

FIFTH ONE-DAY SYMPOSIUM
YOUNG BELGIAN MAGNETIC
RESONANCE SCIENTISTS



Brussels, Friday November 17th 2006
Universitaire Stichting / Fondation Universitaire
Egmontstraat 11 / 11 rue d'Egmont
B-1000 BRUSSELS

Invited Speakers

Jesus Jimenez-Barbero, CSIC, Madrid
Malcolm H. Levitt, University of Southampton

Oral communications

M. Bocconelli (ULB), P. de Tullio (ULg), C. Héroumont (UMH),
K. Houthoofd (KUL), R. Mens (UH), V. Pinoie (VUB), D. Sinnaeve
(UGent), I. Stanculescu (UA), L. Urbanczyk (ULg), E. Vinck (UA)

Event Organized by
Michel Luhmer (ULB) and José C. Martins (UGent)

a joint organisation of

FWO-Vlaanderen Wetenschappelijke Onderzoeksgemeenschap
Gevorderde NMR toepassingen in de materiaal-, chemische en biomedische
wetenschappen, P. Van Hecke (KUL), President
FNRS Groupe de Contact *Résonance Magnétique Pluridisciplinaire*
R. Muller (UMH), President

Details of the program and registration at

<http://www.orgchem.ugent.be/nmrstruc.html#events>

or contact

Michel Luhmer at mluhmer@ulb.ac.be or José Martins at Jose.Martins@UGent.be

Programme

8.15 Registration of the Participants and Coffee/Tea

8.55-10.15 **Morning Session 1**

Chair: José Martins (UGent)

FWO - Onderzoeksgemeenschap NMR

8.55 Introduction

9.00 *Jesus Jimenez-Barbero, CSIC, Madrid*

The Specific Interaction of Carbohydrates with Proteins. Stereochemical, Conformational, and Dynamical Implications of the Binding Processes

9.50 *P. de Tullio (ULg)*

Application of LC-SPE-NMR to the structural determination of KATP channels openers metabolites belonging to the 3-alkylamino-4H-1,2,4-arylthiadiazine 1,1-dioxidesantitative

P. de Tullio, M. Frédérich, P. Chiap, P. Kremers, P. Francotte, P. Lebrun and B. Pirotte.

Drug Research Center, Medicinal Chemistry, Université de Liège

10.15-10.40 **Coffee/Tea Break**

10.40-12.20 **Morning Session 2**

Chair: Michel Luhmer (ULB)

FNRS - Groupe de Contact RMP

10.40 *Davy Sinnaeve (UGent)*

Conformation and self-association of a cyclic lipodepsipeptide investigated by NMR spectroscopy

D. Sinnaeve, P. M. S. Hendrickx, J. van Hemel², B. Sas², F. A. M. Borremans and J. C. Martins.

NMR and Structure Analysis Unit, Universiteit Gent and

²Kemin Pharma Europe, Herentals

Programme Continued

- 11.05 *Raoul Mens (UH)*
Investigation on the morphology and phase separation of MDMO-PPV / PCBM blends
R. Mens, P. Adriaensens, D. Vanderzande and J. Gelan
Institute for Materials Research, Division Chemistry, Universiteit Hasselt
- 11.30 *Céline Héroumont (UMH)*
Investigation of non covalent interactions between some MRI contrast agents and HSA by proton relaxometry and NMR diffusometry.
C. Héroumont, S. Laurent, V. Henrotte, L. Vander Elst and R.N. Muller
Département de Chimie Générale, Organique et Biomédicale, laboratoire de RMN et d'Imagerie Moléculaire, Université de Mons-Hainaut
- 11.55 *Evi Vinck (UA)*
Analyzing the electronic structure of cobalt Jacobsen's catalyst by EPR spectroscopy
E. Vinck, S. Van Doorslaer, D. M. Murphy and I. A. Fallis.
Department of Physics, Universiteit Antwerpen
- 12.20-14.00 **Lunch Break**
- 14.00-15.40 **Afternoon Session 1**
Chair: Robert Muller (UMH)
FNRS - Groupe de Contact RMP
- 14.00 *Marina Bocconcelli (ULB)*
Stability, pairing selectivity and dynamics of natural and chemically modified oligonucleotide duplexes
M. Bocconcelli, K. Snoussi and K. Bartik
Ingénierie Moléculaire et Biomoléculaire, Université Libre de Bruxelles
- 14.25 *Kristof Houthoofd (KUL)*
Solid state NMR study of the adsorption of organic molecules on zeolite NaX, CaX and CaCoX
K. Houthoofd, P. J. Grobet and P. A. Jacobs
Center for Surface Chemistry and Catalysis, Katholieke Universiteit Leuven

Programme Continued

14.50 *Malcolm H Levitt, University of Southampton*
Long-lived nuclear spin states in solution NMR

15.40-16.05 **Coffee/Tea break**

16h05-17h25 **Afternoon Session 2**
Chair: ()
FWO - Onderzoeksgemeenschap NMR

16.05 *Vanja Pinoie (VUB)*
High Resolution MAS NMR as a tool for monitoring supported organotin catalysts
V. Pinoie, K. Poelmans, M. Biesemans, I. Verbruggen and R. Willem
High Resolution NMR Centre (HNMR), Department of Materials and Chemistry (MACH), Vrije Universiteit Brussel

16.30 *Laetitia Urbanczyk (ULg)*
Motional heterogeneity of intercalated species in modified clays and poly(ϵ -caprolactone)/clay nanocomposites
L. Urbanczyk, J. Hrobarikova, C. Calberg, R. Jérôme and J. Grandjean
Center for Education and Research on Macromolecules (CERM) and Chimie organique et spectroscopie multinucléaire (COSM), Université de Liège

16.55 *Ioana Stanculescu (UA)*
The Structure of Calcium Antagonist Tetrandrine Complexes with Alkali Earth Cations studied by 2D-NMR and Computational Methods
I. Stanculescu, L. Pieters² and R. Dommissie
Department of Chemistry, Applied NMR Unit, Universiteit Antwerpen

17.20 Closing Remarks

17.25 End