Newsletter DANNMR

2024 - 3

🚀 Exciting News: New DANNMR PhD course in NMR spectroscopy! 🚀

HAPPY HOLIDAYS

Dear Danish NMR community

A year has passed, and it has brought many magnetic moments to us all, and to DANNMR in particular. A fantastic Danish NMR meeting in January organized by RUC kickstarted 2024, and it was a huge success with almost 100 participants.

Though the year, DANNMR has been stimulating discussions about the next directions for Danish NMR spectroscopy. A collaborative application has been submitted to the Danish National Roadmap for infrastructure with Niels-Chr Nielsen and Jan Ardenkjær spearheading a joint DANNMR suggestion for a future expanded DNP scene in Denmark. At the yearly DANNMR users meeting in Odense, talks on organizations of National NMR centers by Göran Karlström and mind blowing science talk on DNP NMR in biology by Marc Baldus provided the inspiration for discussing strategy and possibilities for DANNMR in the coming 5 years. Many ideas were presented, discussed and matured, and some will materialize in the coming year.

Two important DANNMR actions are relevant to mention. DANNMR is delighted that all our NMR managers are now meeting on a regular basis providing the glue between the technical side of our labs, helping and supporting DANNMR to thrive. Driven by Reinhard Wimmer and hosted by Aalborg University, DANNMR is now able to launch a national PhD course on NMR, and we urge you to get your PhD students enrolled as soon as the course opens for registration.

Finally, and importantly, Danish NMR scientists have made important discoveries and their scientific endeavors been published, testifying to the breadth and depth of what NMR can do. Congratulations to you all!

I wish you a Merry Christmas and a Magnetic New year, and look forward to seeing you all at the Danish NMR meeting in January

Birthe

Announcements

Special issue in 2025 of Magnetic Resonance in Chemistry on NMR and MRI in Scandinavia

*Professor **Jørgen Skibsted** (AU)*

There will be a special issue of Magnetic Resonance in Chemistry (MRC) on NMR/MRI in Scandinavia in 2025. The issue is edited by Dianna Bernin from Chalmers and contributions from Denmark are indeed welcome.

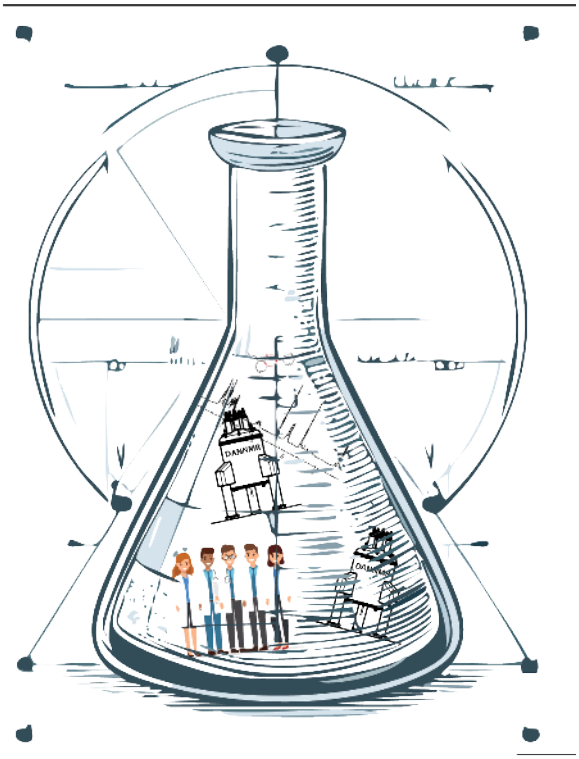
This is a good chance to promote NMR in Denmark, and therefore, you are encouraged to submit a manuscript to this special issue.

The submission deadline is February 15, 2025, and if you are interested in submitting a manuscript, please indicate this by sending an e-mail to Diana Bernin (diana.bernin@chalmers.se) and Jørgen Skibsted (jskib@chem.au.dk).

New DANNMR Ph.D. course: *Theoretical Foundations of Modern NMR Spectroscopy*

Professor ***Reinhard Wimmer*** *(AAU)*

DanNMR members are jointly offering a Ph.D course on the theoretical aspects of NMR. The course will be held for the first time during the autumn semester of 2025.
The course offers a thorough introduction to the basic theory behind NMR spectroscopy, and it will follow the textbook by James Keeler (Understanding NMR Spectroscopy, 2nd Edition, ISBN: 978-0-470-74608-0). It will cover the NMR phenomenon and how we can describe it using vector and quantum mechanical models. The course will cover signal processing, 1D- and 2D-NMR, the product operator formalism and coherence selection as well as basic relaxation theory.
This course is NOT a course in NMR spectrum interpretation.
We offer this course to all students who want to work with NMR and understand a bit better what is actually going on in the sample, when the radiowaves hit, and how this can be turned into the beautiful spectra we see on the screen.
The course is formally hosted by Aalborg University, but taught by NMR-experts from both academic and industrial DanNMR members. Participance is free of charge for Ph.D. students from all Nordic universities.
The course is organized as a combination of online self-study and two mandatory exercise sessions. You can find more information at https://phd.moodle.aau.dk/course/view.php?id=2562 (needs creating a profile first).
We invite everybody who would like to get a bit deeper into NMR to register for the course and we hope to see many eager participants!



Events

46th Danish NMR meeting, Rebild, January 30-31, 2025

Professor ***Reinhard Wimmer*** *(AAU)*

Aalborg University is proud to host next year's Danish NMR Meeting. All information on the meeting will be shared on https://danish-nmr-meeting.dk/

There will be national and international speakers, posters, vendor exhibitions and opportunities for networking. Come and enjoy two days with NMR from all corners of science!

Registration is officially closed, but you can always write to the organizers if you somehow didn't register in time, but do not want to miss out.

> The DANNMR Annual Meeting is a great example of the close collaboration within the Danish NMR community. With participants from all the six Danish universities and a dozen different companies, it is the place to be, if you are working with NMR in Denmark.

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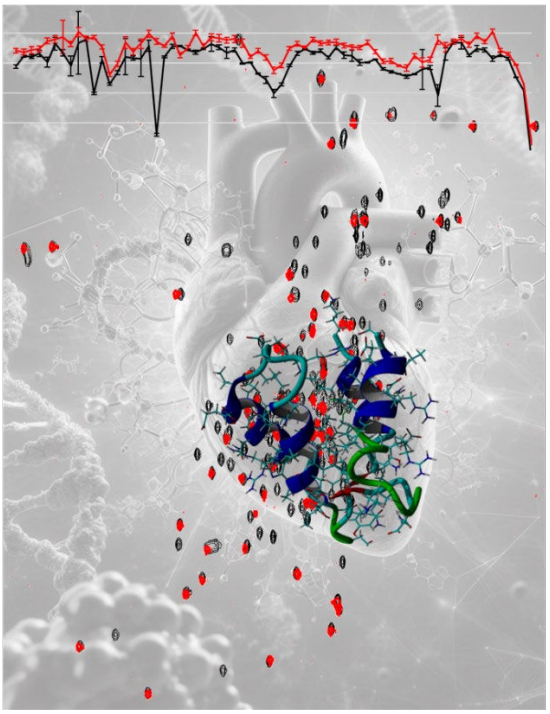
If you have any news for the DANNMR newsletter, please contact: caspar.christensen@bio.ku.dk
Check out our other news at: https://dannmr.dk/

New NMR stories

From the Australian Courts to Danish Laboratories: Calmodulin and Infant Cardiac Arrests

*Professor **Reinhard Wimmer** (AAU)*

In 2023, an Australian woman was released from prison, where she had spent the previous 20 years, wrongfully convicted of having killed her four infants. Scientists discovered that all four children carried mutations in vital genes. Two of the children carried a mutation in one of the calmodulin genes and in vitro experiments showed that this mutation severely impacts the function of calmodulin and that the mutation could have caused cardiac arrest in those two infants.



A mechanistic explanation of the effect of the mutation on the protein structure and dynamics was given in a recent article by a group of researchers around Reinhard Wimmer from Aalborg University and Hideo Iwaï from Helsinki University. The mutated amino acid acts as a C-capping residue and the mutation thus changes structure and stability of the preceding helix. Whereas a salt bridge can stabilize the variant protein in the absence of calcium, leading to a marked rigidification of the molecule, the same is not happening in the calcium-bound form, leading to a destabilization of the protein fold. As a result, calcium binding is impaired for this variant. In addition, replacing a small amino acid with a bulky one, leads to sterical hindrance when the mutated calmodulin interacts with the ion channels that regulate the heartbeat. The work made use of segmental labelling with split inteins, only labelling the mutated domain of calmodulin.

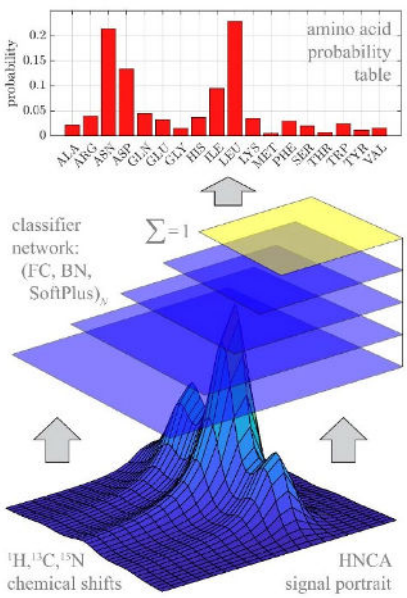
Cell Calcium 117, 102831 (2024),

DOI: 10.1016/j.ceca.2023.102831

Protein NMR assignment by isotope pattern recognition

*Assoc. Professor **Thibault Vinniet** (AU)*

Interesting protein targets are often challenging for resonance assignment, which becomes the bottleneck of NMR investigation. Assist. Professor Thibault Vinniet (iNANO, AU) and colleagues report on a novel way to perform assignment using isotope pattern recognition. ^{13}C-pyruvate can be used instead of glucose, leading to different levels of ^{13}C incorporation at the Cβ position that depend on amino acid type. An HNCA with sufficient resolution thus generates isotope patterns, that can be analyzed by our neural net classifier to obtain amino acid type propensity with higher accuracy than chemical shifts alone. Furthermore, the isotope patterns also help alleviating Cα shift degeneracy and increase the likelihood of finding the right sequential match. Neural nets can be generated on the fly using Spinach and used in the assignment routine of CcpNmr v3 (see details in the publication).



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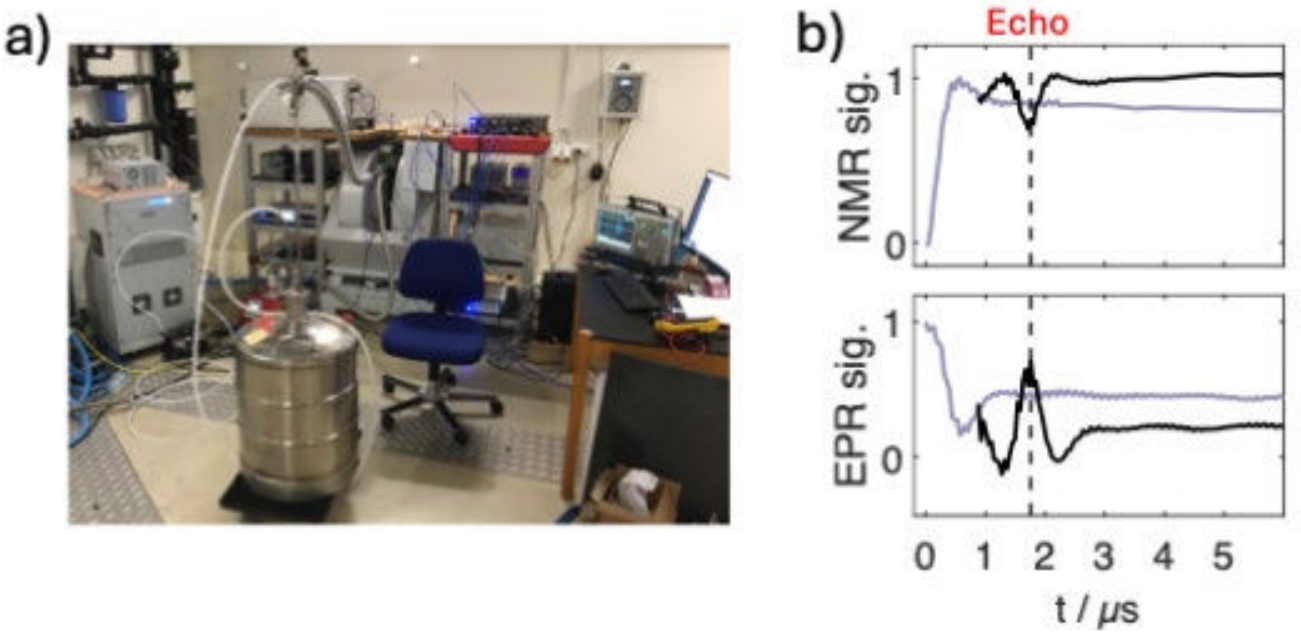
If you have any news for the DANNMR newsletter, please contact: caspar.christensen@bio.ku.dk

Check out our other news at: https://dannmr.dk/

Observation of Dynamic Nuclear Polarization Echoes

Professor ***Niels Christian Nielsen*** *(AU)*

Using front-line home-built dynamic nuclear polarization (DNP) instrument, researchers from iNANO and the Department of Chemistry, Aarhus University, have for the first time observed echo phenomena both on electron and nuclear spins – so-called DNP echoes



Using a home-built X-band pulsed DNP/EPR instrument (a) along with advanced pulse sequence engineering it has been possible to detect so-called DNP echoes (b) causing echo phenomena to appear both with NMR (upper) and EPR (lower) detection.

Echo phenomena is a cornerstone in coherent spectroscopy. Echos – often referred to as time-reversal elements - are key ingredients in advanced NMR, EPR, IR, microwave, and laser spectroscopies. In a study, published in Science Advances (https://www.science.org/doi/10.1126/sciadv.adr2420), Prof. Niels Chr. Nielsen and his research group have, for the first time, demonstrated that it is possible to invert effective electron-nuclear spin hyperfine interactions in pulsed DNP and thereby form so-called DNP echos.

The researchers used advanced spin engineering to generate pulse sequences that inverts the sign of the effective hyperfine coupling interaction. The pulse sequences were implemented on a newly built pulsed DNP/EPR spectrometer using fast arbitrary waveform generators on microwave and radio-frequency channels. This enabled experimental observation the DNP echo phenomena for a sample containing trityl radicals. Echoes formed at the nuclear spin channel (NMR) and electron spin channel (EPR) are illustrated in the figure above.

The realization of DNP echos phenomena may form a breakthrough in the development of pulsed DNP experiments boosting the sensitivity of NMR by orders of magnitude. One could envisage high-sensitivity detection of nuclear spin coupling networks surrounding electron spins. Such experiments could be of great interest for quantum sensing applications.

***Sci. Adv.*10,eadr2420(2024)**

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