

**Chairperson:**

Professor Sharon Ashbrook DPhil FRSC
School of Chemistry
University of St Andrews
North Haugh
St Andrews
KY16 9ST
Phone +44 (0) 1334 463779
Fax +44 (0) 1334 463808
Email: sema@st-andrews.ac.uk

Secretary:

Dr Stephen Byard CChem FRSC
ARCINOVA
Taylor Drive
Alnwick
Northumberland NE66 2DH
Tel: +44 (0) 1665 608544
Fax: +44 (0) 1665 603539
Email: Stephen.byard@arcinova.uk

Treasurer:

Dr John Parkinson CChem FRSC
Department of Pure & Applied Chemistry
University of Strathclyde
Thomas Graham Building
295 Cathedral Street,
Glasgow G1 1XL
Tel: +44 (0) 141 5482820
Fax: +44 (0) 141 5484822
Email: john.parkinson@strath.ac.uk

An Interest Group of the Royal Society of Chemistry
Charity Registration No. 207890

NMR Discussion Group and Molecular Spectroscopy Group Spring Meeting

Low Level Detection and Quantification by NMR Spectroscopy

Date of meeting: Wednesday 29th March 2017

Meeting venue: GlaxoSmithKline
Gunnels Wood Road
Stevenage
Hertfordshire
SG1 2NY^(a)
UK

^(a) SatNav postcode; Use SG1 2FX

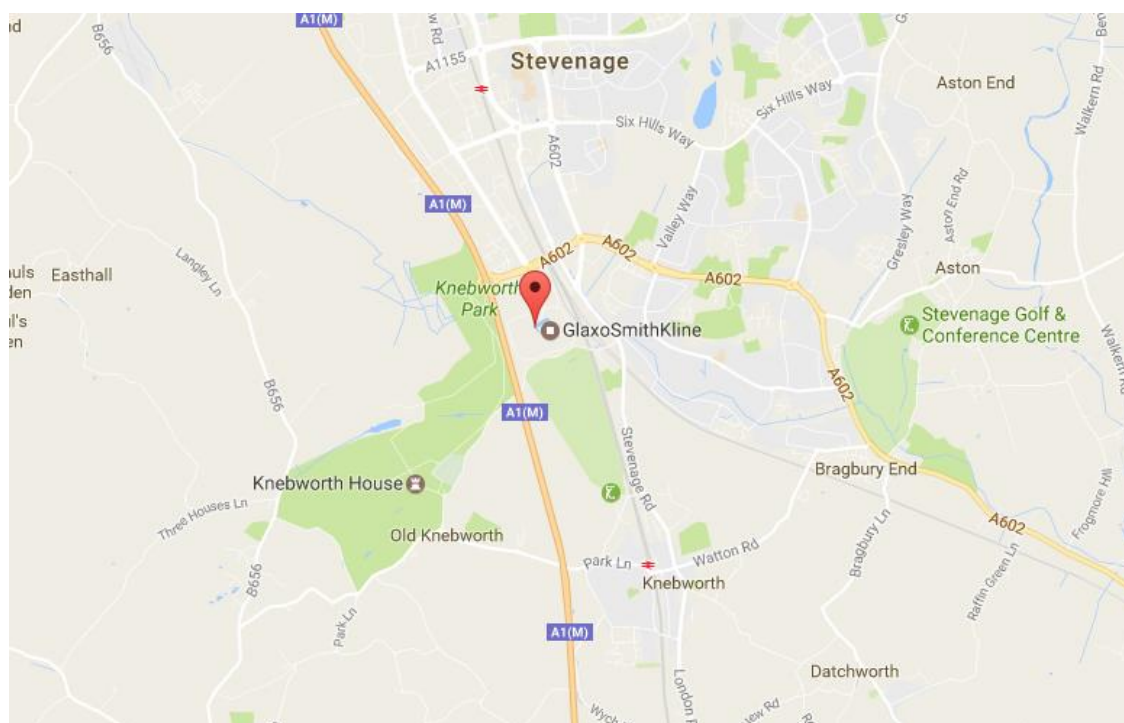
Dear Member,

The Royal Society of Chemistry NMR Discussion Group and Molecular Spectroscopy Group would like to invite you to the 2017 Spring Meeting, which will be held at GlaxoSmithKline (GSK), Stevenage. The theme for the meeting is "Low level detection and quantification by NMR" and different NMR technologies, including solution state NMR, solid state NMR and benchtop/low field NMR will be discussed. The presentations will cover a range of NMR related disciplines, including conventional low level detection and quantification, the use of cryoprobes, quantification of polymorphism using ssNMR and also methods for spectral simplification. Recent developments and applications of hyperpolarisation techniques, within both solution state and solid state NMR, will be presented in conjunction with the effect these sensitivity enhancements have with respect to quantification and limits of detection.

The meeting will take place on **Wednesday 29th March** at the easily accessed GlaxoSmithKline Stevenage site. Limited car parking will be made available on a first-come-first-served basis, and this can be reserved on registration. **When using a SatNav, it is necessary to enter postcode SG1 2FX which will direct you to the main site (Visitors Centre). The Main Site postcode will guide you to the wrong destination.** For delegates who wish to travel to the meeting by rail, the site is conveniently situated close to Stevenage railway station (approximately 15 minutes' walk from GSK).

A map showing the location of the venue is shown below, and can be accessed using the link <https://www.google.com/maps/place/Stevenage+SG1+2FX,+UK/@51.8842263,-0.2707101,12z/data=!4m5!3m4!1s0x4876302f8c3d356f:0x35129499f750b5f0!8m2!3d51.8842263!4d-0.2006723>

Additional, more detailed information, including public transport links, can be obtained from the NMR DG website <http://www.nmrdg.org.uk/>



Registration will close on **Monday 20th March 2017** and the standard fee is £65.00. However, if you are a student or retiree, then a concessionary rate of £45.00 will apply. **Please note that registrations cannot be accepted after the 20th March.** Details of registration can be found on the NMR DG website: <http://www.nmrdg.org.uk/> and registration can be initiated directly using the link <https://events.rsc.org/rsc/1104/register> . For retirees wishing to attend the event, please enter the discount code NMRLD17RET when prompted during the registration process.

For further information, please do not hesitate to send an E-mail to info@nmrdg.org.uk.

Yours sincerely,

The event organizing committee:

Dr Steve Coombes (AstraZeneca) – Molecular Spectroscopy Group Chairperson
Dr Ben Bardsey (GSK) – Molecular Spectroscopy Group Secretary
Dr John Parkinson (University of Strathclyde) – NMR DG Treasurer
Dr Steve Byard (Arcinova) - NMR DG Secretary

NMR Discussion Group and Molecular Spectroscopy Group 2017 Spring Meeting

Low Level Detection and Quantification by NMR Spectroscopy

Wednesday 29th March 2017

GlaxoSmithKline, Gunnels Wood Road, Stevenage, Herts., SG1 2NY

10.00 – 10.25 Registration and refreshments

Morning session chair: tbd

10.25 – 10.30 Introduction and welcome

10.30 – 11.05 **Michael Maiwald , BAM Federal Institute for Materials Research and Testing**

How far does the light shine? A check-up of quantitative high and low field NMR spectroscopy

11.10 – 11.40 **Ian Jones, AstraZeneca, UK**

Development and Validation of a Selective NMR Method for Cleaning Validation in a GMP Pharmaceutical Production Plant

11.45 – 12.20 **Marco Tessari, Radboud University, Netherlands**

Quantitative trace analysis of complex mixtures using SABRE Hyperpolarization

12.25 – 13.25 Lunch and refreshments

Afternoon session chair: tbd

13.25 – 14.00 **Gareth Morris, University of Manchester**

New NMR techniques for high dynamic range samples

14.05 – 14.40 **Ulrich Günther, University of Birmingham**

NMR based metabolic flux analyses in cancer cells

14.45 – 15.15 Refreshments

15.15 – 15.45 **Tran Pham, GlaxoSmithKline, UK**

Use of ssNMR for quantitative analysis of polymorphism in API and drug product

15.50 – 16.20 **Jeremy Titman, University of Nottingham**

Dynamic Nuclear Polarisation Enhanced Solid-state NMR Studies of Surfaces of Materials

16.25 – 16.30 **Closing remarks – Sharon Ashbrook**

16.30 - Departure
