
“NMR and MRI relaxometry in chemistry and bio-medicine“

Programme of the 3rd Workshop of CA15209, 17-19 February 2020

Location: Teatri Väljak 3, II floor 10143 Tallinn, Estonia:

17th February 2020

8:30 - 9:00 Registration

9:00 - 9:15 Introduction Danuta Kruk and Liis Seinberg

Session I: MRI contrast agents

Moderator David J. Lurie

9:15 - 9:35 Giacomo Parigi

Magnetic Resonance Center, University of Florence (Florence, Italy)

Relaxometry characterization of MRI contrast agents

9:35 - 9:55 Mauro Botta

University of Eastern Piedmont (Alessandria, Italy)

Optimizing the rotational dynamics of Gd(III)-based contrast agents

9:55 - 10:15 Pierre Ernotte

University of Mons (Mons, Belgium)

Development of a paraCEST and fluorine MRI contrast agent

10:15 - 10:45 Questions and Discussion

10:45 - 11:15 Coffee break

Session IIa: MRI biomedical applications

Moderator Pedro Sebastião

11:15 - 11:35 Gyula Tircsó

University of Debrecen (Debrecen, Hungary)

Mn(II)-based probes for molecular imaging applications

11:35 - 11:55 Elżbieta Masiewicz

University of Warmia and Mazury in Olsztyn (Olsztyn, Poland)

Revealing the potential of quadrupole relaxation enhancement as a novel mechanism for Fast Field-Cycling MRI in biomedical systems

11:55 - 12:15 Nicholas Senn

University of Aberdeen (Aberdeen, UK)

Detection of exogenous polyhistidine quadrupolar peak in tissue implant scaffold using whole-body Fast Field-Cycling MRI

12:15-12:45 Questions and Discussion

12:45 - 14:15 Lunch

Session IIb: MRI biomedical applications

Moderator Liis Seinberg

14:15 - 14:35 Juan Gallio

International Iberian Nanotechnology Laboratory (Braga, Portugal)

T_1 - T_2 interactions in dual MRI contrast agents, a chemical perspective

14:35 – 15:55 Lionel M: Broche

University of Aberdeen (Aberdeen, UK)

Overview of *in vivo* T_1 relaxation data in human tissues

15:55 - 16:15 James Ross

University of Aberdeen (Aberdeen, UK)

Fast Field-Cycling MRI identifies ischemic stroke at ultra-low magnetic field strength

16:15 - 16:35 Marco Fiorito

University of Basel (Basel, Switzerland)

Low field MR thermometry with a fast, interleaved look-locker based T_1 mapping approach

16:35-17:05 Questions and Discussion

17:05 - 17:35 Coffee break

Moderator Fabio Carniato

17:35 - 17:55 Oleg Petrov

Charles University (Prague, Czech Republic)

Low-field T_1 relaxation time distribution in natural and trypsin-digested bovine articular cartilage

17:55 - 18:15 Evrim Umut

Dokuz Eylul University (Izmir, Turkey)

Water Dynamics in Hydrogel Micro/Nanoparticles as potential drug delivery vehicles

18:15 - 18:35 Simona Baroni

University of Torino (Torino, Italy)

Novel Contrast agents based on quadrupolar peaks

18:35 - 19:55 Simonetta Geninatti Crich

University of Torino (Torino, Italy)

**MRI's contrast agents *in vivo* assessment of Tumour
Associated Macrophages in murine melanoma obtained by
low-field relaxometry in the presence of iron oxide particles**

19:55 - 20:25 Questions and Discussion

“NMR and MRI relaxometry in chemistry and bio-medicine“

18th February 2020

8:30 - 9:00 Registration

Session III NMR Materials Science

Moderator Raivo Stern

9:00 – 9:30 **William Price**

Western Sydney University (Sydney, Australia)

An Introduction to NMR, Diffusion, and MRI

9:30 - 9:50 **Anton Gradišek**

Jožef Stefan Institute (Ljubljana, Slovenia)

Study of internal motions in solids by means of NMR relaxometry

9:50 - 10:10 **Tomaz Apih**

Jožef Stefan Institute (Ljubljana, Slovenia)

A rapid NQDR using field cycling and frequency sweeps

10:10 - 10:30 **Ioan Ardelean**

Technical University of Cluj-Napoca (Cluj-Napoca ,Romania)

Annealing effects on liquid distribution and wettability of silica colloidal crystals

10:30 - 10:50 **Questions and Discussion**

10:50 - 11:20 **Coffee break**

11:20 - 11:40 Rahima Sidi-Boulenouar

CNRS, Université de Montpellier (Montpellier, France)

Multi-Scale Proton Dynamics in Alkali Activated Alumino-Silicates During Sol-Gel Transition

11:40 - 12:00 Jan Lang

Charles University (Prague, Czech Republic)

Spectral lineshape of ^{27}Al satellite transitions from ICR class MOFs

12:00 - 12:20 Fabio Carniato

University Piemonte (Alessandria, Italy)

Structural features of Eu^{2+} -containing cryptates that influence relaxivity

12:20 - 12:50 Questions and Discussion

12:50 - 14:20 Lunch

Session IV NMR Materials Science

Moderator Fabien Ferrage

14:20 - 14:40 Guillaume MÉRIGUET

Sorbonne Université, CNRS (Paris, France)

Study of the specificity of counterion binding to a conjugated polyelectrolyte using a combination of thermodynamics, molecular dynamics and NMR

14:40 - 15:00 Matthias Bechmann

Johannes Kepler University (Linz, Austria)

Dodecahedrane: Symmetry and Dynamics in the Solid State

15:00 - 15:20 Anant Kumar

University of Lisbon (Lisbon, Portugal)

Molecular dynamics study in the nematic and NT-B phases of liquid crystal dimer DTC5C7: A ^1H NMR relaxation study

15:20 - 15:40 Dominique Petit

Ecole Polytechnique CNRS (Palaiseau, France)

Proton Dynamics at Meso-Scale in Fuel Cell Membranes probed by FFC Relaxometry

15:40- 16:00 Adam Svítok

Charles University (Prague, Czech Republic)

New exchange process between isomers of Lanthanide(III) complexes of phosphate dota analogues

16:00 - 16:30 Questions and Discussion

16:30 - 17:00 Coffee break

Moderator Mauro Botta

17:00 - 17:20 Daniela Lalli

University Piemonte (Alessandria, Italy)

^1H and ^{17}O NMR relaxation studies of aqua ions Gd(III) and Mn(II) and Fe(III)

17:20 - 17:40 Duarte de Mesquita e Sousa

University of Lisbon (Lisbon, Portugal)

FFC NMR Relaxometer: a Low Power Lab Bench Solution

17:40 - 18:00 Simone Pisano

Sorbonne University (Paris, France)

Interactions of small molecules in complex mixtures by high-resolution relaxometry

18:00 - 18:20 Małgorzata Florek-Wojciechowska

University of Warmia and Mazury (Olsztyn, Poland)

Dynamics of aqueous solution of gum acacia studied by NMR relaxometry

18:20 - 18:40 Cerar Janez

University of Ljubljana (Ljubljana, Slovenia)

NMR relaxometry investigation of dynamics in polyelectrolyte solution

18:40 - 19:10 Questions and Discussion

19:10 – 19:40 Walking tour in the Old Town by Liis Seinberg

Meeting point in front of My City Hotel

**“NMR and MRI relaxometry in
chemistry and bio-medicine“**

19th February 2020

8:30 - 9:00 Registration

Session V: NMR theory

Moderator Giacomo Parigi

9:00 - 9:20 **Fabien Ferrage**

Sorbonne University (Paris, France)

**A high-field perspective on relaxation at low magnetic fields
with two-field NMR spectroscopy**

9:20 - 9:40 **Pedro Sebastião**

University of Lisbon (Lisbon, Portugal)

**Fast field-cycling NMR relaxometry and liquid crystal
biaxiality**

9:40 – 10:00 **Ernst Rössler**

University Bayreuth (Bayreuth, Germany)

NMR relaxation in liquids: the case glycerol

10:00 - 10:20 **Anne-Laure Rollet**

Sorbonne University (Paris, France)

Multi-scale dynamics of water in green earth tempera painting

10:20 - 10:40 Danuta Kruk

University of Warmia and Mazury (Olsztyn, Poland)

Quadrupole relaxation enhancement as a fingerprint of slow dynamics in biological systems

10:40 - 11:00 Pär Håkansson

University of Oulu (Oulu, Finland)

Toward quantitative model comparison for relaxometry experiments

11:00 - 11:30 Questions and Discussion

11:30 - 12:00 Coffee break

Session VI: NMR experimental Moderator Simonetta Geninatti Crich

12:00 - 12:20 Jean-Baptiste d'Espinose

UMR CNRS (Paris, France)

Hydrophobic silica dispersed in water: interactions and structure

12:20 - 12:40 Tibor Csupász

University of Debrecen (Debrecen, Hungary)

Preparation and coordination chemical characterization of macrocyclic Mn(II) complexes

12:40 - 13:00 Maria Beira

University of Lisbon (Lisbon, Portugal)

Paramagnetic relaxation enhancement and the inconspicuous effect of impurities on PEG-based metallic systems

13:00 - 14:30 Lunch

14:30 - 14:50 Frans A. A. Mulder

Aarhus University (Aarhus, Denmark)

Investigation of co-solute paramagnetic relaxation using field shuttling

14:50 - 15:10 Ville Telkki

University of Oulu (Oulu, Finland)

Novel application of ultrafast Laplace NMR

15:10 – 15:30 Questions and Discussion

Session VII: NMR and Food Chemistry

Moderator Danuta Kruk

15:30 - 15:50 Emin Burcin Ozvural

Cankiri Karatekin University (Cankiri, Turkey)

Analysis of metal margination chemistry before and after digestion by NMR relaxometry

15:50 - 16:10 Berkay Berk

Middle East Technical University (Ankara, Türkiye)

Understand hard candy chemistry by using TD-NMR

16:10 - 16:40 Coffee break

16:40 - 17:00 Valentina Domenici

Pisa University (Pisa, Italy)

^1H NMR relaxation times (T_1 and T_2) and self-diffusion coefficient (D) of Extra Virgin Olive Oils

17:00 - 17:20 Mecit Halil Oztop

Middle East Technical University (Ankara, Türkiye)

Different TD-MRI approach for the determination of honey and crystallization and adultery

17:20 - 17:40 Şirvan Sultan Uğuz

Middle East Technical University (Ankara, Türkiye)

Td-NMR and FCC NMR relaxometry to understand the presence of corn syrup in gelatin based candies

17:40 – 18:00 Questions and Discussion

Moderator Lionel M. Broche

18:00 - 18:20 Goran Angelovski

Max Planck Institute for Biological Cybernetics (Tübingen, Germany)

Calcium-responsive Gd-complexes as functional markers for monitoring of ischemic stroke

18:20-18:40 Quang Hung NGUYEN

UMR CNRS (Paris, France)

Following geopolymerization by proton NMR relaxometry

18:40-19:00 Miłosz Wojciechowski

University of Warmia and Mazury (Olsztyn, Poland)

¹H NMR relaxation of polysaccharides at varying hydration levels

19:00 – 19.30 Questions and Discussion

20th February 2020

9:00 - 13:00 4th Management Committee Meeting

10:30 - 11:00 Coffee break

13:00 - 14:30 Lunch

14:30 - 18:30 4th Working Groups Meeting

16:00 - 16:20 Coffee break