



Member Networks Annual Report Form 2015

To enable us to better support our networks and their activities all member networks (Local Sections, Interest Groups and Analytical Division Regions) are asked to complete this form and return it to networks@rsc.org. The information is shared with the members of your networks, staff and governance Boards and Committees (inc. Division Councils).

Or by post to; Dr Fiona McMillan, Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, CB4 0WF.

This report form will be uploaded to the appropriate web page (signature deleted) unless requested otherwise.

GROUP NAME	NMR Discussion Group
Submitted by	Stephen Byard
Signed (may be signed electronically)	
Date	23 rd April 2016

Please list below the dates of your planned AGM and Committee Meetings (where applicable).

Annual General Meeting (if being held)

Date:	Thursday 15 th December 2016
Venue:	Institute of Structural and Molecular Biology, Birkbeck College, London

Proposed Committee Meetings Dates

Date	Venue
9 th February 2016	Priestly Room, Burlington House, London

Financial Accounts for the year ending 31 December 2015

Summary below:



NMRDG\
Appendix_F_2015.pc



EVENTS

Please attach any meeting reports, newsletters or other reports which are relevant.

Please report below on activities undertaken in the past year. If you have more detailed information about any particularly successful events, or advice to share please use a separate sheet. For more events continue as necessary.

Event Name	2015 Spring Meeting: Diffusion NMR (31st March 2015, University of Birmingham)
Event Type (key)	Scientific Conference - 1 day
Comments	<p>The 2015 spring meeting was a one-day event held at the Department of Chemistry, University of Birmingham, on 31st March 2015, and the theme was 'Diffusion NMR'. The local organiser was Melanie Britton (Department of Chemistry) and, in addition to speakers, vendors and organisers, a total of 53 registered delegates attended the meeting.</p> <p>The meeting was extremely successful and the feedback has been excellent. Following the event, it was suggested by multiple delegates that a meeting with a similar theme could be repeated on an annual basis. Whilst this may not be sustainable, diffusion NMR will be incorporated into future programmes.</p> <p>Speakers included:</p> <ul style="list-style-type: none"> • Prof John Christodoulou, University College London "Protein folding on the ribosome: the crucial role of diffusion NMR" • Dr Iain Day, University of Sussex "Recent developments in size exclusion chromatographic NMR" • Dr Carmine D'Agostino, University of Cambridge "Molecular diffusion in macro, meso and microporous materials: a tortuous tale of PFG-NMR" • Prof Peter Griffiths, University of Greenwich "Self-diffusion measurements - a sensitive and versatile technique to quantify structure and interactions in soft matter" • Prof Gareth Morris, University of Manchester "DOSY: progress and pitfalls" <p>A session of Quickfire poster talks was held, and 5 minute oral presentations</p>

were given by:

- Jane Power, University of Manchester “Broadband DOSY”
- Dr Giuseppe Pileio, University of Southampton “Real-space imaging of macroscopic diffusion and slow flow by singlet tagging MRI”
- Dr Henrik Müller, University of Oxford “Diffusion NMR as a tool for characterising chaperone substrate complexes”
- Mohamed Ainte, University of Cambridge “NMR techniques for measuring transport phenomena in porous materials”
- Dr Davy Sinnaeve, Ghent University “Simultaneous solvent and J-modulation suppression in PFGSTE diffusion measurements”

Commercial sponsorship was received from Bruker, GPE, Jeol, Magritek and Mestrelab.

Event Name	2015 NMR Discussion Group Postgraduate Meeting (24th June 2015, University of Manchester)
Event Type (key)	Education Event/Scientific Conference – 1 day
Comments	<p>The 2015 NMR DG Postgraduate Meeting was held at the Department of Chemistry, University of Manchester, on Wednesday 24th June. As in previous years, the meeting was held in conjunction with the UK NMR Facility Managers Meeting (UK MRM), which took place on Tuesday 23rd June at the same venue. Coordinating the two events in this way was, again, extremely successful and it is intended that this arrangement will be continued for the foreseeable future.</p> <p>The University of Manchester provided excellent facilities for the meeting, with sufficient space for poster presentations adjacent to the lecture theatres. There were 63 participants at the event, comprising 58 from academia, 2 from vendors, 2 from industry and 1 from the Royal Society of Chemistry (as a Sponsor). 28 students submitted abstracts, 8 of which were accepted for oral presentation and all were accepted for poster presentation. It was noted that the standard of both oral and poster presentations was excellent, and the event is now recognised as having an equivalent standard of presentation compared with events comprising programmes delivered by Principal Investigators. The oral presentations covered a good cross-section of NMR disciplines.</p> <p>Two overview lectures were given by established researchers, and the inclusion of these in the programme was again of general interest to the majority of delegates. On this occasion, Mathias Nilsson (The University of Manchester) and David Middleton (The University of Lancaster) gave presentations entitled <i>Pure shift NMR</i> and <i>Adventures in biomolecular design</i>, respectively.</p> <p>Separate registration processes were used for the UK NMR Facility Managers' meeting and the Postgraduate meeting. However, both registration processes were handled by the NMR DG via the RSC website.</p>

The event was supported by Thermo Scientific and the Royal Society of Chemistry.

Prizes were awarded to Davy Sinnaeve (Ghent University) for the best oral presentation and to Giulia Bignami (University of St Andrews) for the best poster presentation. As part of the prize, both Davy Sinnaeve and Giulia Bignami were invited to make presentations at the International joint Anglo-German NMR DG meeting in Darmstadt, with travel, accommodation and registration fees paid for by the NMR DG.

Event Name	Joint Anglo-German NMR DG meeting (7th – 10th September 2015, Darmstadt, Germany)
Event Type (key)	Scientific Conference – Multi-day
Comments	<p>The German NMR Discussion Group (FGMR) and UK NMR Discussion Group hosted a joint meeting on 7th – 10th September 2015 in Darmstadt. The meeting was held in the auditorium and media centre of the Technical University, which is about three miles from the city centre, on the Lichtwiese campus. An associated tour of Merck (Pharmaceutical Company) went ahead as planned.</p> <p>Christina Thiele was the local organiser for the meeting.</p> <p>Representation from the UK was quite reasonable, with approximately 30 UK attendees directly contributing to the programme.</p> <p>Prof Gareth Morris (University of Manchester), NMR DG Chairperson, was involved in the meeting organisation and served as a point of contact on behalf of the NMR DG. The content of the programmes was approximately 70% NMR:30% EPR.</p>

Event Name	2015 Christmas Meeting (Tuesday 15th December 2015, Institute of Structural and Molecular Biology, Birkbeck College, London)
Event Type (key)	Scientific Conference – One-day
Comments	<p>The meeting celebrated the publication of the two-volume text '<i>High Resolution NMR Spectroscopy</i>' in 1965, and the first publication of '<i>Progress in NMR Spectroscopy</i>' in 1966, respectively written and edited by Jim Emsley, Jim Feeney and Les Sutcliffe.</p> <p>Registration costs were maintained at the same rate as the previous year (£45.00 and £25.00 for standard and concessionary rates, respectively). As always, given the programme content, this event is considered to be good value and provide conference access to students or spectroscopists having a limited budget. On this occasion, generous financial assistance was provided by Elsevier.</p> <p>The meeting was attended by 163 delegates. The excellent attendance was a reflection of the programme, celebrating 50 years of Progress in NMR Spectroscopy, and recognising contributions from Jim Emsley, Jim Feeney and Les Sutcliffe. Two speakers each were invited by Jim Emsley, Jim Feeney and Les Sutcliffe and comprised their respective associates. Given the differences in NMR-related research undertaken by the three, the meeting programme was varied and quite balanced. Speakers included Steve Matthews (Imperial College, London), Melanie Britton (University of Birmingham), Angela Gronenborn (University of Pittsburgh, USA), Gordon Roberts (University of Leicester), Geoffrey Luckhurst (University of Southampton) and Denis Merlet (Université Paris-Sud). Presentation titles are listed below:</p> <p>Steve Matthews, Imperial College, London Order and disorder in proteins – beyond nOes</p> <p>Melanie Britton, University of Birmingham Through the chemical looking glass: what MRI can reveal about batteries, corrosion and electroplating</p>

Angela Gronenborn, *University of Pittsburgh*

Synergy between NMR, cryo-EM and large-scale MD simulations – an atomic model of the HIV capsid

Gordon Roberts, *University of Leicester*

Metallo- β -lactamases: structures, zincs and loops

Geoffrey Luckhurst, *University of Southampton*

The fourth nematic liquid crystal. Twist, bend and order identified with ^2H NMR spectroscopy

Denis Merlet, *Université Paris-Sud*

New developments for molecular structural determination of flexible compounds using liquid crystal as NMR solvent

The event was held at the Institute of Structural and Molecular Biology, Birkbeck College, London.

Generous sponsorship for the meeting was provided by Elsevier. Whilst sponsorship for the Christmas meeting is encouraged, the committee have consistently felt that vendor displays are not appropriate for this meeting and should be avoided for future meetings, if requested by vendors. This is based on an assumption that the format of the meeting will remain unchanged.

The BRSG Christmas meeting was held on the previous day to the NMR DG meeting, and was also very well attended. This meeting had a theme of NMR Crystallography. This was quite complementary to the programme organised by the NMR DG and it is evident that delegates benefited from the two events being coordinated in this way. The 2015 BRSG – NMR DG Annual Prize winner, Dr Giuseppe Pileio, Senior Research Fellow at the Department of Chemistry, University of Southampton, gave a presentation at the BRSG Christmas meeting for his work on the theory and application of long-lived nuclear spin states in solution-state NMR. This was extremely well received.

	<p>It is generally recognised that the 2015 NMR DG Christmas meeting was a very successful event and the feedback has been extremely positive.</p>
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AWARDS AND BURSARIES

Please list any awards or bursaries presented by your committee in 2015 and indicate any which will be open for nomination/application in 2016.

The following student travel bursaries were awarded in 2015:

Event	Recipient
SMASH 2015, Baveno, Italy ^(a)	Nicholle Bell Ikenna Ndukwe Andrew Hall Claire Dickson Ruth Dooley Jessica Bame Thomas Leman Aaran Hernandez Cid Jane Power
Joint Anglo-German NMR Discussion Group Meeting, Darmstadt ^(b)	Alison Michan Davy Sinnaeve ^(c) Iva Pritisanic Giulia Bignami ^(c) Nicholle Bell Ikenna Ndukwe
Alpine conference	Scott Sneddon
Euromar, Prague	Martine Abboud
Inter-university collaborative research (UK)	Sarah Newton
ENC, CA, USA	Alex Forse
ICMRM, Munich	Catherine Smith
NMR DG Postgraduate meeting, Manchester	Catherine Smith Jessica Bame Karol Nartowski Paula Sanz Camacho Hannah Davies Hannah Kerr

^(a) Joint NMR DG – SMASH award

^(b) Travel component supported by RSC

^(c) Awarded as part of Postgraduate meeting prize

The 2015 joint BRSG – NMR DG Annual Prize was awarded to Dr Giuseppe Pileio, Senior Research Fellow at the Department of Chemistry, University of Southampton. Giuseppe gave a presentation at the BRSG Christmas meeting for his work on the theory and application of long-lived nuclear spin states in solution-state NMR.



At the 2015 NMR DG Postgraduate meeting, prizes were awarded to Davy Sinnaeve (Ghent University) for the best oral presentation and to Giulia Bignami (University of St Andrews) for the best poster presentation. As part of the prize, both Davy Sinnaeve and Giulia Bignami were invited to make presentations at the International joint Anglo-German NMR DG meeting in Darmstadt, with travel, accommodation and registration fees paid for by the NMR DG.

Student travel bursaries will be offered by the NMR DG throughout 2016, to assist with attendance at both national and international events. Applications can be made directly to the secretary at info@nmrdg.org.uk

The joint BRSG – NMR DG will continue to be awarded on an annual basis. Nominations for the 2017 award will be invited in September 2016.

The NMR DG Postgraduate meeting will take place at St Catherine's College, Oxford, in 2016. Prizes for both best oral and poster presentations will be awarded.

Other information/comments:

The NMR Discussion Group continues to increase engagement with spectroscopists at all levels, both Nationally and Internationally, providing mechanisms for information exchange and scientific advancement. An increased level of support has been delivered to students throughout 2015, assisting with travel to international conferences and also with inter-university collaborations. The NMR DG is also appreciative of the continued support and interactions with the Royal Society of Chemistry, which has been of significant help in allowing us to achieve our aims and objectives.

Continued collaborations with groups who have either similar or complementary interests, including the BRSG (Institute of Physics), Molecular Spectroscopy Group (RSC) and the British Mass Spectrometry Society, are of demonstrable benefit with respect to promoting scientific exchange.

PLANNED ACTIVITIES

Please report below on activities proposed. For more events continue as necessary.

Event Name	Spring meeting 2016 – ‘In Situ Monitoring by NMR’, Department of Chemistry, University of York.
Comments	<p>The 2016 spring meeting will be held at the Department of Chemistry, University of York, on Thursday 17th March 2016 and the theme will be <i>In Situ Monitoring by NMR</i>.</p> <p>Invited speakers include:</p> <p>David Foley, Pfizer USA Understanding chemical reactions in a process development environment using NMR</p> <p>Simon Duckett, University of York Harnessing hyperpolarisation for <i>in situ</i> NMR monitoring</p> <p>Simon Watson/Flavien Susanne, GSK Bench top NMR - Reaction kinetics in the pharmaceutical industry</p> <p>Ulrich Hintermair, University of Bath Reaction monitoring by FlowNMR - new insights into homogeneous catalysis</p> <p>Guy Lloyd Jones, University of Edinburgh Two B or not two B, and other mix-ups</p> <p>Richard Hopkinson, University of Oxford Enzyme binding – to be confirmed</p> <p>Michael Maiwald, BAM Federal Institute for Materials Research and Testing First steps towards field integration of benchtop NMR spectroscopy for online monitoring and process control</p> <p>Bruker, GPE, Mestrelab, Thermo, Oxford Instruments and Magritek have agreed to sponsor the event.</p>

Event Name	2016 NMR DG Postgraduate Meeting (23rd June 2016, Oxford)
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Comments	<p>The 2016 NMR DG Postgraduate Meeting will be held at St. Catherine's College, University of Oxford, on Thursday 23rd June. The meeting will be held in conjunction with the UK NMR Facility Managers Meeting, which will take place on Friday 24th June at the Department of Chemistry, University of Oxford.</p> <p>As on the previous five occasions, two overview lectures will be given by established researchers. Flemming Hansen (University College, London: 'NMR Methods to characterise protein dynamics') and Tim Claridge (University of Oxford) have been invited to give overview lectures.</p> <p>The UK Magnetic Resonance Managers' meeting will take place on Friday 24th June 2016 at the Department of Chemistry, University of Oxford, the day following the Postgraduate meeting. The sessions and speakers have yet to be defined. However, the format adopted for the two previous meetings is likely to be repeated with three to four sessions focussing on current areas of interest.</p>
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Event Name	2016 NMR DG Christmas Meeting (15th December 2016)
Comments	<p>The Christmas meeting will be held at the Institute of Structural and Molecular Biology, Birkbeck College, London, on Thursday 15th December.</p> <p>The two prize winners from the 2016 Postgraduate meeting will be invited to make presentations. Also, Andrew Baldwin, as the 2016 BRSG – NMR DG prize winner for excellence in magnetic resonance has accepted an invitation to present.</p> <p>The meeting will be held in conjunction with the BRSG Christmas meeting, which will take place at the Institute of Physics (IoP) on Wednesday 14th December.</p> <p>Registration fees will be held at the previous levels of £45.00 with a concessionary rate of £25.00.</p>



COMMITTEE

(this information will be used to update our membership database and your web page where appropriate)

Position	Name	Dates on committee
Chair	Prof Sharon E M Ashbrook	2016 - Present
Secretary	Dr Stephen J Byard	2005 - Present
Treasurer	Dr John A Parkinson	2008 - Present
Ordinary Members	Dr Mike Bernstein Dr Melanie Britton Dr Andrew Gibbs Dr Flemming Hansen Prof. Yaroslav Khimyak Dr Harry Parkes	2006 – Present 2012 – Present 2014 – Present 2014 – Present 2012 – Present 1994 – Present
Benevolent Fund Representative (if relevant)	Not applicable	Not applicable
Co-opted members and their affiliation	Prof Gareth A Morris FRS University of Manchester	2014 - Present



COLLABORATION

The issue of communication and collaboration between all member networks has been raised by members at recent events including the regional meetings and the general assembly. There have been instances of committees running very similar events when, had they known about their shared interests, they would have preferred to work together and to share their experiences.

As all of the networks cover such a broad range of topics it would be helpful if you could complete the following information to assist staff in proposing potential collaborations. Please include the topic of an event which you would consider collaborating on with another committee and the contact name for that area (if left blank we will assume that the contact is the Secretary). To facilitate communication if you are happy for us to pass your contact email on to the appropriate person to discuss potential collaboration please indicate below.

This information will be shared with all other member network committees.

Area of interest	Contact Name	Permission to share email YES/NO