	S06 Computational advancements (Congress Hall) chair: Rafael Brüschweiler
15.30	<i>New methods for ultra-wideline solid-state NMR</i> Rob Shurko, Canada	<i>Fast Field-Cycling Magnetic Resonance Imaging</i> David Lurie, UK	<i>Automated biomolecular NMR spectrum analysis for protein structure and dynamics</i> Peter Güntert, Germany
16.00	<i>Probing supramolecular organisation of heterogeneous materials using NMR spectroscopy: from encapsulated pharmaceuticals to soft matter</i> Yaroslav Khimyak, UK	<i>Can the STE sequence be used to observe the bi-exponential IVIM model?</i> Gabrielle Fournet, France	<i>Smoothed optimal control solutions giving robust magnetisation-to-singlet transfer</i> David Goodwin, UK
16.20	<i>High-field NMR observation of proximities between 1H and quadrupolar nuclei provides new insights into the activity of heterogeneous catalysts</i> Olivier Lafon, France	<i>Improving the detection of J coupling resonances at short and moderate echo times for in vivo rat MRS at 9.4 T</i> Yanqin Lin, China	<i>Spectral estimation for ultrahigh-Resolution NMR at full sensitivity</i> Mohammadali Foroozandeh, UK
16.40	<i>Molecular rotors and motors studied by solid-state NMR spectroscopy, MRC Award</i> Martin Dracinsky, Czech Republic	<i>Proton detection of ^{13}C hyperpolarization</i> Felix Kreis, UK	<i>Quick and sensitive serial NMR experiments with Radon transform</i> Rupashree Dass, Poland
17.00	<i>Imidazole-doped cellulose solid state proton conductor: from synthesis to conductive mechanism</i> Jadwiga Tritt-Goc, Poland	<i>In vivo NMR spectroscopy of the human brain at 9.4T</i> Anke Henning, Germany	<i>Principles of protein structural ensemble determination</i> Michele Vendruscolo, UK

17.30-18.00

Coffee break

18.00-18.40 **Plenary Session 2
(Grand Ballroom)**
chair: Anja Böckmann

18.00 *NMR-led investigations of biomolecular complexes*
Józef Lewandowski, UK

19.30-23.00 **Bruker Night - An Evening On The Town**
Venture out and join Bruker Monday evening for fine food and good fun at the Endorfina Foksal Orangery.
Free and open to all EUROMAR2017 Participants. Please register [HERE](#)



Tuesday, 4 July 2017

**08.45-10.05 Plenary Session 3
(Grand Ballroom)**
chair: Christina Redfield

- 08.45 *NMR methods to characterize intrinsically disordered proteins*
Isabella Felli, Italy
- 09.25 *NMR reveals order in disordered proteins*
Robert Konrat, Austria

10.05-10.30 Coffee break

10.30-12.30	S07 Complex biomolecules (Grand Ballroom ABC) chair: Vladimír Sklenář	S08 Methods in solids NMR (Grand Ballroom DEF) chair: Matthias Ernst	S09 Structural EPR 2 (Congress Hall) chair: Gunnar Jeschke
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| 10.30 | <i>Fuzzy intramolecular interactions in Src family kinases</i>
Miquel Pons, Spain | <i>Structural investigation of organic materials by dynamic nuclear polarisation solid-state NMR</i>
Stéphane Viel, France | <i>EPR study of supramolecular assemblies of human ribosome and RNAs</i>
Elena Bagryanskaya, Russia |
| 11.00 | <i>Conformational landscape and active conformation of the Dcp1:Dcp2 mRNA decapping complex</i>
Philip Wurm, Germany | <i>NMR and electron crystallography to address salt/cocrystal/continuum and polymorphs problem</i>
Yusuke Nishiyama, Japan | <i>Determination of helix orientations in highly flexible DNAs by multi-frequency EPR spectroscopy, JMR award</i>
Claudia Maria Grytz, Germany |
| 11.20 | <i>Immersion depths of lipid carbons in bicelles measured by paramagnetic relaxation enhancement</i>
Jobst Liebau, Sweden | <i>Correlation between spin-1/2 and quadrupolar nuclei: high robustness to Magic-Angle Spinning fluctuations</i>
Hiroki Nagashima, France | <i>New Gd(III) tags via C-S conjugation for DEER distance measurements in-vitro and in-cell</i>
Yin Yang, Israel |
| 11.40 | <i>Structural basis and energy landscape for the Ca²⁺-gating and calmodulation of the Kv7.2 K⁺ channel</i>
Oscar Millet, Spain | <i>First straightforward chemical evidence for keto-enol tautomerisation in a crystal lattice traced by solid API – deuterium oxide vapors contacts</i>
Marta Dudek, Poland | <i>Probing the EPR signals within an orthogonal three-spin model system</i>
Alice Bowen, UK |
| 12.00 | <i>Real-time multidimensional NMR: a complementary off-equilibrium tool for structural biology</i>
Bernhard Brutscher, France | <i>What limits nuclear spin singlet state lifetimes?</i>
Alexej Jerschow, USA | <i>DEER and RIDME spectroscopy with high-spin metal centers</i>
Maxim Yulikov, Switzerland |



12.30-13.30	Lunch
12.30-13.30	Jeol Lunch Symposium (Congress Hall) <i>qNMR seamless, bringing qNMR to everyone</i> Dr. Manuel Perez (Mestrelab Research)
13.30-15.30	P02 Poster Session / even numbers (Baltic Ballroom)
13.30-14.30	Spinsolve - Advances in benchtop NMR - 1st workshop (Kopernik Room) Benchtop NMR system have become popular analytical lab instruments in recent years. With the recent launch of the Spinsolve Ultra the magnetic field homogeneity has been improved to match a lineshape that is comparable to superconducting magnets, while the brand new Spinsolve 80 pushes the limits in chemical shift spreading and sensitivity for a benchtop system. During the workshop an overview of applications that can be addressed with benchtop NMR systems will be given and practical demonstrations will be done on a live system. Registration can be done through the following link http://go.magritek.com/euromar-workshop-registration or at the Magritek booth during the conference. Limited to 30 participants.
14.30-15.30	Spinsolve - Advances in benchtop NMR - 2nd workshop (Kopernik Room) Benchtop NMR system have become popular analytical lab instruments in recent years. With the recent launch of the Spinsolve Ultra the magnetic field homogeneity has been improved to match a lineshape that is comparable to superconducting magnets, while the brand new Spinsolve 80 pushes the limits in chemical shift spreading and sensitivity for a benchtop system. During the workshop an overview of applications that can be addressed with benchtop NMR systems will be given and practical demonstrations will be done on a live system. Registration can be done through the following link http://go.magritek.com/euromar-workshop-registration or at the Magritek booth during the conference. Limited to 30 participants.
15.30-17.30	Tutorials (Grand Ballroom) chair: Stefan Jurga
15.30	<i>NMR probe design: Fundamentals and practical details for builders and power users</i> Rachel Martin, USA
16.10	<i>Paramagnetic relaxation in solution: an overview</i> Jozef Kowalewski, Sweden
16.50	<i>Non-uniform sampling: concepts and algorithms</i> Vladislav Orekhov, Sweden
17.30-18.00	Coffee break
18.00-18.40	Plenary Session 4 (Grand Ballroom) chair: Kurt Zilm
18.00	<i>Ultra-High Field NMR magnet development - past and future challenge</i> Patrick Wikus, Germany
19.00-21.00	Jeol Reception



Wednesday, 5 July 2017

**08.45-10.05 Plenary Session 5
(Grand Ballroom)**
chair: Thomas Prisner

- 08.45 *From EPR to DNP: Polarization Transfer between Electron and Nuclear Spin to Study Biomolecules*
Marina Bennati, Germany
- 09.25 *Studies of surfaces and interfacial regions of materials by dynamic nuclear polarization solid-state NMR*
Marek Pruski, USA

10.05-10.30 Coffee break

10.30-12.30 EuroBioNMR Workshop (Kometa Room)
NMR in the European research landscape: the role of EuroBioNMR EEIG
chair: Lucia Banci

- 10:30-10:35 Lucia Banci
- 10:35-10:40 *Presentation of the EuroBioNMR EEIG*, Claudio Luchinat
- 10:40-10:55 *CERM/CIRMMP NMR - access and scientific expertise*, Claudio Luchinat
- 11:00-11:15 *CEITEC NMR - access and scientific expertise*, Vladimír Sklenář
- 11:20-11:35 *NMR Lab of Warsaw University - access and scientific expertise*, Wiktor Koźmiński
- 11:40-11:55 *SONNMRLSF - access and scientific expertise*, Rolf Boelens
- 12:00-12:15 *Using NMR to decipher cancer metabolism*, Ulrich Guenther
- 12:20-12:30 Q & A

10.30-12.30	S10 Hyperpolarization 1 (Grand Ballroom ABC) chair: Malcolm Levitt	S11 NMR imaging (Grand Ballroom DEF) chair: Jim Wild	S12 Biosolids applications (Congress Hall) chair: Tatyana Polenova
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| 10.30 | <i>Hyphenation of Supercritical Fluid Chromatography and (Hyperpolarized) NMR Spectroscopy</i>
Arno Kentgens, The Netherlands | <i>GlucoCEST: Using chemical exchange to assess in vivo metabolism</i>
Xavier G. Golay, UK | <i>NMR studies of antibody light chain aggregates using solution- and MAS solid-state NMR</i>
Bernd Reif, Germany |
| 11.00 | <i>High ¹³C-Overhauser DNP enhancements at high and low magnetic fields</i>
Tomas Orlando, Germany | <i>Imaging of liver fibrosis by Magnetization exchange-based MRI</i>
Gil Navon, Israel | <i>Slow conformational dynamics detected by ¹H solid-state rotating frame relaxation, JMR award</i>
Petra Rovó, Germany |
| 11.20 | <i>Electron decoupling with frequency agile gyrotrons, fluorescent biradical polarizing agents, and DNP in human cells</i>
Alexander Barnes, USA | <i>Stroboscopic RARE: Fluid flow imaging using multiple RARE experiments</i>
Petrik Galvosas, New Zealand | <i>Solid-state NMR approach for structural studies of RNA</i>
Alexander Marchanka, Germany |



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| 11.40 | <i>(Hyper)Polarisation transfer from scalar order to heteronuclear magnetisation, MRC award</i>
Gabriele Stevanato,
Switzerland | <i>Susceptibility contrast by echo shifting in spatially encoded single-scan MRI</i>
Sina Marhabaie, France | <i>Solid-state NMR studies on the Hepatitis B core protein reveal polymorphisms within T4 capsids</i>
Lauriane Lecoq, France |
| 12.00 | <i>Dynamic Nuclear Polarization coupled with rapid dissolution: from technology to new science</i>
Geoffrey Bodenhausen,
France | <i>Hyperpolarized cardiovascular MR imaging</i>
Sebastian Kozerke,
Switzerland | <i>Deuterium NMR Spectroscopy for Structure and Dynamics of Protein</i>
Umit Akbey, Denmark |

12.30-13.30 Lunch

12.30-13.30 Jeol Lunch Symposium (Congress Hall)
CRAFTy applications
Dr. Krish Krishnamurthy (Chempacker LLC)

13.00-15.00 EUROPOL Workshop (Grand Ballroom DEF)

13.30-15.30 P03 Poster Session / all (Baltic Ballroom)

15.30-17.30 S13 Acquisition strategies (Grand Ballroom ABC)
chair: Wiktor Koźmiński

S14 Hyperpolarization 2 (Grand Ballroom DEF)
chair: Geoffrey Bodenhausen

S15 Emerging methods 1 (Congress Hall)
chair: Bernhard Blümich

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| 15.30 | <i>Backbone plus side chain assignments from overnight experiments</i>
Martin Billeter, Sweden | <i>Application of Dissolution Dynamic Nuclear Polarization for Determination of Molecular Structure and Dynamics</i>
Christian Hilty, USA | <i>Recoupling schemes in solid-state NMR: Synchronous, non-synchronous, and for current MAS frequencies</i>
P.K. Madhu, India |
| 16.00 | <i>Information Content of Relaxation Data: New Approaches for Accurate Dynamics Analysis</i>
Albert Smith, Switzerland | <i>Multi-Field Cryogen Free Dissolution-DNP at 3.35, 6.70, and 10.05 T</i>
Sean Bowen, Denmark | <i>Site-specific longitudinal, transverse and cross-relaxation rates measured at 0.33 T in a protein</i>
Fabien Ferrage, France |
| 16.20 | <i>Ultraclean pure shift NMR: cyclic sideband suppression, JMR award</i>
Pinelopi Moutzouri, UK | <i>Casting light on intrinsically disordered proteins by dissolution DNP and exchange with hyperpolarized water</i>
Dennis Kurzbach, France | <i>Billion-fold increase in NMR sensitivity and studies of metal-ion interaction with biomolecules</i>
Magdalena Kowalska, Switzerland |
| 16.40 | <i>Probing translational dynamics in the long-time limit via singlet-enhanced diffusion NMR</i>
Giuseppe Pileio, UK | <i>Increasing the sensitivity of intrinsically disordered protein NMR using hyperpolarized water</i>
Or Szekely, Israel | <i>Photo-Induced Manipulation of Relaxation Times, MRC award</i>
Eduard Stadler, Austria |



17.00 *Alternative sampling and processing approaches to serial NMR experiments*
Krzysztof Kazimierczuk,
Poland

Production of parahydrogen-induced polarization using metal-free catalytic systems: current progress
Vladimir Zhivonitko, Russia

Monatomic spies for molecular imaging
Thomas Meersmann, UK

17.30-18.00

Coffee break

18.00-18.40 **Plenary Session 6**
(Grand Ballroom)
chair: Thomas Vosegaard

18.00 *In-situ solid-state NMR*
Marc Baldus, The Netherlands

19.00-21.00 **AMPERE General Assembly**
(Grand Ballroom)



Thursday, 6 July 2017

**08.45-10.05 Plenary Session 7
(Grand Ballroom)**
chair: Lucio Frydman

- 08.45 *Achieving hyperpolarisation with parahydrogen*
Simon Duckett, UK
- 09.25 *Optimal control of spin dynamics: Widening the perspective to entire pulse sequences*
Steffen Glaser, Germany

10.05-10.30 Coffee break

10.30-12.30	S16 Bioliquids (Grand Ballroom ABC) chair: Isabella Felli	S17 Small molecules 1 (Grand Ballroom DEF) chair: Christina Thiele	S18 Emerging methods 2 (Congress Hall) chair: Fabien Ferrage
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| 10.30 | <i>The awesome power of Fluorine NMR – ligand binding, PREs and other applications</i>
Angela Gronenborn, USA | <i>Ultrafast 2D NMR: an analytical tool for small molecules at low and high magnetic field</i>
Patrick Giraudeau, France | <i>1H NMR at Larmor frequencies down to 3 Hz by means of Field-Cycling techniques</i>
Franz Fujara, Germany |
| 11.00 | <i>The Nedd4-1 WW domain recognizes the PY motif peptide through couple folding-binding equilibria</i>
Vineet Panwalkar, Germany | <i>Benchtop Ultrafast 2D NMR for high-throughput authentication of food samples</i>
Boris Gouilleux, France | <i>Spin isomer conversion in water endofullerene at room temperature</i>
Karel Kouril, UK |
| 11.20 | <i>Studying the large fragments of single-pass membrane proteins by NMR in solution</i>
Konstantin Mineev, Russia | <i>A toolbox of homonuclear experiments providing simplified and highly resolved spectra</i>
Marta Brucka, Switzerland | <i>Towards endoscopic magnetic field sensors based on diamonds for biomedical applications</i>
Arne Wickenbrock, Germany |
| 11.40 | <i>Structural basis for transthyretin amyloidosis</i>
Javier Oroz, Germany | <i>Nanoparticle-small molecule recognition mimics protein-ligand interactions</i>
Federico Rastrelli, Italy | <i>New Pathways to High Pressure NMR in Diamond Anvil Cells</i>
Thomas Meier, Germany |
| 12.00 | <i>Biophysical studies of bacterial surface proteins</i>
Jennifer Potts, UK | <i>Accurate measurement of homonuclear and heteronuclear coupling constants from highly resolved HSQC spectra</i>
Teodor Parella, Spain | <i>Compact NMR: Applications from today and for tomorrow</i>
Bernhard Blümich, Germany |

12.30-13.30 Lunch

13.30-15.30	S19 Biomolecular MR (Grand Ballroom ABC) chair: Miquel Pons	S20 Small molecules 2 (Grand Ballroom DEF) chair: Katalin Köver	S21 MR potpourri (Congress Hall) chair: Elena Bagryanskaya
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| 13.30 | <i>Characterizing transient</i> | <i>Self-induced recognition of</i> | <i>New solution NMR</i> |
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structures of RNA using NMR
Katja Petzold, Sweden

enantiomers in NMR spectroscopy from a peculiar perspective
Csaba Szántay, Hungary

methods and applications: absolute minimal sampling, metabolomics, and IDP-nanoparticle interactions
Rafael Brüschweiler, USA

14.00 *Dead End protects mRNAs from miRNA-mediated repression through an unprecedented mode of tandem RRM-RNA recognition*
Małgorzata Duszczyk, Switzerland

Homo- and heteronuclear relayed FLEX: Detecting non-labile nuclei by FT NMR of a water resonance
Mihajlo Novakovic, Israel

A simultaneous multi-slice selective J-resolved experiment for fully resolved scalar coupling information, JMR award
Qing Zeng, China

14.20 *A structural description of the nucleoskeleton-chromatin interface: role of intrinsically disordered regions*
Sophie Zinn-Justin, France

Burst-Sampled NUS in the Direct Dimension – Providing Sensitivity, Resolution and Speed
Craig Butts, UK

A new concept for fast field-cycling MRI and localized relaxometry
Esteban Anorado, Argentina

14.40 *The RigiFlex approach to ensemble modelling of large biomolecular complexes*
Gunnar Jeschke, Switzerland

A homochiral Polyglutamate with mesogenic sidechains as enantiodifferentiating alignment medium in NMR spectroscopy
Sharon Jeziorowski, Germany

Zero dead time inductive spin detection using LC-tank VCOs
Jens Anders, Germany

15.00 *Functional amyloids involved in programmed cell death investigated by solid-state NMR*
Antoine Loquet, France

Simplifying NMR spectra by interrupted acquisition
Klaus Zangger, Austria

Probing the electronic structure of the copper(ii) complex of a derivative of di-2-pyridyl ketone by continuous wave- and pulse-EPR spectroscopy
George Mitrikas, Greece

15.30-16.00

Coffee break

16.00-18.20 Closing / Plenary Session 8 (Grand Ballroom)

chair: Patrick Giraudeau

- 16.00 Presentation of JMR awards, Lucio Frydman
Presentation of MRC awards, Patrick Giraudeau, Paul Trevorrow
Presentation of JEOL poster awards, Jean-Pierre Munier
Presentation of EPR poster awards, Elena Bagryanskaya
Presentation of Suraj Manrao student poster prizes
Closing remarks, Wiktor Koźmiński, Lucio Frydman, new chair of Euromar Board of Trustees
- 17.00 *Electrically detected magnetic resonance spectroscopy of organic semiconductor materials*
Christoph Boehme, USA
- 17.40 *Broadband Pulses Revisited*
Burkhard Luy, Germany

19.00-21.00 Gala Dinner



EUROMAR
WARSAW 2017

Palace of Science and Culture |

Ratuszowa Hall

Address: Plac Defilad 1 | entrance from Marszałkowska Street | across Marriott

Hotel | walking distance

Admission ticket needed!

Dress code: smart casual