

10th Annual NMR Discussion Group Postgraduate Meeting

The Royal Society of Chemistry NMR Discussion Group celebrated its 10th Annual Postgraduate meeting on 22nd June 2017, at the Department of Pure and Applied Chemistry, University of Strathclyde, Glasgow. With a vibrant ambience and Glasgow's strong chemistry heritage, the university provided an ideal venue. As always, this event was extremely enjoyable and popular, providing an informal setting in which early career researchers were able to showcase their work, either by oral or poster presentations. Most of the academic UK NMR research-based groups were represented at the meeting, covering a wide range of related disciplines, including small molecule characterisation, molecular biology, solid-state characterisation, materials science and imaging. The poster sessions facilitated proactive interactions and exchange of ideas between all presenters, and also with established researchers. The programme incorporated eight oral presentations from early career researchers, again in a relaxed environment, covering a range of subjects:



Ruth Dingle, *Institute of Structural and Molecular Biology, University College London*

Conformational sampling of arginine side-chains

Ieva Goldberga, *Department of Chemistry, University of Cambridge*

Insight into collagen structure from ¹⁵N-labelled synthetic model peptides and mouse bone





Alex Gardner, *Department of Mucosal and Salivary Biology, King's College, London*

Developing and standardising a protocol for quantitative proton nuclear magnetic resonance (^1H NMR) spectroscopy of saliva



Michael A Hope, *Department of Chemistry, University of Cambridge*

Surface selective ^{17}O DNP NMR of CeO_2 nanoparticles



Giulia Bignami, *School of Chemistry, University of St Andrews*

Synthesis and solid-state NMR characterisation of ADORable zeolites

Olga Semenova, *Centre for Hyperpolarisation in Magnetic Resonance, Department of Chemistry, University of York*

Single-shot hyperpolarisation lifetime measurements for monitoring reactivity by benchtop NMR





Serena Monaco, *School of Pharmacy, University of East Anglia*

Inter ligand – STD approach as applied to the characterisation of a novel binding substitute for cholera toxin inhibition

Will Kew, *School of Chemistry, University of Edinburgh*

Scotch whisky as revealed by high-field NMR spectroscopy



In each case, the presentations represented cutting-edge research and were very well-received by meeting participants. The quality of the oral and poster presentations was such that judging was an impossible task and, in addition to winners, a series of runner-up prizes were awarded. The judging panel comprised **Prof Yaroslav Khimyak** (University of East Anglia), **Dr Stephen Byard** (Arcinova) and **Prof Sharon Ashbrook** (NMR DG Chairperson). Both prize winners will be invited to give presentations at the 2017 NMR DG Christmas meeting, which will be held at The Institute of Structural and Molecular Biology, University College London, on Thursday 14th December.

A prize was awarded to **Michael Hope** (University of Cambridge) for the best oral presentation, and this was presented by **Prof Sharon Ashbrook**, the Chairperson of the NMR DG (shown right). The prize was sponsored by the RSC Journal PCCP.

The runner up prize for the best oral presentation was awarded to **Giulia Bignami**, University of St Andrews.





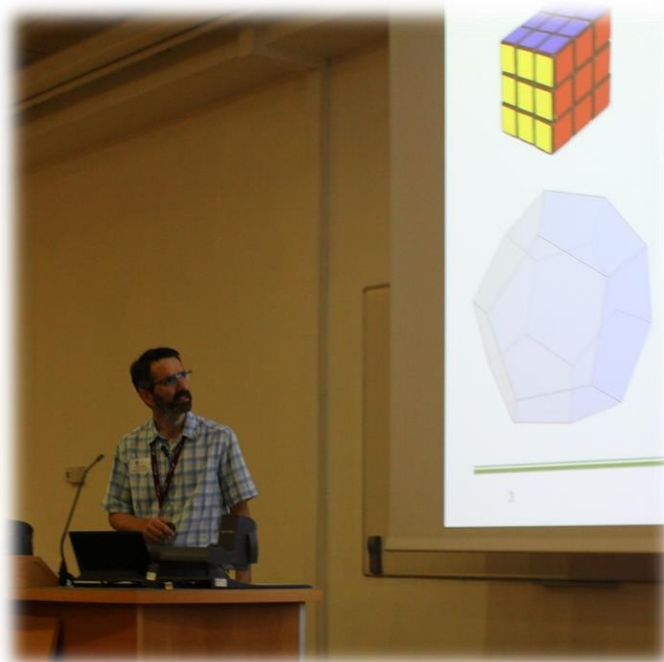
Vanessa Timmermann (School of Chemistry, University of Manchester) was awarded a prize for the best poster presentation, and this was presented by **Dr Nigel Crossley**, of Oxford Instruments, who sponsored the event. Vanessa's research involved evaluation of the solution structure of uranium(IV) DOTA-type complexes by ^1H NMR spectroscopy.



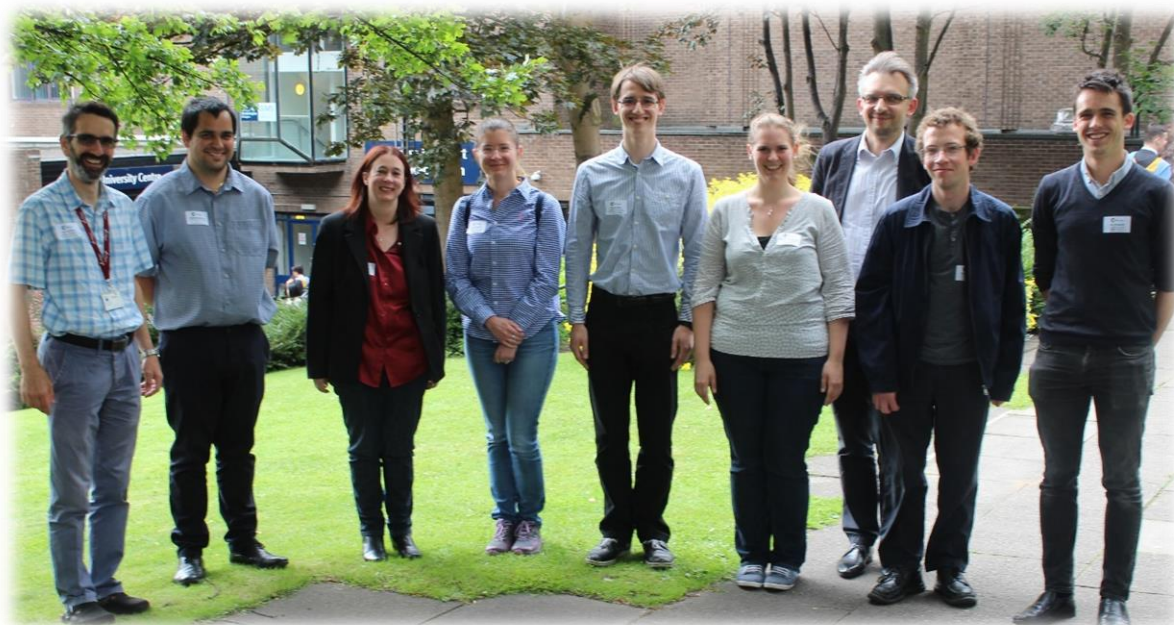
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Three runner-up prizes for best poster presentations were awarded to **Nick Brownbill** (University of Liverpool) for his work on ^{17}O DNP enhanced solid-state NMR spectroscopy at 18.8T, **James Montgomery** (University of St Andrews) for his work on Fractionation and DOSY NMR spectra of model polymers and lignin, and **Matthew Wallace** (University of Liverpool) for his work on rapid measurement of pKa values using NMR imaging techniques.

In recent meetings, 'overview presentations' given by established researchers have been introduced into the programme. On this occasion, **John Parkinson** (University of Strathclyde) opened the meeting with a presentation titled 'NMR Past, Present and Future: One Spin Doctor's Perspective'. John gave a high level account of his career, describing some of the fascinations and influences that had led to his research activities in a broad range of Nuclear Magnetic Resonance based applications. Whilst introducing some of his published data, John also gave an insight into potential technical developments which may be encountered by future spectroscopists.



Jeremy Titman (University of Nottingham) opened the afternoon session with an overview presentation titled ‘What has solid-state NMR ever done for us? Structure, dynamics and polarisation in materials’. Jeremy described some of the early developments that enabled NMR spectra to be acquired on solids, and gave an overview of current applications in different areas, such as pharmaceuticals, nano technology and surface science. He concluded the presentation by describing some work carried out using the recently installed state-of-the-art DNP MAS spectrometer at Nottingham University.



Some organisers, prize-winners and runners-up - From left to right: John Parkinson (University of Strathclyde), James Montgomery (University of St Andrews), Sharon Ashbrook (NMR DG Chairperson), Giulia Bignami (University of St Andrews), Michael Hope (University of Cambridge), Vanessa Timmermann (University of Manchester), Yaroslav Khimyak (University of East Anglia), Matthew Wallace (University of Liverpool) and Nick Brownbill (University of Liverpool).

In particular, the NMR DG would like to acknowledge **John Parkinson** (University of Strathclyde) and **Yaroslav Khimyak** (University of East Anglia) for their contributions towards the organisation of the meeting, and also Oxford Instruments for generous sponsorship and attendance at the meeting.

Steve Byard – NMR DG Secretary, July 2017