

# 9<sup>TH</sup> INTERNATIONAL MEETING

UNIVERSITY OF WARWICK,

10-14 July 1989

## SCIENTIFIC PROGRAMME

The scientific sessions will take place in the Main Hall of the Arts Centre. Coffees and teas will be served in the Mead Gallery at the times stated in the programme.

All eight symposia, which make up the meeting, have Invited Lectures and shorter talks associated with them, and each is in the charge of its chairman.

In addition, the main themes of the meeting will be supported by two poster exhibitions which will allow a wide coverage of related current activity and provide a forum for informal discussion. Time-tabled sessions for formal viewing and discussion of posters are on Tuesday 11 July at 16.10 and on Thursday 13 July at 16.00, with ODD numbered posters being attended on the Tuesday and EVEN numbered posters on the Thursday.

The detailed programme for the meeting is as follows:

PARTICIPANTS ARE REMINDED THAT THE TAKING OF PHOTOGRAPHS DURING LECTURES IS NOT PERMITTED.

### SUNDAY 9 JULY

20.30 Inaugural Reception in Rootes Hall Social Building for all participants, both resident and non-resident

### MONDAY 10 JULY

09.00 Welcome to the University of Warwick

### SYMPOSIUM: 1 STRUCTURAL ELUCIDATION IN THE LIQUID STATE

Chairman: Dr J Feeney National Institute for Medical Research, London

09.05 **INVITED LECTURE:** Some New Techniques and Strategies for Studies of Protein Structure and Dynamics. G Wagner *University of Michigan, USA*

10.00 The Solution Conformation of Porcine C5<sub>ades</sub> Arq by <sup>1</sup>H NMR. M P Williamson *Roche Products, Welwyn Garden City* and V S Madison *Hoffmann-La Roche, New Jersey, USA*

10.30 Coffee

- 11.00      **INVITED LECTURE:** Dynamic Aspects of Structure in Solution. D L Turner *University of Southampton*
- 12.00      Effects of Active Site Amino Substituent on the Conformation and Activity of Staphylococcal Nuclease. S M Stanczyk, J A Wilde, and P H Bolton *Wesleyan University, Connecticut, USA* and M Dell'Acqua, T Pourmotabbed and J A Gerlt *University of Maryland, USA*
- 12.30      LUNCH

### **SYMPOSIUM: 5 NEW EXPERIMENTAL TECHNIQUES**

Chairman: Dr G A Morris *University of Manchester*

- 14.00      **INVITED LECTURE:** Fast Two-Dimensional Correlation Spectroscopy. R Freeman *University of Cambridge*
- 15.00      Selective Excitation by Self-Refocusing 270° Gaussian Pulses, with Applications to Two-Dimensional NMR and Slice Selection without Gradient Reversal in NMR imaging. L Emsley and G Bodenhausen *University of Lausanne, Switzerland*
- 15.30      Tea
- 16.00      Artifacts in COSY. C J Turner *Columbia University, New York, USA* and S L Patt *Varian Associates, Palo Alto, USA*
- 16.30      **INVITED LECTURE:** New 3D and Isotope-edited NMR Techniques for Structure Determination of Proteins. A Bax *NIH, Bethesda, Maryland, USA*
- 17.30      Close
- 19.30      Concert of choral and popular music in Coventry Cathedral sponsored by JEOL (UK) Ltd (Gratis).  
Transport will depart from the coach departure point at 18.45

## **TUESDAY 11 JULY**

### **SYMPOSIUM: 6 POLYSACCHARIDES AND GLYCOPROTEINS**

Chairman: Dr C Brown *Smith Kline and French, Welwyn Garden City*

- 09.00      **INVITED LECTURE:** Glyco Biolog. R A Dwek *University of Oxford*
- 10.00      NMR Analysis of Oligosaccharides in the Characterisation of Antigens and Receptors. E F Hounsell and T Feizi *MRC Clinical Research* and J Feeney *MRC Biomedical NMR Centre*
- 10.30      Coffee

- 11.00     **INVITED LECTURE:** Molecular Recognition by Glyco Peptide Antibiotics. D H Williams University of Cambridge
- 12.00     Application of  $^1\text{H}$ -Detected  $\{^1\text{H}, ^{13}\text{C}\}$ Shift-Correlation and  $\{^1\text{H}, ^1\text{H}\}$  Hartmann-Hahn Spectroscopy to the Study of Plant Cell Wall Xyloglucan Oligosaccharides. H van Halbeek, W S York, A G Darvill and P Albersheim *University of Georgia, USA*

12.30     LUNCH

### **SYMPOSIUM: 7 DATA ANALYSIS AND ARTIFICIAL INTELLIGENCE**

Chairman: Dr R A Hearmon *ICI P & P Division*

- 14.00     **INVITED LECTURE:** CASE : An NMR-Based Automated Structure Elucidation Tool. M E Munk *Arizona State University, USA*
- 14.50     **INVITED LECTURE:** Pattern Recognition in NMR: Multivariate Data Analysis Using Principal Components and Partial Least Squares Models. U Edlund *Umea University, Sweden*
- 15.40     Compensation of Instrumental Imperfections by Deconvolution using an Internal Reference Signal. G A Morris *University of Manchester*
- 16.10     **Tea + POSTER SESSION I**  
Transport will depart from the coach departure point at 19.15

## **WEDNESDAY 12 JULY**

### **SYMPOSIUM: 2 SOLID STATE**

Chairman: Dr C J Groombridge *Royal Holloway and Bedford New College, London*

- 09.00     **INVITED LECTURE:** Shielding Tensors, Their Measurement and Contribution to Chemical Structure. D M Grant *University of Utah, USA*
- 10.00     High Resolution  $^1\text{H}$  and  $^{19}\text{F}$  NMR in Solids. P Jackson, R K Harris and G J Nesbitt *University of Durham*
- 10.30     Coffee
- 11.00     Some Recent High Resolution NMR Studies of Inorganic Solids. R Dupree *University of Warwick*
- 11.30     **INVITED LECTURE:** Measurements of One- and Two-Dimensional Powder Patterns in Rotating Solids. T Terao *Kyoto University, Japan*
- 12.30     LUNCH
- PM        EXCURSIONS

## **THURSDAY 13 JULY**

### **SYMPOSIUM: 3 NON-MEDICAL IMAGING NMR SPECTROSCOPY**

Chairman: Professor E W Randall *Queen Mary College, London*

- 09.00      **INVITED LECTURE:** New Methods for Non Destructive Testing. L D Hall *Addenbrookes Hospital, Cambridge*
- 09.50      NMR Imaging of Liquid to Solid Transitions and Liquid/Solid Interfaces. D Foxall *Spectroscopy Imaging Systems, California, USA*
- 10.30      Coffee
- 11.00      **INVITED LECTURE:** Methods for Solid State NMR Imaging. A N Garroway *US Naval Research Laboratory, Washington DC, USA*
- 11.50      **INVITED LECTURE:** NMR Imaging of Solids with Magic Angle Spinning. W S Veeman *University of Nijmegen, The Netherlands*
- 12.30      LUNCH

### **SYMPOSIUM: 8 LESS COMMON NUCLEI**

Chairman: Dr D G Gillies *Royal Holloway and Bedford New College, London*

- 14.00      **INVITED LECTURE:** Theoretical Aspects of Nuclear Shielding. C J Jameson *University of Illinois, Chicago, USA*
- 15.00      Some New Applications of  $^{14}\text{N}$  NMR. P S Belton *AFRC Institute of Food Research, Norwich*
- 15.30      Deuterium NMR studies of the 1-n-alkyl-p-D-glucopyranosides-Solvents Liquid Crystalline Systems. A Loewenstein and D Igner *Technion, Haifa, Israel, U Zehavi The Hebrew University, Rehovot, Israel, H Zimmermann Max-Planck Institute for Medical Research, Heidelberg, FRG*
- 16.00      **Tea + POSTER SESSION II**
- 19.45 for 20.15      **Conference Dinner** in Chesford Grange Hotel, Kenilworth.  
Transport will depart from the coach departure point at 19.00

## **FRIDAY 14 JULY**

### **SYMPOSIUM: 4 BIOLOGICAL APPLICATIONS**

Chairman: Dr J R Everett *Beecham Pharmaceuticals*

- 09.00      **INVITED LECTURE:** Applications of High Field  $^{19}\text{F}$  and  $^{31}\text{P}$  NMR Spectroscopy in Cancer Research. W E Hull *Heidelberg, FRG*
- 09.50      NMR Studies of Blood Plasma: The Recognition Anions by Plasma Proteins. J D Bill, G Kubal and P J Sadler *Birkbeck College London*

- 10.10 A Pattern Recognition Approach to the use of NMR Spectroscopy in Biochemical Toxicology. K P R Gartland and J K Nicholson *Birkbeck College London* and C Bedell and J Lindon *Wellcome Foundation*
- 10.30 Coffee
- 11.00 Interactions in Membrane Surfaces: A  $^7\text{Li}$ ,  $^{23}\text{Na}$ ,  $^{39}\text{K}$  and  $^{133}\text{Cs}$  Dynamic NMR Study of the Transport of Alkali Metal Ions through Phospholipid Bilayers. A Arumugam and F G Riddell *University of St Andrews*
- 11.20 The Role of Molecular Conformation in Determining the Membrane Permeability of Retrovir. G R Painter, J P Shockcor and C Webster Andrews, *Wellcome Research Laboratories, North Carolina*
- 11.40 **INVITED LECTURE:**  $^{19}\text{F}$  and  $^{31}\text{P}$  NMR Studies of Tumour Therapy in Vivo. J R Griffiths *St Georges Hospital, London*
- 12.40 Closing Remarks
- 12.45 **LUNCH and End of Meeting**

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