

**European Network  
on NMR  
Relaxometry**



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**NEWSLETTER 4  
OF THE COST ACTION**

Date:

**01.04.2018 - 31.08.2018**

Action Chair: prof. dr hab Danuta Kruk

**Short Term Scientific Mission:**

- **DR. Julia Hollenbach**, University of Southampton (Southampton, United Kingdom), duration of the mission: 8 days
- **Dr. Evrim Umut**, University of Warmia and Mazury in Olsztyn (Olsztyn, Poland), duration of the mission: 14 days
- **Enikő Tóth-Molnár, PhD student**, University of Debrecen (Debrecen, Hungary), duration of the mission: 12 days
- **Dr. Anne-Laure Rollet**, Laboratoire PHENIX (UMR 8234 -CNRS/UPMC) (Paris cedex 5, France), duration of the mission: 9 days
- **Calin Cadar, PhD student**, Technical University of Cluj-Napoca (Cluj-Napoca, Romania), duration of the mission: 13 days
- **Dr. Enrico Ravera**, Magnetic Resonance Center (Sesto Fiorentino, Italy), duration of the mission: 6 days
- **Alper Soyler, PhD Student**, Middle East Technical University (Ankara, Turkey), duration of the mission: 14 days
- **Michal Kamenicky, PhD student**, Johannes Kepler University in Linz (Linz, Austria), duration of the mission: 8 days
- **Dr. Elisa Carignani**, Università di Pisa (Pisa, Italy), duration of the mission: 7 days
- **Manuel Petit, PhD student**, BrainTech Lab INSERM U 1205 (Grenoble, France), duration of the mission: 7 days
- **Prof. Hana Lahrech**, BrainTech Lab INSERM U 1205 (Grenoble, France), duration of the mission: 7 days
- **Dr. Małgorzata Starowicz**, PAN in Olsztyn (Olsztyn, Poland), duration of the mission: 6 days

- **Dr. Silvia Casini**, University of Aberdeen (Aberdeen, United Kingdom), duration of the mission: 6 days
- **Natalia Pierunek, PhD student**, Polish Academy of Sciences (Poznań, Poland), duration of the mission: 13 days
- **Esmanur İlhan**, Middle East Technical University (Ankara, Turkey), ), duration of the mission: 10 days
- **Prof. Danuta Kruk**, University of Warmia and Mazury in Olsztyn (Olsztyn, Poland), duration of the mission: 9 days
- **Dr. Robert Kruk**, Institute of Nanotechnology, KIT (Karlsruhe, Germany), duration of the mission: 9 days
- **Dr. Philippe Bodart**, Université de Bourgogne Franche-Comté (Dijon, France), duration of the mission: 11 days
- **Anna Ploch, PhD student**, Medical University of Silesia (Sosnowiec, Poland), duration of the mission: 8 days
- **Betul CILEK TATAR, PhD Student**, Middle East Technical University (Ankara, Turkey), duration of the mission: 7 days
- **Dr. Lionel Broche**, University of Aberdeen (Aberdeen, United Kingdom), duration of the mission: 7 days
- **Stefano Marchesi, PhD student**, Università del Piemonte Orientale “A. Avogadro” (Alessandria, Italy), duration of the mission: 7 days
- **Christian Gösweiner, PhD student**, Graz University of Technology (Graz, Austria), duration of the mission: 7 days
- **Dr. Paweł Rochowski**, University of Warmia and Mazury in Olsztyn (Olsztyn, Poland), duration of the mission: 7 days
- **Dr. Anna Szyk**, Polish Academy of Sciences (Olsztyn, Poland), duration of the mission: 6 days
- **Ziqing Wang, PhD student**, Sorbonne University and Chemistry, École Normale Supérieure (Paris, France), duration of the mission: 6 days
- **Dr. Emin Burcin Ozvural**, Middle East Technical University (Ankara, Turkey), duration of the mission: 7 days
- **Anna Borkowska, PhD student**, Institute of Nuclear Physics Polish Academy of Sciences, (Kraków, Poland), duration of the mission: 7 days
- **Prof. Dominique Champion**, Burgundy university (Dijon, France), duration of the mission: 5 days

### **ITC Grands:**

- **Magdalena Knapkiewicz, PhD student**, Polish Academy of Sciences (Poznań, Poland)
- **Dr. Radosław Kycia**, Cracow University of Technology (Kraków, Poland)

## Co-authored Action publications:

1. **An innovative therapeutic approach for malignant mesothelioma treatment based on the use of Gd/boron multimodal probes for MRI guided BNCT**, J. D. Alberti, A. Deagostino, A. Toppino, N. Protti, S. Bortolussi, S. Altieri, S. Aime, S. Geninatti Crich, **280**, *Controlled Release*, 2018, 31-38, DOI: 10.1016/j.jconrel.2018.04.043
2. **Effect of magnetic coupling on water proton relaxivity in a series of transition metal Gd<sup>3+</sup> complexes**, L. M. Lilley, K. Du, M. D. Krzyaniak, G. Parigi, C. Luchinat, T. D. Harris, T. J. Meade, **57**, *Inorg. Chem.*, 2018, 5810-5819, DOI: 10.1021/acs.inorgchem.8b00120.
3. **Generation of multiparametric MRI maps by using Gd-labelled- RBCs reveals phenotypes and stages of murine prostate cancer**, G. Ferrauto, E. Di Gregorio, S. Lanzardo, L. Ciolli, M. Iezzi, S. Aime, **8**, *Sci. Rep.*, 2018, 10567, DOI: 10.1038/s41598-018-28926-5, Open access
4. **Supramolecular assemblies based on amphiphilic Mn<sup>2+</sup>-complexes as high relaxivity MRI probes**, G. Rolla, V. De Biasio, G.B. Giovenzana, M. Botta, L. Tei, **47**, *Dalton Trans.*, 2018, 10660–10670, DOI: 10.1039/C8DT01250D.
5. **Novel paramagnetic clays obtained through intercalation of Gd<sup>3+</sup>-complexes**, S. Marchesi, F. Carniato, C. Bisio, L. Tei, L. Marchese, M. Botta, **47**, *Dalton Trans.*, 2018, 7896-7904, DOI: 10.1039/C8DT00875B.
6. **Physico-Chemical Changes of Composite Whey Protein Hydrogels in Simulated Gastric Fluid Conditions**, B. Ozel, O. Aydin, L. Grunin, M. H. Oztop, **66**, *J. Agric. Food Chem.*, 2018, 9542–9555, DOI: 10.1021/acs.jafc.8b02829.
7. **Microfriction correction factor to the Stokes–Einstein equation for small molecules determined by NMR diffusion measurements and hydrodynamic modelling**, P. Dvořák, M. Šoltésová, J. Lang, *Mol. Phys.* 2018, DOI: 10.1080/00268976.2018.1510144.
8. **Evidence for the Role of Intracellular Water Lifetime as a Tumour Biomarker Obtained by In Vivo Field-Cycling Relaxometry**, M. R. Ruggiero, S. Baroni, S. Pezzana, G. Ferrante, S. Geninatti Crich, S. Aime, **57**, *Angew. Chem. Int. Ed.*, 2018, 7468-7472, DOI: 10.1002/anie.201713318, open access
9. **Expanding the Family of Pyclyen-Based Ligands Bearing Pendant Picolinate Arms for Lanthanide Complexation**, M. Le Fur, E. Molnar, M. Beyler, O. Fougère, D. Esteban-Gómez, O. Rousseaux, R. Tripier, G. Tircsó, C. Platas-Iglesias, **57**, *Inorg. Chem.*, 2018, 6932-6945, DOI:10.1021/acs.inorgchem.8b00598
10. **Tuning Nuclear Quadrupole Resonance: A Novel Approach for the Design of Frequency-Selective MRI Contrast Agents**, C. Gösweiner, P. Lantto, R. Fischer, C. Sampl, E. Umut, P.-O. Westlund, D. Kruk, M. Bödenler, S. Spirk, A. Petrovič, H. Scharfetter, **8**, *Phys. Rev. X*, 2018, 021076, DOI:10.1103/PhysRevX.8.021076
11. **Aspects of structural order in <sup>209</sup>Bi-containing particles for potential MRI contrast agents based on quadrupole enhanced relaxation**, H. Scharfetter, C. Gösweiner, P. J. Krassnig, C. Sampl, M. Thonhofer, R. Fischer, S. Spirk, R. Kargl, K. Stana-Kleinschek, E. Umut, D. Kruk, *Mol. Phys.*, 2018, DOI:10.1080/00268976.2018.1511869
12. **NMR T<sub>1</sub>–T<sub>2</sub> correlation analysis of molecular absorption inside a hardened cement paste containing silanised silica fume**, C. Cadar, A. Cretu, M. Moldovan, C. Mattea, S. Stapf and I. Ardelean, *Mol. Phys.*, 2018, doi:10.1080/00268976.2018.1513582

13. **The effect of silica nanoparticles on the pore structure of hydrating cement paste: a spatially resolved low-field NMR study**, A. Cretu, C. Mattea, S. Stapf and I. Ardelean, *Mol. Phys.*, 2018, doi:10.1080/00268976.2018.1513581
14. **Coordination Properties of GdDO3A-based Model Compounds of Bioresponsive MRI Contrast Agents**, S. Gündüz, S. Vibhute, R. Botar, F. Kalman, I. Tóth, G. Tircso, M. Regueiro-Figueroa, D. Esteban-Gómez, C. Platas-Iglesias, G. Angelovsky, **57**, *Inorganic Chemistry*, 2018, 5973-5986, DOI:10.1021/acs.inorgchem.8b00473
15. **Lanthanide(III) complexes of monophosphate/monophosphonate DOTA-analogues: effects of the substituents on the formation rate and radiolabelling yield**, S. Procházková, V. Kubíček, J. Kotek, A. Vágner, J. Notni, P. Hermann, **47**, *Dalton Trans.*, 2018, 13006–13015, DOI:10.1039/C8DT02608D
16. **Exploiting the Proton Exchange as an Additional Route to Enhance the Relaxivity of Paramagnetic MRI Contrast Agents**, S. Aime, S. Baroni, D. Delli Castelli, E. Brücher, I. Fábíán, S.C. Serra, A. Fringuello Mingo, R. Napolitano, L. Lattuada, F. Tedoldi, Z. Baranyai, **57**, *Inorg. Chem.*, 2018, 5567-5574, DOI:10.1021/acs.inorgchem.8b00521
17. **Dynamics of two glass forming monohydroxy alcohols by field cycling <sup>1</sup>H NMR relaxometry**, E. Carignani, C. Forte, E. Juszynska-Galazka, M. Garazka, M. Massalska-Arodz, M. Geppi, L. Calucci, **269**, *J. Mol. Liq.*, 2018, 847-854, doi:10.1016/j.molliq.2018.08.112

## Conferences:

1. P. Rathner, M. Stadlbauer, L. Cerofolini, E. Ravera, M. Fahrner, C. Luchinat, G. Parigi, C. Romanin and N. Müller: **STIM1 protein studied by high resolution solid and solution state NMR**, BISSL (Bilateral Impromptu Symposium (Stockholm-Linz) on NMR Spectroscopy), April 2018, Linz, Austria, [https://fodok.iku.at/fodok/sc\\_service.xsql?SCS\\_ID=7188](https://fodok.iku.at/fodok/sc_service.xsql?SCS_ID=7188)
2. M. Bechmann, W. Schöffberger, M. Guggenberger, J. Tsanaktsidis, A. de Meijere, S. I. Kozhushkov, L. A. Paquette, R. Glaser and N. Müller: **Platonic hydrocarbons: Solid-state NMR and DFT calculations of Dodecahedrane**, BISSL (Bilateral Impromptu Symposium (Stockholm-Linz) on NMR Spectroscopy), April 2018, Linz, Austria [https://fodok.iku.at/fodok/sc\\_service.xsql?SCS\\_ID=7188](https://fodok.iku.at/fodok/sc_service.xsql?SCS_ID=7188)
3. M. Kamenicky, A. Rathner, P. Rathner, V. Kopecky, K. Hofbauerova, J. Kohoutova, R. Ettrich and N. Müller: **Initial NMR and other spectroscopic studies of PsbO protein from Photosystem II**, BISSL (Bilateral Impromptu Symposium (Stockholm-Linz) on NMR Spectroscopy), April 2018, Linz, Austria [https://fodok.iku.at/fodok/sc\\_service.xsql?SCS\\_ID=7188](https://fodok.iku.at/fodok/sc_service.xsql?SCS_ID=7188)
4. A. Rathner, K. Chandra, P. Rathner, J. Kohoutova, H. Primasova, L. Cerofolini, C. Luchinat, R. Ettrich, N Müller: **Characterization of extrinsic protein PsbP from Photosystem II by solution NMR spectroscopy**, BISSL (Bilateral Impromptu Symposium (Stockholm-Linz) on NMR Spectroscopy), April 2018, Linz, Austria [https://fodok.iku.at/fodok/sc\\_service.xsql?SCS\\_ID=7188](https://fodok.iku.at/fodok/sc_service.xsql?SCS_ID=7188)
5. P. Rathner: **STIM1 protein studied by high resolution NMR spectroscopy**, 15th International Life Science Meeting”, April 19, 2018, Krems, Austria, <https://www.fh->

[krems.ac.at/en/university/media-portal/press/15th-international-life-science-meeting-at-imc-krems-2018-07-17/](http://krems.ac.at/en/university/media-portal/press/15th-international-life-science-meeting-at-imc-krems-2018-07-17/)

6. P. Rathner [Winner of Dadok Award for this talk]: ***Gain of function mutation in STIM1 protein studied by solid and solution state NMR***, 33rd Central European NMR Meeting, April 23, 2018, Valtice, Czech Republic, <http://www.ncbr.muni.cz/nmrvaltice/history>
7. P. Dvořák, M. Šoltéssová, and J. Lang: ***Determination of the size of small molecules from their diffusion coefficient***, 33rd Central European NMR Meeting, April 23 – 25, 2018, Valtice, Czech Republic, <http://www.ncbr.muni.cz/nmrvaltice/history>
8. P. Pocan, E. Ilhan, E.G. Ates, and M. H. Oztop: ***NMR Relaxation Spectrum Analysis for Soft Candies***, International Eurasian Conference on Biological and Chemical Sciences, April 26-27, 2018, Ankara, Turkey, <https://conferencealerts.com/show-event?id=194877>
9. L. Kubíčková, J. Kohout, P. Brázda, M. Veverka, P. Dvořák, V. Herynek, and K. Závěta: ***Nanomagnets for MRI: Transverse relaxivity of  $\epsilon$ -Fe<sub>2</sub>O<sub>3</sub>***, 12th International Conference on the Scientific and Clinical Applications of Magnetic Carriers, May 22–26, 2018, Copenhagen, Denmark, <https://magneticmicrosphere.com/meeting-twelfth>
10. P. Rathner: ***Stormorken syndrome, a rare genetic disease studied by high field Nuclear Magnetic Resonance***, 1st Austrian-Czech Metabolomics-Workshop, May 24, 2018, Linz, Austria, <http://www.moviss.eu/>
11. M. Kamenicky, A. Rathner, P. Rathner, V. Kopecky, K. Hofbauerova, J. Kohoutova, R. Ettrich and N. Müller: ***PsbO – the biggest extrinsic protein of Photosystem II***, EMBO Workshop: Challenges for magnetic resonance in life sciences, May 27 – 31, 2018, Grosseto, Italy, <http://meetings.embo.org/event/18-nmr>
12. A. Soyler, D. Bouillaud, J. Farjon, P. Giraudeau, and M. H. Oztop: ***Potential of Benchtop Quantitative NMR for Monitoring Enzyme Catalyzed Reactions***, EUROMAR, July 1 -5 2018, Nantes, France (SELECTED FOR BEST POSTER AWARD), [http://www.euromar2018.org/EventPortal/In formation/EUROMAR18/HOME.aspx](http://www.euromar2018.org/EventPortal/In%20formation/EUROMAR18/HOME.aspx)
13. E. Yildiz, S. Guner, G. Sumnu, S. Sahin, and M. H. Oztop: ***Improvement of Gluten- Free Cake Formulation Monitored by NMR Relaxometry***, 5th International ISEKI Food Conference July 3 – 5, 2018, Stuttgart, Germany [https://www.isekiconferences.com/stuttgart 2018/](https://www.isekiconferences.com/stuttgart%202018/)
14. P. Hermann: ***Pyridine or acetic acid as „ideal“ solvents for Kabachnik-Fields and Moedritzer-Irani reactions. Lecture on syntheses of ligands for MRI contrast agents***, 22nd International Conference on Phosphorus Chemistry, July 8-13, 2018, Budapest, Hungary, <http://www.icpc22.mke.org.hu>