

**European Network  
on NMR  
Relaxometry**



COST is supported by  
the EU Framework  
Programme Horizon  
2020

<http://eurelax.uwm.edu.pl>

**NEWSLETTER 5  
OF THE COST ACTION**

Date:

**01.09.2018 - 31.03.2019**

Action Chair: prof. dr hab Danuta Kruk

**Events:**

- **Training School: NMR relaxometry for porous and confined systems**, 5/11/2018 - 7/11/2018 (Paris, France)
- **2nd Workshop of Nuclear Magnetic Resonance Relaxometry**, 4/02/2019 - 6/02/2019 (Prague, Czech Republic)
- **3rd Working Group Meeting**, 7/02/2019 (9.0a.m. - 1.0p.m.) (Prague, Czech Republic)
- **3rd Management Committee Meeting**, 7/02/2019 (2.30p.m. - 6.30 p.m.) (Prague, Czech Republic)
- **Training School: NMR relaxometry and Magnetic Resonance Imaging**, 13/02/2019 - 15/02/2019, Basel (Switzerland)
- **Training School: NMR relaxometry data analysis: theory and software**, 18/02/2019 - 22/02/2019, Pavia (Italy)

**Short Term Scientific Mission:**

- **Magdalena Knapkiewicz, PhD student**, Polish Academy of Sciences (Poznań, Poland), duration of the mission: 8 days
- **Dr. Philippe Bodart**, University of Bourgogne and Agrosup Dijon (Dijon, France), duration of the mission: 10 days
- **Supuksorn Masavang, PhD student**, University of Bourgogne and Agrosup Dijon (Dijon, France), duration of the mission: 10 days
- **Dr. Lionel Broche**, University of Aberdeen (Aberdeen, United Kingdom), duration of the mission: 7 days

- **Peter Urbanovský, PhD Student**, Charles University (Prague, Czech Republic), duration of the mission: 12 days
- **Dr. Maria Enrica Di Pietro**, Department of Chemistry, Materials and Chemical Engineering "Giulio Natta", Politecnico di Milano, Italy, duration of the mission: 8 days
- **Dr. Anton Gradišek**, Jozef Stefan Institute (Ljubljana, Slovenia), duration of the mission: 9 days
- **Baris Ozel, PhD student**, Middle East Technical Univeristy (Ankara, Turkey), duration of the mission: 12 days
- **Elif Gokcen Ates, PhD student**, Middle East Technical Univeristy (Ankara, Turkey), duration of the mission: 12 days
- **Prof. Frans AA Mulder**, Aarhus University, iNANO center (Aarhus, Denmark), duration of the mission: 11 days
- **Dr. Janez CERAR**, University of Ljubljana (Ljubljana, Slovenia), duration of the mission: 11 days

### ITC Grands:

- **Dr. Mecit Halil ÖZTOP**, Middle East Technical University (Ankara, Turkey)

### Co-authored Action publications:

1. **Relaxometric investigations addressing the determination of intracellular water lifetime: a novel tumour biomarker of general applicability**, M. R. Ruggiero, S. Baroni, S. Aime, S. Geninatti Crich, *Mol. Phys.* 2018, DOI: 10.1080/00268976.2018.1527045.
2. **Monitoring the Effects of Ingredients and Baking Methods on Quality of Gluten-Free Cakes by Time-Domain (TD) NMR Relaxometry**, E. Yildiz, S. Guner, G. Sumnu, S. Sahin, M. H. Oztop, **11**, *Food Bioprocess Technol.*, 2018, 1923–1933, DOI: 10.1007/s11947-018-2152-z.
3. **Field-cycling NMR relaxometry: the benefit of constructing master curves**, M. Flämig, M. Hofmann, E. A. Röessler, *Mol. Physics*, 2018, DOI: 10.1080/00268976.2018.1517906.
4. **Characterisation of magnetic resonance imaging (MRI) contrast agents using NMR relaxometry**, S. Aime, M. Botta, D. Esteban-Gómez, C. Platas-Iglesias, *Mol. Phys.*, 2018, DOI: 10.1080/00268976.2018.1516898
5.  **$^1\text{H}$  spin-lattice relaxation in water solution of  $^{209}\text{Bi}$  counterparts of  $\text{Gd}^{3+}$  contrast agents**, D. Kruk, E. Umut, E. Masiewicz, P. Hermann, H. Scharfetter, *Mol. Phys.* 2018, DOI:10.1080/00268976.2018.1517907
6. **Predicting quadrupole relaxation enhancement peaks in proton  $R_1$ -NMRD profiles in solid Bi-aryl compounds from NQR parameters**, C. Gösweiner, D. Kruk, E. Umut, E. Masiewicz, M. Bödenler, H. Scharfetter, *Mol. Phys.*, 2018, DOI:10.1080/00268976.2018.1519201
7. **Quadrupole relaxation enhancement and polarization transfer in DMSO solution of  $[\text{Bi}(\text{NO}_3)_3(\text{H}_2\text{O})_3] \cdot 18\text{-crown-6}$  in frozen state**, D. Kruk, E. Masiewicz, E. Umut, M.

- Schlögl, R. Fischer, H. Scharfetter, *Mol. Phys.* 2018, DOI:10.1080/00268976.2018.1552798
8. ***Use of NMR Relaxometry to Identify Frankfurters of Different Meat Sources***, S. S. Uguz, E. B. Ozvural, M. J. Beira, M. H. Oztop, and P. J. Sebastião, *Mol. Phys.*, 2018, DOI:10.1080/00268976.2018.1542162
  9. ***Local and Global Dynamics in Intrinsically Disordered Synuclein***, N. Rezaei-Ghaleh, G. Parigi, A. Soranno, A. Holla, S. Becker, B. Schuler, C. Luchinat, M. Zweckstetter, **57**, *Angew. Chem. Int. Ed.*, 2018, 15262-15266, doi:10.1002/anie.201808172
  10. ***Dynamics of Dimethylbutanols in Plastic Crystalline Phases by Field Cycling <sup>1</sup>H NMR Relaxometry***, E. Carignani, C. Forte, E. Juszynska-Galazka, M. Garazka, M. Massalska-Arodz, A. Mandoli, M. Geppi, L. Calucci, **122**, *J. Phys. Chem. B*, 2018, 9792-9802, DOI:10.1021/acs.jpcc.8b06391
  11. ***Understanding Overhauser Dynamic Nuclear Polarisation through NMR relaxometry***, G. Parigi, E. Ravera, M. Bennati, C. Luchinat, *Mol. Phys.*, 2018, doi:10.1080/00268976.2018.1527409
  12. E. A. Rössler, M. Hofmann, N. Fatkullin, ***Application of field-cycling <sup>1</sup>H NMR relaxometry for studying translational and rotational dynamics in liquids and polymers***, in: *Field-cycling NMR relaxometry: Instrumentation, model theories, applications*, edited by RSC, 2019
  13. ***NMR Relaxometry Study of Gelatin Based Low Calorie Soft Candies***, Nilgun Efe, Michal Bielejewski, Jadwiga Tritt-Goc, Mecit Halil Oztop, *Molecular Physics (after review)*
  14. ***Determination and quantification of paramagnetic elements in wine by Fast Field Cycling NMR relaxometry***, R. Bodart, A. Rachocki, J. Tritt-Goc, and R. D. Gougeon (*manuscript in preparation*)
  15. ***Local and collective molecular dynamics processes in an antiferroelectric liquid crystal with the SmCa\* phase***, Knapkiewicz, M. Bielejewski, P. Sebastiao, and A. Rachocki (*manuscript in preparation*)
  16. ***Magnetic resonance studies of chemical and textural changes in graviera cheese during maturation***, Ralli, O.V. Petrov, C. Mattea, B. Gizatullin, S. Stapf and A. Spyros, *J. Agric. Food Chem. (manuscript in preparation)*
  17. ***Surface influence on the rotational and translational dynamics of molecules confined inside a mesoporous carbon xerogel***, C. Cadar and I. Ardelean, *Magnetic Resonance in Chemistry*, 2018, *submitted*
  18. M. Hofmann, M. Flämig, E.A. Rössler, *Dynamics of Polymer Systems Studied by Field-Cycling Relaxometry*. Contribution to the book "***NMR Methods for Characterization of Synthetic and Natural Polymers***" edited by RCS, 2018, *submitted*
  19. ***Application of Proton Field-Cycling NMR Relaxometry for Studying Translational Diffusion in Liquids and Polymer Melts***, M. Flämig, M. Hofmann, A. Lichtinger, E.A. Rössler, *Magn. Reson. Chem.* 2018 *submitted*
  20. ***Relaxometric studies of ex-vivo murine breast tissues: new insights for early tumor detection and characterization***, E. Di Gregorio, G. Ferrauto, S. Lanzardo, E. Gianolio, S. Aime, *submitted*

## Conferences:

1. M. Kamenicky, A. Rathner, P. Rathner, J. Kohoutova, V. Kopecky, K. Hofbauerova, L. Cerofolini, G. Parigi, R. Ettrich and N. Müller: ***PsbO – the biggest extrinsic protein of Photosystem II***, Central and Eastern European NMR Symposium, September 5-6, 2018, Vienna, Austria, <https://www.bruker.com/events/ceum.html>
2. P. Rathner, M. Stadlbauer, L. Cerofolini, E. Ravera, M. Fahrner, C. Luchinat, G. Parigi, C. Romanin and N. Müller: ***Investigation of STIM/ORAI PPI using NMR***, Central and Eastern European NMR Symposium, 5-6 September 2018, Vienna, Austria, <https://www.bruker.com/events/ceum.html>
3. E. B. Ozvural, M. Jardim, M. H. Oztop, and P. José: ***Utilization of FFC Relaxometry to Differentiate Frankfurters Made of Different Meat Sources***, MRFOOD 2018, September 17 -21, Rennes, France, <https://www.foodmr.org/>
4. B. Çilek Tatar, M. Jardim, M. H. Oztop, and P. José: ***Analyzing Model Fitting of Fast Field Cycling Nuclear Magnetic Resonance Relaxometry Results of Gluten-free Cakes***, 13th International Conference on Food Physics, October 23 -25, 2018, Antalya, Turkey, <https://icfp2018.org/>

## Projects resulting from Action activities:

1. ***Application of NMR relaxation and diffusion measurements to assess dynamics of complex molecular systems***, CZ, Petr Hermann, National, INTER-EXCELLENCE (INTER-COST), grant No. LTC17067 (Europe in a changing world, inclusive innovative and reflective societies)
2. ***NMR-based metabolomics of cheese products***, EL, Evangelia Ralli, National, 1<sup>st</sup> Call of Scholarships for the support of young PhD candidates (Food security, sustainable agriculture and forestry, marine and maritime and inland water reasearch, and the Bioeconomy)