



NMRDG **Spring 2005 Meeting**

General Information

The site operates a 'no smoking' policy.

Toilets are located at the entrance to the foyer just outside the lecture theatre.

Delegates are asked to make their way into the lecture theatre 5 minutes early to enable a prompt start to the sessions.

Coffee, tea and a buffet meal will be provided in the foyer just outside the lecture theatre.

Post Meeting Discussion

After the formal discussion at the end of the meeting there will be an opportunity for informal discussion over tea and coffee in the foyer. If desired there will be an opportunity to view the NMR facilities at GSK Stevenage. Delegates are asked to vacate the site by 6 pm.

Acknowledgements

The organisers wish to thank ACD/Labs, Bruker BioSpin, GlaxoSmithKline, JEOL UK Ltd, Modgraph, One Moon Scientific Inc, Perch Solutions and Varian Inc for sponsoring this event.

Computer Assisted and Automatic NMR Data Analysis of Small Molecules

Thursday 3rd March 2005

GlaxoSmithKline
Medicines Research Centre
Stevenage, UK



10:00	Tea & Coffee	13:30	Brent Lefebvre (ACD/Labs) <i>"A Complete Solution for Structure Identification"</i>
10:25	Welcome: Duncan Farrant (GSK)		
Session 1	Introduction and NMR data software tools, part 1	14:00	Peter Neidig (Bruker BioSpin) <i>"Semi-Automated Identification, Classification and Identification with AMIX"</i>
Chair:	John Hollerton (GSK)	14:30	Tea & Coffee
10:30	Introduction: Duncan Farrant (GSK) <i>"What are the Questions"</i>	Session 3	Applications of NMR Software to real Problems
10:40	Peter Meadows (JEOL UK Ltd) <i>"Advances in Automated Data Measurement & Analysis"</i>	Chair	Mike Bernstein (AstraZeneca, Charnwood)
11:00	Bruce Johnson (One Moon Scientific Inc) <i>"Computational tools for streamlining the spectroscopic workflow of synthetic chemists"</i>	15:00	John Hollerton (GSK) <i>"High Throughput Structure Verification"</i>
11:20	Matthias Niemitz (PERCH Solutions Ltd) <i>"Automated Spectral Analysis"</i>	15:30	Lee Griffiths (AstraZeneca, Alderley Park) <i>"Automated Analysis of NMR Spectra - In Practice"</i>
11:40	Jeff Seymour (Modgraph Consultants Ltd) <i>"Reliable combined C13 and Proton NMR prediction in a client/server environment"</i>	16:00	Mike Bernstein (AstraZeneca, Charnwood) <i>"Building Blocks for Plate Chemistry Verification"</i>
12:00	Buffet Lunch	16:30	Discussion
Session 2	NMR data software tools, part 2	17:00	Tea & Coffee informal discussion Tour round NMR facilities
Chair:	Duncan Farrant (GSK)	18:00	Depart
13:00	Iain Green (Varian Inc.) <i>"When Does Acquisition End and Processing Begin?"</i>		