ANZMAG 2025 CONFERENCE

PROGRAM HANDBOOK

30 November - 4 December, 2025

Tangalooma Resort Moreton Island, QLD Australia

INDEX - ANZMAG 2025

Welcome to ANZMAG 2025

Tangalooma Island Resort, Queensland

On behalf of the Organising Committee, we are delighted to welcome you to the 13th Australian and New Zealand Society for Magnetic Resonance (ANZMAG) Conference, held at the beautiful Tangalooma Island Resort, just off the coast of Brisbane, Queensland.

This year's conference brings together our vibrant community of researchers, educators, and industry professionals to share ideas, explore new discoveries, and strengthen collaborations across the magnetic resonance field.
We extend a particularly warm welcome to our international participants, whose contributions enrich the discussions and help build lasting global connections.

Thanks to the generous support of our sponsors, invited speakers, and contributors, ANZMAG 2025 continues its proud tradition of fostering the next generation of researchers, providing opportunities for students and early-career scientists to present their work and engage with leading experts. The success of ANZMAG reflects the dedication, collaboration, and generosity of the Australian and New Zealand magnetic resonance community, and we're deeply grateful to all who make this event possible.

We hope you find ANZMAG 2025 both intellectually stimulating and personally rewarding, and that the week ahead inspires new ideas, collaborations, and friendships.

The ANZMAG 2025 Organising Committee

Regards,
Johan Rosengren, Gary Cowin, Jeffrey Harmer, Horst Schirra, Ann Kwan, Gareth Nealon, Vanessa Morris and Conan Wang.
Conference Commitee, ANZMAG 2025

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Conference Venue

Tangalooma Island Resort, Queensland

All scientific sessions, oral presentations, poster sessions and trade displays will be held in the Waterfront Pavillion. All lunches, morning and afternoon teas will also be held here.

Registration Desk

Registration will be open Sunday 30th November, 14:00 -17:00, in the Waterfront Pavillion.
If you arrive outside of these hours, please contact one of our committee members on your arrival.

Name Badges

Your name badge should be worn during all sessions and social events.

WiFi Access

WiFi access details will be made available at the time of registration.

Mobile Phones

To avoid interruptions during scientific sessions, we request that your phone be turned off or on silent.

Program at a Glance

Time	Sunday Nov 30	Monday Dec 1	Tuesday Dec 2	Wednesday Dec 3	Thursday 4 Dec
8:00					
8:30		EPR and DNP of Biological Systems	Free Morning to Swim Snorkle Explore	Protein Structure and Function II	MR Approaches for Materials and the Environment
9:00	Hotel/Ferry Check-in				
9:30					
10:00	Ferry to Tangalooma				
10:30		Morning Tea		Morning Tea	Morning Tea
11:00		Sir Paul Callaghan Medal		ANZMAG Medal	Closing Plenary Session
11:30	Hotel/Ferry Check-in	Screening and Drug Development		Biomolecular Methods & Applications	
12:00					
12:30	Ferry to Tangalooma				
13:00		Lunch	Lunch	Lunch	Lunch
13:30			Soceity AGM		
14:00	Free afternoon to Swim Snorkle Explore	Computational Approaches and PTMs		Metabolomics II	
14:30			Protein Structure and Function I		Ferry from Tangalooma
15:00					
15:30		Afternoon Tea	Afternoon Tea	Afternoon Tea	
16:00		Bruker	Jeol	Fabrum/Bluefors	
16:30		Diffusion and MRI	Metabolomics I	EPR and NMR Methods	
17:00	Opening Plenary Session				
17:30					
18:00		Dinner at own leisure	Dinner at own leisure		
18:30					
19:00	Welcome Function	Dolphin Feeding	Dolphin Feeding	Conference Dinner	
19:30					
20:00		Poster Session	Poster Session	Until late	
20:30					
21:00					

SOCIAL ACTIVITES

Welcome Drinks & Canapes

Tangalooma Island Resort, Conference centre

When: Sunday 30th November
Time: 19:00pm - 21:00pm
Where: Tangalooma Resort, Waterfront Pavillion

Please join us to share some relaxed drinks and canapes as we open the ANZMAG 2025 Conference on Tangalooma Island.

Feed the Dolphins

Tangalooma Island Resort, Wharf

When: Monday 1st December
Time: 19:00pm – 19:30pm
Where: Tangalooma Resort, Jetty

Weather permitting, dolphin feeding will happen on Monday night, otherwise we may need to postpone to the following evening. Meet at ECO Centre at 18:45pm.

Catered Poster Session & Toast to ANZMAG Members

Tangalooma Island Resort, Conference centre

When: Monday 1st December / Tuesday 2nd December
Time: 20:00pm – 21:00pm
Where: Tangalooma Resort, Waterfront Pavillion

Join us for cheese and antipasto plates and enjoy a glass of wine while viewing our posters.

Conference Dinner

Tangalooma Island Resort

When: Wednesday 3rd December
Time: 19:00pm – 23:00pm
Where: Tangalooma Resort, Wheelhouse Restaurant

Join us for a relaxed evening of fresh seafood, great drinks, and plenty of laughs.

Other Activities

Tangalooma Island Resort offers a wide range of land and waterbased activities

Contact reception for bookings and more details.
Visit: tangalooma.com/things-to-do/all-tours-activities

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Head Office:
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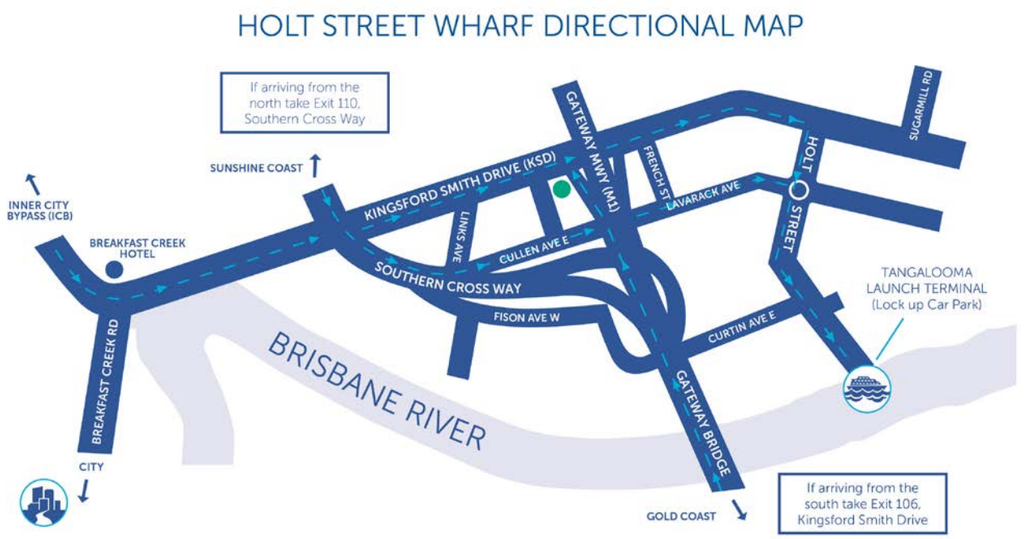
Sunday 30 November, 2025

9:00am	**Hotel/Ferry Check-in** (Holt Street)	10:00-11:15	**Ferry to Tangalooma**
11:30am	**Hotel/Ferry Check-in** (Holt Street)	12:30-13:45	**Ferry to Tangalooma**
Free Afternoon: Swim / Snorkle / Explore			
14:00-17:00	**Registration Open**		
17:00-18:50	**Opening Plenary Session** Chairs: H. Schirra & G. Cowin		
17:00-17:10	**Welcome Remarks**		
17:10-18:00	**Jeremy Nicholson (PL1)** Phenomic Medicine in Clinical Translation – Insights from NMR Spectroscopy and COVID-19		
18:00-18:50	**Leigh Johnson (PL2)** - More info to go here Human ultra-high field MRI: Enabling a research spectrum from fundamental to clinical		
19:00-21:00	**Welcome Function: *Sponsored by Bruker***		



Monday 1 December, 2025

8:30-10:30	**EPR and DNP of Biological Systems** Chairs: N. Cox & M. Sani
8:30-9:00	**Xun-Cheng Su (KL1)** Progress of protein spin labeling in distance measurements by pulsed EPR spectroscopy
9:00-9:30	**Thomas Huber (KL2)** Genetic Alchemy: Conjuring Magnetic Resonance Probes into Proteins
9:30-9:50	**Tatyana Smirnova (IL1)** Local Electrostatics and Hydration at Protein-Lipid interface: Implications for T-Cell Receptor Assembly
9:50-10:10	**Gottfried Otting** 19F-NMR of fluorinated amino acids in proteins
10:10-10:30	**Vishaal Bayya** Protein Structural Analysis using EPR
10:30-11:00	**Morning Tea**
11:00-11:30	**Sir Paul Callaghan Medal** Chair: Ann Kwan
11:30-13:00	**Screening and Drug Development** Chairs: M. Mobli & B. Mohanti
11:30-12:00	**Rihard Aleksis (KL3)** Fast and broadband fragment screening by 19F steady-state free precession NMR
12:00-12:20	**Martin Scanlon (IL2)** Dynamics Driven Drug Discovery
12:20-12:40	**Yun Shi** NMR Reveals Base-Exchange Inhibitors for NAD+ Glycohydrolases
12:40-13:00	**Brooke Kwai** Targeting RNA using fragment-based drug screening
13:00-14:00	**Lunch**

Monday 1 December, 2025 *(continued)*

14:00-15:30	**Computational Approaches and PTMs** Chairs: J. Rosengren & F. Wu
14:00-14:30	**Göran Widmalm (KL4)** Glycan structure by NMR
14:30-14:50	**Martin Stroet (IL3)** Parameterisation of Canonical and Non-Canonical Amino Acids for NMR Structure Determination
14:50-15:10	**Tye Gonzalez** 1H-NERRD: Probing Microsecond Timescale Protein and Bound Ligand Dynamics in Solid-State NMR
15:10-15:30	**Jameel Abduljalil** Deep learning-guided drug target selection: towards discovery of modulators of RNA-binding proteins
15:30-16:00	**Afternoon Tea**
16:00-16:30	**Bruker Workshop**
16:30-18:00	**Diffusion and MRI (Session sponsored by Acryo)** Chairs: P Galvosas & G. Cowin
16:30-17:00	**Bill Price (KL5)** Samples come in all shapes and sizes
17:00-17:15	**Nyoman Kurniavan (IL4)** Microimaging of biological tissues at 16.4 T MRI
17:15-17:30	**Gang Zheng** Application of change point detection in the analysis of tem-poral chemical exchange saturation transfer data
17:30-17:45	**Sarah Stevenson** Assembling a high field NMR platform towards ultra-high-intensity pulse field gradient diffusion NMR
17:45-18:00	**Humna Asad** Magnetic Resonance Pore Imaging with Extended Echo Times in 1D and 2D
18:00-19:00	**Dinner at your own leisure**
19:00-19:30	**Dolphin Feeding**
20:00-21:00	**Poster Session**/mixer with drinks and nibblies ***Sponsored by Novachem***

Tuesday 2 December, 2025

Free Morning: Swim / Snorkel / Explore	
13:00-14:00	**Lunch**
13:30-14:20	**Society AGM**
14:20-15:30	**Protein Structure and Function I** Chairs: A. Bonvin & V. Morris
15:30-14:50	**Fengjie Wu (KL6)** Activation mechanism of G protein-coupled receptor revealed by a novel NMR method
14:50-15:10	**Paul Gooley (IL5)** Conformational modulation of the multifunctional Phosphoprotein of the rabies virus
15:10-15:30	**Pierre de Cordovez** Understanding a novel oxidation-induced amyloid formation mechanism of the tumour suppressor protein p16INK4a
15:30-16:00	**Afternoon Tea**
16:00-16:30	**Jeol Workshop**
16:30-18:00	**Metabolomics I** Chairs: B. Jimenez & J. Nicholson
16:30-17:00	**Philipp Nitschke (KL7)** Biomarker Profiling in Human Serum using Benchtop NMR Spectroscopy
17:00-17:20	**Reika Masuda (IL6)** Structure Elucidation with STOCSY: Insights from Urine NMR Metabolomics in Early Childhood Development
17:20-17:40	**Horst Schirra** Getting to know your roommate – NMR metabolomics as a tool to characterise the role of metabolism in symbiotic relationships
17:40-18:00	**Flynn Watson** NMR as a powerful tool for high-throughput quantitation and metabolite elucidation: Examples from wine
18:00-19:00	**Dinner at your own leisure**
19:00-19:30	**Dolphin Feeding**
20:00-21:00	**Poster Session**/mixer with drinks and nibblies ***Sponsored by Novachem***

Wednesday 3 December, 2025

8:30-10:30	**Protein Structure and Function II** Chairs:. P Gooley and N.Daly
8:30-9:00	**Mehdi Mobli (KL8)** Application of NMR in Receptor–Ligand Interactions: From Venom Peptides to Macrocycles and Fragments
9:00-9:30	**Ann Kwan (KL9)** Targeting the 'untargetables': developing RNA-binding protein inhibitors that outsmart RNAs
9:30-9:50	**David Craik (IL7)** NMR structures of cyclotides: from Oxford sabbatical to a product in Bunnings
9:50-10:10	**Theo Crawford** Structural Basis of DkTx Bivalency
10:10-10:30	**Roland Gamsjaeger** A structural and Biophysical Analysis of the Action of the NSP9 Protein from SARS COV-2 - Implications for Future Drug Discovery Efforts
10:30-11:00	**Morning Tea**
11:00-11:30	**ANZMAG Medal** Chair: David Craik
11:30-13:00	**Biomolecular Methods & Applications** Chairs: G. Nealon & C. Wang
11:30-12:00	**Vanessa Morris (KL10)** Unravelling molecular interactions of the Alzheimer's disease protein TREM2
12:00-12:15	**Karyn Wilde (IL8)** Enabling research using NMR spectroscopy: ANSTO's National Deuteration Facility
12:15-12:30	**Ishanti Liyanage** Benchtop NMR: A Tool for Measuring Vapor Pressure
12:30-12:45	**Ritchy Leroy** TOPicity SECRET
12:45-13:00	**Howard Foster** Universally quantitative band-selective pure shift NMR
13:00-14:00	**Lunch**

Wednesday 3 December, 2025 *(continued)*

14:00-15:30	**Metabolomics II** Chairs: H. Schirra & P. Nitschke
14:00-14:30	**Beatriz Jimenez (KL11)** Tools to exploit the Biological Information residing in NMR spectra of Human Biofluids and their Clinical Applications
14:30-14:45	**Samantha Lodge (IL9)** Monitoring health using the blood lipoproteins in adults and children
14:40-15:00	**Luke Husdell** NMR spectroscopy as an analytical tool for Australian mono-floral honeys
15:00-15:15	**Sarah Walsh** Bacterial bodyguards: Characterising the virus-repressing effect of Wolbachia in Drosophila melanogaster using NMR-based metabolomics
15:15-15:30	**Jessica Broadway** Metabolic Analysis of Wound Response in Wolbachia infected Drosophila melanogaster
15:30-16:00	**Afternoon Tea**
16:00-16:30	**Fabrum/Bluefors Workshop**
16:30-18:00	**EPR and NMR methods** Chairs: G. T. Huber and G. Otting
16:30-17:00	**Martyna Judd (KL12)** Mixing and Matching: two tales of resonances structures for multipurpose EPR and NMR measurements of biological systems.
17:00-17:20	**Adrienne Rancz (IL10)** Relayed DNP NMR Reveals the Nanoscale Structure of Lipid Nanoparticles in mRNA Vaccines
17:20-17:40	**Nick Cox** MEASURING 10-30 ÅNGSTRÖM-SCALE DISTANCES IN PROTEINS USING 19F ENDOR
17:40-18:00	**Marc-Antoine Sani** Enhancing the water channelling effect of the antimicrobial peptide maculatin 1.1
19:00-23:00	**Conference Dinner: *Sponsored by Acryo***

Thursday 4 December, 2025

8:30-10:30	**MR approaches for materials and the environment** P Chairs:. A. Rawal and R. Mulder
8:30- 8:55	**Siegfried Stapf (KL13)** Phase separation of miscible fluids in mesoporous media monitored by NMR relaxometry and diffusometry
8:55-9:20	**Einar Fridjonsson (KL14)** pH controlled modification of metal oxide surfaces in porous media monitored by low field 1H NMR relaxometry
9:20-9:40	**Qin Li (IL11)** The Intricacy between Magnetic Fields and Fluidic Processing in Vortex Fluidic Devices (VFD)
9:40-10:00	**Peggy Schoenherr** Magnetic resonance device for landmine detection
10:00-10:15	**Emanuel Bertizzolo** Optimising Anaerobic Digestate Dewatering with Low-Field NMR Relaxometry: Insights into Solid-Liquid Separation Dynamics
10:15-10:30	**Yady Garcia Castillo** Effect of the polymer nature on the properties of composite solid electrolytes based on the organic ionic plastic crystal HMGFSI
10:30-11:00	**Morning Tea**
11:00-13:00	**Closing Plenary Session** Chairs: J. Harmer & J. Rosengren
11:00-11:50	**Alex Smirnov (PL3)** Ultra-High-Q / High-Finesse Frequency-Agile Photonic Band-Gap Resonators with mm-Wave EPR and DNP
11:50-12:40	**Alexandre Bonvin (PL4)** Solving 3D puzzles of biomolecular interactions by physics- and AI-based integrative modelling
12:40-12:50	**Closing Remarks**
13:00-14:00	**Lunch**
14:30	**Ferry departs from Tangalooma Jetty**

Conference Speakers

Plenary Speakers

PL 1. Jeremy Nicholson

Imperial College London, London, UK

Nicholson obtained his BSc in marine biology with honours from Liverpool University and his PhD in biochemistry from St Thomas' Hospital Medical School (King's College, London University). He has worked at Birkbeck College, London University and at the London School of Pharmacy, becoming full Professor in 1992. In 1998, he became Professor and Head of Biological Chemistry at Imperial College London. Nicholson was appointed Head of the Department of Surgery and Cancer at Imperial College London in 2009. In December 2012, Nicholson became the Director of the MRC-NIHR National Phenome Centre and launched the International Phenome Centre Network (IPCN) in 2016. Nicholson moved to Perth, Western Australia in 2018 to take up the role of Pro Vice Chancellor of Health Sciences at Murdoch University. Nicholson is the founder director, chief scientist and chief scientist officer at Metabometrix Limited, an Imperial College London spin-off company incorporated in April 2000 and specializing in molecular phenotyping, clinical diagnostics and toxicological screening via metabonomics and metabolomics. He is also a founder and scientific advisor of Melico Sciences Limited incorporated in 2017 and specializing in metabolic life coaching. Nicholson is known for having been an early pioneer in NMR-based metabolomics. His research interests include spectroscopic and chemometric approaches to the investigation of disturbed metabolic processes in complex organisms.

PL 2. Leigh Johnston

The University of Melbourne, Melbourne Australia

Leigh Johnston is the Director of the Melbourne Brain Centre Imaging Unit and Head of the Department of Biomedical Engineering at the University of Melbourne. She is the Director of the UoM node of the National Imaging Facility, and Chair of the Victorian Biomedical Imaging Capability. Leigh's research interests focus on the design of MRI and PET acquisition and analysis methods that enable improved brain imaging.

PL 3. Alex I. Smirnov

Department of Chemistry, North Carolina State University, Raleigh, North Carolina, USA

Dr. Alex I. Smirnov is the Governor Robert W. Scott Distinguished Professor of Chemistry, College of Sciences at North Carolina State University (NCSU), USA. He received Ph.D. in Chemical Physics in 1990 from the Moscow Physical Technical Institute & Institute of Chemical Physics of the Soviet Academy of Science, Moscow, Russia. Before joining NCSU in 2000 he was an Associate Director of the Illinois EPR Research Center – a National Institutes of Health (NIH) Research Resource at the University of Illinois at Urbana-Champaign, IL, USA. In 1998 Dr. Smirnov was awarded a Young Investigator Medal from the International Electron Paramagnetic Resonance (EPR) Society - a triennial award. He is also a recipient of the NCSU Alumni Association Outstanding Research Award in 2014. To this date Prof. Smirnov coauthored >180 peer reviewed papers. Prof. Smirnov's main research activities are devoted to interdisciplinary areas of nanotechnology, physical chemistry and biophysics of interfaces, lipid bilayers and membrane proteins, quantum sensing, magnetic resonance and development of high field EPR and DNP NMR instrumentation.

PL 4. Alexandre Bonvin

Utrecht University, Utrecht, Netherlands

Alexandre Bonvin is professor of Computational Structural Biology and scientific director of the Bijvoet Centre for Biomolecular Research at Utrecht University. Bonvin researches how biomolecules such as proteins, nucleic acids and lipids interact with each other. In his research, Bonvin tries to uncover the social life of proteins, or how they recognise each other in order to carry out their work. The form of the proteins plays an important role in this, and these can only be researched using advanced computer models. Bonvin's computer models provide an insight into the various processes that take place within the body, in minute detail. His research is the start of a chain process which enables the targeted development of new medications. As the coordinator of the European WeNMR project (worldwide e-Infrastructure for NMR and structural biology), Bonvin also ensures that the latest computer models and technologies are made available to fellow researchers around the world. In this way, his fundamental research makes an important contribution to applied science.

Conference Speakers

Keynote Speakers

KL 1. Xun-Cheng Su

Nankai University, Tianjin, China

The main interest in Su's group is development of lanthanide binding tags in site-specific labeling of proteins and nucleic acids for biological magnetic resonance. The lab has been focusing on the generation of stable C-S bonds between proteins, and spin labels for in-cell NMR and EPR analysis of proteins and nucleic acids. The group developed a unique thiol-specific reactive group, phenylsulfonyl pyridine moiety, and this method has been widely used in site-specific labeling of proteins with paramagnetic tags. Recently, this lab developed a method in determining 3D structures of transient protein complexes that are short-lived species in low abundance by combination of site-specific tagging proteins and paramagnetic NMR. In addition, the group is developing 19F-NMR methods in quantitative determination of biological small molecules under physiological conditions and monitoring the activity of biomolecules in live cells.

KL 2. Thomas Huber

Australian National University, Canberra, Australia

Thomas Huber received his Diploma of Chemistry from the Technical University Munich and completed his PhD at ETH-Zurich. He has since held positions in physical chemistry at ETH-Zurich (1997), in the Supercomputer Facility at ANU (1998-2000), in the Department of Mathematics at UQ (2001-2005) and in the School of Molecular Bioscience at UQ (2006-2010) before his appointment as an Associate Professor and Future Fellow (2010-2014) at the Research School of Chemistry. Thomas was appointed Professor in 2013.

His computational structural biology group develops innovative tools to determine the 3D structure of biological macromolecules form sparse experimental data of different length scale.

KL 3. Rihards Aleksis

Latvian Institute of Organic Synthesis, Riga, Latvia

Dr. Rihards Aleksis carried out his Bachelor's and Master's theses at the Latvian Institute of Organic Synthesis (LIOS), studying protein-ligand interactions, protein structure and dynamics using liquid-state NMR. He then pursued a PhD at Stockholm University under the guidance of Prof. Andrew J. Pell, developing solid-state NMR methods for quadrupolar nuclei and applying them to paramagnetic materials. He subsequently joined Prof. Lucio Frydman's group at the Weizmann Institute of Science as a postdoctoral researcher, where he developed sensitivity-enhanced methods for both liquid- and solid-state NMR as well as magnetic resonance imaging. He has recently returned to LIOS as a researcher, focusing on advancing NMR methodologies for applications in structural biology and materials science.

KL 4. Göran Widmalm

Stockholm University, Stockholm, Sweden

Göran Widmalm obtained his Ph.D. in Organic Chemistry at Stockholm University in 1988 under the supervision of Prof. P.-E. Jansson. His thesis work dealt with structural determination of polysaccharides using a large arsenal of chemical methods, NMR spectroscopy and the development of a computerized approach to structural determination of oligo- and polysaccharides (CASPER). He was a postdoctoral fellow at the Biophysics Laboratory, CBER/FDA in Bethesda (NIH campus), MD, USA where he carried out molecular dynamics simulations of biomolecules having Dr Richard W. Pastor as a mentor and performed NMR experiments under the guidance of Dr William M. Egan and Dr R. Andrew Byrd. He returned to Stockholm University as an assistant professor and became Docent in 1991. Between 1995 and 1998 he was an associate professor and since 1999 he holds a position as full professor of Bioorganic chemistry. His research interests span from structural investigation of complex glycans, complemented by bioinformatics, to ligand–receptor interaction studies by employing a range of NMR spectroscopy techniques and computational chemistry methods.

Conference Speakers

Keynote Speakers

KL 5. Bill Price

University of Western Sydney, Sydney, Australia

Professor William (Bill) S. Price completed his PhD and DSc (i.e., higher doctorate) at the University of Sydney. After postdoctoral study at the Institute of Atomic and Molecular Science in Taipei, Taiwan and the National Institute of Material and Chemical Research in Tsukuba, Japan he joined the Water Research Institute in Tsukuba, Japan in 1995. In 2000 he spent a year at the Royal Institute of Technology (KTH). In 2001 he returned to Japan as Professor of Chemistry at Tokyo Metropolitan University. At the end of 2003 he returned to Australia and Western Sydney University where he is currently chair of Medical Imaging Physics.

He is a Fellow of the Royal Society of Chemistry, the Royal Australian Chemical Institute (RACI), and the Australian Institute of Physics. He has published one book ('NMR Studies of Translational Motion', Cambridge University Press, 2009), 31 book chapters and almost 200 journal publications. He is Editor-in-Chief of the (UK) Royal Society of Chemistry's "New Developments in NMR" book series and Editor of Elsevier/Academic Press's "Annual Reports on NMR Spectroscopy" His research has resulted in numerous awards including the ANZMAG Medal, the RACI's Rennie Memorial Medal, and (twice) the RACI Ollé Prize for Chemical Literature (1999 & 2010). His research interests span biochemistry, chemistry and physics and include probing molecular dynamics in biological (e.g., tumours) and chemical systems using magnetic resonance measurements of translational diffusion and relaxation, and MRI technique and contrast agent development.

KL 6. Fengjie Wu

University of Basel, Basel, Switzerland

Fengjie Wu is an Ambizione fellow supported by Swiss National Science Foundation (SNSF) and junior group leader at Biozentrum, University of Basel, Switzerland. He received his Ph.D. in 2020 from the University of Melbourne under the supervision of Prof. Paul Gooley and A/Prof. Daniel Scott. He then moved to Basel and did his postdoc with Prof. Stephan Grzesiek, where he developed the "GPS-PCS" NMR method that solves the assignment problem for large proteins. He also develops new isotopic labeling methods for eukaryotic expression system. Over the last ten years, Fengjie has been focusing on applying NMR to understand the mechanism of biological systems, in particular the G protein-coupled receptors.

KL 7. Philipp Nitschke

Australian National Phenome Centre, Perth, Australia

Philipp Nitschke is a specialist in NMR method development and structural elucidation and serves as the NMR Coordinator at the Australian National Phenome Centre (ANPC). His work primarily focuses on using Nuclear Magnetic Resonance (NMR) spectroscopy for biomedical research, particularly in the areas of metabolomics, inflammation biomarkers, and diagnostic tool development. Dr. Nitschke is involved in identifying and validating novel NMR-based biomarkers for various medical conditions, including SARS-CoV-2 infection and cardiovascular disease risk. A significant aspect of his work involves translating sophisticated, high-field NMR diagnostic techniques to more accessible, affordable, benchtop NMR systems. This aims to enable broader access to advanced molecular diagnostics in routine healthcare settings.

KL 8. Mehdi Mobli

The University of Queensland, Brisbane, Australia

Prof. Mehdi Mobli (BSc ChemEng, Chalmers, 2000, Sweden) earned his PhD in physical organic chemistry from the University of Liverpool (UK) in 2004 through a collaborative project with GSK, where he focused on developing nuclear magnetic resonance (NMR) methods for automated characterisation of drug-like molecules. He pursued postdoctoral research at the University of Connecticut Medical School (USA), the University of Manchester (UK), and the University of Queensland, contributing to fast acquisition methods in multidimensional NMR spectroscopy and the structural characterisation of venom peptides. He also serves as a founding Executive Editor of Magnetic Resonance (Copernicus), sits on the advisory board of the Biological Magnetic Resonance Data Bank (BMRB) and the Protein Databank (PDB), and is a member of the Board of Directors of the Australia and New Zealand Society for Magnetic Resonance (ANZMAG).

Conference Speakers

Keynote Speakers

KL 9. Ann Kwan

University of Queensland

Ann Kwan is an Associate Professor at the University of Sydney and has a strong interest in protein biochemistry and biophysics. Her research focuses on tackling antimicrobial resistance and targeting challenging biomolecular interactions using multidisciplinary approaches, including NMR spectroscopy, structure-based drug discovery, in silico screening, and other innovative complementary biophysical methods. Her recent work explores building a multi-pronged discovery pipeline that integrates AI-guided triaging, fragment expansion, cyclic peptide evolution, and modified nucleic acid engineering to generate potent and selective inhibitors against antimicrobial targets that were previously considered 'undruggable'.

KL 1O. Vanessa Morris

University of Canterbury, Christchurch, New Zealand

Vanessa joined the School of Biological Sciences at the University of Canterbury in 2018, after a world tour working and studying in Australia, Germany and Canada. She is interested in proteins that self-associate and can form large aggregates. Her lab is focused on studying the structures, mechanisms, and interactions of such aggregating proteins, in particular proteins that form amyloid fibrils. Protein aggregation is often involved in disease, including Alzheimer's disease and motor neuron disease, but also has functions in important biological processes. In order to study these Vanessa employs a wide range of structural and biophysical techniques including NMR spectroscopy (both solid-state and solution state), fluorescence-based aggregation assays, electron microscopy.

KL 11. Beatriz Jimenez Garrido

The University of Adelaide, Adelaide, Australia

Beatriz have worked in a variety of fields with NMR being a constant theme. She started her career as inorganic chemist working on the characterisation of the metal centre of metaloproteins and soon after developed a strong interest structural biology and the characterisation of protein function. This led to work in NMR pulse sequence development, in order to be able to optimise the experiments and obtain more information. Given her interest in how NMR can be used to answer biologically relevant questions, she soon became interested in Metabonomics and have now been working in the field for a number of years, first at Imperial College where she was in charge of the NMR section of the Clinical Phenotyping Center, and now at the University of Adelaide.

KL 12. Martyna Judd

Northwestern University, Evanston, Illinois, USA

Martyna Judd is a Postdoctoral Researcher in Prof. Songi Han's laboratory in the Department of Chemistry at Northwestern University (USA). She received her PhD in 2025 from the Australian National University in Prof. Nick Cox's group, where she developed new methods for high-field EPR spectroscopy. These included new approaches to distance measurements in proteins at W-band (94 GHz) using 19F ENDOR , as well as hardware development for general-purpose Q-band (34 GHz) EPR resonators. She joined the Han Lab at Northwestern in June 2025, where she is now researching improving methods and probe design for measuring 19F using static and MAS NMR/DNP at high magnetic fields, with a focus on biological and pharmaceutical applications.

Conference Speakers

Keynote Speakers

KL 13. Siegfried Stapf

TU Ilmenau, Ilmenau, Germany

Siegfried completed his PhD at Universität Ulm in 1997, before undertaking post doctoral work at University of Nottingham and his habilitation at RWTH Aachen. In 2007 he was appointed full professor in technical physics / polymer physics at TU Ilmenau. His research interests are in molecular dynamics in soft matter: polymers, elastomers, mesophases. Fluids under confinement and mechanical stress. Quantification of order phenomena – self organization and nanoscopic domains. Establishing and applying NMR techniques over a broad time scale (field cycling) and integration with classical methods for a consistent description of soft matter dynamics. Linking NMR with Electron Spin Resonance (ESR) and Dynamic Nuclear Polarization (DNP). Development of advanced NMR imaging methods for the visualization of complex flow phenomena. Quantification and analysis of flow: relation between matrix structure and transport, rheology with transfer towards rock/soil and environmental issues.

KL 14. Einar Fridjonsson

University of Western Australia, Perth, Australia

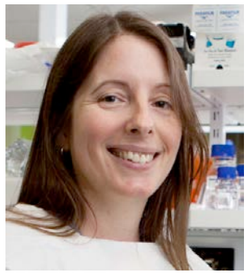
Dr. Einar Fridjonsson is an Associate Professor and Program Chair at the Department of Chemical Engineering at the University of Western Australia. He specialises in the application of Nuclear Magnetic Resonance for engineering applications. Areas of interest include flow metering, separation processes for water management, technical aspects of the future hydrogen economy and materials for mining operations, in particular cemented paste backfill and tailings management. Dr Fridjonsson conducted his PhD research under the supervision of Prof. Joe Seymour and Prof. Sarah Codd at the Magnetic Resonance Laboratory at MSU-Bozeman, and subsequently was a Research Associate at the MRRC at the University of Cambridge, before his current appointment at the University of Western Australia.

Winner of ANZMAG Medal

Congratulations

Norelle Daly

James Cook University, Cairns, Australia



Norelle Daly is a Professor at the Centre for Biodiscovery and Molecular Development of Therapeutics at James Cook University. She completed her PhD at The University of Queensland on 'Structural Studies of the Ligand-Binding Repeats of the LDL receptor'. Following these studies she was involved in establishing a new field of research involving plant derived cyclic peptides. This work resulted in several granted patents and the establishment of a small biotechnology company associated with The University of Queensland.
She was a recipient of a Research Excellence Award from The University of Queensland and has previously held an NHMRC Industry Fellowship and a Queensland Smart State Fellowship. In March 2012 she took up her ARC Future Fellowship at the Queensland Tropical Health Alliance. Her research interests include exploring the potential of natural products as novel drug leads for the treatment of cancer and inflammatory diseases. (See page 101)

Winner of Sir Paul Callaghan Medal

Congratulations

Ivanhoe Leung

University of Melbourne, Melbourne, Australia

Dr. Leung is a Senior Lecturer in Biological Chemistry at the University of Melbourne. Dr. Leung attained his undergraduate and doctorate degrees at the University of Oxford, and began his independent research career at the University of Auckland in 2013. In 2018, he was appointed co-Deputy Director of the Centre for Green Chemistry Science at the University of Auckland. In 2021, Dr. Leung joined the University of Melbourne, where he is now part of the School of Chemistry and Bio21 Molecular Science & Biotechnology Institute. Dr. Leung's research focuses on the study of enzyme structure, function, and modulation with an aim to help solve some of the world's most urgent challenges in health and sustainability. One of his main research interests is the study of multi-copper oxidase including polyphenol oxidase (PPO) and laccase.
(See page 101)

Congratulations

ANZMAG would like to congratulate the following students and early career researchers that have been awarded travel bursaries to attend the conference, and thank the sponsors making these possible.

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Jameel Abduljalil	University of Sydney, AUS	Acryo
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Viator Munjuni	Victoria University of Wellington, NZ	NDF at ANSTO
Sydney Austad	University of Canterbury, NZ	AXT/OXFORD

Delegates List

NAME	INSTITUTION	EMAIL
Jameel Abduljalil	University of Sydney	jabd0952@uni.sydney.edu.au
Peter Airey	AXT	peter.airey@axt.com.au
Rihard Aleksis	Latvian Institute of Organic Synthesis	aleksis@osi.lv
Liz Ankers	Deakin University	elizabeth.ankers@deakin.edu.au
Humna Asad	Victoria University of Wellington	humna.asad@vuw.ac.nz
Sydney Austad	University of Canterbury	sydney.austad@pg.canterbury.ac.nz
Sri Balaji Ponraj	Bruker Pty Ltd	sri_balaji.ponraj@bruker.com
Nigel Bartlett	Fabrum	Nigel@fabrum.nz
Vishal Bayya	University of Queensland	uqvbayya@uq.edu.au
Emanuel Bertizzolo	University of Western Australia	emanuel.gomesbertizzolo@research.uwa.edu.au
Adrian Blaser	University of Auckland	a.blaser@auckland.ac.nz
Alexandre Bonvin	Utrecht University	a.m.j.j.bonvin@uu.nl
Jessica Broadway	Griffith University	jessica.broadway@griffithuni.edu.au
Swetha Chazhikulam	University of Queensland	s4856683@student.uq.edu.au
Richard Clark	University of Queensland	richard.clark@uq.edu.au
Gary Cowin	University of Queensland	g.cowin@uq.edu.au
Nick Cox	Australian National University	nick.cox@anu.edu.au
David Craik	University of Queensland	d.craik@uq.edu.au
Theo Crawford	University of Queensland	t.crawford@uq.edu.au
Matthew Crowther	CSIRO	matthew.crowther@csiro.au
Norelle Daly	James Cook University	norelle.daly@jcu.edu.au
Anthony Day	University of NSW	a.day@unsw.edu.au
Pierre de Cordovez	University of Canterbury	pierre.decordovez@canterbury.ac.nz
Robert de Gille	CSIRO	robert.degille@csiro.au
Howard Foster	howard.foster@qut.edu.au	Queensland University of Technology
Einar Fridjonsson	einar.fridjonsson@uwa.edu.au	University of Western Australia
Petrik Galvosas	petrik.galvosas@vuw.ac.nz	Victoria University of Wellington
Roland Gamsjaeger	r.gamsjaeger@westernsydney.edu.au	Western Sydney University
Yady Garcia Castillo	y.garciacastillo@uq.edu.au	University of Queensland
Tye Gonzalez	tye.gonzalez@tu-dortmund.de	Technical University Dortmund

NAME	INSTITUTION	EMAIL
Paul Gooley	prg@unimelb.edu.au	University of Melbourne
Dean Greenslade	n10185925@qut.edu.au	Queensland University of Technology
Paul Hammond	p.hammond@student.uq.edu.au	University of Queensland
Hideyuki Hara	hideyuki.hara@bruker.com	Bruker Japan K.K.
Jeffrey Harmer	jeffrey.harmer@cai.uq.edu.au	University of Queensland
Rebecca Hawker	r.hawker@uq.edu.au	University of Queensland
Kyle Hearn	kyle.hearn@rmit.edu.au	RMIT
Andrew Heath	andrewh@novachem.com.au	Novachem
Naina Holkar	Naina.Holkar@bruker.com	Bruker Scientific India Pvt Ltd
Thomas Huber	t.huber@anu.edu.au	Australian National University
Luke Husdell	l.husdell@uq.edu.au	University of Queensland
Laurence Jennings	laurence.jennings@outlook.com	University of Queensland
Beatriz Jimenez	beatriz.jimenez@adelaide.edu.au	University of Adelaide
Leigh Johnston	l.johnston@unimelb.edu.au	University of Melbourne
Paul Jonsen	paul.jonsen@talaverascience.com	Talavera Science
Martyna Judd	martyna.judd@northwestern.edu	Northwestern University
William Keane	bkeane@jeol.com.au	JEOL
Faisal Khan	f.khan@jeol.com.au	JEOL
Nyoman Kurniawan	University of Queensland	n.kurniawan@uq.edu.au
Brooke Kwai	Monash University	brooke.kwai@monash.edu
Ann Kwan	University of Sydney	ann.kwan@sydney.edu.au
Ritchy Leroy	University of Reims	leroy.ritchy@gmail.com
Ivanhoe Leung	University of Melbourne	ivanhoe.leung@unimelb.edu.au
Qin Li	Griffith University	qin.li@griffith.edu.au
Feng Liu	University of Queensland	feng@eecs.uq.edu.au
Wendy Loa	Griffith University	w.loa@griffith.edu.au
Samantha Lodge	Murdoch University	sam.lodge@murdoch.edu.au
Vitaly Lozbin	JEOL	vlozbin@jeol.com.au
Thai Ly	CSIRO	thai.ly@csiro.au
Bertram Manz	Magritek Ltd	bertram@magritek.com

Delegates List

NAME	INSTITUTION	EMAIL
Reika Masuda	Murdoch University	reika.masuda@murdoch.edu.au
Thomas Miljenović	The University of Queensland	Tomas@miljenovic.com
Mehdi Mobli	University of Queensland	m.mobli@uq.edu.au
Biswaranjan Mohanty	University of Sydney	biswaranjan.mohanty@sydney.edu.au
Vanessa Morris	University of Canterbury	vanessa.morris@canterbury.ac.nz
Viator Mujuni	Victoria University of Wellington	viator.mujuni@vuw.ac.nz
Roger Mulder	CSIRO	roger.mulder@csiro.au
Asish Nanda	Acryo	ananda@acryo.com.au
Swapnil Nanda	Acryo	sales@acryo.com.au
Jennifer Naughton	University of Queensland	uqjnaug1@uq.edu.au
Gareth Nealon	University of Western Australia	gareth.nealon@uwa.edu.au
Jeremy Nicholson	Imperial College	j.nicholson@imperial.ac.uk
Philipp Nitschke	Murdoch University	philipp.nitschke@murdoch.edu.au
Philip Norcott	Flinders University	philip.norcott@flinders.edu.au
Gottfried Otting	Australian National University	gottfried.otting@anu.edu.au
Nigel Ottman	Bluefors	Nigel.ottman@bluefors.com
Barbara Perrone	Bruker Switzerland AG	barbara.perrone@bruker.com
Gregory Pierens	University of Queensland	g.pierens@uq.edu.au
William Price	University of Western Sydney	w.price@westernsydney.edu.au
Sunnia Rajput	University of Melbourne	rajput.s@unimelb.edu.au
Isanthi Ranathunga Liyanage	University of Canterbury	ira50@uclive.ac.nz
Adrienn Rancz	CRMN Lyon	adrienn.rancz@ens-lyon.fr
Nageshwar Rao Yepuri	ANSTO	raoy@ansto.gov.au
Aditya Rawal	University of New South Wales	a.rawal@unsw.edu.au
Andreas Rimensberger	Bruker Switzerland AG	andreas.rimensberger@bruker.com
Lewis Robertson	CSIRO	lewis.robertson@csiro.au
Johan Rosengren	University of Queensland	j.rosengren@uq.edu.au
Marc Antoine Sani	University of Melbourne	msani@unimelb.edu.au
Hiroaki Sasakawa	JEOL	hsasakaw@jeol.co.jp

NAME	INSTITUTION	EMAIL
Hiroaki Sasakawa	JEOL	hsasakaw@jeol.co.jp
Martin Scanlon	Monash University	martin.scanlon@monash.edu
Horst Schirra	Griffith University	h.schirra@griffith.edu.au
Anneka Schmidt	University of Queensland	anneka.schmidt@uq.edu.au
Peggy Schoenherr	CSIRO	peggy.schoenherr@csiro.au
Martin Shaddock	Bruker Pty Ltd	martin.shaddock@bruker.com
Yun Shi	Griffith University	y.shi@griffith.edu.au
Alex Smirnov	North Carolina State University	aismirno@ncsu.edu
Tatyana Smirnova	North Carolina State University	tismirno@ncsu.edu
Siegfried Stapf	TU Ilmenau	siegfried.stapf@tu-ilmenau.de
Siegfried Stapf	TU Ilmenau	siegfried.stapf@tu-ilmenau.de
Sarah J. Stevenson	Victoria University of Wellington	sarah.stevenson@vuw.ac.nz
Martin Stroet	University of Queensland	m.stroet@uq.edu.au
Xun-Cheng Su	Nankai University	xunchengsu@nankai.edu.cn
Devika Suresh	University of Queensland	s4859716@student.uq.edu.au
Yasvir Tesiram	Bruker Pty Ltd	yas.tesiram@bruker.com
Mahesh Upadhyay	James Cook University	mahesh.upadhyay@my.jcu.edu.au
Sarah Walsh	Griffith University	sarah.walsh3@griffithuni.edu.au
Conan Wang	University of Queensland	c.wang@imb.uq.edu.au
Flynn Watson	Australian Wine Research Institute	flynn.watson@awri.com.au
Ewald Weber	University of Queensland	ewald@uq.edu.au
Renee Webster	CSIRO	Renee.Webster@csiro.au
Göran Widmalm	Stockholm University	goran.widmalm@su.se
Karyn Wilde	ANSTO	raoy@ansto.gov.au
Fengjie Wu	University of Basel	fengjie.wu@unibas.ch
Jan Phillip Wurm	Bruker BioSpin GmbH & Co. KG	philip.wurm@bruker.com
Philip Wurm	Bruker BioSpin GmbH & Co. KG	philip.wurm@bruker.com
Gang Zheng	University of Western Sydney	g.zheng@uws.edu.au

ANZMAG 2025 CONFERENCE

ABSTRACTS

PL 1. Phenomic Medicine in Clinical Translation – Insights from NMR Spectroscopy and COVID-19

Jeremy K. Nicholson

Faculty of Medicine, Imperial College London, London, UK.

Systems biology and advanced spectroscopic tools can be applied at both individual and population levels to understand integrated biochemical function in relation to disease pathogenesis. Metabolic phenotyping offers an important window on systemic activity and both advanced spectroscopic approaches can be used to characterize disease processes and responses to therapy. Humanity faces many challenges in the modern world, including those posed by zoonotic diseases, the most recent notable example being COVID-19 caused by the SARS CoV-2 virus. The study of COVID-19 provided some remarkable new insights into other major diseases and disease risk biochemistry related to longer term cardiovascular and neurological effects, diabetes and ageing. NMR spectroscopy provided some crucial insights into these processes, which are now realising a translational value and new diagnostic strategies beyond COVID itself for studying cardiovascular risks and general viral infectivity. These discoveries involved the identification and structural characterisation of novel biomarkers, the development of new NMR pulse sequences to maximise signal recovery and the transfer of diagnostic and prognostic models from high field instruments to benchtop NMR spectrometers that can be readily deployed into clinical and low technology environments.

PL 2. Human ultra-high field MRI: Enabling a research spectrum from fundamental to clinical.

Leigh Johnston

Department of Biomedical Engineering & Melbourne Brain Centre Imaging Unit, University of Melbourne, Melbourne, Australia

Ultra-high field MRI has been in Australia for over 10 years, and in that time has become a mainstay of brain imaging. This talk will cover the opportunities afforded by 7 Tesla imaging, from exquisite high resolution structural imaging, BOLD fMRI, CEST, Sodium, Magnetic Resonance Spectroscopy and Spectroscopic imaging, to the design of parallel transmit solutions for field inhomogeneity issues at ultra-high field, all for improved cognitive neuroscience, mental health and neurological research outcomes.

PL 3. Ultra-High-Q / High-Finesse Frequency-Agile Photonic Band-Gap Resonators with mm-Wave EPR and DNP

Alex Smirnov

North Carolina State University, Raleigh, North Carolina, USA

Resonators and resonance circuits are essential components of all the EPR and NMR spectrometers that are based on induction detection. The resonators, characterized by Q-factors, provide major boost in sensitivity. Unfortunately, frequency-dependent losses in metals at ambient temperatures limit attainable Q-factors. This is one of the reasons why Q-factors of commercial EPR resonators, even at X-band (9.5 GHz), rarely exceed Q≈10,000 and fall to just ca. 1,000-2,000 at 34 and 95 GHz and even lower at higher frequencies.

One way to increase Q-factors and boost EPR sensitivity is to employ superconducting materials, but then the sample must be also maintained at cryogenic temperatures. Here we demonstrate further advances in the radically new mm-wave resonators that are based on one-dimensional photonic crystals (1). Such resonators are composed of low-loss discs of λ/4 in thickness with alternating dielectric constants and feature high Q-factors >1,000 and finesse up to half of the Q-factor (2).

Here we introduce a new PBGR design with fully adjustable coupling - from under-coupled to critically matched and then to fully over-coupled conditions – achieved by varying an additional gap in the photonic crystal. A 34 GHz PBGR was constructed from 2" sapphire discs and yielded the record unloaded Q=27,300±2,300 at critical coupling (β=1.06±0.18) at room temperature. This is a factor of 20 higher than Q-factors of commercial Q-band resonators. The resonator was integrated and tested with a commercial Bruker E580 Q-band EPR spectrometer. Even though the orientation of spin polarizing magnetic field was suboptimal with respect to the excited microwave mode, a factor of 8 improvement in concentration sensitivity of the echo-detected nitroxide signal was demonstrated when compared to a Bruker resonator. An initial demonstration of dual-mode resonator with mode frequency separation that can be chosen to fit the needs of double electron-electron resonance (DEER) experiments will also be presented.

The PBGR design provides for large volume samples and is readily adapted to higher frequencies such as 95, 200 GHz, and above, and is uniquely suited for increasing electronic B1e field – an essential prerequisite for pulse DNP. Specifically, we demonstrate generating B1e amplitudes up to 75-140 MHz at 197 GHz with the help of PBGRs and a pulsed amplifier with Psat approaching 140 W. Such B1e field are more than sufficient to match the 13C nuclear Larmor frequency at 7 T (3). Simultaneous coherent manipulation of the electronic and nuclear spins was demonstrated by 13C-detected electron Rabi nutations in synthetic diamond.

Supported by NIH R01GM153951 to AIS and AAN.

References:
1 S Milikisiyants, AA Nevzorov, AI Smirnov, J. Magn. Reson. 296 152 (2018).
2 AA Nevzorov, A Marek, S Milikisiyants, AI Smirnov, J. Magn. Reson, 323, 106893 (2021).
3 AA Nevzorov, S Milikisiyants, A Marek, I Kaminker, AI Smirnov, J. Phys. Chem. Lett. 16, 5321 (2025).

PL 4. Solving 3D puzzles of biomolecular interactions by physics- and AI-based integrative modelling

Alexandre M.J.J. Bonvin

Utrecht University, Utrecht, Netherlands

Understanding the structure, interactions, and dynamics of biomolecular macromolecules is key to unraveling cellular processes and advancing drug discovery. Accurate modelling of these complexes benefits greatly from incorporating diverse sources of experimental or predictive information. To this end, we have developed HADDOCK (https://www.bonvinlab.org/software), a versatile integrative modelling platform available as a web service (https://wenmr.science.uu.nl). HADDOCK, which was born out of an NMR problem, can seamlessly combine data from biochemical, biophysical, and bioinformatics approaches to improve both sampling and scoring of biomolecular assemblies.

Over more than two decades of continuous development, we have witnessed the transformative rise of AI in structure prediction. While AI has made remarkable progress, physics-based modelling remains essential, often in combination with experimental, with many challenges still requiring their complementary strengths. In my talk, I will first discuss the raise of AI on the basis of the blind prediction experiments CASP/CAPRI, highlighting the still open challenges. I will then present recent advances in HADDOCK and showcase its applications, including examples where AI-generated predictions are combined with physics-based integrative modelling. In particular, I will highlight studies on antibody complexes, demonstrating the synergy between AI and physics-based approaches.

KL 1. Progress of protein spin labeling in distance measurements by pulsed EPR spectroscopy

Xun-Cheng Su

Nankai University, Tianjin, China

Pulsed electron paramagnetic resonance (EPR) plays a significant role in the study of the structures, interactions and dynamics of biological molecules, and it provides complementary information of biomolecules to the high-resolution nuclear magnetic resonance (NMR). Pulsed EPR provides valuable distance restraints of two spin labels site-specifically anchored in a protein or protein complex.

The distance distributions provide insights into the dynamics and structural changes of the spin-labeled proteins, which is generally achieved via site-specific labeling approach. Despite great efforts towards distance measurements by pulsed EPR have been made, the correlations between protein dynamics and distance distributions remain elusive.

In this report, we undertook the detailed analysis between the spin labeling approaches, rigidity of the spin labels and the measured distance distributions in different proteins covering single domain and multidomain proteins. We found the rigidity of spin labels plays an important role in the measured distance distributions, which are not simply correlated to degree of protein dynamics.

KL 2. Genetic Alchemy: Conjuring Magnetic Resonance Probes into Proteins

Thomas Huber

Australian National University, Canberra, Australia

Genetic code expansion is a well-established method for precisely modifying proteins with novel chemical functionalities. It enables the creation of custom proteins in living cells by selectively replacing a natural amino acid with a non-standard one. This non-canonical amino acid then may be used as sensitive probe to observe the protein's structure, dynamics and function, or act as reactive handle for further functionalization.

Here, I will present our developments to genetically encode non-canonical amino acids to install magnetic resonance probes in proteins. I will: (i) highlight the extraordinary flexibility and specificity of this technique; (ii) demonstrate the facile production of proteins with minimal modifications in high purity and yield; and (iii) showcase some of our genetically encoded reactive amino acids and their applications in magnetic resonance spectroscopies.

KL 3. Fast and broadband fragment screening by ^{19}F steady-state free precession NMR

Rihard Aleksis[1], Laura Ruduša[1], Raitisv Bobrovs[1], Kostiantyn Melnykov[2], Yaroslav Filatov[2], Serhiy Ryabukhin[2], Dmytro Volochnyuk[2], Kristaps Jaudzems[1]

[1]Latvian Institute for Organic Synthesis, Riga, Latvia

[2] Enamine Ltd

Fragment-based drug discovery (FBDD) has become a cornerstone for identifying lead compounds in modern drug development. Nuclear magnetic resonance (NMR) is central to FBDD, offering an arsenal of techniques for ligand–protein interaction studies. However, the full potential of NMR is hindered by its inherently low sensitivity and limited screening throughput. Steady-state free precession (SSFP) has recently re-emerged as a powerful tool across multiple areas of magnetic resonance due to its enhanced sensitivity [Phys. Rev. 112, 1693 (1958)]. In SSFP, a train of pulses separated by short repetition times drives the formation of a steady-state magnetization that can be detected rapidly and continuously. This enables superior signal-to-noise ratios per square-root unit time compared to conventional NMR experiments, which require long recovery delays between scans.

Here, we explore the application of ^{19}F SSFP to fragment-based screening. First, we employed SSFP to screen a fluorinated compound library (240 fragments) against *E. coli* Seryl-tRNA synthetase, a validated antibacterial drug target. Our results reveal that SSFP provides broadband excitation (>120 kHz) and yields a 3.3-fold higher sensitivity than state-of-the-art Carr-Purcell-Meiboom-Gill (CPMG) method[Angew. Chem. 59, 14809 (2020)] typically used for ^{19}F NMR screening. Therefore, the NMR experimental time was reduced by an order of magnitude, enabling the screening of ca. 1400 ligands per day for identification of site-specific binders. Notably, SSFP screening throughput is 30% faster than cutting-edge hyperpolarization approaches such as photo-chemically induced dynamic nuclear polarization [J. Am. Chem. Soc. 145, 12066 (2023)].
Finally, we demonstrate the utility of SSFP in challenging systems by screening against the intrinsically disordered Tau protein, implicated in Alzheimer's disease. SSFP identified three times more binders than CPMG, underscoring its robustness and sensitivity for difficult drug targets.

Therefore, SSFP opens new opportunities for rapid, robust and cost-effective screening even for challenging drug targets, and we anticipate it will become the standard experiment for ligand-detected screening.

KL 4. Glycan structure by NMR

Göran Widmalm

Stockholm University, Stockholm, Sweden

Carbohydrate molecules, known as glycans in a biological context, often have highly complex structures and contain branches, which is unique to this class of biomolecules. They are essential components of living organisms and are, among other things, involved in the storage and transport of energy, cell-cell interactions and regulation of gene expression. Altered glycan patterns can affect inflammatory responses, facilitate cancer cell metastasis or promote viral immune escape.

NMR spectroscopy studies of glycans commonly utilize the spin-½ nuclei, ^{1}H and ^{13}C, and when present ^{15}N and ^{31}P, but other nuclei such as ^{19}F and ^{77}Se have also been employed in investigations of carbohydrates and their interactions with proteins. The limited spectral dispersion of oligo- and polysaccharides where most ^{1}H chemical shifts are found in the spectral region ~3 – 4 ppm and most ^{13}C chemical shifts are found in the spectral region ~60 – 80 ppm make resonance assignments a challenging process (1,2).

Concatenation of NMR modules into a single 2D NMR experiment improves efficiency and results in time saving due to the fact that two or more experiments share a common recovery delay prior to each subsequent scan of the 2D NMR experiment. This concept has been extended to parallel NOAH (NMR by Ordered Acquisition using ^{1}H-detection) supersequences utilizing sequential, parallel and time-shared acquisitions by which ten spectra can acquired in a single measurement, referred to as a p-NOAH 10 (3). A p-NOAH 5 measurement was also tailored to produce NMR data for the computer program CASPER (4,5).

Resonance overlap in NMR spectra of oligosaccharides can be greatly reduced, and resolution improved, by utilizing pure shift methods. Even though many correlations are resolved in ^{1}H,^{13}C-HSQC NMR spectra some may still remain, among other things, due to ^{1}H,^{1}H couplings, though these may be refocused and the resulting pure shift ^{1}H,^{13}C-HSQC NMR spectra are thus devoid of the homonuclear proton-proton couplings. However, peak-picking of cross-peaks in 2D NMR spectra is often time-consuming, limiting the potential of CASPER as an efficient analysis tool. Since pure shift methods aim to collapse multiplets into well-resolved singlets, pure shift data are ideal for use in conjunction with CASPER, allowing for efficient analysis by using automated peak-picking routines (6). Further refinement of ^{1}H NMR chemical shifts and $^{n}J_{HH}$ may be carried out by spin-simulation resulting in data useful for conformational analysis of the glycans.

References:

1. C. Fontana, G. Widmalm, Chem. Rev. 2023, 123, 1040-1102.
2. G. Widmalm, JACS Au 2024, 4, 20-39.
3. Ē. Kupče, J.R.J. Yong, G. Widmalm, T.D.W. Claridge, JACS Au 2021, 1, 1892-1897.
4. M. Lundborg, G. Widmalm, Anal. Chem. 2011, 83, 1514-1517.
5. K. M. Dorst, G. Widmalm, Methods Mol. Biol. 2025, 2961, 23-38.
6. M. J. Smith, E. L. Gates, G. Widmalm, R. W. Adams, G. A. Morris, M. Nilsson, Org. Biomol. Chem. 2023, 21, 3984-3990.

KL 5. Samples come in all shapes and sizes

William S Price, Afsaneh Lahooti, Yves De Deene, Timothy Stait-Gardner

Nanoscale Group, Western Sydney University, Sydney, Australia

Non-linear static (B_0) and oscillating (B_1) magnetic fields and non-constant magnetic gradients (g) are the bane of magnetic resonance. The engineering of the hardware can never be perfect (e.g., B0 should have spatial homogeneity and time stability exceeding 10-8 T) and the problems are exacerbated when the sample shape results in large background gradients due to the inclusion of magnetic susceptibility interfaces in the detected volume. In MRI and Diffusion NMR this results in distorted images with unexpected intensities and with erroneous estimates of diffusion coefficients.

This lecture starts from a personal historical perspective and considers some steps that can be taken to ameliorate these effects including specialised sample holders and preparation including the imaging of flat samples. These techniques are of increasing importance when one wants to precisely correlate the MR dataset with pathology of deformable (e.g., human biopsy) samples.

KL 6. Activation mechanism of G protein-coupled receptor revealed by a novel NMR method

Fengjie Wu

Biozentrum, University of Basel, Basel, Switzerland

The regulation of G protein-coupled receptor (GPCR) signaling by different orthosteric ligands is thought to occur via shifts of dynamically interconverting, conformational distributions. Such changes in dynamical distributions have been detected so far only by very sparse, often non-native experimental probes at low-resolution.

Recently we in silico predicted and in practice created a global positioning system (GPS) that relies on pseudocontact shifts (PCSs) induced by paramagnetic thulium tag attached at various sites to an antibody in order to precisely position magnetic nuclei at distances >60 Å within a protein of interest (1). Using this new NMR technology, we could follow 81 ^{1}H-^{15}N NMR correlations in the beta1-adrenergic receptor (b1AR) at ambient conditions in response to various orthosteric ligands in absence or presence of a G protein-mimicking nanobody. The comparison reveals the dynamics and mechanism of the central, highly conserved xWIPF3 motif, contiguous regions of rigid and loose conformational coupling separated by conserved prolines during signal transmission, as well as the plasticity of the intracellular face in response to transducer binding (2).

References:

1. Wu, F.-J. et al. J. Am. Chem. Soc. (2022) DOI:10.1021/jacs.2c09692.
2. Wu, F.-J. et al. Science (2025) DOI: 10.1126/science.adq9106.

KL 7. Biomarker Profiling in Human Serum using Benchtop NMR Spectroscopy

Philipp Nitschke

Murdoch University / Australian National Phenome Centre, Perth, Australia

NMR Spectroscopy is a major technology for metabolic analyses of biofluids, especially for lipoprotein quantification in e.g. human plasma. Although, NMR spectroscopy can give quick results at low preparation cost per sample for its biomarker panels, it is still held back by the high capital cost, large instrument footprint, and requirement for cryogenic liquids. Low cost, benchtop NMR systems have been on the rise within the last decade but haven't seen much attention in the field of metabolomics. In fact, the trend in metabolomics rather evolved towards even bigger magnets making use of increased spectral dispersion to accurately extract information from complex biological samples.

Yet here we want to demonstrate that benchtop NMR can provide key metabolic markers in human plasma within competitive time frames opening the path for widespread application. In addition, we want to show that benchtop NMR systems provide the necessary stability for inter-lab comparisons as a fundamental requirement for large scale applications.

KL 8. Application of NMR in Receptor–Ligand Interactions: From Venom Peptides to Macrocycles and Fragments

Mehdi Mobli

The University of Queensland, Brisbane, Australia

The function of cell-surface receptors and ion channels is tightly regulated by endogenous ligands, including disulfide-constrained peptides such as oxytocin and insulin. The high potency and selectivity of these peptides have driven their neo-functionalisation for predation and defence by plants, parasites, and venomous animals.[1-2] This evolutionary innovation has inspired interest in the biochemical and biophysical characterisation of bioactive disulfide-rich peptides and their receptors, with the ultimate goal of developing systems suitable for drug discovery.

However, this field faces significant challenges, particularly in producing highly constrained peptides and their membrane-embedded receptors in forms amenable to structural and functional studies. To overcome these hurdles, we employ advanced protein engineering and biochemical strategies, including protein splicing for peptide assembly and lipid nanodisc encapsulation for stabilising membrane proteins.[3-4] These approaches enable us to study the structure, conformational dynamics, and interactions of these complex systems under near-native conditions using biomolecular NMR spectroscopy.[3-5]

In this talk, I will present recent results demonstrating how state-selective venom peptides can serve as powerful tools for the isolation and stabilisation of ligand-binding domains of ion channels. By combining ion channel deconstruction with state-selective venom peptides, we aim to provide robust platforms for targeting these challenging but important drug targets using traditional biophysical screening approaches.

References:
1. Maxwell, M. J., et al., Nat Commun 2023, 14 (1), 1036.
2. Jami, S., et al., Nat Commun 2023, 14 (1), 2442.
3. Jia, X., et al., Commun Chem 2023, 6 (1).
4. Ramanujam, V., et al., Angew Chem Int Ed 2024, 63 (3), e202314621.
5. Kuschert, S., et al., Magn Reson 2023, 4 (1), 57–72.

KL 9. Targeting the 'untargetables': developing RNA-binding protein inhibitors that outsmart RNAs

Ann Kwan

The University of Sydney, Sydney, Australia

RNA-binding proteins (RBPs) play crucial roles in cellular processes across all life forms, regulating RNA metabolism and influencing diseases. Targeting RNA-binding domains (RBDs) can offer new therapeutic and biotech opportunities, but the effectiveness of small-molecule inhibitors has often been limited by the extended interaction surface and/or binding dynamics. Here, I will showcase the approaches and strategies that we have used and developed to target two representative RBPs, consisting of one antibiotic target (FtsY from E. coli) and one antiviral target (Nsp9 from SARS-CoV2).

We have discovered nucleic acid mimics that bind to the FtsY-NG domain and Nsp9 RNA-interaction sites with sub to mid micromolar affinity and some with whole-cell activity. Characterisation of selected NA mimics and their interactions with the targets using biophysical and biochemical methods will be presented. The pros and cons for the different approaches for finding RBP modulators and their potentials for targeting different classes of RBPs will be discussed.

KL 10. Unravelling molecular interactions of the Alzheimer's disease protein TREM2

Vanessa Morris[1], Siddhant Kumar[1], Harrison Cooper[1], Zac Tillett[1], Renwick Dobson[1], Campbell Sheen[2], Christoph Goebl[3]

[1]University of Canterbury, Christchurch, New Zealand
[2]Callaghan Innovation, New Zealand
[3]University of Otago, Christchurch, New Zealand

Dementias such as Alzheimer's disease are one of the leading causes of death worldwide, but there are no effective treatments against the disease. Development of therapies has been hampered by a lack of understanding of basic disease mechanisms. Two hallmarks of Alzheimer's disease are abnormal aggregation of the protein amyloid-beta and chronic inflammation in the brain. Here, we aimed to link these two key features by characterising interactions of the immune receptor protein TREM2 with ligands including amyloid-beta. TREM2 is expressed on the surface of microglia, the brain's resident immune cell, and mutations in this protein cause a ~3 fold increase in the risk of developing Alzheimer's disease. Using solution NMR spectroscopy, along with analytical ultracentrifugation and amyloid aggregation assays, we have performed a detailed characterisation of TREM interactions with amyloid-beta and polysaccharide ligands using both the wildtype and R47H disease variant of TREM2. We have used specific methionine-labelling of TREM2 produced from human cells to map the ligand-binding interfaces, finding differences between mutant and wildtype TREM2. We also found that TREM2 naturally self-associates to form oligomers, and that disease mutations and certain ligands disrupt oligomer formation, which may be important for downstream immune signalling. Finally, we discovered that amyloid-beta and polysaccharide ligands compete for binding with TREM2, rather than facilitating the binding of each other, as previously thought. These findings allow for better understanding of the natural function of TREM2, and how it can be disrupted in Alzheimer's disease, paving the way for future therapeutic developments.

KL 11. Tools to exploit the Biological Information residing in NMR spectra of Human Biofluids and their Clinical Applications

Beatriz Jimenez Garrido

[1]The University of Adelaide, Adelaide, Australia
[2]Imperial College London, London, UK

The NMR spectrum of human biofluids is exceptionally rich in biological information but remains challenging to fully interpret. This complexity increases when aiming to demonstrate to clinical practitioners that metabolic profiles derived from NMR spectroscopy contain translatable information that can enhance diagnostic accuracy and patient management.

Metabolic profiling provides a systems-level overview of metabolite concentrations in biological samples, enabling the identification of biochemical alterations associated with different health states. Assessing these profiles at specific time points can reveal potential disease biomarkers, while longitudinal analyses can capture temporal metabolic changes, offering a dynamic view of disease progression or recovery.

Phenome Centres, such as the National Phenome Centre (NPC) at Imperial College London, have been instrumental in establishing standardised protocols and generating large, high-quality metabolic profiling datasets.[1,2] This valuable resource has facilitated the development of advanced bioinformatics tools designed to extract biologically meaningful information from complex NMR spectra.[3,4]

In this presentation, I will introduce several of these tools for data processing, enhancement, and interpretation.[5,6] Finally, I will use sepsis as a clinical case study to demonstrate how metabolic profiling of biofluids can improve understanding of the biochemical processes underlying complex physiological conditions and ultimately support clinical decision-making.[7]

References:
1 Dona AC, Jiménez B, Schäfer H, Humpfer E, Spraul M, Lewis MR, Pearce JT, Holmes E, Lindon JC, Nicholson JK. Anal Chem. 2014; 86:9887.
2 Jiménez B, Holmes E, Heude C, Tolson RF, Harvey N, Lodge SL, Chetwynd AJ, Cannet C, Fang F, Pearce JTM, Lewis MR, Viant MR, Lindon JC, Spraul M, Schäfer H, Nicholson JK. Anal Chem. 2018; 90: 11962
3 Sands CJ, Wolfer AM, Correia GDS, Sadawi N, Ahmed A, Jiménez B, Lewis MR, Glen RC, Nicholson JK, Pearce JTM. Bioinformatics. 2019; 35: 5359
4 Takis PG, Jiménez B, Al-Saffar NMS, Harvey N, Chekmeneva E, Misra S, Lewis MR. Anal Chem. 2021; 93: 4995
5 Yan Y, Jiménez B, Judge MT, Athersuch T, De Iorio M, Ebbels TMD. Bioinformatics. 2025; 41: btaf045
6 Yan Y, Judge MT, Athersuch T, Xiang Y, Liu Z, Jiménez B, Ebbels TMD. Anal Chem. 2024; 96: 11707
7 Antcliffe DB, Harte E, Hussain H, Jiménez B, Browning C, Gordon AC. Intensive Care Med. 2025; 51: 529

KL 12. Mixing and Matching: two tales of resonances structures for multipurpose EPR and NMR measurements of biological systems

Martyna Judd,[1,2] Anton Savitsky,[3] Nick Cox,[2] Toby Zens,[4] Songi Han.[1]

[1]Department of Chemistry, Northwestern University, Evanston, IL, USA
[2]Research School of Chemistry, Australian National University, Canberra, ACT, Australia
[3]Department of Physics, Technische Universität Dortmund, Dortmund, Germany
[4]JEOL Ltd. Peabody, MA, United States

While magnetic resonance spectroscopies are powerful tools for studying biological questions including protein structure or drug activity, the complex nature of biological systems increasingly necessitates combining data from NMR and/or EPR experiments to reconstruct the full picture. Effective multi-experiment approaches demand hardware that balances diverse experimental needs while maximizing signal sensitivity for in vivo measurements. This talk will describe two recent developments of novel resonance structures of interest to both the EPR and NMR communities.

First, we describe a modular, high-sensitivity Q-band EPR resonator, which harnesses the superior sensitivity of dielectric resonators (DRs) structures, while overcoming two typical DR limitations: i) lack of frequency tunability; and ii) inability to accommodate oversized samples. The resonator is a 2.0 mm I.D. sapphire tube (that can be used as the sample tube) housed inside a brass cavity shield.[1] The resonator operates in the TE01d3 mode, where this field structure interacts with the top and bottom walls of the metallic shield such that varying the cavity length tunes the sapphire resonator frequency. Three-fold sensitivity enhancement is achieved compared to a TE011 cavity resonator,[2] and 37-fold overall signal enhancement compared to a Bruker dielectric resonator, taking into account the enhanced sample filling factor. The resonator can accommodate ENDOR and CW EPR modulation coils, and can be modified with a dielectric coupling element[2] which allows tuning its bandwidth between ~7~100 MHz. Thus, seamless tuning between complementary experiments with orthogonal hardware requirements (e.g. ENDOR and DEER) can be achieved, and the boosted resonator sensitivity pushes the theoretical concentration limit for these techniques towards in-cell sub-micromolar conditions.

Second, we describe a double resonance, magnetically coupled $^{1}H/^{19}F$ NMR circuit for MAS DNP measurements at 600 MHz.[3] $^{1}H/^{19}F$ cross-polarisation. Proton-decoupled/CP ss-NMR measurements with DNP are fast becoming gold standard not only for biomolecules, but also of drug targets as pharmaceutical formulations and in vivo.[4] In the current probe design, magnetic coupling between an inner sample solenoid coil and outer loop gap resonator is used to split the sample coil resonance, generating two close-frequency resonances within a single sample coil. Inductive coupling reduces the number of lead connections necessary for tuning and matching and thus maximises the circuit filling factor to achieve higher sensitivity at both resonances. The design process, calculations and experimental results are described.

In conclusion, concurrent NMR and EPR hardware developments will be critical to unlocking molecular-scale insights into protein complexes of new drug targets, enabling multiple complementary perspectives on the same system, and accelerating the path from fundamental understanding to therapeutic design.

Operating in the TE01d3 Mode. Unpubl. Manuscr. 2025.

References:
1 Judd, M.; Jolley, G.; Williams; Hill, M.; Cox, N.; Savitsky, A. Dielectric Tube General-Purpose Q-Band EPR Resonator
2 Judd, M.; Jolley, G.; Suter, D.; Cox, N.; Savitsky, A. Dielectric Coupler for General Purpose Q-Band EPR Cavity. Appl. Magn. Reson. 2021. https://doi.org/10.1007/s00723-021-01404-4.
3 Zens, Toby.Jeol Ltd. Solid Sample Magnetic Coupling High Resolution Nuclear Magnetic Resolution Probe and Method of Use. US Patent no. US11927653B1, 2023.
4 Li, M.; Xu, W.; Su, Y. Solid-State NMR Spectroscopy in Pharmaceutical Sciences. TrAC Trends Anal. Chem. 2021, 135, 116152. https://doi.org/10.1016/j.trac.2020.116152.

KL 13. Phase separation of miscible fluids in mesoporous media monitored by NMR relaxometry and diffusometry

Siegfried Stapf, Niklas Siebert, Carlos Mattea, Anam Sara, Pascal Merle, Christian Dressler

TU Ilmenau, Ilmenau, Germany

The distribution of mixtures of fluids in geometric confinement is affected by the interaction of the individual components with the interface. Radial density functions of the molecular distribution reveal that, depending on fluid combinations, density variations occur from between one to several molecular diameters away from the surface. Molecular dynamics therefore may be significantly altered in mesoporous materials with pore diameters below 50 nm. Properties such as wettability and proticity, and their influence on NMR relaxation times of the adsorbed molecules, are reasonable well understood for single-phase liquids, T_1 dispersion and T_2 make distinction between polar and non-polar fluids possible. Self-diffusion, on the other hand, of sufficiently small molecules is independent of polarity and is only governed by the tortuosity of the matrix. A comparison of relaxation and diffusion of liquid mixtures in confinement and in the bulk thus serves as a suitable test for anomalies in the mixing behavior.

Binary mixtures of liquids were prepared with one component perdeuterated, and were filled into porous glass as well as several types of silica gels. Samples included acetone/cyclohexane, THF/cyclohexane and acetone/water, all of them being fully miscible in the bulk. Relaxation times T_1 and T_2 of ^1H as well as ^2H were determined for Larmor frequencies between 1 kHz and 300 MHz employing field-cycling relaxometry. Diffusion coefficients were obtained from PFG methods on 1T and 7T scanners. For selected fluids, MD simulations were carried out for cylindrical silica pores of similar size, from which radial density profiles and diffusion coefficients were computed.

For acetone/cyclohexane, a pronounced increase of the apparent tortuosity – the ratio of bulk to confined diffusivity – by a factor of at least 200 was found in acetone while being absent in cyclohexane. Similar observations were made for water/acetone, suggesting demixing with a trend of surface affinity in the order water>acetone>cyclohexane. Very long bulk-like NMR relaxation times confirm that cyclohexane is removed from the silica surface unless it constitutes the only phase present, while ^2H relaxation confirms this is not a dipolar correlation effect. MD radial density profiles clearly confirm the preferred adsorption of the more polar liquid and the removal of the non-polar species. The dramatic reduction in D, observed for the first time in the case of acetone, suggests that the spatial distribution of this component falls below the percolation threshold.

KL 14. pH controlled modification of metal oxide surfaces in porous media monitored by low field ^1H NMR relaxometry

C. I. Karunarathne[1], R. Wilkinson[1], M. L. Johns[1], E. O. Fridjonsson[1]

[1]School of Engineering, Department of Chemical Engineering, The University of Western Australia

Porous media are prevalent in both natural formations and engineered systems, playing a key role in processes such as mineral carbonation and groundwater flow. However, understanding the physiochemical interactions within their complex pore networks remains challenging. Nuclear Magnetic Resonance (NMR) techniques, particularly, transverse relaxation time (T_2) measurements offer a powerful, non-invasive means of inferring pore-scale behaviour [1]. These measurements are highly sensitive to factors such as surface chemistry, mineral deposition and magnetic susceptibility. In systems containing iron oxides, these effects are even more pronounced due to the paramagnetic nature of Fe^{3+}. Additionally, surface charge, and thus surface relaxivity is influenced by pH, electrolyte concentration, and the isoelectric point (IEP) of the mineral surface. This study investigates how NMR T_2 relaxation of hematite-containing porous media responds to changes in pH and electrolyte concentrations, using a low-field NMR rock core analyser. A stepwise increase in NMR T_2 relaxation time was observed when mine tailings were mixed with $MgCl_2$, attributed to acidification and formation of magnesium oxychloride. To further investigate these effects, a model system of borosilicate glass beads and hematite was used. These suggested that at acidic conditions, the formation of amorphous hydroxyl surface groups reduced surface relaxivity, while at basic conditions, FeOOH formation increases surface relaxivity [2]. This study highlights the importance of monitoring surface IEP effects in systems containing metal oxides, and emphasizes importance of pH monitoring for accurate interpretation of NMR data.

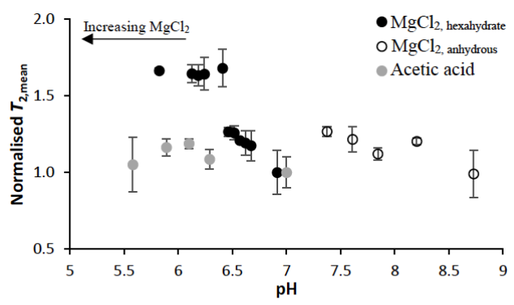


Fig. 1: Normalised $T_{2,mean}$ as a function of pH for tailings mixed with $MgCl_{2,hexahydate}$, $MgCl_{2,anhydrous}$ and acetic acid solutions.

References:
1 Robinson et al., Phys. Rev. Lett. (2023).
2 Parks, Chem. Rev. (1965).

IL 1. Local Electrostatics and Hydration at Protein-Lipid interface: Implications for T-Cell Receptor Assembly

Tatyana Smirnova,[1] Maxim Voinov,[1] Sergey Milikisiyants,[1] Gabriel Cook,[2] Alex Smirnov,[1]

[1]North Carolina State University, Raleigh, North Carolina, USA
[2]Oklahoma State University, Stillwater, USA

The ionization states of amino acid residues are critical for membrane protein assembly and function, yet they remain challenging to resolve experimentally. This difficulty is amplified in studies of membrane proteins due to limited data on transmembrane gradients in polarity, electric potential, and hydration at the protein-lipid interface. Here we investigate how electrostatic interactions — previously implicated as the key drivers in membrane assembly of the T-cell receptor (TCR) — can be modulated through changes in membrane lipid composition. To probe these interactions, we employed novel pH-sensitive, ionizable electron paramagnetic resonance (EPR) spin labels to map the heterogeneous dielectric environment along transmembrane protein-lipid interfaces. Using a series of model transmembrane α-helical WALP peptides, we established the depth-dependent profile of effective pKa values across the membrane. Our findings demonstrate that the effective pKa of ionizable sidechains embedded in the membrane interior can be significantly shifted by altering the surface charge density of the lipid bilayer. We also demonstrate HYSCORE method to evaluate the water penetration profile along the peptide-lipid interface and discuss the implications for the modulation of sidechain pKa.

To explore the biological relevance of these observations, a pH-sensitive nitroxide-labeled peptide corresponding to the transmembrane domain of TCRa was incorporated into liposomes. EPR measurements provided insights into the sidechain's protonation state, membrane insertion, and helix-helix interactions. Increased negative surface charge on the membrane was found to modulate the protonation state of buried ionizable residues, influencing transmembrane domain association. Using Double Electron-Electron Resonance (DEER) spectroscopy, we demonstrated that neutralizing the charge of an ionizable sidechain enhanced the tendency of transmembrane domains to cluster—an effect likely important in TCR assembly and turnover.

EPR spectroscopy using ionizable probes offers a powerful method for elucidating how local environmental changes at protein-lipid interfaces can fine-tune the pKa of ionizable residues and drive structural dynamics in membrane proteins. This material is based upon work supported by the National Science Foundation under Grant No.2305172.

IL 2. Dynamics Driven Drug Discovery

Martin Scanlon,[1] Biswaranjan Mohanty,[2] Wesam Alwan,[1] Yildiz Tasdan,[1]

[1]Monash University, Melbourne, Australia
[2]The University of Sydney, Sydney, Australia

Antimicrobial resistance (AMR) represents one of the most urgent public health challenges of our time. There is a clear and urgent need for new antimicrobial drugs with novel mechanisms of action that can be used either on their own or in combination with current antibiotics. Conventional antibiotics have been discovered through their ability to kill bacterial or inhibit growth. However, targeting bacterial viability often drives drug resistance due to the enormous selective advantage survivors have over their competitors in a population. An alternative to killing bacterial pathogens or stopping their growth, is to search for drugs that disarm them, rendering them avirulent and harmless. Targeting virulence offers several potential advantages, including an increased repertoire of pharmacological targets and novel mechanisms of action, a higher bar to resistance, and, potentially, preservation of the existing beneficial gut microbiota.

An important feature of many virulence factor proteins produced by Gram-negative bacteria is the requirement for structural bracing by disulfide bonds. These disulfide bonds are introduced catalytically by enzymes of the disulfide bond (DSB) system. There is now overwhelming evidence that DsbA is a master regulator of bacterial virulence. Moreover, it has been shown that deletion of DsbA in pathogenic strains of some multi-drug-resistant Gram-negative bacteria both reduces pathogenesis and restores sensitivity to existing antibiotics. Therefore, inhibitors of DsbA have the potential to simultaneously cripple bacterial virulence and induce hypersensitivity to existing antibiotics.

Previous efforts to develop inhibitors of DsbA have met with limited success. This is due in part to the relatively flat and featureless nature of the substrate binding – which is consistent with DsbA's ability to accommodate a broad range of substrates with little sequence preference. Paradoxically, DsbA appears to have exquisite selectivity for a membrane-bound partner protein – DsbB – that is required to complete the catalytic cycle that drives disulfide bond formation in Gram negative bacteria.

To better understand this paradox, we characterised μs-ms dynamics that are present in the protein using NMR spectroscopy. This allowed us to identify a "cryptic pocket" in DsbA, which is more accessible when the active site cysteines are in their oxidised disulfide-bonded form. From this understanding of the dynamics, we were able to identify small molecules that bound within the cryptic pocket. Moreover, this information informed our strategy for expanding from the cryptic pocket to generate functional inhibitors of DsbA that show activity in cellular assays and restore antibiotic sensitivity to AMR strains of bacteria.

IL 3. Parameterisation of Canonical and Non-Canonical Amino Acids for NMR Structure Determination

Martin Stroet,[1] Tye Gonzalez,[2] K. Johan Rosengren,[1] Mehdi Mobli,[1] and Alan Mark[1]

[1]The University of Queensland, Brisbane, Australia
[2]TU Dortmund, Dortmund, Germany

Peptides and proteins containing non-standard amino acids play key roles in cell regulation, antimicrobial defence and bioengineering. However, their structural characterisation by NMR is often prohibitively challenging using standard tools. We have developed a general procedure for generating atomic descriptions required to incorporate ncAAs within popular NMR structure determination software such as CYANA and CNS. This procedure is made publicly available via the existing Automated Topology Builder (ATB) server (https://atb.uq.edu.au) with all submitted ncAAs stored in a dedicated database. We validate the ATB-CNS amino acids parameters on a variety of peptides that contain standard and non-canonical amino acids, as well as determining the structure of a novel conotoxin containing an N-terminal pyroglutamic acid and C-terminal amidation. We show that the ATB-CNS amino acids par! ameters produce peptide structures of equal quality to the established PARALLHDG5.5 force field, demonstrating its versatility in accommodating both canonical and non-canonical amino acids. Automating the generation of structural templates for ncAAs will extend the utility of NMR spectroscopy to studies of more complex biomolecules, with applications in the rapidly growing fields of synthetic biology and chemical biology.

IL 4. Microimaging of biological tissues at 16.4 T MRI

Nyoman Kurniawan,[1] Roger Bourne,[1] Aurel Amar,[1] Adam Phipps,[2] David Reutens,[1]

[1]The University of Queensland, Brisbane, Australia
[2]University College London, London, UK

Background: Pathology and structural studies of biological tissues often rely on information provided from histology. While histology techniques can be tailored to highlight distinct molecular properties of the tissues, they are often destructive, requiring a significant manual handling time and may only provide limited spatial information.

Purpose: MR Imaging at the ultra-high field (UHF) provides unprecedented gain in signal, which in combination with strong MR gradients can be used to examine complex biological structures in 3D ex vivo. In this work, we present examples of microimaging and high-resolution diffusion MRI of fixed biological tissues, and comparison with phase contrast microCT (MCT) and histology.

Methods: Human prostate and kidney tissue samples were imaged using a vertical Bruker 16.4 T Avance II MRI at The University of Queensland, equipped with micro 5 and micro 2.5 gradients and 5 – 25 mm microimaging coils. MR sequences included diffusion tensor imaging (DTI) and T1/T2*-weighted gradient echo imaging. The MR image resolutions ranged between 20 – 40 micron 3D isotropic resolutions, acquired over 2-24 h of scanning. MCT was performed at the Australian Synchrotron facility.

Results: Kidney glomeruli could be visualised with high degree of visibility, producing accurate enumeration similar to that produced by the reference stereology method. DTI fibretracking revealed extensive network of prostate fibromuscular structures, which was comparable to that generated using an MCT tensor analysis.

IL 5. Conformational modulation of the multifunctional Phosphoprotein of the rabies virus

Paul R. Gooley,[1,2,] Shatabdi Chakraborty,[1,2] Ashish Sethi,[3] Stephen M. Rawlinson,[4] Gregory W. Moseley[4]

[1]Department of Biochemistry and Pharmacology, University of Melbourne
[2]Bio21 Molecular Science and Biotechnology Institute, University of Melbourne
[3]Australian Nuclear Science Technology Organisation, The Australian Synchrotron
[4]Department of Microbiology, Biomedicine Discovery Institute, Monash University

Multifunctionality of viral proteins is essential for viruses to coordinate infection, replication and subvert the host-cell antiviral mechanisms. This is particularly critical for viruses such as the lyssaviruses, including rabies, that have small genomes of only five genes. One of these genes of the rabies virus, the P gene, expresses a multifunctional protein, the phosphoprotein (P protein), in five N-terminally truncated isoforms that have various and different roles in replication and immune evasion. We have focused on full-length protein, P1, and the truncate P3 (missing the first 53 residues), as P3 gains unique phenotypes that are lacking in P1, including interactions with multiple cellular membrane-less organelles (MLOs, liquid-liquid phase-separated (LLPS) structures such as microtubules and nucleoli), important to immune evasion. Indeed, we and others have shown that P1 and P3 can phase separate independently in vitro but may require additional co-factors in the cell. In our research we have found that P3 and not P1 binds RNA which may be an important property for in cell phase separation. What is conformationally different about the two proteins is unclear. To characterize the differences and macromolecular interactions we are using biophysical methods including NMR, SAXS and quantitative cross-linking Mass Spectrometry. Further, as the name of the protein implies, phosphorylation may play an important role in protein localization and thus function by modulating the structure of nuclear import and export sequences of P1 and P3.

IL 6. Structure Elucidation with STOCSY: Insights from Urine NMR Metabolomics in Early Childhood Development

Reika Masuda

Murdoch University, Perth, Australia

Nuclear magnetic resonance (NMR) spectroscopy is widely used for untargeted metabolomic investigations, but the inherent complexity of spectra and resonance overlap pose significant challenges for metabolite identification. Statistical Total Correlation Spectroscopy (STOCSY) provides a data-driven strategy to overcome these limitations by exploiting covariance across large datasets. Importantly, STOCSY not only highlights correlations within a molecule through shared spin systems, thereby supporting structure elucidation, but also captures biologically meaningful associations: when two metabolites co-vary across a dataset, their corresponding spectral signals appear highly correlated. This dual functionality makes STOCSY a valuable tool for both chemical and biological interpretation in metabolomics.

In this preliminary study, we applied STOCSY to urine ^{1}H NMR data collected longitudinally from four infants at three developmental stages: 7–10 days, 6 months, and 12 months. To explore biomarkers of early childhood development, spectra were first projected using Age as the explanatory variable. This projection revealed age-dependent metabolic variation, providing a foundation for STOCSY analysis. STOCSY was then used to disentangle overlapping resonances, improve confidence in metabolite annotation, and identify co-varying metabolites that reflect coordinated biological processes.

Our findings demonstrate that STOCSY can resolve spectral complexity while simultaneously uncovering meaningful biological patterns. In the context of early childhood, this approach provided insights into pathways linked to growth, nutrition, and microbial co-metabolism. Beyond this proof-of-concept, STOCSY has the potential to be applied in healthy aging studies, where subtle but biologically relevant metabolic changes can provide new perspectives on resilience, healthspan, and disease susceptibility. Overall, this work highlights STOCSY as an accessible and versatile method for enhancing both structural and functional interpretation in NMR-based metabolomics.

IL 7. NMR structures of cyclotides: from Oxford sabbatical to a product in Bunnings

David J Craik

Institute for Molecular Bioscience, ARC Centre of Excellence for Innovations in Peptide and Protein Science, The University of Queensland, Brisbane, Australia

Naturally occurring macrocyclic peptides offer great potential as leads for drug design and as next-generation crop protection products [1-3]. Our work focuses on a class of macrocyclic peptides known as cyclotides that are exceptionally stable and are resistant to enzymatic or thermal degradation by virtue of their cyclic cystine knot structural motif. They are excellent scaffolds for the incorporation of bioactive peptide epitopes to stabilise them. More than two dozen examples have now been reported where biologically active epitopes have been grafted onto cyclic peptide frameworks to produce drug lead molecules with potential in the treatment of cancer, cardiovascular disease, infectious disease, autoimmune disease (multiple sclerosis) and pain. This presentation will describe our work on the discovery, structural characterisation and applications of cyclotides in medicine and agriculture, including the role of cyclotides as the active insecticidal ingredients in an eco-friendly pesticide product recently launched and sold in all Bunnings stores across Australia for the home gardener market. NMR has played a vital role in the discovery and characterisation of cyclotides and I will give a historical overview of aspects of cyclotide discovery, which started on a sabbatical leave in the laboratory of Professor Iain Campbell at Oxford University.

References:
1 Craik D J: Seamless proteins tie up their loose ends. Science, 311, 1563-1564 (2006).
2 De Veer S J, Kan M-W, Craik D J: Cyclotides: From structure to function. Chemical Reviews (2019) 119, 12375-12421.
3 Wang C K, Craik D J: A designer's guide to the making of macrocycles. Nature Chemical Biology (2018) 14, 417-427.

IL 8. Enabling research using NMR spectroscopy: ANSTO's National Deuteration Facility

Karyn Wilde, Tamim Darwish

National Deuteration Facility - ANSTO, Lucas Heights, Australia

Deuteration can provide greater contrast and improved resolution to assist investigations into the relationship between molecular structure and function of molecules of both biological and synthetic origin. Molecular deuteration of organic compounds and biomolecules significantly increases options available in characterisation and complex structure function investigations using nuclear magnetic resonance (NMR) through reduction of spectral complexity and signal linewidths in both solution and solid-state NMR spectra and in other techniques including neutron scattering, infrared and mass spectrometry (MS), whilst also creating functional materials with superior properties in life sciences, pharmaceutical and advanced technology applications.

The NCRIS-supported National Deuteration Facility (NDF) at the Australian Nuclear Science and Technology Organisation (ANSTO) is the only facility of its kind in the Southern Hemisphere with specialised expertise and infrastructure to provide deuteration through both biological and chemical techniques for a diversity of molecules that may otherwise not be available commercially. The NDF has developed a suite of capabilities in both chemical deuteration of small organic molecules and in vivo biological isotopic labelling of biomolecules providing access to a broad range of deuterated molecules for research and industry, accessible through various NDF user program access modes.

With the application of various stable isotope labelling schemes for proteins well established within the biomolecular NMR community, the NDF utilises adaptation of their reliable and robust methods for the deuteration of a broad range of proteins by high-cell density, high-yield recombinant expression in Escherichia coli BL21, to produce uniformly double ($^{13}C/^{15}N$, $^{2}H/^{15}N$) and triple labelled ($^{2}H/^{13}C/^{15}N$) proteins, as well as ^{13}C- Ala, Ile, Leu Val (AILV) methyl labelled proteins and proteins with selective amino-acid labelling, for the support of structural and functional investigations. Selected examples of protein labelling and their application will be highlighted. The NDF is developing further synthetic biology capabilities to complement bacterial protein labelling and the existing NDF deuteration of molecules including cholesterol utilising bio-engineered yeast and other microbes.

IL 9. Monitoring health using the blood lipoproteins in adults and children

Samantha Lodge

Australian National Phenome Centre, Perth, Australia

Routine blood lipid tests are completed by clinicians to monitor the cardiovascular risk of an individual. However, these tests are not precise and provide only total cholesterol and High-Density Lipoprotein (HDL) measured levels, while the rest of the parameters, normally Low-Density Lipoprotein (LDL) and triglycerides, are obtained by calculation using the Friedewald equation. Using NMR, 112 lipoprotein parameters can be obtained, as well as lipoprotein lipid composition information and NMR derived inflammatory markers all in one 4-minute experiment.

We have determined the healthy ranges and perturbations caused by both chronic and acute inflammation in adults and this work is ongoing in children. Indeed, we have shown these parameters can give an indication of the health status of an individual at a more granular level than previously possible. For example, in paediatric burn trauma shifts in these parameters are observed in the acute injury phase. It is known that burn injuries subject children to long term health complications including stress disorders, gastrointestinal diseases, immune dysfunction and cardiovascular disease.

We have found that at 1 year post burn injury while all clinical measures appear in the normal range for these healed children their lipoprotein profile is altered. While total LDL remains at a normal level there is a shift from larger LDL to smaller denser LDL particles. Additionally, the apolipoprotein B100/ A1 ratio is elevated. Furthermore, all major lipoprotein classes exhibited compositional changes, including an increased triglyceride content in Very Low-Density Lipoprotein (VLDL) and HDL and a rise in cholesterol ester levels in Intermediate Density Lipoprotein (IDL). These changes all indicate an increased atherogenic profile which may have implications for long-term cardiovascular health.

While this work was completed on high field 600 MHz NMR instruments, we have translated the methods to be able to monitor these parameters on a benchtop NMR, where high field associated limitations in terms of cost, maintenance and accessibility can be vastly reduced. This development has significant implications for making a powerful diagnostic tool widely available, enhancing the potential for longitudinal personalized medicine through molecular phenotyping in the clinic.

IL 10. Relayed DNP NMR Reveals the Nanoscale Structure of Lipid Nanoparticles in mRNA Vaccines

Adrienn Rancz,[1] Judith Schlagnitweit,[1] Salah-Eddine Akrial,[1] Landry Gayet,[1] Frédéric Ronzon,[2] David Gajan,[3] Loïc Salmon,[1] Guido Pintacuda,[1] Anne Lesage[1]

[1]Centre de RMN à Hauts Champs de Lyon CRMN, Lyon, France
[2]Sanofi Pasteur, Marcy l'Étoile, France
[3]Laboratory of Catalysis, Polymerization, Processes and Materials, CP2M UMR 5128 Université de Lyon, Institut de Chimie de Lyon, CNRS, Université Lyon 1, 69616 Villeurbanne, France

Lipid nanoparticles (LNPs) are advanced and effective mRNA delivery vehicles, as shown with the vaccines against SARS-CoV-2. However, their architecture is still poorly understood due to their complex lipid composition and self-assembly process. Dynamic nuclear polarization (DNP) solid-state NMR has previously been used to probe siRNA and mRNA LNPs, leveraging hyperpolarization transfer from exogenous radicals in the frozen solution surrounding the particles to the radical-free LNPs via proton spin diffusion.[1,2] This approach enables the spatial mapping of different components based on DNP enhancement factors (e) and polarization build-up time (TB). While siRNA NMR signal could be resolved, no nucleotide resonances were previously detected in mRNA-loaded LNPs.

Here, we applied relayed DNP to explore mRNA LNP-vaccines with pharmaceutically-relevant composition and concentration. ^{13}C-enhanced NMR spectra were acquired at 9.4 T and 10 kHz MAS, and assigned based on reference spectra from pure lipid components. All lipid resonances were identified, enabling compound-specific measurements of e and TB. Notably, the mRNA ribose C1' resonance was resolved and assigned via 2D correlation experiments, confirmed by comparison with empty LNPs. Numerical simulations of e and TB using differential equation modelling[3] suggest a layered architecture, with an inner mRNA domain surrounded by the cationic lipids, phospholipids, cholesterol, and PEG-lipids, providing new insight into the structural organization of mRNA-LNPs.

References:
1 J. Viger-Gravel et al, J. Phys. Chem. B, 2018, 122, 2073
2 G. Porat-Dahlerbruch et al, Small Methods, 2024, 9, 2400622
3 A. C. Pinon et al, J. Phys. Chem. C, 2017, 121, 29, 15993

IL 11. The Intricacy between Magnetic Fields and Fluidic Processing in Vortex Fluidic Devices (VFD)

Qin Li[1], Colin Raston[2], James Scott[1], Dechao Chen[1], Ahmed Naseer[1], James Watts[1], Badriah M. Alotaibi[2], Matt Jellicoe[2], Zoe Gardner[2]

[1]Queensland Quantum and Advanced Technologies Research Institute, School of Engineering & Built Environment, Griffith University [2]Flinders Institute for Nanoscale Science and Technology, College of Science and Engineering, Flinders University

The vortex fluidic device (VFD) is a dynamic thin film microfluidic platform, in which the film is uniform in thickness along the upper side of the tube when the tube is tilted at 45° and rotating at a high speed (1.5 – 9 k rpm). Within the thin liquid film, localized extreme high-shear stress regimes exist predominantly in the form of typhoon-like spinning top (ST) flows and double-helical (DH) flows. This intensified vortex thin film has been shown to be able to catalyse chemical reactions and form carbon dots at room temperature [1], cut [2] and unzip carbon nanotubes [3], synthesize magnetic gold nanoparticles [4]. More interestingly, we found the fluid field in VFD exhibit sensitivity to earth magnetic field, which can be observed from the VFD-processed materials. Carbon nanotubes in VFD can be either turned into toroids or twisted in a shape of 8, which can be either left- or right-hand lemniscates [5]. These new discoveries made from the VFD poses a question: what exactly is going on in VFD? This talk aims to provide some insights.

References:
1 D Chen, M Usman Zia, TMD Alharbi, JR Harmer, CL Raston, Q Li; Room‐Temperature Vortex Fluidic Flow Chemistry Synthesis of Full Color Carbon Dots; ChemSusChem, 2025, e202402182.
2 Alharbi, Thaar MD, Qin Li, and Colin L. Raston. "Thin film mechano-energy induced slicing of carbon nanotubes under flow." ACS sustainable chemistry & engineering 9.48 (2021): 16044-16051.
3 Thaar MD Alharbi, AEH Alotaibi, Dechao Chen, Qin Li, Colin L Raston, Unzipping multiwalled carbon nanotubes under vortex fluidic continuous flow, ACS Applied Nano Materials, 2022, 5 (9), 12165-12173.
4 Badriah M. Alotaibi, Soraya Rapheima, …, Qin Li, Mats R. Anderson, Nadim Darwish, Colin L. Raston Vortex Fluidic Mediated Synthesis of Enhanced Hydrogen Producing Magnetic Gold, Small Science, 2025, 2400449
5 Matt Jellicoe, Zoe Gardner,…, Qin Li, Jamie S. Quinton and Colin L. Raston, Chiral lemniscate formation in magnetic field controlled topological fluid flows, Small, 2025, 21, 240980.

OL 1. ^{19}F-NMR of fluorinated amino acids in proteins

Gottfried Otting,[1] Yi Jiun Tan,[1] Elwy H. Abdelkader,[1] Haocheng Qianzhu,[1] Nathan Paul,[1] Thomas Huber,[1] Nicholas F. Chilton,[1] Ansis Maleckis,[2]

[1]Australian National University, Canberra, Australia
[2]Latvian Institute of Organic Synthesis, Riga, Latvia

The incorporation of fluorinated amino acids into proteins provides multiples probes for facile interrogation by 1D ^{19}F-NMR spectroscopy. Uniform substitution of canonical leucine, valine and isoleucine residues by fluorinated analogues can be achieved by cell-free protein synthesis from amino acids. For fluorinated aromatic amino acids, aminoacyl-tRNA synthetases have been developed that afford site-specific incorporation in response to an amber stop codon.

We present a way for assigning the ^{19}F-NMR spectra of fluorinated leucine, valine and isoleucine without site-directed mutagenesis. Our work shows that CH_2F groups barely perturb the protein structure, adopt preferential but rarely single rotamers and their ^{19}F chemical shifts are sensitive to small changes in rotamer populations. Through-space ^{19}F-^{19}F scalar couplings are readily observed between fluorine atoms forming direct contacts at least transiently. A single pentafluorophenylalanine residue replacing a phenylalanine also does not disrupt the protein structure and provides ready access to aromatic ring-flip rates as a probe of the 'liquidity' of the hydrophobic core.

References:
1 Maleckis, A., Abdelkader, E. H., Herath, I. D., and Otting, G.: Synthesis of fluorinated leucines, valines and alanines for use in protein NMR, Org. Biomol. Chem., 20, 2424-2432, https://doi.org/10.1039/D2OB00145D, 2022.
2 Tan, Y. J., Abdelkader, E. H., Tarcoveanu, E., Maleckis, A., Nitsche, C., and Otting, G.: (2S,4S)-5-Fluoroleucine, (2S,4R)-5-fluoroleucine, and 5,5′-difluoroleucine in E. coli PpiB: protein production, 19F NMR, and ligand sensing enhanced by the gamma-gauche effect, Biochemistry, 63, 1376-1387, https://doi.org/10.1021/acs.biochem.4c00080, 2024.
3 Tan, Y. J., Abdelkader, E. H., Herath, I. D., Maleckis, A., and Otting, G.: Through-space scalar 19F-19F couplings between CH2F groups of leucine residues in a protein, Magn. Reson., 6, 131-142, https://doi.org/10.5194/mr-6-131-2025, 2025.
4 Qianzhu, H., Tan, Y. J., Abdelkader, E. H., Huber, T., Otting, G.: Genetic encoding of fluorinated analogues of phenylalanine for 19F-NMR spectroscopy: detection of conformational heterogeneity in flaviviral NS2B-NS3 proteases, ACS Sens. 10, 3152-3161, https://doi.org/10.1021/acssensors.5c00432, 2025.
5 Abdelkader, E. H., Chilton, N. F., Maleckis, A. and Otting, G: Gamma-effects identify preferentially populated rotamers of CH2F groups: side-chain conformations of fluorinated valine analogues in a protein, Magn. Reson. Discussion, https://doi.org/10.5194/mr-2025-12,2025.

OL 2. Protein Structural Analysis using EPR

Vishaal Bayya

University of Queensland, Brisbane, Australia

Protein structure and dynamics are crucial to function and require a range of biophysics techniques for its elucidation. This information is critical, for example, in the study of therapies and treatments for various diseases. Knowing protein structure enables scientists to design drugs that target specific proteins, leading to more effective treatments. Protein structure is also important in understanding cellular signalling and metabolic pathways and in designing proteins with novel functions. The three most successful and widely used structural determination techniques are NMR, X-ray crystallography and Cryo-EM.

DEER, a form of EPR spectroscopy is a complementary technique and offers several advantages over the above techniques for studying protein structure and dynamics. Key features of DEER include the ability to study proteins in solution, there is no size limit, so large proteins are amenable, no crystallisation is required, and the spin label pair report on a distance distribution making the technique ideal to study disorder and protein conformations. In DEER, spin labels are typically attached to the protein via site-directed mutagenesis. However, there are issues with existing spin labels, with the biggest issue being the dependence on cysteine residues for tagging; this renders proteins with numerous surface-exposed cysteines not applicable to the technique as they have to either be removed, which is expensive and time-consuming, and/or they may be critical to the protein's structure and function. Currently, there is no generally applicable 'off the shelf' labelling technique that does not rely on cysteine labelling. To address these limitations, non-canonical amino acids (ncAAs) can be genetically incorporated into proteins to provide an alternative site-directed mutagenesis methodology that circumvents the cysteine labelling limitation.

This research aims to develop a new generally applicable spin label technique for proteins based on ncAAs, expanding the applicability of the existing techniques to facilitate a comprehensive analysis of all potential protein systems. This methodology involves (1) the synthesis of spin labels with ideally short linkers, keeping the mobility of the spin label minimal, (2) genetically inserting suitably functionalised ncAAs for a bioorthogonal click chemistry reaction with the spin label, and (3) performing DEER measurements on model proteins to characterise the accuracy and sensitivity of the new labelling approach. Phase two of the research plan would then implement this new spin labelling methodology in applications to protein systems of interest, such as the non-ribosomal peptide synthetase (NRPS) which makes the antibiotic teicoplanin (studies within the EPR group). This 200 kDa protein has many surface-exposed cysteines that are functional and is believed to exist in a range of conformations in solution, presumable explaining why it has not been able to be crystallised and has not been able to be studied by Cryo-EM.

OL 3. NMR Reveals Base-Exchange Inhibitors for NAD+ Glycohydrolases

Yun Shi, Tamim Mosaiab, Veronika Mosaic, Paige Harten, Thomas Ve

Griffith University, Brisbane, Australia

Nicotinamide adenine dinucleotide (NAD+) is a ubiquitous biomolecule essential for all cellular life. Beyond its role as a redox cofactor in energy metabolism, NAD+ serves as a substrate for NAD+-dependent signalling pathways. NAD+ glycohydrolases, such as SARM1 and CD38, consume NAD+ and represent promising therapeutic targets for a range of diseases. Using NMR spectroscopy and other biophysical techniques, we have identified a base-exchange mechanism that enables the in situ generation of SARM1 inhibitors from small-molecule fragments. Building on this mechanism, we propose an NMR-first, fragment-based approach to discover additional base-exchange inhibitors targeting various NAD+ glycohydrolases.

OL 4. Targeting RNA using Fragment-Based Drug Screening

Brooke X.C. Kwai[1,2], Indu R. Chandrashekaran[1,2], Biswaranjan Mohanty[1,3], Menachem Gunzburg[1,4], Bradley C. Doak[1,4], Ashish Sethi[5], Sean Harrison[6], Pedro Serrano[6], Shubhadra Pillay[7], Elisa Barile[7], Martin J. Scanlon[1,2,4]

[1]Medicinal Chemistry, Monash Institute of Pharmaceutical Sciences, Monash University, Victoria, Australia. [2]ARC Centre for Fragment-Based Design, Monash University, Victoria, Australia [3]Sydney Analytical Core Research Facility, The University of Sydney, New South Wales, Australia [4]Monash Fragment Platform, Monash Institute of Pharmaceutical Sciences, Monash University, Victoria, Australia.[5]Australian Synchrotron, Australian Nuclear Science and Technology Organisation, Victoria, Australia. [6]Drug Discovery Sciences, Takeda Pharmaceuticals International Company, Massachusetts, USA. [7]Takeda California, Inc., San Diego, USA

Non-coding RNAs account for up to 80 % of the human genome.[1] It has become increasingly clear that non-coding RNAs play a diverse and critical role in many important cellular functions.[2] Although modulation of non-coding RNAs using small molecules has been demonstrated to be a promising therapeutic strategy, the structure-interaction relationships of RNA targeting small molecules remain largely unexplored.[3] We hereby present a fragment-based drug discovery approach where NMR identified hits were validated and ranked by SPR, and binding poses were modelled using NMR NOESY data in combination with molecular docking to evaluate and elaborate fragment hits against a theophylline aptamer model system. The methods used in this study have the potential to be applied to a variety of novel RNA targets.

References:
1 Djebali S, Davis CA, Merkel A, et al. Landscape of transcription in human cells. Nature. 2012;489(7414):101-108. doi:10.1038/nature11233
2 Rizvi NF, Smith GF. RNA as a small molecule druggable target. Bioorg Med Chem Lett. 2017;27(23):5083-5088. doi:10.1016/j.bmcl.2017.10.052
3 Childs-Disney JL, Yang X, Gibaut QMR, Tong Y, Batey RT, Disney MD. Targeting RNA structures with small molecules. Nat Rev Drug Discov. 2022;21(10):736-762. doi:10.1038/s41573-022-00521-4

OL 5. ^{1}H-NERRD: Probing Microsecond Timescale Protein and Bound Ligand Dynamics in Solid-State NMR

Tye Gonzalez

Technische Universität Dortmund, Dortmund, Germany

Generative protein folding tools such as AlphaFold-2/3 or Boltz1 deliver highly accurate static snapshots of biomolecular architecture. However, they remain blind to the conformational heterogeneity that govern free-energy landscapes.

For protein-protein interactions this shortcoming is often tolerated due to the enthalpic component dominating the free energy of binding. In small-molecule binding, however, the entropic and conformational motion contribution is much more significant. Here we aid in this understanding through ^{1}H-NERRD (proton Near Rotor-Resonance Relaxation Dispersion) under fast magic-angle spinning as a sensitive probe in solid-state NMR.

By modulating the spin-lock tilt angle we decouple auto- from cross-relaxation pathways, suppressing spin-diffusion artefacts and isolating true microsecond dynamics. Global fits of dispersion profiles yield both the correlation time (τ_c) and order parameter (S^2) in a single experiment. In addition, ^{1}H-NERRD is also sensitive to translational motion and nearby motion in a way that ^{15}N and ^{13}C methods are effectively blind to. The quantitative dynamic fingerprints we obtain highlight the importance of conformational heterogeneity in ligand binding.

OL 6. Deep learning-guided drug target selection: towards discovery of modulators of RNA-binding proteins

Jameel Abduljalil, Sandro Ataide, Ann Kwan

School of Life and Environmental Sciences, Faculty of Science, The University of Sydney, Sydney, Australia

RNA-binding proteins (RBPs) are the cornerstones of transcription, translation, and RNA metabolism, yet their molecular interactions with RNA remain only partially understood and difficult to model in comparison to protein-protein complexes. RBPs often have structurally diverse binding pockets with highly dynamic interaction modes with their RNA partners. These features pose challenges and opportunities for drug discovery targeting RBPs. Nuclear magnetic resonance (NMR) spectroscopy is one of the experimental approaches to probe the interactions of RBPs:RNA complexes or their potential modulators, as it can capture both transient and long-lived interactions at the atomic level.

To systematically explore bacterial RBPs, we analyzed 2622 protein:RNA structures deposited in the Protein Data Bank and extracted the physicochemical and geometric features of the binding interfaces. Using deep embedding clustering, we grouped 162 unique complexes into five distinct clusters whose interaction profiles seem to align with previously reported biophysical data, including in-house lab data. As a proof of concept, we selected representative RBPs from two clusters to target via small molecules that can either compete with the RNA for binding the protein or perturb protein:RNA binding dynamics. Deep learning models trained on molecular docking affinity data were developed to virtually screened ZINC20 database (~329 M molecules). Potential binders were narrowed down via pharmacokinetic filters and molecular dynamics simulations. Ongoing NMR experiments, including CPMG, saturation transfer difference, and waterLOGSY, are now being applied to validate the binding of candidate modulators. This integrated framework highlights how deep leaning and computational modeling can be harnessed for pre-clinical antibiotic discovery and expanding the scope of druggable proteins.

OL 7. Application of change point detection in the analysis of temporal chemical exchange saturation transfer data

Gang Zheng

Western Sydney University, Sydney, Australia

As a new form of magnetic resonance imaging (MRI) contrast enhancement scheme, temporal chemical exchange saturation transfer (CEST) can provide rich pathological and pharmacokinetic (PK) information. However, the detailed analysis of temporal CEST data is significantly ham-pered by low signal-to-noise ratio (SNR) conditions. Here, pruned exact linear time (PELT)-based change point detection (CPD) was innovatively applied to simulated and experimental temporal CEST data to obtain change point distributions. Excitingly, different simulated PK scenarios (i.e. curve types) gave rise to distinct change point distribution patterns and similar change point dis-tribution patterns were observed for dynamic glucose-enhanced (DGE) CEST data, validating the applicability of PELT-based CPD to temporal CEST data. The application of PELT-based CPD to extremely noisy temporal thiol-CEST data provided interesting findings, thanks to its great noise tolerance also demonstrated on simulated data and experimental data with added pseudo-white noise.'

OL 8. Assembling a high field NMR platform towards ultra-high-intensity pulse field gradient diffusion NMR

Sarah J. Stevenson,[1] Petrik Galvosas[1,2*]

[1]School of Chemical and Physical Sciences, Victoria University of Wellington, New Zealand
[2]MacDiarmid Institute for Advanced Materials and Nanotechnology, New Zealand

Access to the cutting edge of strong magnetic field gradient NMR hardware opens the exciting possibility for material science studies: observing smaller diffusivities / decreased displacements lengths for porous media (such as zeolites and metal organic frameworks [1]) and producing higher resolution images (especially when paired with magnetic resonance pore imaging using averages over identical pores to improve signal-to-noise ratios [2]). Both commercial NMR equipment manufacturers and individual research groups have therefore been motivated to build Nuclear Magnetic Resonance (NMR) systems with usable strong gradients (10 T/m or higher) [3-6]. Set-ups often lacked the durability, stability, and reliability to be experimentally used near their quoted maximums. Most impressively gradient strengths of up to 200 T/m have been achieved and diffusivities as smaller as 2.4x10-16 m^2/s have been observed, however these systems are not in operation anymore [7,8].

Present state of the art includes ultra-high-intensity pulsed field gradient NMR gradient probes from the Leipzig University (Germany)[1,6]. The Magnetic Resonance Physics group at Victoria University of Wellington (VUW, New Zealand) aims to enhance its research capabilities for tracing particle displacements using a 35 T/m and 70 T/m (prototype) Leipzig probe. The probes' 100 A current requirement necessitated a custom NMR platform. This contribution reports on the multiyear PhD journey commissioning and integration of two Leipzig probes with a custom high-field Kea[2] spectrometer (Magritek), analogue input Techron 7790 series gradient amplifier (AE Techron), 500 W RF amplifier (Tomco), and an Oxford 9.4 T vertical wide-bore superconducting magnet with a Bruker AVANCE I shim rack and BVT3000 variable temperature unit.

The necessary set-up processes will be justified and outlined, including the unexpected challenges which had to be navigated. Stability validations for the NMR instrumentation revealed dependencies on room temperature, facilitating the need to record room temperature during experiments to gauge the trustworthiness the of data collected. The impact this could have on the NMR results was experimentally confirmed. The current gradient amplifier arrangement is nominally able to produce magnetic field gradients of up to 22.75 T/m and 56.7 T/m for the two probes, with potential to increase this capability by different gradient configurations.

References:
1 D. Mehlhorn et al. ChemPhysChem, 15, 1681-1686 (2014)
2 S. A. Hertel et al. Phys Rev E, 92, 012808 (2015)
3 Doty Scientific, https://dotynmr.com/products/diffusion-pfg-probes
4 K. Zick, Diffusion NMR User Manual – Section 11, Bruker, 4 (2016)
5 JEOL, https://www.jeol.com/products/scientific/probes/GR5AT.php
6 P. Galvosas et al. J Magn Reson, 151, 260-268 (2001)
7 M. E. Komlosh and P. T. Callaghan, J Chem Phys, 109, 10053–10067 (1998)
8 N.L. Zakhartchenko et al. Magn Reson Imaging, 16, 583–586, (1998)

OL 9. Magnetic Resonance Pore Imaging with Extended Echo Times in 1D and 2D

Humna Asad,[1,2] Philipp Matern,[3] Daniel J. Holland,[4] Petrik Galvosas[1,2]

[1]Victoria University of Wellington, Wellington, New Zealand
[2]MacDiarmid Institute, New Zealand
[3]Heidelberg University, Heidelberg, Germany
[4]University of Canterbury, Christchurch, New Zealand

Magnetic Resonance Pore Imaging (MRPI) [1–3] maps the internal structure of porous media by enabling reconstruction of average pore shapes. To date, this has been demonstrated mainly for closed pores, but the approach can be extended to open pores [4]. MRPI builds upon the pulsed–gradient spin–echo (PGSE) concept introduced by Stejskal and Tanner [5] but extends one of the diffusion encoding gradients to average out NMR phases to the centre-of-mass position in the pore. Thus, achieving sufficiently long diffusion times under the extended gradient may be challenging due to transverse magnetization decay and artifacts such as gradient–induced dephasing [6,7]. Recently, we have shown that, under favourable conditions and in specific geometries, spin–echo times (TE) can be pushed to ~ 2 s [8].

Here, we deploy these extended echo times to re-implement 1D and 2D experiments in glass capillaries, pushing both PGSE and MRPI to long echo times while maintaining high signal-to-noise ratios. In 1D PGSE experiments, 10 µm capillaries were measured up to TE ≈ 1 s, and 50 µm capillaries up to TE ≈ 2 s. At these echo times, PGSE diffusive–diffraction produced clear pore–diffraction signatures. Beyond diffusive–diffraction, we performed 1D MRPI at similar long echo times (thus raising DT /L2), the signal E(q) converged toward the pore form factor S0(q), from which we obtained the 1D pore-shape density projection via Fourier transform. Furthermore, in 2D MRPI experiments, echo times of 300–400 ms yielded pore reconstructions with ~ 1 µm resolution in both x and y directions, surpassing typical limits for MRI. These results demonstrate that, under optimal experimental conditions (shimming, careful sample preparation and alignment), long-TE MRPI is feasible without severe signal loss and without employing a CPMG-backbone variant of the MRPI pulse sequence. By increasing the total long–gradient time T – and thus the ratio DT / L2–we broaden the applicability of MRPI to pore-filling fluids with low molecular mobility. This capability may enable measurements of slow diffusive processes in closed pores and, by extension, in open porous systems.

References:
[1] Laun, F.B. et al., Phys. Rev. Lett. 107, 048102 (2011)
[2] Hertel, S.A. et al., Phys. Rev. E 92, 012808 (2015).
[3] Hertel, S.A., Microporous Mesoporous Mater. 205, 183–190 (2015).
[4] Laun, F.B.; Müller, L.; Kuder, T.A., Phys. Rev. E 93, 032401 (2016).
[5] Stejskal, E.O.; Tanner, J.E., J. Chem. Phys. 42, 288–292 (1965).
[6] Bertleff, M. et al., J. Magn. Reson. 278, 39–50 (2017).
[7] Callaghan, P.T., Translational Dynamics and Magnetic Resonance
[8]Galvosas, P. et al., EUROMAR 2025 Book of Abstracts, 335 (2025).

OL 10. Understanding a novel oxidation-induced amyloid formation mechanism of the tumour suppressor protein p16^{INK4a}

de Cordovez, P.[1], Heath, S.G.[1], Gray, S.G.[2], Gölitz, A.[1], Demeler, B.[3,4], Morris, V.K.[2,5], Göbl C.[1,5]

[1]Mātai Hāora - Centre for Redox Biology and Medicine, University of Otago, Christchurch, NZ, [2]School of Biological Sciences, University of Canterbury, Christchurch, NZ, [3]Department of Chemistry and Biochemistry, University of Lethbridge, Canada, [4]Department of Chemistry, University of Montana, USA, [5]Biomolecular Interaction Centre, University of Canterbury, Christchurch, NZ.

Amyloids are highly ordered protein aggregates that display a characteristic cross β-sheet structure, and they are known as the hallmark of neurodegenerative disorders, such as Parkinson's or Alzheimer's disease. We have recently found that the tumour suppressor protein p16^{INK4A} can fold into amyloid structures, but unlike the great majority of amyloid-prone proteins, p^{16INK4A} does not spontaneously form fibrils[1]. Instead, we found that amyloid formation is induced by the oxidation of the protein's single cysteine residue. Under mild oxidative conditions, monomeric proteins form an intermolecular disulfide bridge, and the resulting dimeric species then aggregates to form the amyloid structures. The amyloid structure is mainly stabilised by the disulfide bond and fibrils will disassemble under reducing conditions and restore the fully functional monomeric protein.

We are using this unique and strictly inducible system to study amyloid fibril growth by monitoring the transition from the stable, purely α-helical monomeric protein to the fully grown β-stranded amyloid fibrils. Using several solution NMR techniques, we were able to highlight the critical role played by the protein C-terminus in the aggregation process. Combined with electron microscopy, analytical ultracentrifugation, and biochemical assays, we also characterized the structural changes and the resulting kinetics of the amyloid formation. We were able to detect a partial unfolding of the intermediate dimeric species, which rapidly aggregates into higher order assemblies. These early oligomeric species were shown to be highly transient, whereas the first detectable stable aggregates appeared to be substantially bigger structures. This novel inducible amyloid system thus offers a powerful model to dissect the early stages of amyloid formation and provides detailed insights into protein unfolding, oligomerization and fibril growth.

References:
1. Heath, S.G. Gray, S.G., Hamzah, E.H., O'Connor, K.M., Botha A.D., de Cordovez, P. et al. Amyloid formation and depolymerization of the tumor suppressor protein p16INK4a is strictly controlled by an oxidative thiol-based mechanism. Nature Communications. 2024. 15: 5535.

OL 11. Getting to know your roommate – NMR metabolomics as a tool to characterise the role of metabolism in symbiotic relationships

Horst Joachim Schirra[1,2,3,*], Sarah Walsh[2], Luke Husdell[3,2], Denni Currin-Ross[3], Jessica Broadway[1], Eric Caragata[4], Jeremy C. Brownlie[1,5]

[1] School of Environment and Science, Griffith University, [2]Institute for Biomedicine and Glycomics, Griffith University, [3]Centre for Advanced Imaging, The University of Queensland, [4]Florida Medical Entomology Laboratory, University of Florida, [5]Australian Research Centre for Human Evolution, Griffith University

Model organisms are useful tools for uncovering fundamental biological processes in systems that are comparatively less complex than higher animals/humans. Here we discuss several examples of using NMR-based metabolomics as a key platform technology to exploring the role of metabolic processes in host-symbiont interactions in various insect models:
(1) Infecting Drosophila with the endosymbiont Wolbachia wMel depresses the insulin/insulin-like-growth factor cascade, whilst inducing the hypoxia signaling pathway. This causes ROS production and ROS adaptations, next to other metabolic changes that steer metabolism away from oxygen-intensive pathways and enable mutually beneficial metabolite exchange between symbiont and host. These responses signify a reprogramming of the host's mitochondrial metabolism rather than an immune response. (2) In contrast, infection with wMelPop in the mosquito Aedes. aegypti triggers host immune responses, including melanogenesis and ROS production. wMelPop is more aggressive, whereas wMel is more likely to form stable inheritable infections. (3) Wolbachia infection in Drosophila temporarily suppresses viral infections. Understanding the basis for this effect is of great interest in the context of inhibiting the spread of insect-borne viral diseases. Metabolomics characterisation of coinfection of Drosophila with wMel and Drosophila C virus provides evidence for metabolic competition between the endosymbiont and the virus as the underlying basis for the inhibition of viral replication. (4) Such viral infection studies involve injecting Drosophila with the virus. Thus, the metabolic response to viral infection is confounded by a concurrent wounding/wound-healing response. We have studied the metabolic profile of this wounding/wound-healing response and provide a basis for interpreting both processes in viral infection studies. We also show Wolbachia is accelerating wound healing next to providing viral protection.

These examples show the breadth and depth of insights into the role metabolism plays in host-symbiont interactions that can be gained through metabolomics/systems biology.

Keywords:
Drosophila melanogaster; Aedes aegypti; Wolbachia pipientis; host-symbiont interactions; metabolic regulation.

OL 12. NMR as a powerful tool for high-throughput quantitation and metabolite elucidation: Examples from wine

Flynn T Watson[1,2,3], Don Teng[1,2], Keren Bindon[1], Stella Kassara[1], Natoiya D R Lloyd[1,2], William S Price[3], Allan Torres[3], Mathias Nilsson[4], Gareth A Morris[4], Damian Espinase Nandorfy[5], and Markus J Herderich[1,2,6]

[1]The Australian Wine Research Institute, [2]Metabolomics Australia, [3]Nanoscale Organisation and Dynamics Group, School of Science, Western Sydney University, [4]Department of Chemistry, The University of Manchester, [5]Food Nutrition and Dietetics, La Trobe University, [6]Discipline of Wine Science and Waite Research Institute, The University of Adelaide

A primary strength of NMR metabolomics, when compared to other technologies, is its ability to accurately quantify compounds against a single internal reference. Sample preparation for solution-state NMR analysis of wine is straightforward, requiring minimal preparation, which reduces perturbation of the matrix. Multi-frequency presaturation effectively eliminates the signals from water and ethanol, the major constituents, allowing access to macro-components such as sugars and acids, for example.

Spectra of complex mixtures, such as wine, often show significant overlap due to the narrow proton spectral range and high number of metabolites present, complicating compound assignment. This ambiguity can be resolved through use of additional spectroscopic experiments, statistical approaches, or a combination thereof. For example, GEMSTONE-TOCSY can be used to selectively excite and propagate magnetisation to reduce spectral complexity, enabling unambiguous metabolite assignment [1]. Traditional methods including 2D-TOCSY can be used in combination with non-traditional computational strategies like statistical TOCSY (STOCSY) [2]. Once assigned, compounds can be quantitated through manual peak integration or automated processing workflows, with automation enabling robust high-throughput capabilities for wine metabolite analysis. Often, provided spectra have been acquired in a standardised manner, quantitation can be performed retrospectively, a capability not available in other metabolomic technologies.

Our work has presented the unambiguous assignment of pyroglutamic acid in wine using a combination of traditional and advanced NMR experiments, and explored the efficacy of a statistical method (STOCSY) [3]. Further, we have presented an automated quantification method for proline, a structurally analogous compound to pyroglutamic acid with favourable sensorial properties [4]. This automated data processing workflow delivered accurate measurements across 1000 samples with high reproducibility. These studies exemplify NMR's comprehensive utility from metabolite discovery through to efficient quantitative analysis in complex sample matrices.

References:
1 P. Kiraly et al., "Single-Scan Selective Excitation of Individual NMR Signals in Overlapping Multiplets," Angew. Chem. Int. Ed., vol. 60, no. 2, pp. 666-669, Jan 11 2021, doi: 10.1002/anie.202011642.
2 O. Cloarec et al., "Statistical total correlation spectroscopy: an exploratory approach for latent biomarker identification from metabolic 1H NMR data sets," Anal. Chem., vol. 77, no. 5, pp. 1282-9, Mar 1 2005, doi: 10.1021/ac048630x.
3 F. T. Watson, M. Nilsson, M. Herderich, A. Torres, W. S. Price, and G. A. Morris, "Identification and quantitative measurement of pyroglutamic acid in 1H NMR spectra of wine," Food Research International, 2025, doi: 10.1016/j.foodres.2025.116247.
4 F. T. Watson et al., "Robust, automated quantitation of proline in wine," Food Chem., vol. 493, no. Pt 1, p. 145386, Jul 3 2025, doi: 10.1016/j.foodchem.2025.145386.

OL 13, Structural Basis of DkTx Bivalency

Theo Crawford,[1] Venkatraman Ramanujam,,[1] Ben Cristofori-Armstrong,[1] Jen R. Deuis,[1] Xinying Jia,[1] Michael Maxwell,[1] Sina Jami,[1] Linlin Ma,[2] Irina Vetter,[1] Mehdi Mobli[1]

Australian Institute for Bioengineering and Nanotechnology, The University of Queensland
Griffith Institute for Drug Discovery, Griffith University, Brisbane, Australia

Bivalency is a highly advantageous property of biomolecules, conferring enhanced target specificity and binding kinetics. Several venom peptides, composed of two independently folded disulfide-rich domains connected by a linker, have been shown to act via a bivalent mechanism. These peptides exhibit remarkable avidity, often described as irreversible binding, despite their individual domains displaying relatively weak affinity.

Current theories propose a sequential binding mechanism, where one domain engages the receptor first, followed by the second domain due to increased local concentration. However, synthetic attempts to replicate bivalency by covalently linking peptides with flexible linkers have largely failed to reproduce the enhanced and prolonged pharmacological effects observed in naturally evolved bivalent peptides. The role of the linker in facilitating domain alignment and receptor engagement remains poorly understood yet may hold the key to designing more effective bivalent molecules.

We investigated the structural and dynamic properties of the linker in double-knot toxin (DkTx), a bivalent TRPV1 channel agonist, using multidimensional NMR spectroscopy. The solution structure reveals residual order in the linker, stabilised by aromatic stacking between tyrosine residues in the first domain and the linker. NMR spin-relaxation experiments show that disrupting this interaction increases linker disorder, resulting in impaired bivalent binding with reduced potency and avidity. Notably, the loss of avidity occurs even at concentrations above the EC50 of the individual domains, conflicting with the sequential binding hypothesis. At higher peptide concentrations, avidity is partially restored, suggesting that domain pre-orientation enhances bivalent receptor engagement.

Our findings demonstrate that domain pre-organisation, facilitated by evolved linker constraints, plays a critical role in enabling bivalent peptide function for DkTx. These insights suggest that future engineering efforts could benefit from incorporating structured linkers inspired by naturally evolved multidomain peptides to enhance potency and avidity.

OL 14. A structural and biophysical analysis of the action of the nsp9 protein from sars cov-2 - implications for future drug discovery efforts

Serene El-Kamand,[1] David Baker,[1] Rowan Heggen,[1] Shradha Ajith,[1] Bing Wang,[2] Gayathri Mani,[1] Mar-Dean Du Plessis,[1] Thomas Allport,[3] Irina Artsimovitch,[2] Lorna Wilkinson-White,[3] Sandro Ataide,[3] Ann Kwan,[3] Liza Cubeddu[1,3] and Roland Gamsjaeger[1,3]

[1]School of Science, Western Sydney University, Australia
[2]Department of Microbiology, Ohio State University, USA
[3]School of Life and Environmental Sciences, University of Sydney, Australia

Severe acute respiratory syndrome coronavirus 2 (SARS CoV-2) is an RNA virus from the betacoronavirus family that cause serious respiratory illness in humans. One of the conserved non-structural proteins encoded for by the coronavirus family is non-structural protein 9 (nsp9). Nsp9 plays an important role in the RNA capping process of the viral genome, where it is covalently linked to viral RNA (known as RNAylation) by the conserved viral polymerase, nsp12. Nsp9 has also recently been implicated in the priming of viral RNA, a process that is mediated by a human host protein, termed Staphylococcal nuclease domain-containing protein 1 (SND1). In two related papers published earlier, we first revealed the RNA recognition interface of nsp9 and in a follow-up study, determined the biophysical basis of the interaction between nsp9 and nsp12. We are currently determining the molecular details of nsp9 and SND1 involvement in viral RNA production. Our approach centres on a combination of nuclear magnetic resonance (NMR) spectroscopy, biolayer interferometry (BLI), surface plasmon resonance (SPR) and biochemical assays. Our findings will significantly contribute to the ongoing global efforts to develop novel drugs against the highly contagious SARS CoV-2 virus.

OL 15. Benchtop NMR: A Tool for Measuring Vapor Pressure

Isanthi Ranathunga Liyanage, Prof. Daniel Holland, Prof. Richard M. Hartshorn

University of Canterbury, Christchurch, New Zealand

Measuring the vapor pressure of a liquid is crucial for understanding its volatility, predicting its phase behaviour, and informing safe handling, process optimization, and environmental assessment.
Traditional techniques for measuring vapor pressure - such as the manometric method, isoteniscope method, ebulliometer, and headspace gas chromatography, often require specialized equipment, complex sample preparation and larger sample volumes. This means these techniques are unsuitable for the analysis of novel species. Here, we present a method to measure vapor-liquid equilibria that uses benchtop ^{1}H NMR spectroscopy. The method is based on the principle that the vapor signal intensity is directly proportional to the partial pressure of species in the vapor phase. Here, the vapor samples were generated directly inside a standard 5 mm NMR tube by placing 0.1 mL of a volatile liquid (1-heptane, ethanol, cyclohexane, methanol, methylcyclopentane, 1-hexane, acetone, diethyl ether, methyl formate) inside a customized 3D-printed tube insert. The vapor-phase ^{1}H NMR spectra of known pure liquid samples were recorded at thermal equilibrium (26.5 °C) using a 60 MHz benchtop NMR spectrometer. The distinct chemical shifts of the vapor signals confirm clear differentiation from their corresponding liquid-phase resonances. Despite using a low-field NMR instrument, the vapor ^{1}H NMR spectra of each compound were acquired with a good signal-to-noise ratio, demonstrating sufficient resolution for quantitative analysis. A graph (Figure 1) was generated by plotting the normalized peak area for each sample as a function of its corresponding vapor pressure at 26.5 °C, obtained from the NIST database. A key finding of this study is the robust linear correlation between peak area and vapor pressure ($y = 0.0375x$, $R^2 = 0.9997$), confirming that benchtop ^{1}H NMR can reliably quantify vapor pressure through direct spectral measurements. This method will now be expanded to obtain vapor-liquid equilibrium (VLE) data for binary liquid mixtures.

OL 16. TOPicity SECRET

Ritchy Leroy

University of Reims, Reims, France

Understanding and predicting chemical equivalence is essential for interpreting NMR spectra.
A computational approach has been developed in Python to automatically identify chemically equivalent atoms within molecular structures through the analysis of topicity relationships (homotopic, enantiotopic, and diastereotopic). From these equivalence relationships, the expected number of distinct NMR signals on every nuclei can be predicted in function of media.The method identifies chemically equivalent atoms by applying virtual isotopic substitution, allowing the analysis of topicity relationships within the molecular structure.This approach provides a reliable framework for anticipating signal counts, useful for teaching, spectral assignment, structure validation and filtering NMR database.

OL 17. Universally quantitative band-selective pure shift NMR

Howard M. Foster,[1,2] Mathias Nilsson,[1] Ralph W. Adams,[1] and Gareth A. Morris[1]

[1]Department of Chemistry, The University of Manchester, Manchester M13 9PL, United Kingdom
[2]Current institution – Central Analytical Research Facility, Queensland University of Technology, Brisbane, Australia

NMR spectroscopy is an intrinsically quantitative analytical technique, in that signal integrals are proportional to the numbers of spins which give rise to those signals. In practice, however, typically only the simple pulse-acquire experiment is "universally" quantitative, meaning that the relative integrals of different signals faithfully represent the relative numbers of spins which contribute to those signals. Unfortunately, extracting quantitative information from 1H pulse-acquire spectra is frequently hindered by signal congestion, owing to the narrow chemical shift range and extensive signal multiplicity in 1H NMR. Pure shift NMR techniques[1] offer a route to alleviating signal overlap by suppressing the effects of homonuclear scalar coupling, but in doing so they introduce site-dependent signal losses and thus are not, in the general case, universally quantitative.

One strategy for obtaining universally quantitative data from multiple-pulse NMR experiments is to measure the degree to which the pulse sequence attenuates each signal integral. So long as the pulse sequence elements that cause signal loss act independently, repeating each element a variable number of times prior to acquisition permits extrapolation back to the loss-free integral. This concept, originally introduced in the time-zero extrapolated HSQC (HSQC0) experiment,[2] is applied here to band-selective pure shift NMR.[3,4] We have proposed the name EXQUISITE (extrapolating quantitative integrals by successive iteration) for the general application of this principle.

Our first implementation of the EXQUISITE method with band-selective pure shift NMR yielded relative signal integrals within ±0.5 % of those obtained from a pulse-acquire experiment for a three-component mixture.[5] In that initial form however, the total experiment time increases linearly with the number of EXQUISITE iterations performed. Here, we introduce a novel acquisition strategy for EXQUISITE pure shift NMR that records the data for all iterations sequentially within each individual scan. Applied to overlapping signals from a three-component mixture, this method afforded relative integrals with a quantitative accuracy better than ±1 %. Consequently, this acquisition mode is close to a "something for nothing" approach to quantitative band-selective pure shift NMR, given that the required measurement time is essentially the same as that for the conventional pure shift NMR experiment.

References:
1 K. Zangger, Prog. Nucl. Magn. Reson. Spectrosc., 2015, 86–87, 1–20.
2 K. Hu, W. M. Westler, J. L. Markley, J. Am. Chem. Soc., 2011, 133, 1662–1665.
3 L. Castañar, P. Nolis, A. Virgili, T. Parella, Chem. - Eur. J., 2013, 19, 17283–17286.
4 J. Ying, J. Roche, A. Bax, J. Magn. Reson., 2014, 241, 97–102.
5 H. M. Foster, M. Nilsson, R. W. Adams, G. A. Morris, Anal. Chem., 2024, 96, 9601–9609.

OL 18. NMR spectroscopy as an analytical tool for Australian mono-floral honeys

Luke Husdell[1,2,] Deni Taleski[3], Natasha Hungerford[4], Henry Smith[2], Horst Joachim Schirra[5,2,1]

[1]Centre for Advanced Imaging, The University of Queensland, [2]Institute for Biomedicine and Glycomics, Griffith University, [3]National Measurement Institute, Department of Industry, Science, Energy and Resources, North Ryde, NSW, [4]Queensland Alliance for Agriculture and Food Innovation, The University of Queensland, [5]School of Environment and Science, Griffith University

Creating a standard workflow for analysing complex food matrices is critical to combatting food fraud.
To use NMR spectroscopy for this, it is important to be able to analyse individual compounds within a complex mixture, thus requiring a method that can detect key analytes and resolve overlapping signals. Here we developed a decomposition workflow for one-dimension ^{1}H-NMR spectra using orthogonal information from a paired J-res inspired by recently described method[1]. To evaluate this method, we applied this workflow to a set of analytes spiked into honey, and then to a larger set of 130 commercially available honeys. Results from these spiked standard additions were comparable to commercially available NMR tools, as were the results for some, but not all, analytes in the larger dataset. Additionally, using multivariate analysis, we were able to determine a set of candidate signals which may be used for fingerprinting these mono-floral honeys.
This work presents the first steps towards building a standard method for analysing Australian honeys using NMR spectroscopy.

References:
1 Teipel, J. C., et al. (2020). Foods, 9(10), 1355.

OL 19. Bacterial bodyguards: Characterising the virus-repressing effect of Wolbachia in Drosophila melanogaster using NMR-based metabolomics

Sarah M. Walsh,[1,2] Tyson Thomson,[3] Karyn N. Johnson, [3] Jeremy C. Brownlie,[1] Horst Joachim Schirra[1,2,4]

Institute for Biomedicine and Glycomics, Griffith University

Wolbachia, an intracellular bacterial symbiont, exhibits antiviral effects in insects and has been employed to limit the spread of arboviruses. However, the mechanisms underlying this interference are not consistently understood. Our study employs nuclear magnetic resonance (NMR)-based metabolomics to characterise the bi- and tripartite host-*Wolbachia*-virus interactions using the model insect *Drosophila melanogaster*, the protective *Wolbachia* strain wMel and the pathogenic *Drosophila* C virus (DCV).

The findings reveal that wMel-infected flies showed increased simple carbohydrate catabolism and elevated purine metabolite levels relative to uninfected *Drosophila*. DCV infection perturbed nucleotide synthesis and nucleotide abundance in *Drosophila* compared to uninfected *Drosophila*, driving metabolism to likely meet the viral replication demands imposed on the host. Notably, co-infected Drosophila exhibited a metabolic profile more similar to wMel-infected flies than DCV-infected flies, suggesting wMel generates a metabolic environment where there is competition for host metabolites between wMel and DCV inhibiting viral replication. The study also suggests that wMel competes with the host for oxygen, creating a hypoxic environment that generates reactive oxygen species (ROS). ROS are effector molecules well known to trigger specific immune pathways that have been previously proven to contribute to *Wolbachia*-mediated antiviral protection.

We therefore propose that *Wolbachia*-mediated antiviral protection should be viewed as a multimodal response resulting from wMel's influence on host metabolism, rather than a single mechanism. Results suggest that wMel drives metabolism in a direction that at least temporarily inhibits DCV replication and is metabolically similar to single wMel infections; in doing so, it concomitantly triggers immune pathways that contribute towards *Wolbachia*-mediated pathogen blocking. This perspective may guide future research and contribute to the continued success of *Wolbachia*-based vector control strategies against RNA arboviruses, potentially leading to novel approaches for defending against such pathogens and improving vector control strategies.

OL 20. Metabolic Analysis of Wound Response in *Wolbachia* infected Drosophila melanogaster

Jessica Broadway, Sarah Walsh, Jeremy C. Brownle, Horst Joachim Schirra

School of Environment and Science, Griffith University

Viral studies of *Drosophila melanogaster* typically involve virus injection with a small needle, causing post-injury a wounding/wound healing response, in addition to the effects of viral infection. However, the metabolic response to the needle injury is understudied, and many viral investigations neglect potential effects of this response. Furthermore, the wMel strain of the endosymbiont bacterium *Wolbachia* pipientis provides anti-viral protection in *Drosophila*. Here we used NMR-based metabolomics to characterise the acute wounding response in *Drosophila* and the relationship between wound healing and the *Wolbachia* strain wMel.

The most notable response to wounding was found on the initial day of injury and lessened with time in both uninfected and *Wolbachia* infected flies. Metabolic changes in injured flies revealed evidence of inflammation and Warburg-like metabolism as a response to wounding. In addition, at five days post injury *Wolbachia* infected injured flies were metabolically more similar to the uninjured flies than uninfected injured flies were at the same time point, indicating an interaction between *Wolbachia* infection and wound healing.

This study is the first metabolomic characterisation of the wound response in *Drosophila* and its findings are crucial to the metabolic interpretation of viral experiments in *Drosophila* in both past and future studies.

OL 21. Measuring 10-30 ÅNGSTRÖM-SCALE distances in proteins using ^{19}F Endor

Nick Cox

Research School of Chemistry, Australian National University, Canberra, Australia

Proteins are large, flexible molecules that are challenging to characterize. One approach to characterize protein structure and dynamics is to attach paramagnetic tags (molecules that contain an unpaired electron) to the protein, which can then be used to characterize the local protein structure and discrete distances between tags. Recently, it has been shown that such tags can also be used to detect fluorine, using a technique called ENDOR (1, 2). As approximately 50% of all pharmaceuticals contain fluorine, this method allows the identification of drug binding sites within protein targets, both at substrate and allosteric sites, driving efficient drug discovery and optimization. In this talk I will describe how 19F ENDOR can be used to measure sparse structural constraints in proteins. In metalloproteins, where the position of the spin tag is fixed, we can measure short (<12 Å) distances and precisely constrain the position the fluorine in the protein (1). In these experiments the fluorine is carried by the side chain of a genetically encoded non-natural amino acid (1, 3, 4). For proteins labelled with spin tags attached the protein surface, we can measure distances between the spin tag and the fluorine up to 30 Å (5). Furthermore, by using multiple spin tags, we can triangulate the position of the fluorine to within the protein (5). We can also pull-out dynamics, resolving the conformational space accessed by surface exposed side-chains (3, 4). These measurements can be performed at low concentration (10 µM), require little sample (3 µL) and on proteins in solution, embedded in membrane fragments and in whole cells (6).

References:
1 M. Judd, E. H. Abdelkader, M. Qi, J. R. Harmer, T. Huber, A. Godt, A. Savitsky, G. Otting and N. Cox, Physical Chemistry Chemical Physics, 2022, 24, 25214-25226.
2 A. Meyer, S. Dechert, S. Dey, C. Höbartner and M. Bennati, Angewandte Chemie International Edition, 2020, 59, 373-379.
3 M. Judd, E. H. Abdelkader, H. Qianzhu, E. Habel, C. Lindsay, A. Brancewicz, T. Huber, G. Otting and N. Cox, Chemistry - A European Journal, 2025, accepted.
4 E. Habel, M. Judd, J. R. Harmer, T. Huber and N. Cox, 2025, submitted.
5 M. Judd, E. H. Abdelkader, M. Qi, J. R. Harmer, T. Huber, A. Godt, A. Savitsky, G. Otting and N. Cox, Journal of the American Chemical Society, 2025, 147, 16826-16835.
6 M. Seal, W. Zhu, A. Dalaloyan, A. Feintuch, A. Bogdanov, V. Frydman, X.-C. Su, A. M. Gronenborn and D. Goldfarb, Angewandte Chemie International Edition, 2023, 62, e202218780.

OL 22. Enhancing the water channelling effect of the antimicrobial peptide maculatin 1.1

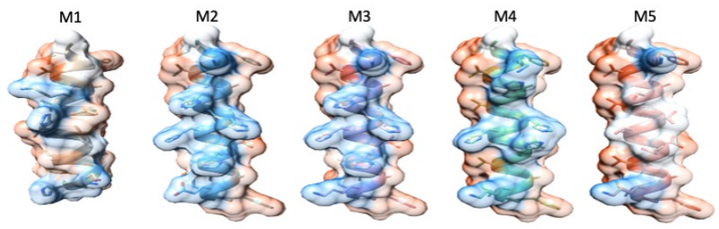
F. Separovic,[1,2,] D. W. Keizer,[2] and M.-A. Sani,[2,*]

[1]School of Chemistry, The University of Melbourne, Melbourne, Australia
[2]Bio21 institute, The University of Melbourne, Melbourne, Australia

Maculatin 1.1 (M1) is a 21 amino acids long residue cationic peptide found on the skin of Australian tree frogs. It has been shown to have antimicrobial properties, ranging from the low micromolar activity against Gram-positive and mid to high micromolar range against Gram-negative bacteria. Mac1 is a typical linear amphipathic peptide with random coil conformation in buffer but an alpha helical structure in contact with lipid membranes. The peptide can insert into the hydrophobic core of lipid bilayers, in a transmembrane orientation, and release large molecular weight molecules in a concentration dependent manner. It has even been shown to perturb nucleic acids in live bacteria.

In this study, we examine the hydrophilic residues along the hydrophilic side of Mac1 as to a potential for water channelling. Several alterations to the peptide primary sequence were made to amplify this effect, e.g. by using a core of histidine residues (Fig. 1). The 3D structures of the peptides were determined by solution-state NMR spectroscopy in dodecylphosphocholine micelles, complemented by circular dichroism. The peptides retained their helical structure in the lipid environment, and exposure to solvent was pH dependent as showed by PRE effect. ^{31}P and ^{2}H solid-state NMR were used to determine the pH-dependent impact of the peptides on the structure of phospholipid membranes made of POPC, POPC/cholesterol or POPE/POPG, mimicking the compositions of mammalian or bacterial cell membranes. Using ^{15}N labelled histidine residues, the interactions with water and location with the lipid bilayer was assessed by ^{1}H-edited and ^{31}P-^{15}N REDOR NMR experiments, respectively.

Finally, combining ^{15}N labelled E. coli cells and ^{13}C labelled M2 peptide, the mapping of the intracellular contacts was performed using REDOR experiments. Overall, the new analogues showed interesting pH modulations that could be fine-tuned for antimicrobial activities.



Name	Sequence
M1	G L F G V L A K V A A H V V P A I A E H F-NH_2
M2	G L F K V L A H V A H H V V H A I A E I F-NH_2
M3	G L F K V L A H V A H H V V H A I A K I F-NH_2
M4	G L F K V L A H V A H H V V H V I A K I F-NH_2
M5	G L F K V L A S V A T S V V T V I A K I F-NH_2

OL 23. Magnetic resonance device for landmine detection

Peggy Schoenherr,[1] Lewis Robertson,[1] Matthew Gerges,[2] Nick Cutmore,[2] David G. Miljak[1]

[1]Commonwealth Scientific and Industrial Research Organisation (CSIRO), Lucas Heights, Australia
[2]MRead Ltd Sydney, Australia

Landmines remain a persistent threat in over 60 countries and regions, posing serious risks to civilian populations and hindering regional development. Traditional clearance methods—such as metal detection and ground-penetrating radar—suffer from high false-positive detection rates and have seen limited technological progress in the last century. To address these limitations, the introduction of a sensor based on nuclear quadrupole resonance (NQR) offers a promising technological advancement.

CSIRO has developed a novel handheld landmine detector based on NQR, offering direct detection of the commonly used explosive compound RDX (cyclotrimethylenetrinitramine) at depths of up to 13 cm. Conveniently, and unlike nuclear magnetic resonance, NQR does not require a static magnetic field. It exploits quadrupole resonances in nuclei with spin $I > ½$, arising from interactions between the nuclear quadrupole moment and the surrounding electric field gradient. In RDX, detection is based on the 5.192 MHz NQR transition of ^{14}N ($I = 1$), selected for its favourable relaxation properties.

Developed as a minimum viable product for Australian company MRead Ltd., the device is battery-powered, largely automated, and designed for field use. Drawing on CSIRO's expertise in magnetic resonance technologies for mining, the team addressed longstanding NQR challenges—including noise suppression, temperature drift, and electronic limitations—to enable reliable outdoor operation. This was confirmed in two successful field trials conducted on a test field in Brisbane, Australia, and on minefields in Cuito Cuanavale, Angola, in collaboration with the HALO Trust and MRead. These promising results demonstrate the potential of NQR-based sensing to enhance landmine clearance efficiency and accelerate the safe return of land to affected communities. Future projects will target improvements to the sensor and expand detection capabilities to include new explosives such as TNT, aiming to support the clearance of all types of landmines.

OL 24. Optimising Anaerobic Digestate Dewatering with Low-Field NMR Relaxometry: Insights into Solid-Liquid Separation Dynamics

E. G. Bertizzolo[1], N. N. A. Ling[1], M. L. Johns[1], E. O. Fridjonsson[1]

[1]The University of Western Australia

Introduction:

Efficient management of anaerobic digestate (AD) can enhance nutrient recovery, making it a viable biobased fertiliser[1]. Dewatering is a critical first step, yet routine monitoring methods (e.g. total solids, turbidity, zeta potential) can be both time- and energy-intensive and can struggle monitoring complex solid/liquid structures. In this research, we investigate low-field nuclear magnetic resonance (LF-NMR) relaxometry as a complementary, non-invasive method to characterise and optimise the dewatering of two industrial AD samples.

Materials and Methods:

The AD samples were sourced from industrial red meat processing (RM-AD) and food waste (FW-AD) facilities and were flocculated using a cationic polymer (EM640CT @ 0.41% active content) across 0 – 4.5 wt% and 0 – 25.5 wt%, respectively. Samples were monitored using T_2 CPMG (25,000 echoes, 300 µs of echo time and 4 scans) and T_2-T_2 CPMG-CPMG (32 log-spaced steps between 10 and 25,000 echoes, 300 µs echo time and mixing time (t_{mix}) of 100 ms).

Results and Discussion:

Representative RM-AD and FW-AD samples are shown (Fig. 1). The RM-AD samples showed visual improvement in solid/water separation with increasing flocculant dosing, while the FW-AD samples showed poor separation performance. Fig. 2 shows the T_2 distributions as function of increasing flocculant dosing with RM-AD samples showing significant change in distributions with increasing long T_2 component (i.e. free-water), this is contrasted with the FW-AD samples whose T_2 distributions showed minimal change with increasing flocculant dosing.

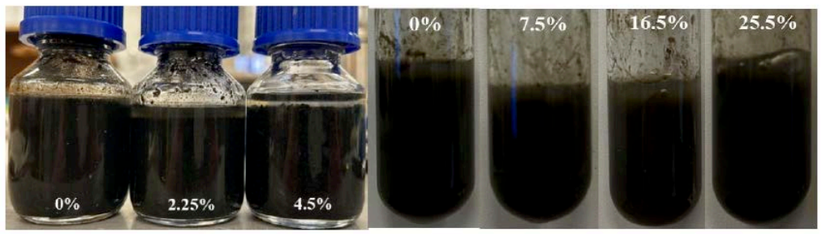


Figure 1. (L) RM-AD and (R) FW-AD samples.

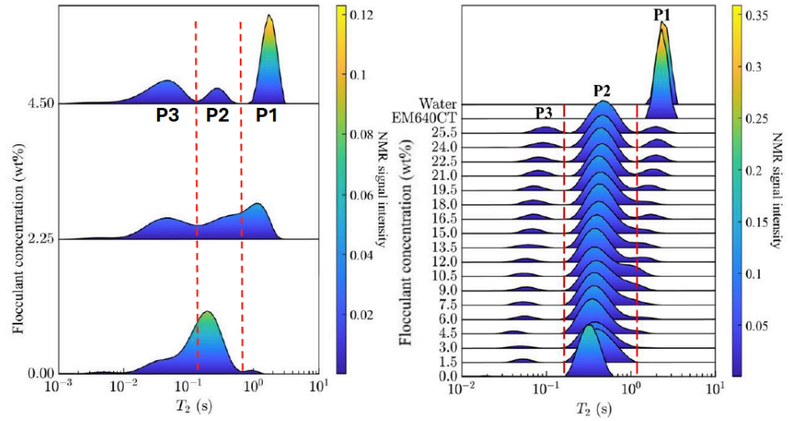


Figure 2. T_2 distributions of (L) RM-AD and (R) FW-AD.

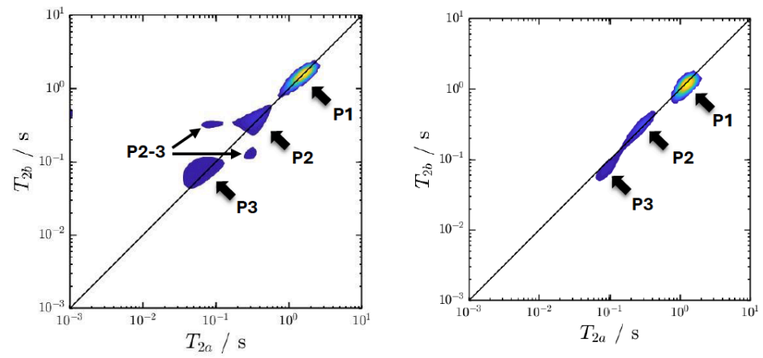


Figure 3. T_2-T_2 maps of (L) RM-AD dose with 4.5 wt% and (R) FW-AD with 25.5 wt%.

Conclusions and Future Works:

This research provides results on the dewatering behaviour of industrial RM-AD and FW-AD samples monitored using LF-NMR relaxometry. The use of 1D and 2D relaxometry enables characterisation of changes in water/solids structures as function of flocculant dosing within the digestates. Results showed a strong correlation between increasing T_2 relaxation (i.e. free water content) and dewatering performance. T_2-T_2 maps of RM-AD samples showed emergence of exchange peaks (P2-3) upon optimal flocculant dosing. Future research will investigate the dewatering performance of the FW-AD using a range of chemical flocculants, this will allow further study of LF-NMR relaxometry as a monitor for dewatering performance of industrial AD samples.

References:

1 Fagerström, A., Seadi, T. A., Rasi, S. & Briseid, T. The Role of Anerobic Digestion and Biogas in the Circular Economy. (IEA Bioenergy Task 37, 2018).

2 Bertizzolo, E. G. et al. Monitoring settling of anaerobic digestates using low-field MRI profiling and NMR relaxometry measurements. Water Research 245, 9 (2023). https://doi.org:https://doi.org/10.1016/j.watres.2023.120660

3 Callaghan, P. T.

OL 25. Effect of the polymer nature on the properties of composite solid electrolytes based on the organic ionic plastic crystal HMGFSI

Yady Garcıa,[abg] Antonela Gallastegui,[cd] Vera Bocharova,[e] Luca Porcarelli,[ac] Colin Kang,[a] Haijin Zhu,[af] David Mecerreyes,[cd] Maria Forsyth,[acd] and Luke A. O'Dell[a].

[a]Institute for Frontier Materials and the ARC Industry Transformation Training Centre for Future Energy Technologies Deakin University, Geelong, VIC 3216, Australia.
[b]Griffith Institute for Drug Discovery, Griffith University, Nathan, Queensland, Australia
[c]POLYMAT University of the Basque Country UPV/EHU, Joxe Mari Korta Center, 20018 Donostia-San Sebastian, Spain

The design of solid electrolyte composites for Li-ion batteries integrating polymers and organic ionic plastic crystals (OIPCs) requires an understanding of the synergy between their components to achieve the desired ionic conductivity. Here, we study composites between the OIPC hexamethylguanidinium bis(fluorosulfonyl) imide HMGFSI and polymers functionalised with the comonomer lithium 1-(3-(methacryloyloxy)propylsulfonyl)-1-(trifluoromethylsulfonyl)imide (LiMTFSI). These polymers have different macromolecular structures (i.e., homopolymers, copolymers, linear polymers, or polymer nanoparticles) and concentrations of lithium (Li). Characterisation of the composites by differential scanning calorimetry, X-ray diffraction, solid-state nuclear magnetic resonance spectroscopy, and electrochemical impedance spectroscopy showed that the composite containing large polymer nanoparticles with a low Li concentration had the highest ionic conductivity and structural disorder at low temperatures as well as a higher fraction of ions (i.e., Li+ and FSI−) that become highly dynamic. The role of the polymer nature and Li content in promoting interactions that led to different ion dynamics in the composites was discussed. Understanding the complex interplay between the composite components and the effect on properties such as thermal stability, structure and ion conduction, and dynamics assists in optimizing the overall performance of solid electrolyte composites.

P 1. When to use the 'big magnets': a sensitivity study for novice NMR users

Rebecca R. Hawker and Laurence K. Jennings

Collaborative Research Platform for NMR Spectroscopy at The University of Queensland, Brisbane, Australia

It is commonly known that you observe higher sensitivity (i.e. higher signal-to-noise ratios) by moving to higher fields,[1] and by using cryogenically cooled probes.[1,2] One question that newer NMR users often don't know is when they should use the higher field instruments. This is often due to lack of knowledge of cost, instrument availability and understanding. Common questions NMR Facility Manager's hear include: "how much sample do I need?" or "I only have 1 mg, is that ok?" and as signal is dependent on the molar concentration, the answers is always dependent on molecular size.

To address some of these questions a comparative study was undertaken at the newly formed Collaborative Research Platform for NMR spectroscopy at The University of Queensland. Samples of ca. 1 mg and 10 mg of molecules with small and larger molecular weights were compared across spectrometers at 400 MHz up to 900 MHz, comparing lower-field room temperature probes with higher-field helium cryoprobes.

This simple study aims to give some data for NMR users to determine optimal sample amounts, spectrometer selection and cost-efficiency. As an 8-hour ^{13}C spectrum at 100 MHz is likely not the best use of spectrometer time and user money when compared with a 30 min spectrum at 226 MHz.

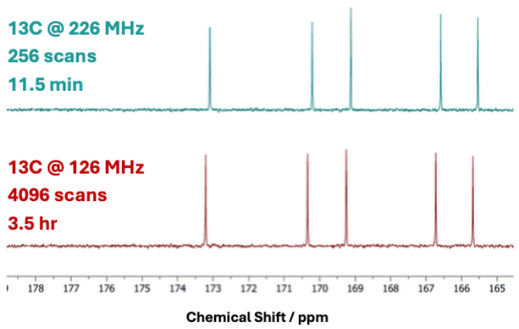


Figure 1. $^{13}C\{^{1}H\}$ spectra of a Taxol sample (60 mM) at 900 MHz (TCI-CP) with 256 scans and 500 MHz (RT probe) with 4096 scans with comparable signal-to-noise ratios.

References:
1. Timothy D. W. Claridge, High Resolution NMR Techniques in Organic Chemistry, 3rd ed., Elsevier: Oxford, 2016.
2. Bruker Corporation. Cryoprobes. https://www.bruker.com/en/products-and-solutions/mr/nmr/cryoprobes.html.

P 2. Metabolic response of cells to mechanical stimulus studied with Rheo-NMR

Frederick D. Nightingale[1], Kenneth Chen[1], Josephine Miller[1], Petrik Galvosas[1,2]

[1]School of Chemical and Physical Sciences, Victoria University of Wellington, New Zealand,
[2]MacDiarmid Institute for Advanced Materials and Nanotechnology, New Zealand

Red Blood Cells show increased metabolic rates under deformation. Specifically lactate production from glucose in RBCs suspended in gelatine gels have shown an increase of 90% in production rate [1].
The findings highlight that mechanical deformation activates ion channels, notably Piezo 1, leading to calcium influx and enhanced glycolytic activity. These insights explain the link between mechanical stimuli and cellular metabolism, advancing understanding of erythrocyte behaviour under flow conditions [1].

Here, the metabolic response of red blood cells (RBCs) to mechanical shear stress is investigated using Rheo-NMR techniques [2]. Experiments involved applying high shear rates in excess of $1000s^{-1}$ to Red Blood Cell suspensions within specialized NMR-compatible rheological cells. In order to measure metabolic activity, particularly lactate production was monitored with ^{13}C NMR spectroscopy and ^{133}Cs NMR exchange NMR.

Previous results found a significant metabolic rate increases (up to 250%) at shear rates exceeding $1000s^{-1}$, with variations observed depending on the shear cell geometry [3]. This increased metabolic rate should be accompanied by an increased ion flux through the cell membrane via Piezo 1. Therefore, ^{133}Cs ion exchange spectroscopy was used to monitor ion flux under various shear rates.

The research presented here highlights the potential of Rheo-NMR as a powerful tool for studying biomechanical effects on cell physiology, with implications for blood flow dynamics and related medical applications.

References:
1. Kuchel, P. W., and Shishmarev, D., Science Advances, 3, eaao1016, (2017)
2 Callaghan, P. T., Rep. Prog. Phys. 62 599-670, (1999)
3 Milius, J., MSc thesis, Metabolic Response of Erythrocytes under Shear Stress. (2019).

P 3. Characterising multiphase flow using two dimensional T_2 – propagator correlation NMR

Viator Mujuni[1] and Petrik Galvosas[1]

[1]School of Chemical and Physical Sciences, Victoria University of Wellington, New Zealand

Quantifying fluid flow in industrial settings ought to be robust and low cost, requirements often met by low field NMR systems. However, additional demands may need to be satisfied if flowing materials are composed of more than one component (multiphase flow). To determine specific volume flow rates in such conditions, discriminating material properties for the different phases need to be found [1,2]. The individual components of the sample can be characterized and analysed by determining their corresponding distinct relaxation rates [3].

Here, we suggest using the correlation of fluid displacement with T_2 relaxation, to determine the T_2 of the stationary fluid components near the pipe wall. This would in turn enable us to measure velocities of individual components by determining component specific signal decays due to outflow [1]. A suitable method would be the Laplace Nuclear Magnetic Resonance Propagator (LNMRP) technique [4] which allows us to extract the T_2 values of fluids under rest and link flow rates with the respective individual components.

One drawback of LNMRP technique is that it requires a considerably long experimental time, a common difficulty for multidimensional (NMR) experiments [5]. To mitigate this issue, we apply sparse sampling methods in which only a fraction of the full dataset is collected [6] and reconstructed by different mathematical strategies such as multi-dimensional decomposition, linear prediction, zero filling or Poisson gap algorithms.

Current implementations utilise high field wide bore spectroscopy NMR systems which allow us to develop the method under near ideal environment (homogeneous B_0 and B_1 fields, presence of 3D gradient system). Furthermore, conditions found in low field NMR systems may be mimicked using gradient and shim controls, which may help to port the method to low field instruments.

References:
1 Feng D, Chunming X, Shiwen C, Guanhong C, Mengying W, Huabing L, Jianjun Z, Qun L, Gang C, Dongping X, Ye T, and Lizhi X, Pet. Explor. Dev., vol. 47, pp. 855–866, 2020.
2 Zargar M, Johns ML, Aljindan J, Noui-Mehidi N, and O'Neill K, SPE Prod & Oper, vol. 36, pp. 423–436, 2021.
3 Callaghan PT, Translational dynamics and magnetic resonance: principles of pulsed gradient spin echo NMR. New York: Oxford University Press, 2011.
4 Britton MM, Graham RG, and Packer KJ, J. Magn. Reson., vol. 169, pp. 203–214, 2004.
5 Telkki VV, Urbańczyk M, and Zhivonitko V, Prog. Nucl. Magn. Reson. Spect., vol. 126–127, pp.101-120, 2021.
6 Mitchell J, Fordham EJ, Graf von der Schulenburg DA, Holland DJ, Sederman AJ, Johns ML, and Gladden LF, in AIP Conference Proceedings, Cambridge: AIP, 2008, pp. 71–74.

P 4. Structural investigation of the Non-Ribosomal Peptide Synthetase complex responsible for teicoplanin glycopeptide antibiotic biosynthesis

Jennifer D. Naughton[1], Madeline Pesch[2], Callum Macfarlane[3], Theo Crawford[1], Mehdi Mobli[1], Martin Stroet[3], Max J. Cryle[2], Jeffrey R. Harmer[1]

[1]Centre for Advanced Imaging, Australian Institute for Bioengineering and Nanotechnology, University of Queensland, Brisbane, Australia
[2]Department of Biochemistry and Molecular Biology, Biomedicine Discovery Institute, Monash University, Melbourne, Australia
[3]Centre for Organic Photonics and Electronics, School of Chemistry and Molecular Biosciences, University of Queensland, Brisbane, Australia

Escalation of antibiotic resistance is an ever-mounting concern in clinics worldwide. Glycopeptide antibiotics (GPAs), like teicoplanin, serve as last-resort treatments for multi-drug resistant Gram-positive bacterial infections. The extreme difficulty and associated high cost to produce these glycopeptide antibiotics via total synthesis means production scale up for medicinal use is unfeasible, making investigation of GPA's complex natural biosynthesis mechanisms greatly necessary to enable more viable antibiotic production and discovery options. Teicoplanin biosynthesis combines two powerful secondary metabolism enzymatic classes through initial non-ribosomal peptide synthesis (NRPS), followed by oxidative aromatic cross-linking cyclisation reaction cascades, which represent major synthetic challenges. The cytochrome P450 (Oxy) enzymes responsible for mediating these cross-linking reactions exhibit a conserved order of crosslinking activity, occurring while the antibiotic heptapeptide remains tethered to the peptidyl carrier protein (PCP) domain within the seventh and final NRPS module. These NRPS domain/enzyme complexes display multiple conformations facilitated by flexible linkers, demonstrating the dynamic nature of this system[1]. However, despite their importance, structural insights remain lacking regarding these domain arrangements during enzyme binding[2].

Our study aims to address this gap by investigating spatial positioning of the teicoplanin PCP-X didomain relative to the bound enzyme during the first cross-linking reaction step. To elucidate the PCP-X/Oxy complex structure via DEER EPR spectroscopy with excess enzyme, the didomain constructs were spin-labelled with MTSL nitroxide and loaded with the GPA teicoplanin peptide via Sfp transferase. Distance distribution measurements between label positions, obtained at Q-band frequency, were combined with computational modelling and molecular dynamic simulations to produce a tertiary structure of the enzyme-bound protein complex. This structural model provides one of the initial insights into the domain-enzyme arrangements during the first cross-linking reaction of teicoplanin biosynthesis. These findings advance our understanding of NRPS structural dynamics during this highly complex GPA production pathway and provide foundational information that can be utilised for synthetic production of existing and potentially novel derivative GPAs, an essential step in combating antibiotic resistance.

References:
1 Ho YTC, Zhao Y, Tailhades J, Cryle MJ. A Chemoenzymatic Approach to Investigate Cytochrome P450 Cross-Linking in Glycopeptide Antibiotic Biosynthesis. Methods Mol Biol. 2023;2670:187-206.
2 Haslinger K, Brieke C, Uhlmann S, Sieverling L, Süssmuth RD, Cryle MJ. The Structure of a Transient Complex of a Nonribosomal Peptide Synthetase and a Cytochrome P450 Monooxygenase. Angewandte Chemie International Edition. 2014;53(32):8518-22.

P 5. The orphan opioid peptide synenkephalin as a novel biomarker for cardiorenal function

Anneka C. Pereira Schmidt[1], Theo Crawford[1], Jessica J. Harrison[2], Jody Hobson-Peters[2], Mehdi Mobli[1]

[1]Australian Institute for Bioengineering and Nanotechnology, The University of Queensland, Brisbane, Australia
[2]School of Chemistry and Molecular Biosciences, The University of Queensland, Brisbane, Queensland

Synenkephalin is a 73-amino acid peptide produced by the proenkephalin gene, which also encodes the enkephalin opioid peptides. It belongs to a family of yet uncharacterised disulfide-rich peptides, the so-called 'synpeptides', that are co-expressed with the endogenous opioid peptides. These synpeptides do not contain the opioid receptor binding motif, and they may serve a unique biological purpose. Their disulfide-rich structures – imparting stability and resistance to proteolysis – are highly suggestive of some physiological role. Given its stoichiometric co-expression with enkephalins, synenkephalin may serve as a surrogate biomarker for diseases associated with elevated enkephalin production, such as renal dysfunction and cardiorenal syndromes – conditions for which early and accurate diagnostic tools are currently limited. This work aims to develop a blood-based diagnostic assay for synenkephalin detection. For this, three different strategies have been taken to generate binders against synenkephalin: monoclonal antibodies raised in mouse, nanobodies raised in alpaca, and de novo designed binders generated using a RoseTTAFold-based diffusion model. These candidates are currently being screened for binding performance, including NMR-based affinity characterisation and epitope mapping, and the most promising will be selected for assay development. This work lays the foundation for a novel diagnostic approach targeting synenkephalin, with potential applications in early detection and monitoring of renal-related diseases.

P 6. NMR insights into the dynamic monomer-dimer equilibrium of the second bromodomain in BET proteins

Biswaranjan Mohanty, Karishma Patel, Xufei Jing, Josh Maxwell, Xavier Reid, Richard Payne, Joel Mackay

The University of Sydney, Sydney, Australia

Bromodomain and extra-terminal (BET) proteins BRD2, BRD3, and BRD4 regulate gene expression by recognizing acetylated lysine residues on histone tails through their two bromodomains (BD1 and BD2). They are recognized as important therapeutic targets in several diseases, most notably cancer. While many biochemical and structural studies have focused on isolated BD1 and BD2 constructs, the question of whether the these domains can self-associate remained unresolved. Using solution NMR spectroscopy, we show that BD2 domains undergo concentration-dependent dimerization, whereas BD1 domains remain monomeric even at concentrations as high as 500 μM. All three BRD2-BD2, BRD3-BD2 and BRD4-BD2 proteins exhibited reversible monomer-dimer formation with monomer-dimer dissociation constant of 150 - 200 μM. Furthermore, we investigated the binding of an acetylated peptide to BRD3-BD2 under conditions favouring predominantly monomeric and dimeric states. Our results indicate that dimerization modestly reduces peptide-binding affinity. These findings establish the oligomerization potential of BD2 independent of ligand binding or phosphorylation, which may have direct implications for understanding ligand binding and thus for their physiological significance as epigenetic regulators.

P 7. Characterization of a Novel β-Hairpin Peptide from the Fire Sea Urchin Asthenosoma varium

Mahesh Upadhyay,[1] David Wilson,[1] Richard Harris,[2,3] Robert Courtney,[1] Jamie Seymour,[1] Ira Cooke,[4,5] Sina Ehlert[6] and Norelle L. Daly[1]

[1]Australian Institute of Tropical Health and Medicine (AITHM), James Cook University, Cairns, QLD, Australia. [2]Australian Institute of Marine Science (AIMS), Cape Cleveland, 4810, Australia [3]School of Science, Technology and Engineering, University of the Sunshine Coast, Sippy Downs, Queensland 4556, Australia. [4]Molecular Genetics Unit, James Cook University, Townsville, QLD 4811 Australia. [5]Department of Marine Biology and Aquaculture, James Cook University, Townsville, 15 QLD 4811 Australia. [6]College of Science and Engineering, James Cook University, Townsville, QLD, Australia

Marine-derived peptides represent a prolific source of structurally diverse and biologically active molecules with significant potential for therapeutic development. While extensive research has focused on peptides from cone snails and corals, sea urchins remain comparatively understudied despite their biochemical complexity.

In this study, extracts from *Asthenosoma varium* were analyzed using multidimensional NMR spectroscopy and complementary mass spectrometric techniques to explore their molecular diversity. The extract revealed a range of low to mid molecular weight peptides with varied structural features. Among these, a novel peptide exhibiting a β-hairpin structural motif was characterized, marking one of the first reports of such a structure from a sea urchin. Unlike many disulfide-rich marine peptides, this molecule lacks cysteine residues, suggesting an alternative mode of structural stabilization.

Further investigations are underway to elucidate its biological role and therapeutic potential. These findings expand our understanding of marine peptide diversity and highlight *A. varium* as an untapped source of bioactive molecules for drug discovery.

P 8. Single-Sided Portable NMR: The Role of RF Non-Ideality in Understanding Diffusion Attenuation of the Magnetisation Profile

Dean Greenslade

Queensland University of Technology, Brisbane, Australia

In recent years, an increasing amount of research has been conducted into the application of single-sided portable NMR to medical imaging. Portable NMR is potentially complementary to conventional, high-field MRI by being both more mobile and cost-efficient while reporting on the same quantitative tissue characteristics as conventional MRI (e.g. diffusion coefficients or spin-relaxation times). This makes it an attractive imaging modality in remote-community or away-from-hospital settings, where high-field MRI is not easily available, as well as for routine screening tasks, where high-field MRI may not be cost-efficient.

While the underlying physics of conventional MRI and portable NMR are the same, there are significant practical differences, the most significant being the presence of a strong, permanent magnetic field gradient in single-sided portable NMR instrumentation. Consequently, rather than producing near-ideal 90- or 180-degree radio-frequency pulses, portable NMR yields a spatially dependent distribution of rotation angles at each pulse.

This spatial dependence introduces complex winding of the magnetisation profile during RF pulses, in turn leading to elevated diffusion attenuation during free precession periods. Several sets of experiments have shown a clear bias between the measured diffusion coefficient of an agar gel sample as measured by stimulated echo pulse sequence with a CPMG echo train versus direct acquisition of the stimulated echo. Additionally, it has been observed that the apparent diffusion coefficient is dependent on various temporal parameters such as the CPMG echo time and the diffusion time.

We will discuss our attempts to analyse, through simulations, the stimulated echo pulse sequence and the mechanics of how these dependencies arise. The aim being to explain how and to what degree RF pulses can distort the measured diffusion coefficient. Direct acquisition stimulated echo, despite providing a lower SNR than the CPMG-detected STE, was identified as the best way to analyse this given that it largely eliminates contributions from contaminant coherence transfer pathways.

P 9. Investigation of the metabolic defluorination of fluorobeta-alanine as a possible mechanism for generation of cardiotoxic metabolites in cancer patients

Adrian Blaser, Shreeya Bhardwaj, Sihan Wang, Kathryn Burns, Malcolm Tingle, Nuala Helsby

University of Auckland, Auckland, NZ

Clinical use of the anticancer drug 5-fluorouracil is associated with cardiotoxicity, with approximately 5% of patients experiencing symptoms such as severe chest-pain or life-threatening myocardial infarction. This cardiotoxicity is assumed to involve the metabolic biotransformation of the drug into fluoroacetate which then inhibits aconitase and perturbs the mitochondrial Kreb's cycle. However, fluoroacetate has only been observed in patients following administration of 5-fluorouracil formulations which contained impurities such as fluoroacetaldehyde. Notably, the major circulating metabolite of 5-fluorouracil in humans is fluorobeta-alanine (FBAL). It has previously been demonstrated that rat liver AGXT2 enzyme can defluorinate FBAL to release free fluoride ion [PMID: 7503799]. Our hypothesis is that it is the generation of fluoride ion, not fluoroacetate formation, that is the likely cause of 5-fluorouracil induced cardiotoxicity.

The in vitro hepatic metabolism of FBAL (in rat and human liver homogenates) was investigated and the rate of fluoride release quantified using fluoride ion specific potentiometry. ^{19}F-NMR (400 MHz, 26000 scans) with comparison to authentic standards, was used to further characterise the metabolic fate of FBAL in these samples.

Rat liver homogenate catalysed concentration-dependent FBAL defluorination with a Vmax of 5.84 nmol/h/mg and KM of 5.54 mM. Human liver homogenate data will also be discussed. Following metabolism FBAL, ^{19}F-NMR could detect formation of fluoride (δ– 45.6 ppm) in rat liver and a number of new signals easily distinguished from the FBAL substrate (δ-112.8 ppm) were observed (e.g. δ -112.4, -113.0 and -113.1 ppm). These were also observed in human liver. The -113.1 ppm signal is consistent with literature value for 3-fluoro-2-hydroxypropanoic acid (FHPA). Authentic fluoroacetate standard gave a δ-147.7 ppm and this signal was not observed following human or rat liver metabolism. Initial ^{19}F-NMR analysis of urine samples from patients receiving 5-fluorouracil confirmed detection of fluoride ion as well as the signal tentatively identified as FHPA, but fluoroacetate was not detected. Further identification of the products of FBAL metabolism by mass-spectrometry are planned.

Conclusions: These initial results suggest that FBAL is not extensively metabolised to fluoroacetate, however fluoride ion formation was observed. Clinical investigations are ongoing to determine relationships between extent of fluoride ion formation and cardiotoxicity.

We acknowledge funding from Te Aka Matepukupuku (UoA University Research Centre).

P 10. Oxidation of the cell death protein caspase-9 by hypothiocyanous acid triggers formation of amyloid aggregates that influence cell death outcomes

Sydney Austad,[1] Abigail Schwartfeger,[1] Christoph Goebl,[2] Mark Hampton,[2] Vanessa Morris[1]

[1]University of Canterbury, Christchurch, New Zealand
[2]University of Otago, Christchurch, New Zealand

Both nonlytic and lytic (inflammatory) programmed cell death are essential in humans for developing and maintaining healthy tissue, mounting immune responses, and preventing cancers, and their dysregulation is implicated in many diseases. Central to these cell death pathways is a family of cysteine protease enzymes called caspases. Proteolytic self-cleavage activates caspases and determines the type of cell death. Recent published work by our group demonstrated that caspase-8 is regulated by treatment of cells with the immune-derived oxidant hypothiocyanous acid. This treatment inhibits nonlytic apoptosis and instead promotes lytic necroptosis. Likewise, we demonstrate here that caspase-9, an initiator of apoptosis via the intrinsic pathway following DNA damage or mitochondrial distress, is also sensitive to inactivation by hypothiocyanous acid. This project aims to characterise the structural and functional changes occurring upon oxidation and inactivation of caspase-9 by hypothiocyanous acid and how these changes influence biochemical outcomes and cell death.

Using a variety of established biophysical methods, we have found that hypothiocyanous acid oxidation of recombinant human caspase-9 results in the formation of a catalytically inactive dimer which is prone to aggregation. These aggregates are insoluble and demonstrate several amyloid-like characteristics, such as loss of alpha-helical character in far-UV CD spectroscopy, binding of the amyloid dye Thioflavin-T, and fibrilisation in atomic force microscopy (AFM). X-ray fibre diffraction reflections are also consistent with spacing of beta-sheet structures of amyloids. Additionally, we observed formation of insoluble caspase-9 aggregates in human cells upon stimulation of apoptosis and subsequent oxidation of whole cells with hypothiocyanous acid. Overall, this work demonstrates a propensity of the cell death protein caspase-9 to form amyloids upon cysteine oxidation, representing a novel, redox regulation mechanism.

P 11. Mixing polymer cocktails: Diffusion and relaxation distributions of mixed and polydisperse poly (ethylene oxide) melts

Siegfried Stapf,[1] Kevin Lindt,[1] Carlos Mattea,[1] Sarah Maihiot,[2]

[1]TU Ilmenau, Ilmenau, Germany
[2]Bruker Biospin, Germany

Theoretical predictions and experimental evidence for polymer melt dynamics have benefitted from a combination of several NMR techniques: whereas pulsed and constant field gradient diffusometry determines mean-squared displacements (MSD) between about 1 ms to 1 s, relaxometry of attached protons and other nuclei covers a much wider range of times but gives more indirect information about motion. Common to the vast majority of studies is the restriction to ideal, monodisperse linear molecules with a well-defined length, a situation that can be approximated by some technical polymers but is never perfectly met. Important questions remain largely unanswered: how does a distribution of molecular weights affect the measured quantities, and are diffusion and relaxation affected in different ways?

PEO melt samples of narrow dispersity (typically 1.1 or better) in bulk and in mixtures of 10% ^{1}H-containing in 90% ^{2}H-containing PEO were studied by PFG diffusometry, relaxometry and echo analysis (e.g. Hahn, solid) and were compared to artificially broadened molecular weight distributions obtained from mixing several samples with defined molecular weights. Measurements were predominantly carried out on the ^{1}H resonance, i.e. the minority component. Diffusion data were obtained by a Bruker Diffusion Observe Broadband Probe providing a maximum pulse gradient strength of either 17 or 29 T/m at a resonance frequency of 500 MHz and at variable temperatures above the bulk melting point of PEO between 343 and 373 K. Echo and relaxation dispersion data were collected on a Bruker Avance III 7T spectrometer and a Stelar Spinmaster Relaxometer in the field range 0.2 mT to 0.5 T.

This study focused on the change of diffusion and relaxation properties of a component A in a matrix B, or of a defined mixture, relative to the theoretical predictions for melts below and above the critical molecular weight of about 5 kDa for PEO. For diffusion, the conditions of the majority matrix (90 vol%) dominate the minority component, i.e. short chains in a matrix of long chains are severely restricted in their mobility whereas long chains in a matrix of short chains show a much increased mobility compared to the bulk. A weaker weight dependence in mixtures of species in a lighter matrix, compared to simple melts, provides important information for fundamental variations of the established reptation theory. Relaxation qualitatively follows this trend and supports the concept of Rouse dynamics and chain reptation, respectively, as deuteration is sufficient to suppress intermolecular relaxation contributions. For these mixtures, relaxation is mostly exponential, while deviations from simple Gaussian diffusion decays are identified even for the narrowest molecular weight distributions. The latter effect becomes much more pronounced in polymer mixtures of different weight, suggesting diffusometry as a possible tool for the quantification of polymer polydispersity in the melt.

P 12. Quantitative NMR of Magnetite at Laboratory and Bulk Scale

Matthew Crowther, Richard Yong, Thai Ly, Andrew Curtain

CSIRO, Australia

Magnetite (Fe_3O_4) is a key naturally occurring source of iron used in the steel industry to meet the rising global demand for steel due to rapid industrialisation. Methods to reduce processing of low yield material are desirable as it decreases waste and energy usage increasing the profitability of mines. One such method is bulk ore sorting, applicable if the desirable mineral content of bulk ore can be quantified. The use of magnetic resonance is well suited for bulk scale quantification and has been previously demonstrated for on-line monitoring system for chalcopyrite, an important copper-bearing mineral [1]. Magnetite is an excellent candidate for such a measurement due to its ferrimagnetic structure providing a static magnetic field on the 57Fe nuclei, and the existence of the ferromagnetic enhancement factor providing a significant increase in NMR signal magnitude and corresponding decrease in required power.

A custom built laboratory nuclear magnetic resonance spectrometer was used to quantify the magnetite grade of 35 synthetic magnetite samples and 3 natural samples. An excellent linear correlation between magnetite grade as determined by quantitative x-ray diffraction, and magnetic resonance spin-echo signal was achieved with R^2=0.98 and R^2=1.00 respectively to two decimal places. A bulk spectrometer intended for use around iron ore belts was built and the two bulk samples from Braemar iron formation were subjected to magnetite magnetic resonance. An excellent correlation between magnetite mass and magnetic resonance spin-echo signal was achieved. The theoretical lower detection limit based on the results obtained was calculated to be 1.1kg of pure magnetite in 1s of measurement time. As such, magnetic resonance of magnetite presents an excellent opportunity for bulk quantification or beneficiation processes.

References:
1 P. Coghill, N. Cutmore, J. Lehmann-Horn, B. Lovric, A. McEwan, D. Milinkovic, D. Miljak, G. Roberts and R. Yong, "Demonstration of a Magnetic Resonance Analyser for Bulk Copper Ore Sorting," 2018.

P 13. Nuclear Quadrupole Resonance Detection of Land Mines Exposed to Temperature Gradients

Lewis Robertson,

CSIRO, Lucas Heights, Australia

Land mine contamination remains a global humanitarian challenge, responsible for thousands of annual casualties. Nuclear Quadrupole Resonance (NQR) offers a promising alternative to conventional land mine detection methods by directly sensing explosive compounds, reducing false positives with the goal of expediting clearance efforts.

In the field, land mines are exposed to environmental conditions such as sunlight and ambient temperature fluctuations. These conditions can create stark temperature gradients in the soil, particularly near the surface. Due to the temperature dependence of NQR transitions this can lead to an inhomogeneous broadening of the spectral line. If this broadening is not accounted for, then in extreme cases it can render the explosive undetectable. While various techniques exist in the literature to measure strongly broadened spectral lines, they are often challenging to implement in practical systems.

In this study, we present a series of controlled laboratory experiments investigating the performance of free induction decay (FID) and echo sequences targeting the ^{14}N transition at 5.192 MHz in the explosive compound RDX under varying thermal conditions. The temperature gradients applied in the laboratory were designed to realistically mimic those encountered in sun-exposed soil environments. These measurements demonstrate that both FID and echo sequences have complementary attributes useful for RDX detection. The results reveal a clear transition in performance between FID and echo modes as temperature gradients increase, allowing application of optimised measurement strategies based on environmental parameters.

Understanding how environmental factors, such as temperature gradients, influence NQR measurements is crucial for explosives detection under real-world conditions.

P 14. Application of 2D and 3D Diffusion-Ordered NMR Spectroscopy Techniques to Chemical Forensic Profiling of Organophosphorus Nerve Agents

Renee Webster

CSIRO, Australia

The ongoing use of chemical warfare agents (CWAs) in conflicts, assassinations, and terrorist attacks means that the detection and identification of these compounds are crucial. Many traditional analytical techniques are destructive and require lengthy sample preparation, therefore the development and validation of new analytical methods is essential. Here, compounds that are both precursor and degradation products of novichok analogues have been characterised using 2D ^{1}H-^{13}C heteronuclear multiple quantum coherence (HMQC) nuclear magnetic resonance (NMR). The detection and identification of these compounds is vital for understanding the structures of Novichok analogues and to allow efficient analysis and identification using a non-destructive method. Furthermore, mixtures of compounds related to the Chemical Weapons Convention (CWC) were analysed using 2D ^{1}H diffusion-ordered spectroscopy (DOSY) and 3D ^{1}H-^{13}C DOSY-HMQC NMR experiments, which proved useful for analysing compounds related to organophosphorus nerve agents (OPNAs), indicating their potential effectiveness in assessing real CWAs.

P 15. Investigation of the Nuclear Quadrupole Resonance Characteristics of Two Common Landmine Constituents

Robert de Gille, Lewis Robertson, David Miljak, Peggy Schoenherr

CSIRO, Australia

Landmine contamination is a persistent and distressing problem which calls for the technological development of landmine detectors. The chemical specificity of nuclear quadrupole resonance (NQR) can be leveraged to directly measure explosive materials, circumventing the challenges of high false positive rates associated with traditional detectors. However, the task of landmine detection using NQR is complicated by the lack of control over the environmental conditions of minefields.

The resonance frequencies and relaxation rates of the nuclear quadrupole resonances of Royal Demolition Explosive (RDX) and trinitrotoluene (TNT), the most ubiquitous substances in landmines, depend on environmental conditions including temperature. Here, various resonances of the two substances are characterised in a temperature and humidity-controlled environment, replicating conditions that are found in the subsurface, outdoor settings where landmines are located. The T_1, T_2, and T_2* relaxation rates along with the transition frequencies are monitored over varied environmental conditions.

Significant changes in the relaxation rates are observed with changing experimental conditions in both substances. Differences in relaxation rates determine the optimal pulse sequence and pulse sequence parameters to maximise the signal to noise ratio achievable by an NQR detector. Due to these factors, this work forms an important design consideration for landmine detectors, including our recently developed RDX detector. The results form a crucial reference for optimising the sensitivity and robustness to enable the usage of NQR sensors in a wide range of environments.

P 16. Chemical Synthesis and Characterisation of the Structurally and Functionally Unique Peptide Natural Product Recifin A

K. Johan Rosengren, Richard J. Clark

The University of Queensland, School of Biomedical Sciences, Brisbane, Australia

Recifin A is a 42 amino acid cysteine-rich peptide isolated from the marine sponge Axinella sp. It represents the inaugural member of a newly identified structural class termed the "tyrosine-lock"[1]. This unique fold features a central four-stranded β-sheet stabilized by three disulfide bonds. The disulfides are arranged such that they together with connecting backbone segments form an embedded ring that wraps around one of the β-strands, encapsulating a buried tyrosine side chain, and resulting in a tightly constrained molecular architecture.

Functionally, recifin A acts as a selective allosteric inhibitor of tyrosyl-DNA phosphodiesterase 1 (TDP1), a DNA repair enzyme implicated in the repair of topoisomerase I-induced DNA damage1. By binding to a site distinct from the active site, recifin A modulates TDP1 activity, thereby enhancing the cytotoxic effects of topoisomerase inhibitors such as topotecan and irinotecan. This mechanism positions recifin A as a promising candidate for combination cancer therapies aimed at overcoming resistance to these chemotherapeutic agents.

The total chemical synthesis of recifin A was achieved using native chemical ligation chemistry and solid-phase peptide synthesis (SPPS), followed by oxidative folding under controlled redox conditions to promote correct disulfide bond formation[2]. Despite the complex fold the native structure is remarkably favoured during folding, and synthetic recifin A and analogues were structurally validated via NMR spectroscopy. Pharmacological studies revealed initial structure activity relationships that suggest that the intrinsically disordered regulatory domain of TDP-1 wraps around recifin A, creating a large contact area.

The discovery of recifin A underscores the potential of marine-derived peptides in drug development and introduces the tyrosine-lock fold as a novel scaffold for therapeutic intervention. Its unique structural features and functional properties make it a valuable subject for further research in the design of targeted cancer therapies.

References:
1. Krumpe LRH, Wilson BAP, Marchand C, Sunassee SN, Bermingham A, Wang W, Price E, Guszczynski T, Kelley JA, Gustafson KR, Pommier Y, Rosengren KJ, Schroeder CI, O'Keefe BR. Recifin A, Initial Example of the Tyr-Lock Peptide Structural Family, Is a Selective Allosteric Inhibitor of Tyrosyl-DNA Phosphodiesterase I. J Am Chem Soc. 2020 142(50):21178-21188.
2. Smallwood TB, Krumpe LRH, Payne CD, Klein VG, O'Keefe BR, Clark RJ, Schroeder CI, Rosengren KJ. Picking the tyrosine-lock: chemical synthesis of the tyrosyl-DNA phosphodiesterase I inhibitor recifin A and analogues. Chem Sci. 2024 15(33):13227-13233.

P 17. Alpha-Methylation of the Peptide Backbone as a Method for Stabilising Helical Structure

Devika Praseetha Suresh,[1] Mohammed Akhter Hossein,[2] Ross Bathgate,[2] K. Johan Rosengren,[1]

[1]The University of Queensland, School of Biomedical Sciences, Brisbane, Australia.
[2]Florey Institute, Melbourne, Australia

Peptides occupy a central position in chemical biology and therapeutic design, but their tendency to adopt unstable or disordered conformations in solution remains a major challenge. Many bioactive peptides rely on well-defined secondary structures, such as alpha-helices, to bind to their receptors effectively. However, outside of their native contexts, such peptides often lose their structural order, limiting their biological activity. Alpha-methyl amino acids have been proposed as effective helix-inducing elements. Earlier work on the relaxin-3 B-chain using alpha-methyl phenylalanine suggested enhanced helicity. The results prompted a systematic examination of the generalisability of alpha-methyl amino acid-mediated stabilisation across diverse peptide systems.

To assess this, four peptide scaffolds representing distinct biological classes were analysed: the antimicrobial peptide magainin-2, the neuropeptides NPY and galanin and the metabolic hormone GLP-1. In each system, alpha-methyl amino acids were placed at i,i+4 positions to probe their ability to reinforce local helical structure and each analogue was compared with its unmodified counterpart. Comprehensive 2D NMR characterisation under aqueous conditions was done using TOCSY, NOESY, ^{1}H-^{13}C HSQC and ^{1}H-^{15}N HSQC spectra, to assign backbone resonances, assess NOE cross-peak patterns and analyse secondary chemical shift trends. These data revealed consistent local helix reinforcement adjacent to alpha-methylated sites across all peptide families, despite their divergent sequence contexts. Among the systems examined, NPY analogue exhibited the most pronounced ordering, prompting further structural analysis. Assigned chemical shifts were used for TALOS-N evaluation. But predicted torsion angles near alpha-methylated positions showed inconsistencies with observed NOE patterns. Therefore, angle restraints were not used and structures were calculated in CYANA using NOE-derived distance restraints only. This produced well-converged structural ensembles with a clearly defined helical segment centred around the modified positions. For comparison, the structures calculated for the control NPY analogue did not display significant helical character in the same region, demonstrating the local stabilising effect of alpha-methylation.

Taken together, these observations indicate that alpha-methylation can reinforce short-range ordering reliably, although the degree of helicity enhancement varies with each peptide's intrinsic conformational tendencies and sensitivity to its solvent environment. Consistent behaviour across distinct peptide systems suggests the potential of alpha-methylation as a generalisable stabilisation strategy in peptide design. More broadly, the study highlights the use of NMR spectroscopy to analyse residue-specific conformational responses to chemical modification. It can serve as a key tool for guiding future peptide engineering and ligand design efforts.

P 18. Structural Design of Relaxin-3 Variants Using Alpha-Methylated Amino Acids

Swetha G. Chazhikulam,[1] Mohammed Akhter Hossein,[2] Ross Bathgate,[2] K. Johan Rosengren,[1]

[1]The University of Queensland, School of Biomedical Sciences, Brisbane, Australia.
[2]Florey Institute, Melbourne, Australia

Relaxin-3 is a neuropeptide central to regulating stress, arousal, and mood via the RXFP3 receptor, making it an emerging target in therapies for neuropsychiatric and metabolic disorders. The relaxin-3 B-chain represents a minimal structural scaffold crucial for receptor recognition. Given its bioactive conformation when complexed with the A-chain is largely helical, but this secondary structure is lost when removed from the A-chain, it serves as a valuable model for studying α-helical stabilization strategies in short peptides. Previous studies have shown that α-methylation, particularly with alpha-methyl-phenylalanine (alphaF), can enhance helical stability through a combination of steric restriction and Pi-Pi stacking interactions. This study aimed to evaluate whether stabilization could be achieved using combinations of positively charged and aromatic amino acids with alpha-methylation, utilizing a combination of steric restriction and cation-pi interactions.

A series of relaxin-3 B-chain analogues with alpha-methyl substitutions were analysed using multidimensional nuclear magnetic resonance (NMR) spectroscopy, including total correlation spectroscopy (TOCSY), nuclear Overhauser spectroscopy (NOESY) and heteronuclear single quantum coherence (HSQC) experiments. Secondary chemical shift analyses revealed that all analogues preserved some aplpa-helical profile characterized by negative secondary chemical shifts for HA and CB nuclei, and positive secondary chemical shifts for CA. This confirms that alpha-methylation support helicity regardless of side-chain variation. However, no distinct NOE cross-peaks or spectral features indicative of stable cation-pi interactions were detected between the modified amino acids, suggesting that the proposed electrostatic reinforcement did not materialize. Instead, helix preservation and reinforcement were primarily attributed to alpha-methyl-induced backbone rigidity and local hydrophobic packing between aromatic residues.

Comparative analysis against previously studied alpha-methylated alanine and phenylalanine analogues indicated that phenylalanine substitution produced the most pronounced helical signatures, consistent with enhanced structural preorganisation arising from cooperative Pi-Pi stacking and alpha-methyl backbone restriction. These findings reinforce the utility of alpha-methylation as a robust helix-supporting strategy and provide a structural framework for developing next-generation relaxin analogues. Future studies should explore alternative charged residues and positioning in order to optimise the potential for further side chain interactions.

P 19. Fully Automated Resonance Assignment of Peptides Using Natural Abundance Heteronuclear 2D NMR Experiments

Paul Hammond, K. Johan Rosengren

The University of Queensland, School of Biomedical Sciences, Brisbane, Australia.

NMR spectroscopy has long been the leading choice for determining the structure of peptides in solution, generating excellent quality spectra with rich structural information due to peptides favourable fast tumbling properties. However, most peptides studied by NMR are derived from natural sources or have been chemically synthesised, therefore are not isotopically enriched making 'triple-resonance' experiments unfeasible. Instead, the analysis of peptides is largely a manual process relying primarily on homonuclear proton experiment. Here, we aim to demonstrate that with modern spectrometers with cryoprobes sensitivity is sufficient so that homonuclear and heteronuclear datasets can be recorded to employ automatic resonance assignment algorithms in CYANA, enabling near complete assignment of ^{1}H, ^{13}C and ^{15}N atoms. We recorded TOCSY, NOESY, HSQC, HSQC-TOCSY and HMBC data, the combination of which overcomes resonance overlaps and resolving most ambiguities. We show that the automatic assignments made are consistent with manual efforts and additionally, assignments made and used to generate structural restraints can be used to generate structures that are of similar quality to those produced through manual analysis. Our findings illustrate an effective strategy for the automation of chemical shift assignment of non-enriched two-dimensional NMR datasets, which reduces the time and cost of bioactive peptide discovery and drug development.

P 20. Fluid Flow Regimes in Triply Periodic Minimal Surface Structures Studied by Dynamic NMR Microscopy and CFD

Daniel A. Clarke,[1,2] Petrik Galvosas,[1] and Daniel J. Holland[3]

[1]School of Chemical and Physical Sciences, Victoria University of Wellington, Wellington, New Zealand
[2]Division of Physical Chemistry, Lund University, 221 00 Lund, Sweden
[3]Department of Chemical and Process Engineering, University of Canterbury, Christchurch, New Zealand

Magnetic Resonance Imaging (MRI) in combination with pulsed field gradients allows the spatially resolved detection of flow and random motion using Dynamic NMR Microscopy [1] . This technique measures coherent motion (flow) via phase shifts in the NMR signal, while random motion (diffusion and dispersion) is extracted from signal attenuations. Dynamic NMR Microscopy can be tuned to measure fully resolved averaged propagators or only its lower order moments, i.e., focussing on mean velocities and dispersion. It may also be optimised for high spatial or temporal resolution.

Triply Periodic Minimal Surface structures (TPMS) are ordered periodic porous materials defined by mathematical expressions to form internal surfaces with minimal local energies. These structures may offer improved performance for instance for heat exchangers or chromatographic columns. We studied the time averaged mean velocities and velocity fluctuations in TPMS systematically, covering creeping flow at Reynolds numbers as low as Re = 1.25 [2], inertial flow at Re = 17.6 and 32 [2], the transition into unsteady laminar flows between Re = 101 and Re = 152 [3], and turbulent flows of up to Re = 1470 [4]. MRI velocity data were cross-validated by Computational Fluid Dynamics (CFD) simulations, where concordant results validated the simulation methods and the MRI experiment design.

In addition to time averaged data we recently recorded velocity vector images with a temporal resolution of 12 ms (at a spatial resolution of 32x32) and 21 ms (at a spatial resolution of 64x64) for flows in TPMS with Reynolds numbers of up to 2500, revealing time resolved details of the flow under unsteady and turbulent regimes [5].

References:
1. Callaghan, P. T.; Eccles, C. D. and Xia, Y., J. Phys. E 21 820-822 (1988)
2. Clarke, D. A.; Dolamore, F.; Fee, C. J.; Galvosas, P. and Holland, D. J., Chem. Eng. Sci. 231 116264 (2021)
3. Clarke, D. A.; Galvosas, P. and Holland, D. J., AIChE J. 69 18097 (2023)
4. Clarke, D. A.; Coe, M. J.; Galvosas, P. and Holland, D, J., submitted to Chem. Eng. J.
5. Clarke, D. A.; Galvosas, P. and Holland, D, J., in preparation

Integrating molecular data to visualise metabolic flux by NMR

Winner of 'Sir Paul Callaghan Medal'

Ivanhoe Leung

The University of Melbourne, Melbourne, Australia

From the simplest microbe to the most complex organism, all life on Earth depends on capturing nutrients from the environment and converting them into molecules that provide energy and support growth. This process, known as metabolism, must be maintained in balance (homeostasis) for cells to function and survive. Bacteria maintain metabolic homeostasis through a tightly coordinated network of sensing, signalling, and response mechanisms.

Deciphering how this intricate web operates as an integrated whole is not trivial. I have recently developed a method to integrate different levels of molecular information to illustrate how Mycobacterium tuberculosis (Mtb), one of the most adaptable bacteria in terms of nutrient use, can co-metabolise glucose and fatty acids simultaneously. By combining detailed enzymology, including how key metabolic enzymes are regulated by metabolites, with transcript and metabolite data measured under different growth conditions, I developed an integrated model that uses NMR spectroscopy to visualise how nutrients are channelled through the metabolic network. This integrated picture revealed a previously unrecognised "mixer-tap" mechanism that explains how Mtb dynamically divides nutrients between different metabolic routes in response to their availability.

Structural characterisation of a cysteine-rich conotoxin, sigma(σ) S-GVIIIA extracted from the defensive venom of the marine cone snail Conus geographus

Winner of 'ANZMAG Medal'

Norelle Daly

James Cook University, Cairns, Australia

The activity of the serotonin type 3 (5-HT3) receptor is associated with neurodegenerative, inflammatory and metabolic diseases, neuropsychiatric disorders and cancer. Structural analysis of modulators of this receptor is likely to aid in future medicinal chemistry studies aimed at developing lead molecules targeting this receptor. Here we report the structure of a cone snail venom peptide, sigma(σ)S-GVIIIA, purified from the crude venom of Conus geographus, which was shown to be an antagonist of the 5-HT3 receptor more than 25 years ago. This lag in structural characterisation studies is likely due to challenges in isolating the native peptide and to difficulties in producing synthetic peptide due to the presence of ten cysteine residues involved in five disulfide bonds. Using NMR spectroscopy, we show that σS-GVIIIA adopts a growth factor cystine knot (GFCK) fold. This is the first example of a cone snail venom peptide experimentally determined to contain the GFCK structural motif, and the first example of a 5-HT3 receptor antagonist containing this motif. Our study also highlights complexities in the use of artificial intelligence-based structure prediction models. Peptide structure predictions using AlphaFold 3 were consistent with our NMR structure when the input sequence contained the well-conserved precursor sequence, but were inconsistent when the precursor sequence was not included in the input sequence. AI-based structure prediction of proteins is a rapidly advancing field, but this inconsistency emphasises the need for more experimental structural training data when novel structures are involved, as was the case here for a cysteine-rich peptide.

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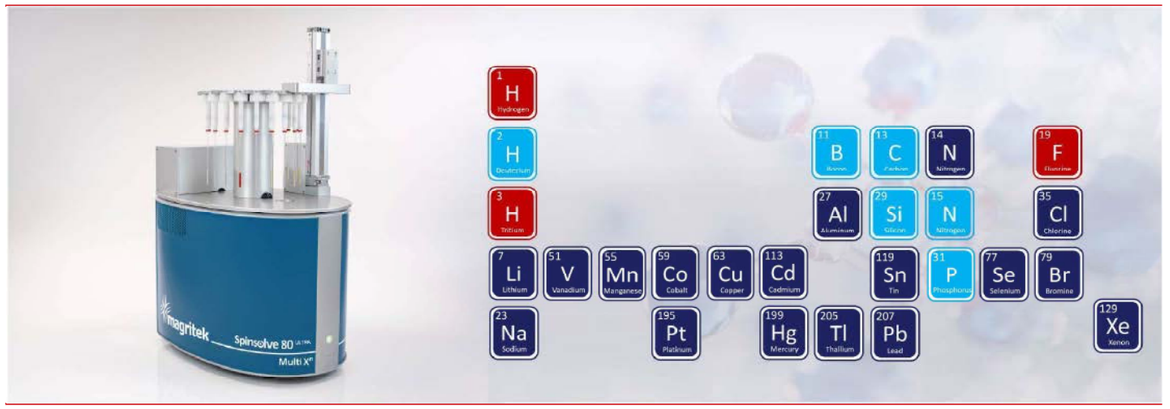

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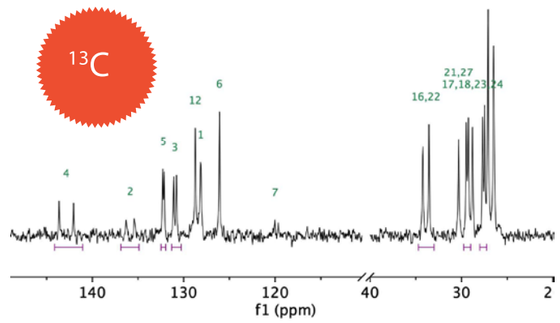

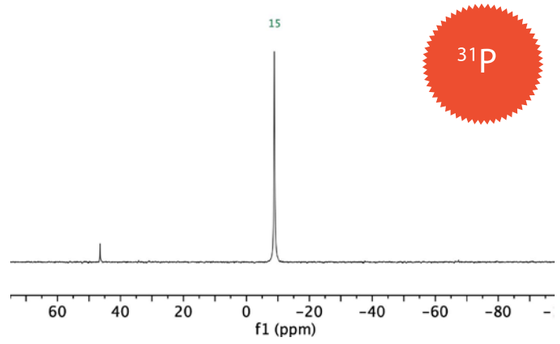

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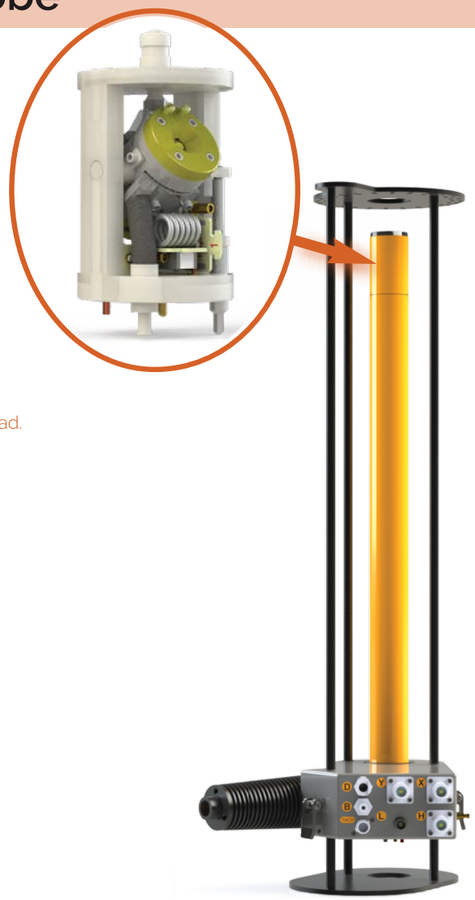

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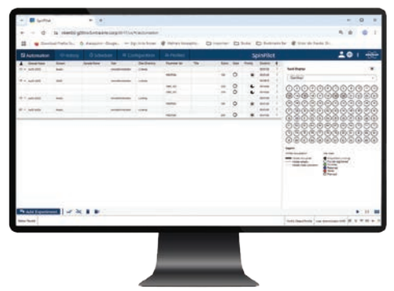

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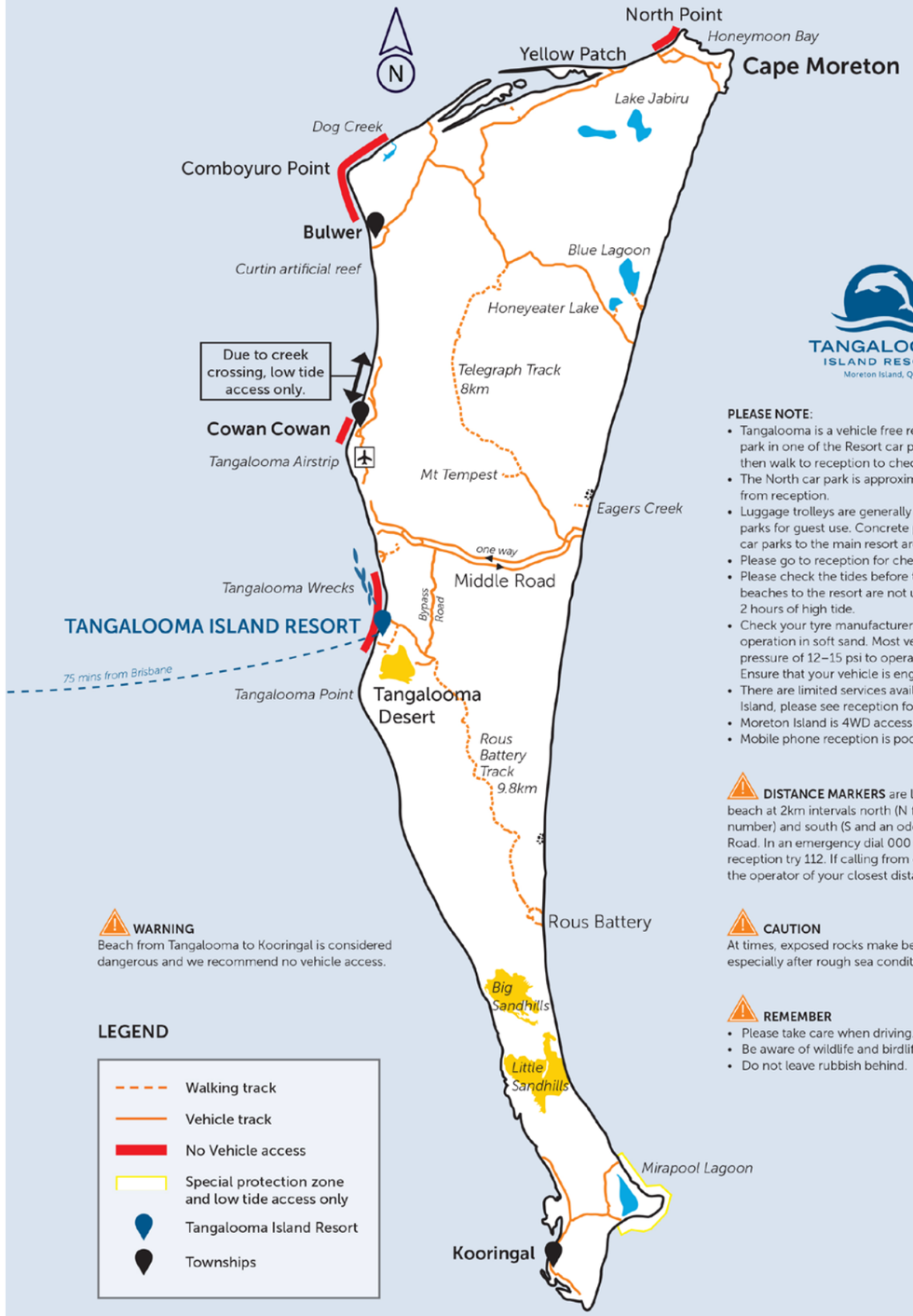

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- The North car park is approximately 600 metres from reception.
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At times, exposed rocks make beaches impassable, especially after rough sea conditions.

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- Be aware of wildlife and birdlife.
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e: j.rosengren@uq.edu.au
e: g.cowin@uq.edu.au
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