

## **The 2013 NMRDG Meeting.**

**Friday 8 November 2013, Eindhoven**

It is a pleasure to invite you to the next scientific symposium of the NMR Discussion Group, to be held at the TU/e in Eindhoven on Friday 8 November 2013. Leo Pel will act as host. This year we have compiled a programme with considerable attention to new NMR groups and activities in the Netherlands to present their work (Maastricht University, Spinnovation, Belastingdienst, Wageningen University). The lecture hall, lunches, coffee, tea and refreshments are offered by TU/e in collaboration with the NMR-DG. We are grateful to Bruker, Agilent, Anaspec, Buchem, Eurisotop, Magritek, Praxair and Sigma Aldrich for their financial contribution. Hence there will be no registration fees for the symposium.

### Registration

We have restricted this mailing to our e-mail addressable members. We therefore urge all of you to make people at your institute aware of this NMR-DG meeting. For those of you who received the information of the coming symposium through colleagues, please, tell us your email address to ensure that you receive forthcoming mailings. To make the necessary preparations for the lunch and the poster session, the registration deadline has been set at Friday, October 25. Registration is possible via our website <http://www.nmrdg.nl>.

### Poster session

Please send us full details on the posters to be presented on behalf of your institute or company (Title, Authors, Name of the presenter and Affiliation) not later than Friday, November 1 to [science.secr.nmr@uu.nl](mailto:science.secr.nmr@uu.nl). The titles of the posters will be emailed in the week before the meeting. The NMR-DG will award the best poster presentation with a prize.

### Location

Location: Department of Mechanical Engineering (Werktuigbouwkunde)

Building Gemini, Den Dolech 2 (De Wielen), 5612 AZ Eindhoven

Route description: <http://www.tue.nl/en/university/departments/mechanical-engineering/the-department/contact-and-accessibility/>

We hope that this symposium will be as successful as many of the preceding ones and will attract a large audience. You can contribute to this success by ensuring that everybody that may be interested in the symposium knows of it. In this way you help to realize the aims of the NMR-DG Meetings: to be a platform for exchanging experiences between all NMR Users in the Netherlands and Belgium, whatever their specific interest, from universities, large research and technological institutes and industries. The NMR-DG does not charge membership fees. Persons interested in attending the symposium that are not members of the NMR-DG are welcome to attend the symposium, free of charge, provided they register for attending the symposium.

November 2013

Pieter Magusin, John van Duynhoven and Rolf Boelens.

## 48<sup>th</sup> meeting of the Dutch NMR-DG at TU/e

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9.30-10.00 Reception with coffee etc.

10.00 Opening and welcome

10.05 Leo Pel (Tue) *NMR at Tue*

10.35 Marcellus Ubbink (LU) *Taming the mighty electron spin: Protein complexes studied with paramagnetic NMR*

11.05 Frederic Girard (Spinnovation) *Overview of NMR-based technologies Applications in the (Bio-) Pharmaceutical Industry*

11.35-11.50 Coffee

11.50 Adriana Carvalho-Souza (DSM) *Quantitative NMR a powerful tool to study enzyme-assisted biomass conversion into ethanol*

12.20 Hans Ippel (Maastricht University) *Human galectin-3, a chimera-type adhesion/growth-regulatory lectin that acts as potent cellular effector*

12.50-14.00 Lunch & poster session

14.00 Lavinia Utiu (RU) *Linking chemical structure to physical properties in polypropylenes*

14.30 Markus Weingarth (UU) *Supramolecular Organization of Ion Channels*

15.00-15.15 Coffee

15.15 Martin Berkheij (Dutch Customs Laboratory) *NMR at Customs: a new weapon in the fight against tax evasion and unknown substances*

15.45 Adrik Velders (WU) *1D & 2D heteronuclear NMR spectroscopy on nanoliter samples*

16.15-16.30 Closure

16.30-17.30 Drinks offered by Tue

## Posters Dutch NMR-DG, 8 November 2013, Eindhoven University

1. N. Eshuis, N. Hermkens, B.J.A. van Weerdenburg, M.C. Feiters, F.P.J.T. Rutjes, S.S. Wijmenga, M. Tessari, *Institute for Molecules and Materials, Radboud University Nijmegen*, "Towards nanomolar detection by NMR through Sabre Hyperpolarization".
2. Niels de Roo, Ewoud van Velzen, Velitchka Mihaleva, Laura Mariani, Ferdi van Dorsten, John van Duynhoven and Peter Hoos, *Unilever Research and Development Vlaardingen, Microbiology and Analytical, Olivier van Noortlaan 120, 3133 AT Vlaardingen*, "qNMR approaches for polar low molecular weight compounds in complex food samples, a case study"
3. Velitchka V. Mihaleva<sup>1,2</sup>, Daniël B. van Schalkwijk<sup>3</sup>, Albert A. de Graaf<sup>3</sup>, John van Duynhoven<sup>2,4,5</sup>, Ferdinand A. van Dorsten<sup>2,4</sup>, Jacques Vervoort<sup>1,2</sup>, Age Smilde<sup>2,6</sup>, Johan A. Westerhuis<sup>2,6</sup>, Doris M. Jacobs<sup>2,4</sup>, *1-Laboratory of Biochemistry, Wageningen University, Dreijenlaan 3, 6703 HA Wageningen, 2-Netherlands Metabolomics Centre, Einsteinweg 55, 2333 CC, Leiden, 3-TNO, Microbiology and Systems Biology, Utrechtseweg 48, 3700 AJ Zeist, 4-Unilever R&D, Olivier van Noortlaan 120, 3133 AT Vlaardingen, 5-Laboratory of Biophysics, Wageningen University, Dreijenlaan 3, 6703 HA Wageningen, 6-Swammerdam Institute for Life Sciences, Universiteit van Amsterdam, Science Park 904, 1098 XH Amsterdam*, "A systematic approach to obtain validated PLS models for predicting lipoprotein subclasses from serum NMR spectra".
4. Velitchka V. Mihaleva<sup>1,3</sup>, Samuli-Petrus Korhonen<sup>5</sup>, John van Duynhoven<sup>2,3,4</sup>, Mathias Niemitz<sup>5</sup>, Jacques Vervoort<sup>1,4</sup>, Doris M. Jacobs<sup>3,4</sup>, *1-Laboratory of Biochemistry, Wageningen University, Wageningen, 2- Laboratory of Biophysics and Wageningen NMC Centre, Wageningen University, Wageningen, 3- Unilever R&D Vlaardingen, Vlaardingen, 4- Netherlands Metabolomics Centre, Leiden, 5- PERCH Solutions Ltd., Kupio, Finland*, "A high-throughput and robust Quantum Mechanical Total Line Shape fitting approach for quantitative profiling of the serum metabolome".
5. Marco Tessari, *Institute for Molecules and Materials, Radboud University Nijmegen*, "Improved Chemometric Analysis and Botanical Differentiation of Honey Samples from Resolution-Enhanced PURE SHIFT NMR Spectra".
6. P.A.J. Donkers, L. Pel and O.C.G. Adan, *University of Technology Eindhoven, Department of Applied Physics, Eindhoven*, "Dehydration of MgSO<sub>4</sub>.7H<sub>2</sub>O studied by NMR".
7. C.J. Kuijpers, H.P. Huinink, O.C.G. Adan and N. Tomozeiu, *University of Technology Eindhoven, Department of Applied Physics, Eindhoven*, "Towards Green Inks".
8. Marco Tassi, Gunter Reekmans, Martine Vanhamel, Prof. Adriaenssens, Prof. Carleer, *Universiteit Hasselt, TANC - Applied and analytical chemistry-, Agoralaan Building D, 3590 Diepenbeek, Belgium*, "<sup>31</sup>P SS-NMR and ATR-IR characterization of TiO<sub>2</sub> fuctionalized with phosphonic acids for solid phase extraction and purification applications"
9. Ö.Geziçi, P.A. van Meel, P.A.J. Donkers, S.J.F. Erich, H.P. Huinink, O.C.G. Adan, *University of Technology Eindhoven, Department of Applied Physics, Eindhoven*, "Understanding Water Transport Through Coatings into Wood".
10. P.C.M.M. Magusin, *KU Leuven University, Centre for Surface Science and Catalysis, Leuven*, "Inorganic materials for heterogeneous catalysis and energy storage investigated with MAS NMR".
11. Tessa Sinnige<sup>1</sup>, Markus Weingarth<sup>1</sup>, Jan Tommassen<sup>2</sup>, Marc Baldus<sup>1</sup>, *1- NMR Spectroscopy group, Bijvoet Center for Biomolecular Research, Utrecht University, Padualaan 8, 3584 CH Utrecht, 2- Institute of Biomembranes, Utrecht University*, "Plasticity of the  $\beta$ -barrel assembly machinery investigated by NMR".
12. Ewoud J.J. van Velzen, John P.M. van Duynhoven, Niels de Roo, and Peter Hoos, *Unilever R&D, Microbiology and Analytical, Vlaardingen*, "qNMR Targeted Profiling of Food Compounds".
13. Merijn Blaakmeer<sup>1</sup>, Ernst R.H. van Eck<sup>1</sup>, V. Busico<sup>2</sup>, Arno P.M. Kentgens<sup>1</sup>, *1-Institute for Molecules and Materials (IMM), Radboud University Nijmegen, Heyendaalseweg 135, 6525 AJ Nijmegen, 2-Laboratory of Stereoselective Polymerizations (LSP), Federico II University of Naples, Via Cintia, 80126 Naples, Italy, #-Dutch Polymer Institute (DPI), P.O. Box 902, 5600 AX Eindhoven*, "Novel Quadrupolar NMR Methodology for the Study of MgCl<sub>2</sub>-Supported Ziegler-Natta Catalysts".
14. V. Breukels<sup>1</sup>, C.F.J. Janssen<sup>2</sup>, J.J.A. van Asten<sup>1</sup>, A. Capozzi<sup>4</sup>, J.W.M. van Os<sup>3</sup>, P.J.M. van Bentum<sup>3</sup>, A. Comment<sup>4</sup>, J.A. Schalken<sup>2</sup> and T.W.J. Scheenen<sup>1</sup>, *1-Dept. of Radiology, RadboudUMC, Nijmegen, 2-Dept. of Urology, RadboudUMC, Nijmegen, 3-Institute for Molecules and Materials, Radboud University Nijmegen, 4-Laboratory for Functional and Metabolic Imaging, École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland*, "Studying prostate cancer metabolism using dissolution DNP enhanced NMR".
15. D.W. de Kort<sup>a,d</sup>, F. Hoeben<sup>b,d</sup>, H.M. Janssen<sup>b,d</sup>, J.P.M. van Duynhoven<sup>a,c,d</sup>, H. Van As<sup>a,d</sup>. *a-Wageningen University, Laboratory of Biophysics; b-SyMO-Chem B.V., Eindhoven; c-Unilever R&D, Vlaardingen; d-TI-COAST, Amsterdam*, "Nanoprobe diffusometry at low and high field strengths for exploring the nanoporous structures in soft materials".
16. D.W. de Kort<sup>a,e</sup>, G.J.W. Goudappel<sup>b,e</sup>, Y. Mulla<sup>a</sup>, A. Kuijk<sup>b</sup>, S. Veen<sup>b</sup>, K.P. Velikov<sup>b,d</sup>, F.J.M. Hoeben<sup>c,e</sup>, H.M. Janssen<sup>c,e</sup>, H. Van As<sup>a,e</sup>, J.P.M. van Duynhoven<sup>a,b,e</sup>. *a-Wageningen University, Laboratory of Biophysics; b-Unilever R&D, Vlaardingen; c-Symo\_Chem B.V., Eindhoven, d-Utrecht Univerity, Soft Condensed Matter Group, e-TI-COAST, Amsterdam*, "Shear-induced aggregation of bacterial-cellulose dispersions as viewed by rheo-MRI"

- and nanoprobe diffusometry".
17. Shanthi Pagadala, Erik Nonhebel, Henk Van As, *Wageningen University, Laboratory of Biophysics and Wageningen NMR Centre*, "The use of high-field DOSY and low field 2D-correlated T<sub>2</sub>-D-NMR to study thylakoid membrane dynamics in chloroplasts".
  18. A. Prisova, F.J. Vergeldt, H. Van As, *Wageningen University, Lab of Biophysics and Wageningen NMR Centre*, "Phloem sap flow assessed by MRI".
  19. A.P.A. Faiyas, S.J.F. Erich, H.P. Huinink, M. van Soestbergen, O.C.G. Adan, and T.G. Nijland, *University of Technology Eindhoven, Department of Applied Physics, Eindhoven*, "How Methylhydroxyethylcellulose influences drying in porous media".
  20. Manvendra Sharma, James Leggett, Gerrit Janssen, Arno Kentgens, Jan van Bentum, *Radboud University, Institute for Molecules and Materials, Department of Solid State NMR*, "Rapid Melt DNP: A Novel Approach for DNP".
  21. Koen C.H. Tijssen, Michael C.D. Tayler, J.W.G. (Hans) Janssen, P.J.M. (Jan) van Bentum, Wilhelm T.S. Huck, Arno P.M. Kentgens, *Institute for Molecules and Materials (IMM), Radboud University Nijmegen, Heyendaalseweg 135, 6525 AJ Nijmegen* "Stripline NMR on Microsized Samples: Investigation of Reaction Kinetics and Molecular Diffusion".
  22. J. (Ole) Brauckmann<sup>1</sup>, René Verhoef<sup>2,1</sup>, Ernst R.H. van Eck<sup>1</sup>, Arno P.M. Kentgens<sup>2</sup>, *1-Solid State NMR, Institute for Molecules and Materials (IMM), Radboud University Nijmegen, Heyendaalseweg 135, 6525 AJ Nijmegen, 2-Teijin Aramid BV, Velperweg 76, 6802 ED Arnhem*, "High Resolution Solid State NMR of Aramids".
  23. Klaartje Houben, Elwin van der Crujisen, Markus Weingarth, Marc Baldus, *NMR Spectroscopy group, Bijvoet Center for Biomolecular Research, Utrecht University*, "Probing dynamics of a potassium channel (KcsA) using solid-state NMR".