

The 2009 NMRDG Meeting.

Friday 16 October 2009, Leiden

It is a pleasure to invite you to the next scientific symposium of the NMR Discussion Group, to be held at Gorlaeus Laboratories at Leiden University on Friday 16 October 2009. Kees Erkelens and Joerg Matysik will act as host. The lecture hall, lunches, coffee, tea and refreshments are offered by Leiden University in collaboration with the NMR-DG. We are grateful to Bruker Nederland, Unilever and Buchem BV 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 9, 2009, 5.00 PM. Registration is possible via our website <http://www.nmr-dg.nl>.

C.J. Gorter-NMRDG Award

At the meeting the third "C.J. Gorter - NMR-DG Award" will be handed out. The Award winner will present his research in a lecture.

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, October 9 to secr@nmr.chem.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

Gorlaeus Laboratoria, Einsteinweg 55, 2333 CC Leiden, lecture hall 3. University site map and route description: [http://lic.leidenuniv.nl/en/contact/travel-directions\[1\]](http://lic.leidenuniv.nl/en/contact/travel-directions[1]). After the last roundabout, the car park is directly on the left opposite to the Gorlaeus Laboratories

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.

September 2009

Pieter Magusin, John van Duynhoven and Rolf Boelens.

44^d meeting of the [Dutch NMR-DG](#) at Leiden University

Friday, 16 October 2009 in Leiden

Location: Gorlaeus Laboratoria, Einsteinweg 55, 2333 CC Leiden, lecture hall 3

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09.30 Reception with coffee

10.00 **Jaap Brouwer** (Leiden University), Opening and Welcome

10.05 **Jörg Matysik** (Leiden University), Magnetic resonance in Leiden

10.20 **Subramanian Srinivasan** (University of Technology, Eindhoven), Hydrogen siting and dynamics in magnesium-based hydrogen-storage materials.

10.45 **Raluca Fratila** (University of Twente), Multinuclear nanoLiter NMR spectroscopy in a microfluidic chip.

11.10 **Suresh K. Vasa** (Radboud University, Nijmegen), Opportunities for studying single-crystals using μ -MAS NMR.

11.35 **Qamar Bashir** (Leiden University), Paramagnetic NMR combined with Monte Carlo Simulations to study a protein ensemble.

12.00-13.30 Poster session and lunch buffet offered by Leiden University

13.30 **Andrew Webb** (Leiden University Medical Center), NMR of very small samples.

14.00 **Jeroen A. Pikkemaat** (Philips Research), Structure and function of MRI contrast agents.

14.25 **Johan Hollander** (Zobio), Target Immobilization and NMR Screening of Fragments in Early Drug Discovery

14.50 **Kamil Tamiola** (University of Groningen), Random coil NMR chemical shift database derived from intrinsically disordered proteins.

15.15 Laudatio for the winner of the "C.J. Gorter - NMR-DG Award 2009"

15.25 Lecture by the **Award Laureate**

15.55-16.10 Closure

16.10-17.30 Drinks offered by Leiden University.

Posters Dutch NMR-DG, 16 October 2009, Leiden University

1. P.H.J. Keizers, B. Mersinli, W. Reinle, Y. Hiruma, F. Hannemann, M. Overhand, R. Bernhardt, M. Ubbink, *Leiden University/ Saarland University*, "Solution structure of the adrenodoxin - adrenodoxin reductase complex"
2. Gert-Jan W. Goudappel, Song Miao, Andreas Mayr, Monika Schaezel, *Unilever R&D Vlaardingen/ Unilever Deutschland GmbH*, "Water (re)distribution phenomena in savoury products – Understanding the effect of ingredients and processing on ageing"
3. G.H.A. van der Heijden, L. Pel, H.P. Huinink, en K. Kopinga, *Technical University Eindhoven*, "Fire spalling of concrete, as studied by NMR"
4. Tamerlan Saidov, Leo Pel, *Technical University Eindhoven*, "Sodium sulfate crystallization strain in porous media, NMR study"
5. Viktor Baukh, Henk Huinink, Olaf Adan, Bart Erich and Leo van der Ven, *Eindhoven University*, "Imaging and T_2 relaxometry of water in multilayer coatings"
6. Nico Reuvers, Henk Huinink and Olaf Adan, *Technical University Eindhoven*, "Water uptake in thin Nylon films"
7. Erik Saaltink, Viktor Baukh, Henk Huinink, Olaf Adan and Ruud van Overbeek, *Technical University Eindhoven*, "The ingress of tributyl phosphate in a heated coating"
8. Kashif Kamran, Leo Pel, Alison Heritage, Henk Huinink and Klaas Kopinga, *Technical University Eindhoven*, "NMR study of the electrokinetic desalination of Na/Al salt mix in porous building materials"
9. Sonia Gupta, Leo Pel, Alison Heritage, *Technical University Eindhoven*, "Drying Behavior of Porous building materials"
10. J. van Duynhoven, E. van Velzen, F. van Dorsten, R.Kemperman, E.Vaughan, A.Smilde, D.Jacobs, J.Westerhuis, *Unilever R&D Vlaardingen*, "NMR-based nutrikinetik approach for the assessment of inter-individual variation in the bioconversion of dietary polyphenols in humans"
11. J. van Duynhoven, I.Visser, M.Klinkenberg, *Unilever R&D Vlaardingen*, "Quantitative Assessment of surfactants in complex formulations by NMR"
12. Agnieszka Szczygiel, Leo Timmermans, Bernd Fritzing, Iwan Moreels, Zeger Hens, José C. Martins, *Gent University*, "New perspectives for STD NMR and transfer NOE spectroscopy for the characterization of dispersant-nanoparticle interactions in colloidal dispersions"
13. Tatiana Didenko, Afonso Duarte, Elif Karagoz, Rolf Boelens and Stefan Rüdiger, *Utrecht University*, "Structural changes in 170kD protein studied by DOSY NMR"
14. Jörg Matysik, *Leiden University*, "The solid-state photo-CIDNP effect"
15. B.C. Anger, M.S. Solum, R.J. Pugmire and B. Saam, *Leiden University*, "Intrinsic Gas-Phase Spin Relaxation of ^{129}Xe "
16. Fu Chen, Eva Schieferstein, Jörg Matysik, *Leiden University*, "Solid-state ^{13}C MAS NMR investigation of European coals"
17. Chen Song, Christina Lang, Jon Hughes, Wolfgang Gärtner, Jörg Matysik, *Leiden University*, "Exploring chromophore-binding pocket: High-resolution solid-state (^1H) - (^{13}C) interfacial correlation NMR spectra"
18. Smitha Thamarath Surendran, A. Alia, Eugenio Daviso, Geertje J. Janssen, Anton Savitsky, John H. Golbeck, Jörg Matysik, *Leiden University*, " ^{13}C -photo-CIDNP MAS NMR investigations on heliobacterial cells"
19. Geertje J. Janssen, Eugenio Daviso, Gunnar Jeschke, Jörg Matysik, A. Alia, *Leiden University*, "Solid state photo-CIDNP ^{13}C MAS NMR studies on photosystem II in native photosynthetic membranes from plants"
20. Karthick Babu Sai Sankar Gupta, Eugenio Daviso, Anna Diller, Peter Gast, Huub J.M. de Groot, A. Alia, Gunnar Jeschke and Jörg Matysik, *Leiden University*, "Laser-flash photo-CIDNP MAS NMR experiments on photosynthetic reaction centers: Observation of spin diffusion in real time at the atomic scale"
21. M.Jupin, P.Michiels, M.Spraul, F.Girard and S.Wijmenga, *Radboud University Nijmegen*, "Detection of interacting metabolites in blood plasma by disturbing the binding equilibrium"
22. A.J.Kolkman, N.Eshuis, L.Blanchet, E.V.Vottero, K.A.M.Ampt, J.N.M.Commandeur, H. Irth, N.P.E.Vermeulen, L.M.C.Buydens, M.Honing and S.S.Wijmenga, *Radboud University Nijmegen*, "NMR and UV study to determine the orientation of Norethisterone in the active site of a mutant of the

bacterial Cytochrome P450BM3"

23. A.Smolinska, K.Ampt, A. van Gool, T.Leider, M.Stoop, R.Weahrens, L.Buydens, S.Wijmenga, *Radboud University Nijmegen*, "Nuclear Magnetic Resonance of human CSF. Identification and quantification."
24. Bob C.Hamans, Anna Andreychenko, Arend Heerschap, Sybren S.Wijmenga, Marco Tessari, *Radboud University Nijmegen*, "Single-scan multinuclear NMR at earth magnetic field using Para-hydrogen Induced Hyperpolarization"
25. J. A.Villanueva-Garibay, G.Annino, P.J.M. van Bentum, A.P.M.Kentgens, *Radboud University Nijmegen*, "Liquid-State ^1H NMR-Dynamic Nuclear Polarization Enhancements at High Field: Experimental Evidences Beyond the Standard Models"
26. Suresh K.Vasa, Andreas Brinkmann, Hans Janssen, Dennis L.A.G.Grimminck, Ernst Van Eck, W.Leo Meerts and Arno Kentgens, *Radboud University Nijmegen*, "Proton microMAS NMR : A study of nano-liter volume solid samples"
27. Dennis L.A.G.Grimminck, W.Leo Meerts, A.P.M.Kentgens, A.Brinkmann, *Radboud University Nijmegen*, "On-spectrometer optimization of Solid-State NMR experiments, using self-learning algorithms"
28. Chandrakala M.Gowda, Erik Schwartz, E.R.H. van Eck, Gilles de Wijs, Andreas Brinkmann, Georg Kresse, Martijn Marsman, Jeroen J.L.M.Cornelissen, Roeland J.M.Nolte, A.E.Rowan and Arno P.M.Kentgens, *Radboud University Nijmegen*, "Structural Study of Carbazole functionalised compounds using Solid State NMR"
29. Jack J.A. van Asten, Vincent Cuijpers, Claudia Soede-Huibregts, Marinette van der Graaf, Albert Verhofstad, Arend Heerschap, *Radboud University Nijmegen*, "High Resolution Magic Angle Spinning MR Spectroscopy on Fine Needle Biopsies to Discriminate Malign and Benign Human Prostate Tissue"
30. Dirk Stratmann, Alexandre M.J.J Bonvin, Rolf Boelens, *Utrecht University*, "Quantitative use of chemical shift perturbation for the modelling of protein complexes"
31. Elena Talnishnikh, Leon Jong, and Henk Van As, Wageningen University, "Low field portable NMR meets leaves"
32. C. Windt, M. Witek, E. Gerkema, J. van Duynhoven, H. Van As, Wageningen University/ Unilver Vlaardingen, "Quantitative imaging of moisture ingress in cereal crackers: an SPI study"
33. N.Homan, H.Van As, Wageningen University, "Flow characteristics in porous system as observed by PFG-MRI"
34. Victoria Gómez, Javier Guerra, Richard Crooks, and Aldrik H.Velders, *University of Twente*, "Let's Dens"
35. Raluca M.Fratila, Victoria Gómez, and Aldrik H.Velders, *University of Twente*, "Multinuclear nanoLiter NMR spectroscopy in a microfluidic chip"
36. I.Pérez-Victoria, A.Piermattei, D.N.Reinhoudt, A.H.Velders, *University of Twente*, "Hydrogen-bond based self-assembled supramolecular receptors formation and host-guest interactions in solution."
37. J. Galindo Millán, A.Ruggi, T.Buckle, D.N.Reinhoudt, F.W.V. van Leeuwen and A.H.Velders, *University of Twente*, "New multimodal systems for magnetic resonance, fluorescent & nuclear imaging"
38. Renee Otten, Kathleen Wood and Frans A. A. Mulder, *Groningen University*, "Comprehensive determination of $^3\text{JHnHa}$ for unfolded proteins using ^{13}C -resolved spin-echo difference spectroscopy"
39. Nur Alia Oktaviani, Djurre de Jong, Renee Otten, Pieter van der Meulen, Ruud M. Scheek and Frans A.A. Mulder, *Groningen University*, "The world's fastest recording of NMR data for (intrinsically) disordered proteins"
40. Fenneke KleinJan, Kathleen Wood and Frans A.A.Mulder, *Groningen University*, "Unfolded, yes, but random? Never!"
41. Jelle Slager, Ruud M.Scheek and Frans A.A.Mulder, *Groningen University*, "Side chain pK_a values determined from backbone chemical shifts"
42. Burçin Acar, Kamil Tamiola and Frans A.A.Mulder, *Groningen University*, "Intrinsically disordered proteins: Defining random coil by chemical shifts"
43. Afonso Duarte, Hans Ippel, Martijn van Rosmalen, G.Elif Karagoz, Rolf Boelens and Stefan Rudiger, *Utrecht University*, "Lego chemistry approach overcame size limit of NMR for large proteins"
44. G. Elif Karagoz, Tessa Sinnige, Hans Ippel, Afonso Duarte, Tanya Didenko, Sandra Kling, Rolf Boelens and Stefan Rüdiger, *Utrecht University*, "NMR dissection of the mechanism of s folding machine"