

Subject: 50th NMRDG meeting, November 6 2015

Dear all,

It is a pleasure to invite you to the 50th scientific symposium of the NMR Discussion Group. The meeting will be organized on **Friday November 6, 2015, in Utrecht**, following the official opening of the uNMR-NL facility in Utrecht on Thursday 5 November, and will be hosted by Prof. Marc Baldus and Prof. Rolf Boelens.

The lecture hall, lunches, coffee, tea and refreshments are offered by Utrecht University in collaboration with the NMR-DG. We are grateful to Bruker, Jeol, ACD/Labs, Anaspec, Buchem, CortecNet, EurisoTop, MR Solutions and Praxair for their financial contribution. Hence there will be no registration fees for the symposium. We have restricted this mailing to our e-mail addressable members, and therefore urge all of you to make people at your institute aware of this NMR-DG meeting.

The latest information of the program can be found at our website, www.nmrdg.nl, where also late registrants can subscribe.

This year will be a special edition of the symposium to celebrate its 50th anniversary. We have composed an attractive [program](#) with distinguished international speakers covering different fields. In addition, four PhD students from the Netherlands were selected to present their research. The lunch break is combined with a poster session. The NMRDG will award the best poster with a prize (sponsored by Anaspec).

The meeting will be closed with a reception (sponsored by Jeol). For the festive buffet, sponsored by Bruker Biospin, in the evening you need to have signed up during registration.

We look forward to welcome you at the 50th NMRDG meeting!

On behalf of the Dutch NMR Discussion Group
Rolf Boelens, John van Duynhoven, Ernst van Eck, Pieter Magusin, Jeanine Prompers

Program 50th NMR-DG meeting

Friday, November 6, 2015

Location lecturehall Cosmos, Victor J. Koningsbergergebouw, Budapestlaan 4a-b, 3584 CD Utrecht

Map <http://www.uu.nl/en/victor-j-koningsberger-building>

Hosts Marc Baldus and Rolf Boelens

09.30 Reception with coffee

10.00 **Welcome** and introduction hosts

10.15 Rob Kaptein (Utrecht) - NMR in The Netherlands: heroes of the past (and present)

10.45 Ad Bax (NIH Bethesda) - NMR under pressure

11.15 Mohammed Kaplan (Utrecht) - Cellular DNP-supported solid-state NMR on eukaryotic systems in native environment

11.30 Axel Haase (TU München) - Hyperpolarised ¹³C NMR: methodology and preclinical applications

12.00 Poster pitches

12.15 **Poster session and lunch buffet**

14.00 Jules Nelissen (TU Eindhoven) - Magnetic Resonance Elastography of pressure ulcers

14.15 Beat Meier (ETH Zürich) - Higher magnetic fields and faster spinning: new opportunities in solid-state NMR

14.45 Daan de Kort (Wageningen) - Yielding and flow of cellulose microfibril dispersions as viewed by rheo-MRI

15.00 **Tea break**

15.30 Christian Griesinger (MPI Göttingen) - Conformational dynamics and kinetics in proteins studied by NMR

16.00 Nan Eshuis (Nijmegen) - NMR Analysis of Sub-Micromolar Mixtures using Para-Hydrogen Induced Hyperpolarization

16.15 Clare Grey (Cambridge University) - Following Function in Real Time: New NMR and MRI Methods for Studying Structure and Dynamics in Batteries and Supercapacitors

16.45 **Closure**

17.00 **Reception**

18.00- Buffet Dinner

Posters

1. D Augustijn, HJ de Groot, A Alia (LIC, Leiden University) Metabolic profiling of intact *Arabidopsis thaliana* leaves using ^1H high-resolution magic angle spinning (HR-MAS) NMR
2. Fatemeh Azadi¹, Karthick Babu Sai Sankar Gupta¹, Diana Simionata², Giorgio Perin², Tomas Morosinotto², Anjali Pandit¹ (¹Leiden University, ²University of Padova, It) In-Situ Solid state NMR spectroscopy on intact photosynthetic thylakoid membranes
3. Merijn Blaakmeer^{1,2}, Giuseppe Antinucci^{2,3}, Ernst van Eck¹, Vincenzo Busico³, Arno Kentgens¹ (¹IMM Radboud University Nijmegen, ²Dutch Polymer Institute Eindhoven, ³Federico II University of Naples, It) Observing surface sites in MgCl_2
4. J Ole Brauckmann^{1,2}, Pegah Zolfaghari¹, Hans Janssen¹, Gilles A de Wijs¹, Arno PM Kentgens¹ (¹IMM Radboud University Nijmegen, ²TI-COAST Amsterdam) ssNMR structural studies of high-performance polyaramid fibres
5. Ivan Corbeski¹, Klemen Dolinar¹, Hans Wienk¹, Rolf Boelens¹, Hugo van Ingen² (¹Utrecht University, ²Leiden University) Interaction of a histone chaperone involved in DNA repair with core histones
6. Daan de Kort, Sandra Veen, Henk Van As, Daniel Bonn, Krassimir Velikov, John van Duynhoven (Wageningen University) Yielding and flow of cellulose microfibril dispersions
7. Riza Dervisoglu, Mark Koenis, Herma M. Cuppen, Ernst RH van Eck, Arno PM Kentgens, Gilles de Wijs (Radboud University Nijmegen) Structural investigation of H-FER zeolite; by DFT-GIPAW and solid state ^{27}Al NMR
8. M Faridounnia¹, H Wienk¹, L Kovačič², GE Folkers¹, NGJ Jaspers³, R Kaptein¹, JHJ Hoeijmakers³, R Boelens¹ (¹Utrecht University, ²Jožef Stefan Institute Ljubljana, ³Erasmus MC Rotterdam) Stability and specificity of the DNA repair complex ERCC1-XPF
9. WMJ Franssen, R Dervisoglu, APM Kentgens (Radboud University Nijmegen) $\text{CH}_3\text{NH}_3\text{PbI}_3$ perovskite formation studied by multinuclear solid state NMR
10. Ulric le Paige¹, Peter 't Hart², Fons Lefeber¹, Nathaniel Martin², Hugo van Ingen¹ (¹Leiden University, ²Utrecht University) An NMR analysis of an isotope-labeled methyllysine analogue
11. Robin Legner, Melanie Voigt, Martin Jaeger (Niederrhein University of Applied Sciences, D) Using Portable NMR and PCA/PLS to determine RONs of fuels
12. Yanzhang Luo, Mohammed Kaplan, Lukas Kapitein, Wieger Hemrika, Marc Baldus, Gert Folkers (Utrecht University) Purification of tubulin from mammalian cells for NMR studies
13. Yuliya Miloslavina¹, Karthick Babu Sai Sankar Gupta¹, Michael Reus², Swapna Ganapathy³, Alfred R Holzwarth², Huub JM de Groot¹ (¹LIC Leiden University, ²MPI Mülheim a/d Ruhr, ³Delft University) Structural heterogeneity of light-harvesting antenna from sulfur bacterium *Chlorobium tepidum*
14. ¹Tania Morán Luengo, ¹Dominique Hagemans, ¹G Elif Karagöz, ²Tobias Madl, ²Rolf Boelens, ¹Stefan GD Rüdiger (¹CPC and ²NMR Utrecht University) The Hsp90-Tau complex
15. Tatiana Nikolaeva, Daan de Kort, Adrian Voda, Ruud den Adel, Henk van As, John van Duynhoven (Wageningen University) A NMR view on multiscale fat crystal networks
16. Cecilia de Agrela Pinto, Karim Hajji, Tessa Sinnige, Jan Tommassen, Marc Baldus (Utrecht University) BAM Complex assembly

17. A Prusova, FJ Vergeldt, AN Bader, J Philippi, E Gerkema, H Van As (Wageningen University) Transport in phloem tissue
18. Indrek Reile, Nan Eshuis, Niels Hermkens, Bram van Weerdenburg, Martin Feiters, Floris Rutjes, Marco Tessari (IMM Radboud University) NMR Detection of Dilute Human Urine Metabolites by ParaHydrogen Induced Polarization
19. Manvendra Sharma, Arno Kentgens, Jan van Bentum (IMM Radboud University Nijmegen) Rapid Melt DNP on a strip
20. Marco Tassi, Gunter Reekmans, Jan D'Haen, Robert Carleer, Peter Adraensens (Hasselt University, B) ^{31}P Solid State NMR as a tool for the characterization of TiO_2 nanopowders modified with phosphonic acids
21. Brijith Thomas, Jeroen Rombouts, Rajeev K. Dubey, Karthick Babu Sai Sankar Gupta, Gert T. Oostergetel, Huub de Groot (LIC Leiden University) Expanding the NMR palette: insights on artificial charge separators
22. Koen Tijssen, Jacob Bart, Hans Janssen, Roald Tiggelaar, Arno Kentgens, Jan van Bentum (Radboud University Nijmegen) Tapered Stripline NMR: Imaging, Reaction Monitoring and Magnetic Field Gradient Compensation with Radiofrequency Gradients
23. Hugo van Ingen (Leiden University) Interactive NMR simulators for education
24. SGJ van Meerten, APM Kentgens, PJM van Bentum (Radboud University Nijmegen) Towards Overhauser DNP in compressed CO_2 at high field
25. D Mance, T Sinnige, M Kaplan, S Narasimhan, M Daniels, K Houben, M Baldus, M Weingarth (Utrecht University) An efficient labeling approach to harness backbone and side chain protons in ^1H -detected solid-state NMR
26. Ruud Aspers, Nan Eshuis, Marco Tessari (Radboud University Nijmegen) Equipment for the production of parahydrogen and continuous hyperpolarization at high magnetic field