

Program

Refreshments and meals will be served in the Exhibition and Poster Area which may be found in the London Suite of the Barceló Hotel with an overflow area in the Paris Suite. All lectures will be presented in the Paris Suite where the conference dinner will also be held. Software workshops will be hosted by the relevant manufacturers in Conference Room 13. Please refer to maps and signage to assist you.

Day 1: 24th February 2010

10:00-12:00 Arrival, Registration (*Rotunda*), Coffee & Exhibition
 12.00-13.00 **Lunch**
 13.00-13.05 Structure 2010 Opening Remarks and Welcome by Prof. Paul Thomas

13.05-14.50 Session 1 Session Chair: Prof. Paul Thomas, University of Loughborough

13.05-13.40 Dr. Don Richards, Pfizer UK
What is Structure Elucidation?

13.40-14.15 Dr. Mark O'Neil-Johnson, Sequoia Sciences, USA
Plant Natural Products in a Drug-Discovery Program: From the Ground Up

14.15-14.50 Prof. Ian Wilson, AstraZeneca UK
Hyphenated and Hypernated Techniques for the Structure Elucidation of Metabolites

14.50-15.20 **Tea**

15.20-17.00 Session 2 Session Chair: Dr. Don Richards, Pfizer U.K.

15.20-16.25 **Pfizer** Sponsored Plenary Lecture delivered by Prof. Herb Hill, Washington State University, USA
Using Mobility Mass Correlation Curves for Structure Identification

16.25-17.00 Prof. Roy Goodacre, University of Manchester, UK
From Data to Knowledge: Mining the Metabolite Profile with Machine Learning



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17.30-20.00 Early Evening Parallel Events

17.30-19.30 Exhibition Area
 Drinks Reception
 (Sponsored by **Bruker UK**)
 Poster Session
 Vendor Exhibition



**18.00-19.50 Software Workshops:
 Conference Room 13**

18.00-18.30 Thermo Scientific
 18.40-19.10 ACD/Labs
 19.20-19.50 Mestrelab Research/Modgraph

20.00-22.00 **Conference Dinner** (Paris Suite)
 Wine Sponsored by **Thermo Scientific**
 Including Award by Dr. Steve Coombes of the Duncan Bryant Memorial Prize on behalf of the RSC Molecular Spectroscopy Group for the best Poster Presentation.



22.00-24.00 Mixing, Vendor Exhibition, Bar

Day 2: 25th February 2010

09.00-10.40 Session 3 Session Chair: Dr. Steve Coombes, AstraZeneca, Macclesfield UK.

09.00-10.05 **AstraZeneca** Sponsored Plenary Lecture delivered by
Prof. Lucio Frydman, Weizmann Institute, Israel.
*NMR, MRI and EPR Coming Together in the Aid of Structure
Elucidation: Ultrafast, Ultrasensitive Multidimensional NMR*



10.05-10.40 Dr. Jean-Claude Wolff, GlaxoSmithKline, UK
Authentic or Fake? A Mass Spectrometric Journey to Establish What is in Your Medicine!

10.40-11.10 **Coffee**

11.10-12.30 Session 4 Session Chair: Dr. Tim Claridge, University of Oxford

11.10-11.45 Prof. Lyndon Emsley, Ecole Normale Supérieure de Lyon, France
NMR Powder Crystallography

11.45-12.30 Dr. David Watkin, University of Oxford
Small Molecule Crystallography: All you ever wanted to know about X-rays but....

12.30-13.45 **Lunch**

13.45-14.55 Session 5 Session Chair: Dr. John Parkinson, University of Strathclyde

13.45-14.20 Dr. Christina Thiele, Technische Universität Darmstadt, Germany
Residual Dipolar Couplings as Novel NMR-Spectroscopic Restraints in Organic Structure Determination

14.20-14.55 Prof. Colin Creaser, University of Loughborough, UK
Structural Studies of Small Molecules by Ion Mobility-Mass Spectrometry

14.55-15.30 Closing Remarks and Tea

15.30 Formal Close of Structure 2010