

## 47<sup>th</sup> Meeting of the Dutch NMR Discussion Group

It is a pleasure to invite you to the next scientific symposium of the NMR Discussion Group, to be held at Unilever R&D Vlaardingen on Friday **2 November 2012**. John van Duynhoven (Unilever) will act as host.

The lecture hall, lunches, coffee, tea and refreshments are offered by Unilever in collaboration with the NMR-DG. We are grateful to Bruker Nederland, Praxair, Euriso-Top, Anaspec, Campro and Oxford 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.

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 Monday October 29, 2012. Registration for the meeting 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 - no abstract, and please as plain text in the email) not later than **Friday, October 26** to Barbara Hendrix: [science.secr.nmr@uu.nl](mailto:science.secr.nmr@uu.nl) (you will get a confirmation on **Monday October 29**). The titles of the posters will be emailed in the week before the meeting. The NMRDG will award the best poster presentation with a prize.

### Location

Unilever R&D, Olivier van Noortlaan 120, 3133 AT VLAARDINGEN. Route description: attached PDF

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.

Board Dutch NMR-DG  
John van Duynhoven (Unilever)  
Pieter Magusin (TU/e)  
Rolf Boelens (UU)

## **47<sup>th</sup> Meeting of the Dutch NMR Discussion Group**

- 09.30 Reception with coffee
- 10.00 Opening and Welcome
- 10.05 John van Duynhoven (Unilever), NMR at Unilever R&D
- 10.20 Dipen Shah (Leiden University/ZOBIO) Rapid ways to determine structures of protein:small molecule complexes by NMR
- 10.45 Carlo van Mierlo (Wageningen University) Distant residues mediate picomolar-binding affinity of a protein cofactor
- 11.10 Mathias Hass (Leiden University) Towards Seeing the Invisible: Protein Dynamics with Paramagnetic Lanthanide Tags
- 11.35 Shimon Vega (Weizman Institute) Solid State Dynamic Nuclear Polarization – some new insights
- 12.10-13.45 Poster session and lunch buffet offered by Unilever, Vlaardingen
- 13.45 Sybren Wijmenga (Radboud University Nijmegen) Chemical Shifts Pure and Alone. Their role in NMR-based Nucleic Acid Structure Determination and Metabolomics.
- 14.20 Klaartje Houben (Utrecht University) The influence of the membrane mimicking environment on membrane protein structure
- 14.45 Gijs van der Heijden (Radboud University Nijmegen) Quantitative analysis of liquid-state dynamic nuclear polarization at 3.4T
- 15.10 Coffee break
- 15.25 Laudatio for winner of the C.J. Gorter NMR-DG award 2012
- 15.30 Lecture by the Award Laureate
- 16.00-16.10 Closure
- 16.10-17.30 Drinks offered by Unilever, Vlaardingen.

## Posters Dutch NMR-DG, 2 November 2012, Vlaardingen, Unilever R&D

### Posters Dutch NMR-DG, 2 November 2012, Vlaardingen, Unilever R&D

1. E. Van Velzen<sup>1</sup>, N. de Roo<sup>1</sup>, L. Mariani<sup>1</sup>, R. Poort<sup>1</sup>, L. van Adrichem<sup>1</sup>, K. Brunt<sup>3</sup>, H. Schols<sup>2</sup>, Y. Westphal<sup>1</sup>, C. Grun<sup>1</sup>, J. van Duynhoven<sup>1,2</sup>, *1-Unilever R&D, Vlaardingen, 2-Wageningen University, 3-Eurofins, Heerenveen*, "qNMR assessment of polysaccharides in complex food matrices".
2. Jia-Ying Guan, Peter Keizers, Wei-Min Liu, Frank Löhr, Ed Heeneman, Harald Schwalbe, Marcellus Ubbink and Gregg Siegal, *Protein Chemistry Group, Leiden University*, "Determination of Ligand Binding Site by Paramagnetic NMR".
3. Yuliya Miloslavina, Karthick Babu Sai Sankar Gupta, Naoto Kuwamura, Kasim Ocakoğlu, Marcus Tank, Alfred R. Holzwarth, Donald Bryant, Huub J.M. de Groot, *Leiden Institute of chemistry, Leiden University*, "Phase-modulated decoupling in solid-state NMR: intersurface linkers and Bacteriochlorophyll e".
4. Silvia Gosiewska, Adriana Carvalho de Souza & Peter Lankhorst, *DSM Biotechnology Center Delft*, "Optimization of Saeman's hydrolysis conditions combined with <sup>1</sup>H NMR detection for quantification of gellan polysaccharide".
5. Adriana Carvalho de Souza, Tim Rietkerk, Coralie G.M. Selin and Peter Lankhorst, *DSM Biotechnology Center Delft*, "A robust and universal NMR method for the compositional analysis of polysaccharides".
6. Adrian Voda, Gert-Jan Goudappel, Ruud den Adel, John van Duynhoven\*, *Unilever Discover Vlaardingen + \*Laboratory of Biophysics, Wageningen University*, "Domain sizes in triglyceride crystal networks by 1H spin-diffusion NMR".
7. Anna Jo Oosthoek - de Vries, Hans Janssen, Jan van Bentum, Han Gardeniers, Arno Kentgens, *Radboud University Nijmegen - solid state NMR*, "Microfluidic stripline NMR: In flow <sup>1</sup>H and <sup>13</sup>C measurements in 1 and 2 dimensions".
8. H. Van As, *Lab of Biophysics and Wageningen NMR Centre, Wageningen University*, "The beauty of simplicity: IR-PFG-CPMG".
9. H. Van As, N. Homan, E. Gerkema, F.V. Vergeldt, *Lab of Biophysics and Wageningen NMR Centre, Wageningen University*, "MRI of water transport in (woody) plants: the short and the long".
10. Nico Reuvers<sup>1</sup>, Henk Huinink<sup>1</sup>, Hartmut Fischer<sup>2</sup>, Olaf Adan<sup>1,2</sup>, *1. TU/e 2. TNO*, "Water and ion transport in nylon films".
11. Vipin Agarwal<sup>1</sup>, Victor Litvinov<sup>2</sup>, Lavinia Utui<sup>1</sup>, Markus Gahleitner<sup>3</sup> and A.P.M Kentgens<sup>1</sup>, *1 - Institute of Molecular Materials (IMM), Radboud University Nijmegen, 2 - DSM Research, Geleen, 3 - Borealis GmbH, Innovation Center Linz, Austria*, "Linking Chemically Specific Structure Information to Physical Properties of Polymers".
12. Marco Tessari<sup>1</sup> and Elisabetta Schievano<sup>2</sup>, *1.-Institute of Molecular Materials (IMM), Radboud University Nijmegen, 2.- Department of Chemical Sciences University of Padova, Italy*, "Pure shift: an NMR tool for food analysis?".
13. S. Venglovska and L. Pel, *Department of Applied Physics, Eindhoven University of Technology*, "Li transport in cementitious materials as observed by NMR".
14. Abhishek Cukkemane, Deepak Nand, and Marc Baldus, *NMR Spectroscopy group, Bijvoet Center for Biomolecular Research, Utrecht University*, "Structural characterization of a cyclic nucleotide-regulated K<sup>+</sup>-channel using solid-state NMR spectroscopy".
15. Sabine Gradmann, Christian Ader, Ines Heinrich, Deepak Nand, Marc Dittmann, Abhishek Cukkemane, Marc van Dijk, Alexandre M.J.J. Bonvin, Martin Engelhard and Marc Baldus, *NMR Spectroscopy group, Bijvoet Center for Biomolecular Research, Utrecht University*, "The FANDAS web portal and its application to NMR studies of Sensory Rhodopsin II in different cellular (-like) settings".
16. Pieter C.M.M. Magusin, *Eindhoven University of Technology*, "Inorganic materials for heterogeneous catalysis and energy storage investigated with dipolar-recoupled MAS NMR".
17. Markus Weingarh<sup>1</sup>, Elwin van der Crujisen<sup>1</sup>, Alexander Prokofyev<sup>1,2</sup>, Deepak Nand<sup>1</sup>, Adrien Melquiond<sup>1</sup>, Olaf Pongs<sup>2</sup>, Alexandre MJJ Bonvin<sup>1</sup> and Marc Baldus<sup>1</sup>, *1. NMR Spectroscopy group, Bijvoet Center for Biomolecular Research, Utrecht University, 2. Saarland University, Faculty of Medicine, Homburg, Germany*, "Supramolecular organisation of membrane proteins by solid state

NMR and Molecular Dynamics simulations".

18. [Ramachandra Dongre](#)<sup>1</sup>, Hans Wienk<sup>1</sup>, Gert Folkers<sup>1</sup>, R. Spurio<sup>2</sup>, Claudio Gualerzi<sup>2</sup> and Rolf Boelens<sup>1</sup>, 1. NMR Spectroscopy group, Bijvoet Center for Biomolecular Research, Utrecht University, 2. University of Camerino, Department of Biology, Italy, "NMR studies of ribosomal Translation Initiation Factor 2 (IF 2)"
19. [P.A.J. Donkers](#), J.F.M. van Rens, L. Pel and O.C.G. Adan, Eindhoven University of Technology, "Thermochemical heat storage for the future"
20. [J.Han](#), [R.Pishkari](#), J.J.A.M.Borgharts, L.Pel, Eindhoven University of Technology, "Combined <sup>1</sup>H, <sup>23</sup>Na and <sup>35</sup>Cl imaging for understanding the transport in concrete".
21. [Tessa Sinnige](#), Markus Weingarth, Jan Tommassen, Marc Baldus, NMR Spectroscopy group, Utrecht University, "High-resolution solid-state NMR studies on BamA - a large membrane protein machine"
22. [D.M. Jacobs](#), Laura Spiesser, Maxime Garnier, Niels de Roo,, Ferdi van Dorsten, Boudewijn Hollebrands, Ewoud van Velzen, Richard Draijer, John van Duynhoven, Unilever R&D Vlaardingen, SPE-NMR metabolite sub-profiling of urine