EUROPEAN COOPERATION
IN SCIENCE AND TECHNOLOGY

2nd Workshop of Nuclear Magnetic Resonance Relaxometry
CA-15209

4.02. Monday

8.00 – 8.30 Registration

8.30-9.00 Petr Hermann, Danuta Kruk, *Introduction*

Session I: Concepts

9.00 – 9.30 **Guillaume Mériguet**
Laboratoire PHENIX (UMR 8234 -CNRS/UPMC) (Paris Cedex 5, France)
How did artists achieve tempera paints?A combined relaxometry and rheology study

9.30 – 10.00 **Ernst Rössler**
University of Bayreuth (Bayreuth, Germany)
Field-cycling NMR relaxometry: The benefit of constructing master curves

10.00 – 10.30 **Thomas Vangijzegen**
University of Mons (Mons, Belgium)
VSION: potential T_1 contrast agents and influence of experimental parameters on their properties in a novel continuous-flow synthetic process

10.30 – 11.00 **Anne-Laure Rollet**
Laboratoire PHENIX (UMR 8234 -CNRS/UPMC) (Paris Cedex 5, France)
Effect of Poymer coating on NMR relaxivity of size-sorted maghemite nanoparticles

11.00-11.30 Coffee break

Session II: Experimental development

11.30 – 12.00 **Ville-Veikko Telkki**
University of Oulu (Oulu, Finland)
Ultrafast relaxation and diffusion experiments

12.00 – 12.30 **Duarte de Mesquita e Sousa**
Instituto Superior Técnico/DEEC/AC Energia & INESC ID (Lisboa, Portugal)
Digital vs. Analog Control of a FFC NMR Power Supply

12.30 – 13.00 **Oleg V. Petrov**
Charles University in Prague (Prague 8, Czech Republic)
Measuring NMR relaxation through principal component analysis

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13.00 – 13.30 **Andreas Petrovic**
Graz University of Technology (Graz, Austria)
A time domain signal equation for multi-echo spin-echo sequences with arbitrary refocusing angle and phase

13.30-15.30 Lunch

Session III: Material Science (I)

15.30 – 16.00 **Valentina Domenici**
University of Pisa (Pisa, Italy)
Study of liquid crystals showing two isotropic phases by 1H NMR diffusometry and ^{1}H NMR relaxometry

16.00 – 16.30 **Anton Gradišek**
Jozef Stefan Institute (Ljubljana, Slovenia)
Molecular dynamics in liquid crystals close to phase transition by NMR relaxometry

16.30 – 17.00 **Pedro Sebastiao**
University of Lisbon (Lisbon, Portugal)
Molecular order and dynamics of water in hybrid cellulose acetate–silica asymmetric membranes

17.00 – 17.30 **Jean-Baptiste Pigot**
Laboratoire PHENIX (UMR 8234 -CNRS/UPMC) (Paris Cedex 5, France)
Study of molecular dynamics within multi-scale porous catalyst

17.30-18.00 Coffee break

18.00 - Poster session

5.02. Tuesday

Session IV: Paramagnetic Contrast agents

8.30 – 9.00 **Peter Urbanovsky**
Charles University (Prague, Czech Republic)
NMR properties of lanthanide complexes of two interconnected DO3AP

9.00 – 9.30 **Graeme J. Stasiuk**
University of Hull (Hull, United Kingdom)
Development of nanoparticle based PDT/MRI theranostic agents

9.30 – 10.00 **Carlos Platas Iglesias**
Centro de Investigacións Científicas Avanzadas (CICA) and University of a Coruña (Coruña, Galicia, Spain)
Gadolinium(III)-based Dual ^{1}H/^{19}F MRI Probes

10.00 – 10.30 **Gyula Tircso**
University of Debrecen (Debrecen, Hungary)
Ligand rigidity and MRI relevant physicochemical performance of some GdDTPA-derivative complexes

10.30 – 11.00 **Mauro Botta**
University of Eastern Piedmont "Amedeo Avogadro" (Alessandria, Italy)
Enhancing the Sensitivity of Gd-based Nanoparticles as MRI probe

11.00-11.30 Coffee break

Session V: Medical applications (I)

11.30 – 12.00 **Simonetta Geninatti Crich**
University of Turin (Turin, Italy)
Assessment of tumour response to chemiotherapy by In vivo fast field cycling relaxometry

12.00 – 12.30 **Hana Lahrech**
BrainTech Lab—INSERM U12O5—Universityof Grenoble Alpes (Grenoble, France)
Infiltrative glioma discrimination by FFC-NMR and quadrupolar peaks 14N-1H origin: a study of three glioma animal models

12.30 – 13.00 **Lionel M. Broche**
University of Aberdeen (Aberdeen, United Kingdom)
Imaging of acute stroke by FFC-MRI: the PUFFINS study

13.00 – 13.30 **Ludovic de Rochefort**
Aix-Marseille University (Marseille, France)
Fast-field cycling magnetic resonance imaging around 1.5T to map NMR relaxation dispersion in vivo

13.30-15.30 Lunch

Session VI: Medical applications (II)

15.30 – 16.00 **Hermann Scharfetter**
Graz University of Technology (Graz, Austria)
Building MRI contrast agents based on quadrupole enhanced relaxation: What have we learned from CONQUER?

16.00 – 16.30 **Danuta Kruk**
University of Warmia and Mazury in Olsztyn (Olsztyn, Poland)
PRE versus QRE

16.30 – 17.00 **David Lurie**
University of Aberdeen (Aberdeen, United Kingdom)
Field-Cycling Overhauser-effect MRI of Free Radicals

17.00 – 17.30 **Olli Gröhn**
University of Eastern Finland (Kuopio, Finland)
MRI of myelin and demyelination by advanced rotating frame and cross relaxation mapping in the brain

17.30-18.00 Coffee break

Session VII: Food (I)

18.00 – 18.30 **Anet Rezek Jambrak**
Faculty of Food Technology and Biotechnology (Zagreb, Croatia)
Nonthermal food processing: Electron spin resonance as a tool to detect free radicals upon high power ultrasound and plasma treatments

18.30 – 19.00 **Mecit Halil Öztop**
Middle East Technical University (Ankara, Turkey)
Use of Solid Echo (SE) and Magic Sandwich Echo (SE) sequences to develop a new tool for quantifying crystallinity in food samples

6.02. Wednesday

Session VIII: Macromolecules

8.30 – 9.00 **Ziqing Wang**
Sorbonne University and Chemistry, École Normale Supérieure (Paris, France)
Interaction of Metabolites with Macromolecules in Biological Fluids Investigated by High-Resolution Relaxometry

9.00 – 9.30 **Natalie Malikova**
Sorbonne University, CNRS, Laboratoire PHENIX (Paris, France)
Ion-specificity and surface water dynamics in protein solutions

9.30 – 10.00 **Giacomo Parigi**
CERM/CIRMMP and University of Florence (Florence, Italy)
Local and global dynamics in intrinsically disordered proteins from FFC relaxometry

10.00 – 10.30 **Anna Borkowska**
University of Warmia and Mazury in Olsztyn (Olsztyn, Poland)
Protein dynamics by means of NMR relaxometry and dielectric spectroscopy

10.30-11.00 Coffee break

Session IX: Theory

11.00 – 11.30 **Pär Håkansson**
University of Oulu (Oulu, Finland)
NMR relaxation study of SF6 and 129Xe in Porous Organic Cages extracting molecular dynamics using microscopic potential energy surface

11.30 – 12.00 **Christian Gösweiner**
Graz University of Technology (Graz, Austria)
Lineshape calculation of NQR spectra based on the Liouville von Neumann equation to reveal molecule dynamics

12.00 – 12.30 **Elżbieta Masiewicz**
University of Warmia and Mazury in Olsztyn (Olsztyn, Poland)
Models of "quadrupole peaks"

12.30 – 13.00 **Danuta Kruk**
University of Warmia and Mazury in Olsztyn (Olsztyn, Poland)
Multiple relaxation pathways in electrolytes

13.00-15.00 Lunch

Session X: Material Science (II)

15.00 – 15.20 **Elisa Carignani**
University of Pisa (Pisa, Italy)
Dynamic properties of ibuprofen by solid state NMR spectroscopy and relaxometry: from pure active ingredients to formulations

15.20 – 15.40 **Max Flämig**
University of Bayreuth (Bayreuth, Germany)
Dielectric relaxation and proton field-cycling NMR relaxometry study of glycerol/dimethyl sulfoxide mixtures down to glass-forming temperatures

15.40 – 16.10 **Dominique Petit**
Ecole Polytechnique-CNRS and University of Montpellier (Montpellier Cedex 5, France)
Multiscale Proton Dynamics in Fuel Cells: From Nanoparticles to Membranes

16.10 – 16.40 **Per-Olof Westlund**
Umeå University (Umeå Sweden)
^2H T_1 nuclear magnetic relaxation dispersion applied and analysed for acetonitrile in a confined space

16.40 – 17.00 **Mária Šoltésová**
Charles University (Prague 8, Czech Republic)
Relation between molecular size and diffusion coefficient for small molecules

17.00 – 17.30 **Manuel Mariani**
University of Pavia (Pavia, Italy)
Spin dynamics of molecular nanomagnets investigated by NMR

17.30-18.00 Coffee break

Session XI: Food (II)

18.00 – 18.30 **Emin Burcin Ozvural**
Middle East Technical University (Ankara, Turkey)
Pectin-Soy Protein Isolate (SPI) Soft Candies: A Characterisation Study by NMR Relaxometry

18.30 – 19.00 **Sirvan Sultan Uguz**
Middle East Technical University (Ankara, Turkey)
Physicochemical characterisation of bovine and porcine gelatin based soft candies by Time Domain (TD) NMR Relaxometry

Posters

1. **Matthias Bechmann**: ***Dodecahedrane: Solid-state NMR and DFT calculations***
   Johannes Kepler University Linz (Linz, Austria)

2. **Miłosz Wojciechowski**: ***Investigation of multinuclear relaxation of Lithium Borohydride***
   University of Warmia and Mazury in Olsztyn (Olsztyn, Poland)

3. **Evrim Umut**: ***Molecular Dynamics in sugar derivative hydrogen microparticles***
   Dokuz Eylül University (Izmir, Turkey)

4. **Michael C. D. Tayler**: ***Relaxometry at very low magnetic fields***
   University of Cambridge (West Cambridge, United Kingdom)

5. **Małgorzata Florek-Wojciechowska**: ***κ -carrageenan gelation in presence of water and milk studied by NMR relaxometry and complementary techniques***
   University of Warmia and Mazury in Olsztyn (Olsztyn, Poland)

6. **Lucia Calucci**: ***^{1}H NMR relaxivity of novel colloidal nanostructured Gd(III)-based potential contrast agents***
   ICCOM-CNR (Pisa, Italy)

7. **Silvia Pizzanelli**: ***Potential nanostructured contrast agents based on Gd(III) complexes with keplerate polyanions***
   ICCOM-CNR (Pisa, Italy)

8. **Filip Koucký**: ***Contrast agents based on d-metal ion complexes***
   Charles University in Prague (Prague 8, Czech Republic)

9. **Jakub Obuch**: ***NMR and Structural Study of Lanthanide Complexes of trans-DOTA-diamide***
   Charles University (Prague, Czech Republic)

10. **Fabio Carniato**: ***Relaxometric characterization of novel Mn(II) picolinate derivatives for MRI applications***
    University of Eastern Piedmont "Amedeo Avogadro" (Alessandria, Italy)

11. **Stefano Marchesi**: ***Relaxometric properties of saponites bearing Ln3+ ions in the inorganic framework***
    University of Eastern Piedmont "Amedeo Avogadro" (Alessandria, Italy)

12. **Michelle Kinnon**: ***Development of a platelet specific MRI imaging agent***
    University of Hull (Hull, United Kingdom)

13. **Simona Baroni**: ***Exploring the tumour extracellular matrix by in vivo Fast Field Cycling Relaxometry after the administration of a Gadolinium based MRI contrast agent***
    University of Torino (Torino, Italy)

14. **Silvia Borsacchi**: ***Dynamics of an anhydrous solid form of Na-Ibuprofen from 1H and 13C nuclear relaxation times***
    Institute for the Chemistry of OrganoMetallic Compounds of CNR, ICCOM-CNR (Pisa, Italy)

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15. **Matteo Avolio**: ***Influence of porosity on the relaxometric and hyperthermic efficiency of elongated magnetic nanoparticles***
University of Pavia (Pavia, Italy)

16. **Yesim Karademir**: ***Detection of adulteration in processed meat products through TD-NMR relaxometry: A preliminary study***
Middle East Technical University (Ankara, Turkey)

17. **Francesca Brero**: ***Magnetic nanoparticles: investigation of the effects of coating on the 1H-NMR relaxation properties***
University of Pavia (Pavia, Italy)

18. **Janez Cerar***: Use of PFG NMR and NOESY experiments in studying polyion-counterion equilibria*
University of Ljubljana (Ljubljana, Slovenia)