

16th 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 ^{13}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 ¹⁹F 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}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 Gönne
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}C and ^1H 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**