



## Member Networks Annual Report Form

*Reporting events held in 2017 and those planned for 2018*

In line with the rules for member networks and 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](mailto:networks@rsc.org) or by post to; Networks Team, Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, CB4 0WF.

### Deadlines

Deadline for receipt of Financial Accounts by RSC Finance Team: **9<sup>th</sup> February 2018**

Deadline for receipt of Annual Report by Networks Team: **26<sup>th</sup> February 2018**

If there is any reason that your committee will **not** be able to meet either or both of these deadlines please inform [networks@rsc.org](mailto:networks@rsc.org) as soon as possible.

This report will be uploaded to your web page to share with the members of your network. Staff will also share a digest of all member networks activities taken solely from these annual reports with appropriate staff and governance boards and committees including Division Councils with similar interests.

<b>Committee</b>	NMR Discussion Group
<b>Completed by</b>	Stephen Byard
<b>Date</b>	28 <sup>th</sup> January 2018

Please list below the dates of all of your planned committee meetings and, if held, AGM.

### **Annual General Meeting (if being held)**

<b>Date:</b>	Thursday 13 <sup>th</sup> December 2018
<b>Venue:</b>	Institute of Molecular and Structural Biology, Birkbeck College, London

### **Proposed Committee Meetings Dates**

<b>Date</b>	<b>Venue</b>
Friday 23 <sup>rd</sup> March 2018	Royal Society of Chemistry, Science Room, Burlington House, London.



## 2017 Events

Please append electronic copies of any meeting reports, newsletters or relevant materials to this report.

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 KEY:

- Education Event (including outreach activities for school students or the general public)
- Public Lecture
- Retired Members Event
- Scientific Conference - 1 day
- Scientific Conference - multi day
- Social Event
- Training/workshop
- Award Lecture
- Other

<b>Event Name</b>	NMR Discussion Group and Molecular Spectroscopy Group Joint Spring Meeting: Low Level Detection and Quantification by NMR Spectroscopy (Wednesday 29 <sup>th</sup> March 2017 – GlaxoSmithKline, Stevenage)
<b>Event Type (key)</b>	Scientific Conference – 1 day
<b>Comments</b>	<p>The 2017 spring meeting was jointly organised by the RSC NMR Discussion Group (NMR DG) and RSC Molecular Spectroscopy Group (MSG). This was a one-day event held at GlaxoSmithKline, Stevenage, on 29<sup>th</sup> March 2017, and the theme was 'Low Level Detection and Quantification by NMR Spectroscopy'.</p> <p>The meeting was attended by 62 participants, and speakers included:</p> <ul style="list-style-type: none"> <li>• <b>Michael Maiwald, <i>BAM Federal Institute for Materials Research and Testing</i></b> How far does the light shine? A check-up of quantitative high and low field NMR spectroscopy</li> <li>• <b>Ian Jones, <i>AstraZeneca, UK</i></b> Development and validation of a selective NMR method for cleaning validation in a GMP pharmaceutical production plant</li> <li>• <b>Marco Tessari, <i>Radboud University, Netherlands</i></b>  Quantitative trace analysis of complex mixtures using SABRE Hyperpolarization</li> <li>• <b>Gareth Morris, <i>University of Manchester</i></b> New NMR techniques for high dynamic range samples</li> <li>• <b>Ulrich Günther, <i>University of Birmingham</i></b></li> </ul>

	<p>NMR based metabolic flux analyses in cancer cells</p> <ul style="list-style-type: none"> <li>• <b>Tran Pham, <i>GlaxoSmithKline, UK</i></b> Use of ssNMR for quantitative analysis of polymorphism in API and drug product</li> <li>• <b>Jeremy Titman, <i>University of Nottingham</i></b> Dynamic Nuclear Polarisation enhanced solid-state NMR studies of surfaces of materials</li> </ul> <p>The NMR DG and MSG are grateful to AstraZeneca for generous sponsorship, and to GlaxoSmithKline for providing excellent conference facilities.</p> <p>Holding joint RSC interest group meetings in this way facilitates exchange between members of the respective groups, in addition to focussing on common interests. Equally, collaborative efforts circumvent potential duplication of subject-specific meetings.</p> <p>A meeting report can be accessed via the link:  <a href="https://sites.google.com/site/rscmolecularspectroscopygroup/home/meeting-reports/nmrdg-and-msg-spring-meeting-report-2017">https://sites.google.com/site/rscmolecularspectroscopygroup/home/meeting-reports/nmrdg-and-msg-spring-meeting-report-2017</a></p>
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<b>Event Name</b>	10 <sup>th</sup> Annual NMR Discussion Group Postgraduate Meeting (Thursday 22 <sup>nd</sup> June 2017, Department of Pure and Applied Chemistry, University of Strathclyde)
<b>Event Type (key)</b>	Education Event/Scientific Conference – 1 day
<b>Comments</b>	<p>The 2017 NMR DG Postgraduate Meeting was held at the Department of Pure and Applied Chemistry, University of Strathclyde, on Thursday 22<sup>nd</sup> June. As in previous years, the meeting was held in conjunction with the UK NMR Facility Managers Meeting (UK MRM), which took place on Wednesday 21<sup>st</sup> 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 Strathclyde provided excellent facilities for the meeting, with sufficient space for poster presentations adjacent to the lecture theatres. There were 71 participants at the event, comprising 63 from academia, 4 from vendors, 3 from industry and 1 retiree. 26 students submitted abstracts, 8 of which were accepted</p>

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 diverse cross-section of NMR disciplines.

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, John Parkinson (The University of Strathclyde) and Jeremy Titman (The University of Nottingham) gave presentations entitled *NMR Past, Present and Future: One Spin Doctor's Perspective* and *What has solid-state NMR ever done for us? Structure, dynamics and polarisation in materials*, respectively.

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.

The event was generously supported by Oxford Instruments and the Royal Society of Chemistry, for which the NMR DG are extremely grateful.

Prizes were awarded to **Michael A Hope**, *Department of Chemistry, University of Cambridge*, for the best oral presentation and to **Vanessa Timmermann**, *School of Chemistry, University of Manchester*, for the best poster presentation. As part of the prize, both Michael Hope and Vanessa Timmermann were invited to make presentations at the NMR DG Christmas meeting in London. The standard of presentations was excellent, thus making the task of choosing prize-winners exceptionally difficult. To this end, additional prizes were awarded for best poster presentations to **Nick Brownbill** *University of Liverpool*, **James Montgomery** *University of St Andrews* and **Matthew Wallace** *University of Liverpool*.

A meeting report was issued for publication, and consent was obtained from all those whose photographs were included in the document (Attached to this report as a .pdf file).



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<b>Event Name</b>	2017 NMR DG Christmas Meeting (Thursday 14 <sup>th</sup> December 2017, Institute of Structural and Molecular Biology, Birkbeck College, London)
<b>Event Type (key)</b>	Scientific Conference – 1 day
<b>Comments</b>	<p>The annual NMR DG Christmas meeting is an extremely popular event, typically comprising presentations covering a diverse range of subjects. This year, the programme comprised lectures concerning subjects including recent developments in small molecule characterisation, structure based design in pharmaceuticals, molecular biology and the continually developing discipline of solid-state characterisation. It was intended that the presentations would be of interest to the majority of spectroscopists of differing backgrounds, either through direct relevance or through potential applicability</p> <p>Registration costs were increased slightly compared with previous years, and concessionary rates were offered to students, retirees and RSC members). The standard fee was £55.00 for non-RSC members or £45.00 for RSC members. However, for students or retirees, a concessionary rate of £30.00 was applied for non-RSC members or £25.00 for non-members. Members of affiliated groups, such as the Institute of Physics, also qualified for the same rates as RSC members.</p> <p>The meeting was attended by 113 delegates. A list of speakers and presentation titles is presented below:</p> <p><b>Burkhard Luy, <i>Karlsruher Institut für Technologie (KIT)</i></b> Fast and Broadband: New Developments in High Resolution NMR Spectroscopy</p> <p><b>Elisabetta Chiarparin, <i>AstraZeneca, UK</i></b> Free Ligand NMR Conformations: A New Perspective in Structure-Based Drug Design</p> <p><b>Vanessa Timmermann, <i>University of Manchester</i></b> Evaluating the Solution Structure of Uranium(IV) DOTA-type Complexes by <sup>1</sup>H NMR Spectroscopy</p> <p><b>Mathias Nilsson, <i>University of Manchester</i></b> Progress in Mixture Analysis of Small Molecules</p> <p><b>Tony Watts, <i>University of Oxford</i></b> Pushing the boundaries in solid state NMR of membrane-embedded proteins: DNP, fast MAS and proton detection</p> <p><b>Jonathan Iggo and Matthew Wallace, <i>University of Liverpool</i></b></p>

Soups, Gels, Gradients and Images: NMR Methods for Studying NMR Invisible Soft Matter and other Things

**Michael Hope, *University of Cambridge***

Investigating the Mechanism and Electronic Properties of Electrochemically Metallised VO<sub>2</sub> using Solid-state NMR

**Steven Brown, *University of Warwick***

Characterising Structure of Organic Molecules in the Solid State: Combining Magic-Angle Spinning NMR, DFT Calculation and Powder X-ray Diffraction

Generous sponsorship for the meeting was provided by John Wiley and Sons. 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 under Extreme Conditions* and was quite complementary to the programme organised by the NMR DG. It is evident that delegates benefited from the two events being coordinated in this way. The 2017 BRSG – NMR DG Annual Prize winner, **Dr Frédéric Blanc**, Senior Lecturer, *University of Liverpool*, gave a presentation at the BRSG Christmas meeting for his work on DNP enhanced solid-state NMR of insensitive nuclei, with applications to oxygen-17 and low-gamma. This was extremely well received.

It is generally recognised that the 2017 NMR DG Christmas meeting was a very successful event and the feedback has been extremely positive.

### Awards and Bursaries

Please list any awards or bursaries presented by your committee in the past 12 months and indicate any which will be open for nomination/application in the next calendar year.

Please ensure that all members of your network are notified of any awards or bursaries for general application.

Student travel bursaries were awarded, as listed in the below table.

Event	Recipient
SMASH 2017, Baveno, Italy <sup>(a)</sup>	Guilherme Dal Poggetto Pinelopi Moutzouri Claire Dickson Olga Semenova Lydia Dewis Serena Monaco Ariana Jones Siyong Zhong
Alpine conference, Chamonix Mont Blanc, France	Nick Brownbill Suzie Pugh Rosalie Cresswell
Euromar, Warsaw, Poland	Guilherme Dal Poggetto Pinelopi Moutzouri Harry MacKenzie
CCPN (Collaborative Computing Project for NMR) Annual Conference, Stirling, Scotland	Ruth Dingle
ENC, CA, USA	Alex Forse
ICMRM, Halifax, Nova Scotia, Canada	Emma Thompson
International Summer School, Germany	Zhipeng Ke
NMR DG Postgraduate meeting, Strathclyde	Giulia Bignami Ruth Dingle Alex Gardner Ieva Goldberga Michael Hope Will Kew Serena Monaco Olga Semenova Vanessa Timmermann

(a) Joint NMR DG – SMASH bursary



The 2017 joint BRSG – NMR DG Annual Prize was awarded to Dr Frédéric Blanc, Senior Lecturer, University of Liverpool for his work on DNP enhanced solid-state NMR of insensitive nuclei, with applications to oxygen-17 and low-gamma. Frédéric gave a presentation at the 2017 BRSG Christmas meeting, which was held at 41 Portland Place, London.

At the 10<sup>th</sup> Annual Postgraduate meeting, prizes were awarded to **Michael A Hope**, *Department of Chemistry, University of Cambridge*, for the best oral presentation and to **Vanessa Timmermann**, *School of Chemistry, University of Manchester*, for the best poster presentation. As part of the prize, both Michael Hope and Vanessa Timmermann accepted invitations to make presentations at the NMR DG Christmas meeting in London. Runner-up prizes were awarded for best poster presentations to **Nick Brownbill** *University of Liverpool*, **James Montgomery** *University of St Andrews* and **Matthew Wallace** *University of Liverpool*.

Student travel bursaries will be offered by the NMR DG throughout 2018, to assist with attendance at both national and international events. Applications can be made directly to the secretary at [info@nmrdg.org.uk](mailto:info@nmrdg.org.uk)

The joint BRSG – NMR DG prize will continue to be awarded on an annual basis. Nominations for the 2019 award will be invited in September 2018.

The NMR DG Postgraduate meeting will take place at the Department of Physics, University of Warwick, in 2018. 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 2017, assisting with travel to international conferences and also with attendance at international summer school. Registration fees will be maintained at the lowest possible rates, and concessionary rates for our events will be offered to both students and retirees, consistent with the group's objective of facilitating social and professional interaction at all levels. 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 British Biophysics Society are of demonstrable benefit with respect to promoting scientific exchange.

### Future Activities

When planning any activities please remember to ensure that all events are logged on our events database and ensure that all contracts are sent to our Legal Team with enough time for amendments and, where necessary, approval by the Board.

Please outline any activities already in planning for the next calendar year.

<b>Event Name</b>	NMR DG Spring meeting 2018 – ‘NMR Studies of Soft Matter’, Department of Chemistry, University of Sheffield, 11 <sup>th</sup> April 2018.
<b>Comments</b>	<p>The theme for the 2018 Spring meeting is ‘NMR Studies of Soft Matter’. The principal objective of the meeting is to explore potential applications of NMR for understanding systems involving multiple phase boundaries and lengths scales, typical of those present in complex molecular and biological materials.</p> <p>Invited speakers include:</p> <p>Melinda Duer, <i>University of Cambridge</i>            David Middleton, <i>University of Lancaster</i>            Matthew Wallace, <i>University of East Anglia</i>            Jesus Angulo, <i>University of East Anglia</i>            Melanie Britton, <i>University of Birmingham</i>            Mike Williamson, <i>University of Sheffield</i>            Oleksandr Mykhaylyk, <i>University of Sheffield</i>            Sarah Mann, <i>University of Warwick</i></p>

<b>Event Name</b>	11 <sup>th</sup> Annual NMR Discussion Group Postgraduate Meeting (21 <sup>st</sup> June, University of Warwick)
<b>Comments</b>	<p>The 2018 NMR DG Postgraduate Meeting will be held at the Department of Physics, University of Warwick, on Thursday 21<sup>st</sup> June. The meeting will be held in conjunction with the UK NMR Facility Managers Meeting, which will take place on Wednesday 20<sup>th</sup> June at the 850 MHz Solid-state Facility, Milburn House, University of Warwick.</p> <p>As on the previous five occasions, two overview lectures will be given by established researchers. Prof Mark Smith, <i>University of Lancaster</i> (Some Recent Observations of Low-<math>\gamma</math> Quadrupolar Nuclei with Solid-state NMR and Thoughts on</p>

	<p>Career Paths for NMR Spectroscopists) and Prof Peter Sadler, <i>University of Warwick</i> (A Periodic Table of NMR and Medicines) have been invited to give overview lectures.</p> <p>The UK NMR Facility Managers Meeting will take place on Wednesday 20<sup>th</sup> June at the 850 MHz Solid-state Facility, Milburn House, University of Warwick. The sessions and speakers have yet to be defined. However, the format adopted for the two previous meetings will be repeated with three to four sessions focussing on current areas of interest.</p>
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<b>Event Name</b>	2018 NMR DG Christmas Meeting (13 <sup>th</sup> December 2018)
<b>Comments</b>	<p>The Christmas meeting will be held at the Institute of Structural and Molecular Biology, Birkbeck College, London, on Thursday 13<sup>th</sup> December 2018.</p> <p>The two prize winners from the 2018 Postgraduate meeting will be invited to make presentations. Also, the 2018 BRSG – NMR DG prize winner for excellence in magnetic resonance will be invited 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 12<sup>th</sup> December 2018.</p>

### Committee

This information will be used to update our membership database and your web page. Please ensure that any changes to the committee are sent to [networks@rsc.org](mailto:networks@rsc.org) as soon as possible.

<b>Position</b>	<b>Name</b>	<b>Dates on committee (20xx – 20xx)</b>
Chair	Prof Simon Duckett	2018 - Present
Secretary	Dr Stephen J Byard	2005 - Present
Treasurer	Dr John A Parkinson	2008 - Present
Ordinary Members	Dr Mike Bernstein	2006 – Present
	Dr Melanie Britton	2012 – Present
	Dr Andrew Gibbs	2014 – Present
	Dr Flemming Hansen	2014 – Present
	Prof. Yaroslav Khimyak	2012 – Present
	Prof Gareth Morris	2014 – Present
	Dr Harry Parkes	1994 – Present
	Prof Sharon Ashbrook	2016 – Present
	Dr Matthew Wallace	2018 – Present
Chemists' Community Fund Representative (if relevant)		



Co-opted members and their affiliation		
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## **Diversity & Inclusion**

Our trustees are aiming to embed diversity and inclusion in all of our activities and networks. Our [online network handbook](#) contains more information to support our networks in achieving this.

Please comment on how your group is showing that it has embraced Diversity and Inclusion within its practices.

The NMR Discussion Group continues to hold events at locations that are geographically accessible to as many members as possible, and venues are selected that provide access to members who may have disabilities. Where possible, locations for annual meetings are varied throughout the United Kingdom to permit attendance by delegates who may wish to limit travel time or avoid use of overnight accommodation. Mechanisms are in place to assist with private communications to ensure that potential delegates can make any specific requirements known. Consideration to all dietary requirements of delegates are given, and specific assistance with requirements of differing faith groups has been provided at meetings.

Events are advertised using all media types, to avoid exclusion of potential delegates. Concessionary rates are offered to students and retirees, and registration rates are maintained at the lowest possible levels. Our events are designed to be inclusive and appealing to all age groups, from early-career researchers to retirees and, correspondingly, maintain social and professional interactions at all levels.

Interested sixth form school pupils are encouraged to attend events, and additional assistance or guidance provided on a dedicated basis where appropriate.

Interactions with NMR Spectroscopists in countries having limited access to instrumentation are both fostered and promoted, and advice provided accordingly to assist with teaching.