

**16<sup>th</sup> International Meeting on NMR Spectroscopy**  
**University of Cambridge**  
**29 June – 3 July 2003**

**Monday 30 June 2003**

Lecture Theatre Concert Hall

09:00 Opening Remarks by **Dr David Neuhaus**

Welcome by **Professor Jeremy Sanders** *University of Cambridge, UK*

**Symposium 1 Macromolecular Techniques**

Chair: **Michael Williamson**

- 09:10 I1 Weak Orientation Allows of a Very Precise View of Biomolecular Structure  
**A Bax**  
*National Institutes of Health, Bethesda. USA*
- 10:00 C1 NMR Structural Studies of Very Large Proteins: The 110kDa Polypyrimidine Tract binding Protein and a 350kDa AAA ATPase-adaptor Complex  
**X Yuan, P Simpson, A Szendroi, I Dreveny, C Mckeown, S Conte, V Pye, S Curry, X Zhang, P Freemont and S Matthews\***  
*Imperial College of Science, Technology and Medicine. iJK*
- 10:25 C2 High Pressure NMR Expands the Protein Structure World  
**K Akasaka**  
*Kinki University. Japan*
- 10:50 **COFFEE** sponsored by Syngenta
- 11:10 I1 GFT NMR Spectroscopy: Rethinking Multidimensional Data Acquisition  
**T Szyperski**  
*University of Buffalo, The State University of New York, USA*
- 12:00 C3 Structure and Function of the Cyclotides: Proteins with a Circular Backbone  
**D J Craik\*, R Clark, N L Daly and U Goransson**  
*University of Queensland, Australia*
- 12:25 **LUNCH**

**Parallel Sessions**

**Lecture Theatre Concert Hall**

**Symposium 2 Molecular Interactions**

Chair: **Glyn Williams**

- 14:00 I3 STD-NMR to Screen Libraries and to Characterise Ligand Binding to Receptors

**B Meyer**

*Institute for Organic Chemistry, University of Hamburg, Germany*

- 14:50 C4 NMR Investigation of the Interaction of Epothilones and Tubilin  
**T Carlomagno, V M Sánchez\*, M J J Blommers and C Griesinger**  
*Max Planck Institut für Biophysikalische Chemie, Göttingen. Germany*
- 15:15 I4 Looking Deeper into Vertebrate Development: Applications of Micro-MRI in Development Biology  
**R Jacobs**  
*California Institute of Technology, USA*

**Lecture Theatre: Recital Room**

**Symposium 3 Ordered Fluids**

Chair: **Jim Emsley**

- 14:00 I5 Aligned Lipid Matrices for the Structural Characterisation of Membrane Proteins  
**T Cross**  
*National High Field Magnet Laboratory, Florida State University, USA*
- 14:50 C5 Dipolar Interactions in Liquid Crystals by Two-dimensional Local Field Spectroscopy  
**S V Dvinskikh\*, Z Luz, H Zimmermann, D Sandström and A Maliniak**  
*Stockholm University, Sweden*
- 15:15 I6 Carbon-13 NMR Studies of Some New and Old Pyramidic Liquid Crystals  
**Z Luz**  
*Weizmann Institute of Science, Israel*
- 16:05 **TEA** sponsored by Syngenta

**Postgraduate Session**

**Lecture Theatre: Concert Hall**

Chair: **David Davies**

- 19:45 PG1 Effects of Coherent CSA-Dipolar Cross-Correlation on <sup>13</sup>C NMR of Labelled Compounds  
**L Duma\*, S Hediger, A Lesage, D Sakellariou, S Brown and L Emsley**  
*Ecole Normale Supérieure de Lyon, France*
- 20:05 PG2 Isolation of Homodalastatin 16, a New Cyclic Depsipeptide From a Kenyan Collection of *Lyngbya Majuscula*  
**M T Davis-Coteman, D M Dzeha\*, C A Gray, S Hess, L K Pannell, D T Hendricks and C E Arendse**

*Kenya Marine and Fisheries Research Institute. Kenya*

- 20:25 PG3 Real-time Chemical Shift Scaling in High Resolution NMR  
**N P Jerome\***, **L-Y Lian** and **G A Morris**  
*University of Manchester UK*
- 20:45 PG4 Solid-state NMR Investigations into the Interactions Between  
Bimetallic Clusters and Mesoporous Silica  
**M D Jones\***, **M J Duer**, **B F G Johnson** and **J M Thomas**  
*University of Cambridge. UK*
- 21:05 PG5 A Novel Lithiated Tubular System  
**N Treitel\***, **M Deichmann**, **T Sternfeld**, **T Sheradsky**, **R Herges** and  
**M Rabinovitz**  
*The Hebrew University of Jerusalem, Israel*

**Tuesday 1 July 2003**

**Lecture Hall: Concert Hall**

**Symposium 4 Biomedical**

Chair: **David Gadian**

- 09:00 I7 Magnetic Resonance Spectroscopy of the Human Brain  
**P Barker**  
*Johns Hopkins University. Baltimore. USA*
- 09:50 C6 Molecular Imaging Using Magnetic Resonance – New Tools for the  
Development of Tumour Therapy  
**K M Brindle**  
*University of Cambridge, UK*
- 10:15 C7 Gene Reporter Molecules: A New Platform Using <sup>19</sup>F NMR  
Substrates for β-Galactosidase  
**J Yu**, **W Cui** and **R P Mason\***  
*University of Texas Southwestern Medical Center at Dallas, USA*
- 10:40 **COFFEE** sponsored by Syngenta
- 11:55 I8 Molecular and Supramolecular Structure of Amyloid Fibrils  
**R Tycko**  
*National Institutes of Health, Bethesda, USA*
- 12:00 C8 Picometer Structural Resolution of the Chromophore of Bovine  
Rhodopsin by Double-quantum Solid-state NMR  
**M Carravetta\***, **X Zhao**, **O G Johannessen**, **M Verhoeven**,  
**PH M Bovee-Geurts**, **P E Verdegem**, **S Kiihne**, **H J M de Groot**,  
**W J de Grip**, **J Lugtenburg** and **M H Levitt**  
*University of Southampton. UK*
- 12:25 **LUNCH**

## Parallel Sessions

**Lecture Theatre: Concert Hall**

### **Symposium 5 Analytical Applications**

Sponsored by Eli Lilly

Chair: **John Shockor**

- 14:00 I9 Multidimensional NMR Studies of Synthetic Macromolecules  
**P Rinaldi**  
*University of Akron, USA*
- 14:50 C9 Use of Entropy Minimisation for Automatic Phase Correction and  
Pure Component Spectral Reconstruction of NMR Spectra  
**L Chen**  
*University of Singapore, Singapore*
- 15:15 I10 New Developments in the Determination of Stereochemistry by  
NMR  
**R T Williamson**  
Wyeth-Ayerst Research, USA

**Lecture Theatre: Recital Room**

### **Symposium 6 'Exotica'**

Chair: **Gareth Morris**

- 14:00 I11 NMR Spectroscopy with an Increase in S/N by More Than 10000  
Times. Is it Possible?  
**K Golman**  
*Amersham Health R & D, Sweden*
- 14:50 C10 Reaction Intermediates in the Headlights: NMR Studies Using  
Parahydrogen  
**S Duckett**  
*University of York, UK*
- 15:15 I12 Explorations in Micro-Spectroscopy and Micro Imaging  
**A Kentgens**  
*University of Nijmegen, Netherlands*

16-05 **TEA** sponsored by Syngenta

16:30 -18:00 **POSTER SESSION II** sponsored by Pfizer

## **IUPAC Workshop**

**Lecture Theatre: Recital Room**

Chair: **R K Harris**

19.45 **Open Forum on Chemical Shift Measurement**

This will be an organised discussion session on all aspects of chemical shift/shielding measurement and reporting not covered in the recently-published IUPAC conventions, including

- (a) MAS for both solids and solutions
- (b) solvent and temperature effects on the reference
- (c) magnetic susceptibility measurements and corrections
- (d) conventions for shielding tensor

Contributions to the discussion will come, inter alia, from E D Becker, R K Harris, K W Zilm, P Granger, S C de Menezes and R E Hoffman. Active participation by those attending will be welcomed. The debate will inform an IUPAC task force on the subject. The formal session will close at ca. 21:15, at which time some refreshments will be available - all participants are invited to remain for further informal discussion.

### **Wednesday 2 July 2003**

**Lecture Theatre: Concert Hall**

#### **Symposium 7 Materials**

Chair: **Malcolm Levitt**

09:00 I13 Going with the Flow: Localising the Physics of Soft Matter  
**P Callaghan**  
*Victoria University of Wellington, New Zealand*

09:50 C11 High-resolution NMR Spectroscopy of Disordered Solids  
**D Sakellariou, S P Brown\*, A Lesage, G de Paepe, S Hediger, M Bardet, C A Meriles, A Pines and L Emsley**  
*University of Warwick, UK*

10:15 C12 Natural Abundance  $^{17}\text{O}$  NMR  
**S E Ashbrook\* and I Farnan**  
*University of Cambridge, UK*

10:40 **COFFEE** sponsored by Syngenta

11:10 I14 Advanced Solid State NMR Techniques for Elucidating Structure and Dynamics of Complex Materials  
**H Spiess**  
*Max-Planck- Institut für Polymerforschung, Mainz, Germany*

12:00 C13 New Applications of Spin Counting Methods to Biomolecules and Polymers  
**C E Hughes\*, A Lange, M Baldus, M H Levitt and J Schmedt auf der Günne**  
*Max Planck Institute for Biophysical Chemistry, Göttingen, Germany*

12:25 **LUNCH**

Excursions & Conference Banquet - full details on timings and departure points can be found on page 14.

### **Thursday 3 July 2003**

**Lecture Theatre: Concert Hall**  
**Symposium 8 Small Molecules**

Chair: **Tim Claridge**

- 09:00 I15 Intermolecular Interactions as Studied by NOE and Diffusion  
**S Berger**  
*University of Leipzig, Germany*
- 09:50 C14 Advances in Prediction of  $^{13}\text{C}$  and  $^1\text{H}$  NMR Spectra Prediction  
**V Rafalovsky\*, G M Banik, L Taylor and E Melanson**  
*Bio-Rad Laboratories Inc, USA*
- 10:15 C15 Resolution Enhancement in Solid-State NMR of Labeled Biomolecules Using Spin-State Selective Techniques  
**Hediger\*, L Duma, A Lesage and L Emsley**  
*Ecole Normale Supérieure de Lyon, France*
- 10:40 **COFFEE** sponsored by Syngenta
- 11:10 C16 Solution Structures of Small Molecules from Residual Dipolar Coupling Constants Measured in Dilute Liquid Crystalline Media  
**T N Pham, D W H Rankin and D Uhrin\***  
*University of Edinburgh. UK*
- 11:35 I16 Applications and Advances with Cryoprobes and Computer-assisted Structure Elucidation  
**G Martin**  
*Pharmacia, USA*
- 12:25 **LUNCH AND CLOSURE OF MEETING**