

# PANACEA news

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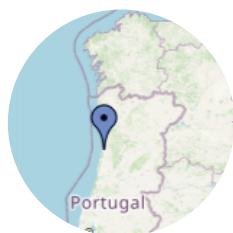
A Pan-European Solid-State NMR Infrastructure  
for Chemistry-enabling Access



Issue 5, May 2024

#### Users meeting

PANACEA 3<sup>rd</sup>  
Annual Users Meeting,  
September 2024,  
Aveiro, Portugal.



#### Meet with PANACEA

Visit us at the 2024  
Spring Meeting of the  
European Materials  
Research Society.



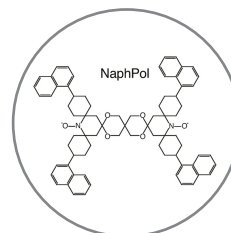
#### Summer school

The PANACEA  
solid-state NMR  
summer school is  
coming up June 2024.



#### Publication

A novel biradical is the  
most promising DNP  
polarizing agent in  
organic solvents to date.



#### Meet our user

Interview with  
Heitor Secco Seleghini,  
University of St  
Andrews, Scotland, UK.



## PANACEA 3<sup>rd</sup> Annual Users Meeting Aveiro, Portugal, September 25 - 26, 2024



We are delighted to officially invite you to attend the PANACEA 3<sup>rd</sup> Annual Users Meeting!

The event will take place from Wednesday September 25<sup>th</sup> to Thursday September 26<sup>th</sup>, 2024, and is hosted by the University of Aveiro in Aveiro, Portugal. This event is a two-day European forum for high-level discussions between academic and industrial users and consortium partners on the latest developments in solid-state NMR spectroscopy and their applications in contemporary chemistry and materials research.

The event will be impulsed by a dynamic program structured into six distinct symposia, each centered around a different research talk for solid-state NMR, additional speakers and a round table discussion.

#### PANACEA key numbers

- 1650 access days
- 27 spectrometers
- > 200 chemistry-related projects
- 4 user meetings
- 4 hands-on trainings
- 1 NMR summer School
- 3 industry-targeted workshops
- 32 taster days for industrials
- 8 summer fellowships for students

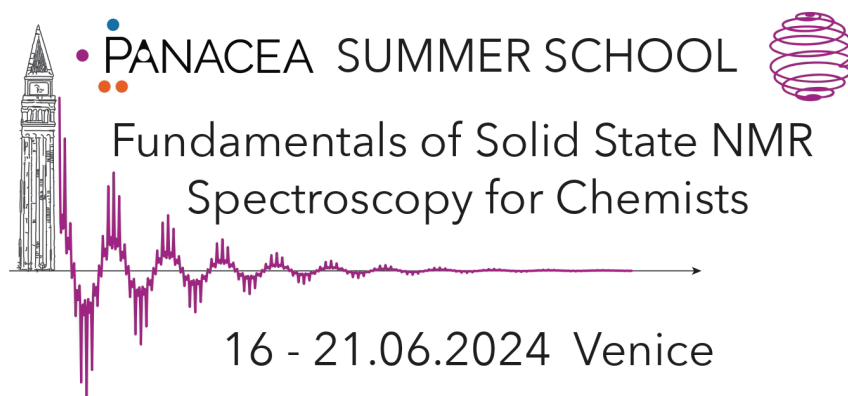
## PANACEA outreach at the Spring Meeting of the European Research Society



We are pleased to announce that PANACEA will be present at the 2024 Spring Meeting of the European Materials Research Society (E-MRS) where two members of the consortium will highlight the access opportunities within PANACEA.

The conference will consist of parallel symposia with invited speakers, oral and poster presentations assorted by a plenary session to provide an international forum for discussing recent advances in the field of materials science.

The high quality scientific program will address different topics organized into 22 symposia arranged in 6 clusters covering the fields of Decarbonized energy and sustainability; Materials for human well-being; 2D materials and surfaces: synthesis, characterization and perspectives; Advanced characterization of materials; Materials sciences for cultural heritage; Electronics, magnetism and photonics.



Just one month remains until the *Fundamentals of Solid-State NMR Spectroscopy for Chemists* Summer school kicks off in the picturesque city of Venice, Italy. Selected from a pool of applicants, our diverse cohort of 70 participants ensures a rich and inclusive learning environment.

The lineup includes eight distinguished speakers. The tailored scientific program will blend lectures, tutorials, and round-table discussions to provide a comprehensive understanding of solid-state NMR principles and their real-world implications.

Philip Grandinetti (Ohio State University, Columbus, USA)  
Clare Grey (University of Cambridge, UK)  
Malcolm Levitt (University of Southampton, UK)  
Jozef Lewandowski (University of Warwick, UK)  
Jennifer Mathies (University of Konstanz, Germany)

Len Mueller (University of California, Riverside, USA)  
Tatyana Polenova (University of Delaware, Newark, USA)  
Michael Hope (University of Warwick, UK)  
Thomas Vosegaard (Aarhus University, Denmark)  
Frank Engelke (Bruker Biospin)

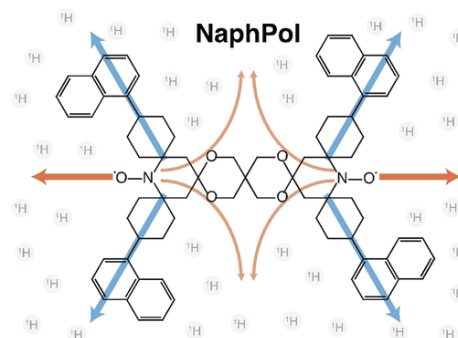
## Publication highlight: novel DNP polarizing agent

An exciting new publication has emerged from within the PANACEA consortium.

In short summary from the published paper, the authors have investigated the effect of biradical protonation/deuteration levels on the outcome of MAS DNP NMR experiments at 9.4 T. A series of seven deuterated and one fluorinated TEKPol biradicals were investigated.

The findings show that the  $^1\text{H}$  DNP build-up times increase substantially with TEKPol isotopologues that have fewer hydrogen atoms in the phenyl rings. This prompted the authors to design a novel biradical, NaphPol and use it to boost NMR sensitivity, making it the best performing DNP polarizing agent in organic solvents to date. For the full paper, see the reference below.

Polarization transfer pathways



Reference: Amrit Venkatesh, Gilles Casano, Yu Rao, Federico De Biasi, Frédéric A. Perras, Dominik J. Kubicki, Didier Siri, Sébastien Abel, Hakim Karoui, Maxim Yulikov, Olivier Ouari, Lyndon Emsley, Deuterated TEKPol Biradicals and the Spin-Diffusion Barrier in MAS DNP, *Angew. Chem. Int. Ed.*, 2023, **62**, e2023048.

## Transnational access: user profile

Heitor Secco Seleghini of University of St Andrews, Scotland, UK has an ongoing PANACEA user project and has recently visited the Lyon facilities.

### What is your field of research?

I am currently working on using solid-state NMR spectroscopy, mainly of quadrupolar nuclei, together with DFT calculations to study disorders in different kinds of solids.

### Could you tell us a bit more about your scientific academic journey?

I did my BSc degree in chemistry at the University of Campinas in Brazil, graduating in 2018. I stayed at the same university to do my masters in physical chemistry, where I worked with computational chemistry, simulating semiconductor oxides. After I finished my masters in 2021, I moved to Scotland to begin my PhD studies under the supervision of professors Sharon Ashbrook and Russell Morris at the University of St Andrews, where I am today.

### How did you hear of PANACEA?

From the UK High-Field Facility which is part of the PANACEA network and at the PANACEA workshop at EUROMAR 2023 in Glasgow, UK.

### What was the purpose of your visit?

We are trying to understand the conformation of a bioactive molecule that is attached to the surface of a metalorganic framework of nanoparticles. However, due to the low amount of signal because of the  $^{13}\text{C}$  natural abundance and quantity of the bioactive molecule in the sample, it is necessary to use DNP-MAS for its signal enhancement and to properly perform the measurements we deem necessary for this project.

### Overall, did you enjoy this access opportunity?

I enjoyed it a lot! Everyone in the CNRS Lyon Facility was really friendly and helpful. I learned a lot about the DNP-MAS technique during the use of the spectrometer. I need to give special thanks to Dr Zhuoran Wang, Dr Anne Lesage and Raphaële Coulon, for all the help in running the experiments and organizing my visit.



Heitor Secco Seleghini  
at work in CNRS Lyon.