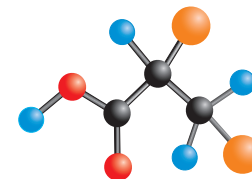


SMASH 2009 Conference Program



Sunday September 20th

4:30 PM - 6:00 PM Registration, Le Majestic
6:00 PM - 8:00 PM Dinner, Le Vista, Hotel Alpina
8:00 PM - 11:00 PM Mixer, Le Vista, Hotel Alpina

Monday September 21st

8:15 AM - 8:30 AM Opening Remarks
8:30 AM - 10:00 AM

Multidimensional NMR of Small Molecules

Chair: Tim Claridge, University of Oxford, UK

Applications of Spectral Aliasing to the Study of Complex Mixtures Using 2D HSQC Spectra

Damien Jeannerat, University of Geneva, Switzerland

Solution State Crystallography - A New Way to Look at Correlation Spectra and NOEs

Craig Butts, University of Bristol, UK

Applications of 2D NMR Methods to Structure Elucidation in Drug Development

Ben Bardsley, GlaxoSmithKline, UK

10:00 AM - 10:30 AM Break

10:30 AM - 12:00 PM

Latest Movements in Solids

Chair: Bénédicte Elena, Ecole Normale Supérieure de Lyon, France

Probing Hydrogen Bonding in Organic Solids: Applications to NMR Crystallography and Pharmaceuticals

Steven P. Brown, University of Warwick, UK

Molecular Dynamics in Solids: A Combined Analysis of Several Relaxation Times and Spectral Properties

Marco Geppi, University of Pisa, Italy

MAS NMR on the Tetrapyrrole Chromophore of the Photoreceptor Phytochrome

Thierry Rohmer, University of Leiden, The Netherlands

12:00 PM - 1:30 PM Lunch, Le Vista, Hotel Alpina

1:30 PM - 3:00 PM

Student and Post-Doctoral Session

Helen Atherton, University of Oxford, UK

Metabolic Markers of Combined Pesticide Exposure

Oliver Jones, University of Cambridge, UK

New Methods for NMR Crystallography of Powdered Solids

Elodie Salager, University of Lyon, France

Solvent Relaxation as a Tool to Screen Small Molecule-Metalloprotein Interactions - A Case Study Using Human Prolyl Hydroxylase Domain 2

Ivan K.H. Leung, University of Oxford, UK

3:00 PM - 3:30 PM Break
3:30 PM - 5:00 PM Workshops (Concurrent)

I. Careers in NMR

Jules Griffin, University of Cambridge, UK

II. Hyphenation and Automation in the NMR Lab

Ron Crouch, Varian Inc., USA

5:00 PM - 6:00 PM Free Time

6:00 PM - 6:30 PM Social Gathering

6:30 PM - 9:00 PM Dinner, Le Vista, Hotel Alpina

After Dinner Speaker: David Davies

University of London, UK

Serendipity in 40 years of NMR

9:00 PM - 11:00 PM Mixer, Le Vista, Hotel Alpina

Tuesday September 22nd

8:30 AM - 10:00 AM

Advances in NMR Analysis

Chair: Gerhard Wagner, Harvard Medical School, USA

New 2D and 3D DOSY Techniques and Applications

Gareth Morris, University of Manchester, UK

Application of Covariance NMR to the Analysis and Molecular Identification of Chemical Mixtures

Rafael Bruschweiler, Florida State University, USA

Efficient Detection and Characterization of Protein-ligand Interactions in H₂O

Alvar Gossert, Novartis, Switzerland

10:00 AM - 10:30 AM Break

10:30 AM - 12:00 PM

Exotica

Chair: Duncan Farrant, GSK, UK

Spectral Editing of Organic Mixtures into Pure Compounds using NMR and Ultra Viscous Solvents

André Simpson, University of Toronto, Canada

NMR with Small Magnets

Bernhard Blümich, Institut für Technische und Makromolekulare Chemie, Germany

Reversible Interactions with para-Hydrogen Enhance NMR Sensitivity by Polarization Transfer

Simon Duckett, University of York, UK

12:00 PM - 1:30 PM Lunch, Le Vista, Hotel Alpina

1:30 PM - 3:00 PM

Human Health and Nutrition

Chair: Sunil Kochhar, Nestle, Switzerland

Assessment of Nutritional Interventions on Health by NMR-Metabolomics

Xavier Correig Blanchar, Universitat Rovira i Virgili, Spain

Nutritional Influences on the Metabolic Profile, Chances and Pitfalls

Manfred Spraul, Bruker BioSpin GmbH, Germany

Metabolic Health Assessment by Nutritional Metabolomics

Serge Rezzi, Nestle Research, Switzerland

3:00 PM - 3:30 PM Break

3:30 PM - 5:00 PM Workshops (Concurrent)

I. Metabolomics

Hector Keun, Imperial College London, UK

II. Pulse Programming

Ulrich Gunther, University of Birmingham, UK

5:00 PM - 6:00 PM Free Time

6:00 PM - 7:30 PM Dinner, Restaurant La Calèche

8:00 PM - 10:00 PM Poster Session & Mixer, Le Majestic

10:00 PM - 11:00 PM Mixer, Le Majestic

Wednesday September 23rd

8:30 AM - 10:00 AM

Metabolomics

Jean Charles Portais, INSA-Toulouse, France

Identification of Biomarkers for Toxicity by NMR-Based Metabolomics

Nelly Aranibar, Bristol-Myers Squibb, USA

Metabolic Profiling Techniques to Assess and Manage Quality in Fruit Production

Dominique Rollin, INRA Bordeaux, France

NMR-based Fluxomics: Current Challenges and Perspectives

Stéphane Massou, INSA Toulouse, France

10:00 AM - 10:30 AM Break

10:30 AM - 12:00 PM

Sensitivity Enhancement and Novel Developments in NMR

Chair: Adrian Davis, Pfizer, UK

Industrial Process Control Employing NMR/MRI Based Sensors

Michael J. McCarthy, University of California-Davis, USA

Ultra-fast and Ultra-sensitive 2D NMR of Hyperpolarized Solutions

Patrick Giraudeau, Weizmann Institute, Israel

High-Field in-situ DNP - Applications from Small Molecules to Large Biomolecules

Thorsten Maly, MIT, USA

12:00 PM - 12:15 PM Closing Remarks

12:15 PM - Box Lunches