

**13<sup>th</sup> INTERNATIONAL MEETING  
UNIVERSITY OF EXETER  
6-11 July 1997**

**SCIENTIFIC PROGRAMME**

*\* Denotes the presenter of the contributions*

**MONDAY 7 JULY**

09.00      Welcome and Opening Remarks  
              Sir Rex Richards *Chancellor, Exeter University*

**SYMPOSIUM 1 - NMR OF BIOLOGICAL MACROMOLECULES**

**Chairman:**      Dr D Neuhaus *Medical Research Council, UK*

09.15      **I.1 Characterization of the Structure and Dynamics of Protein Folding Intermediates by Heteronuclear NMR.** P E Wright *The Scripps Research Institute, USA*

10.05      **O.1 Studies of Dynamics and Interactions Involving Arginine Residues in Proteins Using <sup>1</sup>H/<sup>15</sup>N HSQC Experiments.** J Feeney\*, A R Gargaro, P M Nieto, B Birdsall, W D Morgan, V I Polshakov and T A Frenkiel *National Institute for Medical Research, UK*

10.25      **O.2 *In situ* NMR Analysis of Dual-labelled Glycoprotein Glycans.** C T Weller\*, J Lustbader, K Seshadri, J M Brown, C A Chadwick, C E Kolthoff, S Ramnarain, R Canfield and S W Homans *University of St Andrews, UK*

10.45      *COFFEE/TEA*

11.15      **I.2 Structure-Function Studies of a Theophylline-binding RNA.** A Pardi *University of Colorado at Boulder, USA*

12.05      **O.3 Using NMR to Locate the Binding site of CapZ, the Actin Capping Protein, on the S100B Dimer.** P M Kilby", L J Van Eldik and G C K Roberts *Roche Products, UK*

12.25      *LUNCH*

**SYMPOSIUM 2 - NMR IN PHYSICAL CHEMISTRY**

**Chairman:**      Dr D G Gillies *University of Surrey, UK*

14.00      **I.3 NMR of Liquid Crystals.** J W Emsley *University of Southampton, UK*

14.50      **O.4 N-15 NMR Investigations of the Acidity of Nanostructured Ceramics Formed Using Lyotropic Crystal Templates.** M Edgar\*, M Schubert, C G Goltner and H H Limbach *Freie Universität Berlin, Germany*

- 15.10      **O.5 Host-Guest Interaction between Water-Soluble Calix[4]arenes and Organic Ammonium Ions Investigated by Measurement of Relaxation Data.** A Dölle\* and J Antony *RWTH Aachen, Germany*
- 15.30      **O.6 Coupling Constants, Proton-deuteron Exchange and Proton and Deuteron Relaxation in Water.** N M Sergeyev\*, N D Sergeyeva, Yu A Strelenko and W T Raynes *Moscow State University, Russia*
- 15.50      COFFEE/TEA
- 16.20      **I.4 The Role of NMR in Surfactant Science.** O Söderman *University of Lund, Sweden*
- 17.10      **O.7 NMR Self-Diffusion Measurements on Cosmetic and Dermatologic Emulsions.** D Emeis\* and P Arlt *Beiersdorf AG, Germany*
- 17.30      *SESSION ENDS*

## **TUESDAY 8 JULY**

### **SYMPOSIUM 3 - EXPERIMENTAL TECHNIQUES**

**Chairman:**      Professor J C Lindon *Birkbeck College, London, UK*

- 09.00      **I.5 Diffusion and Mobility Ordered NMR: Opportunities and Limitations.** C S Johnson Jr *University of North Carolina, USA*
- 09.50      **O.8 Automated 'Gradient' Shimming with Normal Spectrometer Hardware.** G A Morris\* and P B Chilvers *University of Manchester, UK*
- 10.15      COFFEE/TEA
- 10.45      **O.9 The Detection of Transition Metal Dihydrides by Parahydrogen Induced Polarisation.** S B Duckett\*, S K Hasnip and C J Sleigh *University of York, UK*
- 11.10      **O.10 A Three-Dimensional Version of the H-Ca-N-HN Experiment.** T D Spitzer\* and K L Facchine *Glaxo Wellcome, USA*
- 11.35      **I.6 New Methods for Probing Protein Structure and Dynamics.** A Bax *National Institutes of Health, Bethesda, USA*
- 12.25      *LUNCH*

### **SYMPOSIUM 4 - NMR IN ORGANIC CHEMISTRY**

**Chairman:**      Dr I H Sadler *University of Edinburgh, UK*

- 14.00      **I.7 Probe and Pulse Sequence Developments: Applications to the Solution of Complex Natural Product Structures.** G E Martin *Pharmacia and Upjohn, USA*

- 14.50      **O.11 An Investigation of the Advantages and Limitations of  $f_1$  Forward Linear Prediction in Processing 2D Data Sets.** W F Reynolds\*, M Yu and R G Enriquez *University of Toronto, Canada*
- 15.10      **O.12 Structure and Thermodynamics of Drug:DNA Complexation.** D B Davies\*, S F Baranovsky, V I Pahomov, L N Djimant, A N Veselkov *Birkbeck College, London, UK*
- 15.30      **I.8 NMR in Combinatorial Chemistry.** M J Shapiro *Novartis Pharmaceutical Corporation, USA*
- 16.20      *TEA AND POSTER SESSION*

## **TUESDAY EVENING - POSTGRADUATE SESSION**

**Chairman:**      Professor L H Sutcliffe *Institute of Food Research, UK*

- 20.00      **O.13 Assignment and SCS of Ketones in Bicycloheptane, Cyclohexane, Decalin and Steroid Systems.** M Ainger\* and R J Abraham *University of Liverpool, UK*
- 20.20      **O.14 NMR-Investigation of the Conformation-Activity Relationships of Reactive Site Loops from Bowman-Birk Inhibitor Proteins Using Small Synthetic Protein Mimetics.** ABE Brauer\*, J D McBride, M Nievo, S J Matthews, R M Cooke and R J Leatherbarrow *Imperial College, London, UK*
- 20.40      **O.15 New Multinuclear Experiments on Solid Organotin Fluorides.** J C Cherryman\* and R K Harris *University of Durham, UK*
- 21.00      **O.16 Protein Dynamics via  $^{13}\text{C}$ O Spin-Lattice Relaxation Measurements.** M L Tillett\*, T J Norwood and L-Y Lian *University of Leicester, UK*
- 21.20      **O.17 The Structure and Dynamics of the Solid Amino Acid Derivatives and their Interactions Studied by NMR.** Y Wang\* and P S Belton *Institute of Food Research, UK*
- 21.40      **O.18 MRI Studies on L-2-Chloropropionic Acid Toxicity in Rat Brain.** R E Williams\*, M Prior, H S Bachelard, J C Wateron, D Checkley and E A Lock *University of Nottingham, UK*
- 22.00      *SESSION ENDS*

## **WEDNESDAY 9 JULY**

### **SYMPOSIUM 5 - SOLIDS**

**Chairman:**      Dr J J Titman *University of Nottingham, UK*

- 09.00      **I.9 Removal and Reintroduction of Spin Interactions in Solid-state NMR.** B H Meier *University of Nijmegen, The Netherlands*
- 09.50      **O.19 Hydrogen Bond Exchange Dynamics in Solids.** F G Riddell\*, K S Cameron and R A Spark *University of St Andrews, UK*
- 10.10      **I.10 Structures of Solid State Proteins by NMR.** A McDermott *University of Columbia, USA*
- 11.05      *COFFEE/TEA*
- 11.20      **I.11 Solid-state NMR: Multiple-quantum NMR and High Resolution NMR Imaging.** W S Veeman *University of Duisburg, Germany*
- 12.15      *LUNCH*

## **EXCURSIONS**

### **THURSDAY 10 JULY**

#### **SYMPOSIUM 6 - NMR IN INORGANIC CHEMISTRY**

**Chairman:** Professor R K Harris *University of Durham, UK*

- 09.00      **I12 Relaxometric Studies of Gadolinium (III) Complexes Relevant to their Application as Contrast Agents in MRI.** S Aime *University of Turin, Italy*
- 09.50      **O.20 Quantitative 2D-EXSY Studies of Novel Fluxionality in Metal Complexes of Pyridine-based Ligands.** K G Orrell\*, A Gelling, M D Olsen, A G Osborne and V Sik *University of Exeter, UK*
- 10.10      **O.21 Gradient Pulsed  $^1\text{H}$ - $^{119}\text{Sn}$  HMQC NMR Spectroscopy in Structural Organotin Chemistry.** R Willem\*, M Biesemans, M Gielen, F Kayser, and J C Martins *Vrije Universiteit Brussel, Belgium*
- 10.30      *COFFEE/TEA*
- 11.00      **I13 Ordering and Exchange among Oxygens in Silicates: Inferences from  $^{17}\text{O}$  NMR.** J Stebbins *Stanford University, USA*
- 11.50      **O.22 Two-Dimensional MQMAS NMR of Quadrupolar Nuclei.** S Wimperis\* and S P Brown *University of Oxford, UK*
- 12.10      **O.23 Two-Dimensional NMR Studies of Alkali Metal Silicate Glasses.** M J Duer\*, S R Elliott and L F Gladden *University of Cambridge, UK*
- 12.30      *LUNCH*

#### **SYMPOSIUM 7 - NMR IMAGING**

**Chairman:** Dr W Vennart *University of Exeter, UK*

- 14.00 I14 **Recent Developments and Applications of Rapid NMR Imaging Techniques.** D Firmin *Royal Brompton Hospital, UK*
- 14.50 0.24 **Cardiac MRI in the Mouse.** P D Hockings\*, D G Reid, I Mitchell, L Freeman, N Toseland, M Benson and P Groot *SmithKline Beecham Pharmaceuticals, UK*
- 15.10 O.25 **Towards Stray-field Imaging of Nuclei of Integer Spin.** E W Randall\*, T G Nunes and P R Bodart *Queen Mary & Westfield College, UK*
- 15.30 I15 **Recent Advances in fMRI Techniques.** R Turner *Institute of Neurology, University of London, UK*
- 16.10 TEA AND POSTER SESSION

## **FRIDAY 11 JULY**

### **SYMPOSIUM 8 - BIOMEDICAL NMR SPECTROSCOPY**

**Chairman:** Dr J R Everett *Pfizer Central Research, UK*

- 09.00 I.16 **How NMR has Revolutionised Medical Diagnosis.** I C P Smith *National Research Council, Canada*
- 09.50 I.17 **MRS in Human Disease: What has been Achieved and Where are we Going?** P Styles *John Radcliffe Hospital, UK*
- 10.35 COFFEE/TEA
- 11.05 I.18 **Diagnostic <sup>1</sup>H NMR Spectroscopy of Biofluids and Tissue Biopsies.** J Nicholson *Birkbeck College, London, UK*
- 11.50 CLOSING REMARKS
- 12.00 MEETING ENDS

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