

The 46th NMR Discussion Group, 28 October 2011, Den Haag

Dear NMR colleagues,

It is a pleasure to invite you to the next scientific symposium of the NMR Discussion Group, to be held in The Hague on Friday **28 October 2011**. Dick Schipper en Marcel van Tilborg (DSM) will act as host. The lecture hall, lunches, coffee, tea and refreshments are offered by DSM in collaboration with the NMR-DG. We are grateful to Bruker Nederland, Praxair, Buchem and Euriso-Top 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. 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 14, 2011. Registration is possible via our website.

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 21** to Barbara Hendricx: secr@nmr.chem.uu.nl (you will get a confirmation on Monday October 24). 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

Van der Valk Hotel Den Haag – Nootdorp, Gildeweg 1, 2632 BD Den Haag.

Route description: <http://www.hoteldenhaag.nl/nl/route/route>

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.

Programme

09.30 Reception with coffee

10.00 Marcel van Tilborg (DSM), Opening and Welcome

10.25 Dick Schipper (DSM, Delft)

10.55 Victor Litvinov (DSM, Geleen) Morphology, Phase Composition, and Molecular Mobility in Polyamide Films in Relation to Oxygen Permeability.

11.20 Mithun Goswami (Radboud University, Nijmegen) NMR of Quadrupolar Systems - Dealing with low Sensitivity and large Linewidths.

11.45 Bela Bode (Leiden University), Photo-CIDNP MAS NMR sheds light on the primary charge separation in plant photosynthesis.

12.10-13.00 Poster session and lunch buffet offered by DSM, Delft

13.00 Hugo van Ingen (Utrecht University) Influence of strong $^3J_{HH}$ coupling on measurement of $^1J_{CH}$ coupling constants in carbohydrates.

13.25 Leo Pel (TU Eindhoven), Fire behaviour of building materials as studied by NMR

13.50 Justin van der Hooft (Wageningen University), The use of MSn and MS guided HPLC-SPE-NMR for metabolite identification in complex extracts from plants and human body fluids.

14.15 Coffee break and poster session continued

15.00 Alia Oktaviani (University of Groningen), Comprehensive determination of protein tyrosine pKa values for photoactive yellow protein using indirect ^{13}C NMR spectroscopy

15.25 Bharat Somireddy Venkata (Leiden University) Binding orientations of a peptide on the c-Src SH3 domain studied by paramagnetic NMR.

15.50 Tobias Madl (Utrecht University), Dissecting the potential of solvent PREs for structural analysis of large proteins and their complexes using sparse data

16.15-16.20 Closure

16.20-17.30 Drinks offered by DSM, Delft.

Posters Dutch NMR-DG, 28 October 2011, Den Haag, Van der Valk Hotel

1. Tim Rietkerk, Leo van der Ven, Nico van Beelen^a, *Akzo Nobel Car Refinishes, Sassenheim*, "¹H-DOSY NMR for the polymer mass distribution of paint polymers".
2. Ard J. Kolkman, Jurjen Draaisma, Sybren S. Wijmenga and Marco Tessari, *Radboud University Nijmegen*, "Spectral simplification by collapsing J-multiplet structures: an improved technique for dilute samples"
3. M. Jupin¹, S. Wijmenga¹, P. Michiels² and F. Girard², ¹*Radboud University Nijmegen/*²*Spinovation Nijmegen*, "Investigation into endogenous metabolites interactions in blood plasma and blood plasma mimics"
4. Niels de Roo, Peter van Geffen, Peter Hoos, Ferdi van Dorsten, John van Duynhoven, Ewoud van Velzen, *Unilever R&D, Vlaardingen*, "qNMR in applied foods research",
5. Niels de Roo, Imane Mahlous, Monique Klinkenberg, Pauline Alexandre, Doris Jacobs, Hans-Gerd Janssen, John van Duynhoven, *Unilever R&D, Vlaardingen*, "Towards identification of polyphenol metabolites in bodyfluids by SPE¹-LC-SPE²-cryoNMR-TOF MS".
6. A. Voda, F. Vergeldt, G. van Dalen, A. Duijster, R. van der Sman, L. van Vliet, H. Van As, J. van Duynhoven, *Unilever Discover, Vlaardingen & Wageningen University & University of Technology, Delft*, "Rehydration behaviour of freeze-dried vegetables assessed by NMR and MRI".
7. Bas van Meerten, Dennis Grimminck, Margriet Verkuijlen, Leo Meerts, Arno Kentgens, Radboud University, IMM, Solid State NMR, "Fitting of MQ-MAS NMR data using a genetic algorithm".
8. K.C.H. Tijssen, J. Bart, J.W.G. Janssen, P.J.M. van Bentum and A.P.M. Kentgens, Radboud University, IMM, Solid State NMR, "Fast reaction monitoring using tapered stripline imaging".
9. A.J. Oosthoek - de Vries, J. Bart, P.J.M. van Bentum, J.W.G. Janssen, K. Koch, P. Nieuwland, B. van den Broek, F. Rutjes, J.G.E. Gardeniers, A.P.M. Kentgens, Radboud University, IMM, Solid State NMR, "Microfluidic stripline NMR for tiny samples and in flow monitoring".
10. P.J.M. van Bentum, G.H.A. van der Heijden, J. A. Villanueva-Garibay, A.P.M. Kentgens, Radboud University, IMM, Solid State NMR, "Quantitative analysis of high field liquid state DNP"
11. M. Jupin¹, S. Wijmenga¹, P. Michiels² and F. Girard², ¹Radboud University, IMM, Biophysical Chemistry|
²Spinovation Analytical – Integrated NMR Services, "Investigation into endogenous metabolites interactions in blood plasma and blood plasma mimics".
12. Jealemy Galindo Millán, Melanie Brasch, Jordi Cabanas-Danés, Melissa Koay, David N. Reinhoudt, Aldrik H. Velders, Pascal Jonkheijm, Jurriaan Huskens, and Jeroen Cornelissen, *University of Twente*, "Metal Complex-Based Templates for Multimodal Magnetic Resonance/Optical Imaging Systems"
13. A.P.A Faiyas, S.J.F Erich, H.P Huinink, O.C.G Adan, *Eindhoven University of Technology*, "Effect of pore liquid viscosity on the drying of porous media".
14. Vijay K. Anuganti, P. Steunenberg, M. Sobik, Aldrik. H. Velders, *University of Twente*, "Covalent functionalization of Multi-Walled Carbon Nanotubes with Ir(III) complexes."
15. Kiran Sunku^a, Anjali Pandit^b, Huub de Groot^a. □^a Leiden University. □^b VU University Amsterdam, "Structural comparison of LHCII in fluorescent and fluorescent-quenched states".
16. Viktor Baukh, Henk Huinink, Olaf Adan, Bart Erich and Leo van der Ven, *Eindhoven University*, "NMR study of water transport in multilayer coatings".