

NMR applied to structure and reactivity in solution

A meeting organised by

NMR Discussion Group *and* Physical Organic Chemistry Group

RSC | Advancing the
Chemical Sciences

4 July 2011

GlaxoSmithKline Stevenage, Gunnels Wood Road, Stevenage SG1 2NY,
R&D Lecture Theatre



Agilent Technologies



Programme

10.30 Registration and coffee

Session 1: Reactions in solution

(Chair: Craig Butts)

- 11.00 Mathias Nilsson, University of Manchester
New NMR tools for reaction monitoring, mixture analysis and structure elucidation
- 11.35 Quickfire poster 1 Rob Evans, University of Manchester
Estimating diffusion coefficients for small molecules
- 11.40 Quickfire poster 2 Ralph Adams, University of Manchester
Resolving natural product epimer spectra by chiral matrix-assisted diffusion-ordered NMR spectroscopy
- 11.45 Quickfire poster 3 Chris Collett, University of St Andrews
Mechanistic studies of NHC mediated reactions
- 11.50 Quickfire poster 4 Catharine Jones, University of Bristol
Interproton distances from nuclear Overhauser effect (NOE) data
- 11.55 Quickfire poster 5 Tim Claridge, University of Oxford
1D HOESY sequences for ^{19}F - ^1H heteronuclear NOE experiments
- 12.00 Stefan Berger, University of Leipzig
Attempts to observe a Diels-Alder reaction before it happens
- 12.35 Lunch
- 13.15 Poster viewing

Session 2: Structure and association in solution

(Chair: Mike Williamson)

- 14.35 Jonathan Yates, University of Oxford
Computational approaches to NMR-based conformational analysis
- 15.10 Chris Hunter, University of Sheffield
Association in solution as probed by chemical shifts
- 15.45 Tea break
- 16.15 Award of poster prize (sponsored by Mestrelab)
- 16.25 Craig Butts, University of Bristol
High accuracy NOEs - a tool for small molecule conformational dynamics
- 17.00 Finish