

### Presentation

Nuclear Magnetic Resonance (NMR) is a powerful tool for the analysis of food and biological samples. Quantitative and non-targeted NMR methods allow for the determination of multiple parameters in a single analysis, providing a comprehensive picture of the sample composition. This is particularly relevant in the context of food safety and health protection, where the identification and quantification of specific compounds is essential to ensure compliance with regulations and to prevent potential health hazards.

In this NMR Day, we will discuss the latest advances in quantitative and non-targeted NMR methods for the analysis of food and biological samples. We will focus on the use of these techniques for the characterization of food quality parameters, such as composition, authenticity, and freshness. We will also highlight the potential of NMR for the analysis of biological fluids for the diagnosis and monitoring of diseases.

It will be emphasized the importance of method validation, interlaboratory comparisons, and international standardization in NMR analysis for the protection of health and food. These practices ensure the accuracy and reliability of NMR results and enable the comparison of data obtained from different laboratories.

Overall, this NMR Day will show the versatility and potential of quantitative and non-targeted NMR for the protection of health and food, providing insights into the latest developments and applications of this powerful analytical technique.

### Scientific Committee

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# Politecnico di Bari Via Edoardo Orabona, 4, 70126 Bari BA

## Sponsors



# Program

10:00 - Opening

**Francesco Cupertino**, Rector of the Polytechnic University of Bari

**Leonardo Damiani**, Director of DICA-TECh of the Polytechnic University of Bari **Gianluca Maria Farinola**, President of

the Italian Society of Chemistry (SCI)

Michele Chierotti, President of the
GIDRM

**Cristina Airoldi,** Coordinator of the GIRM of the Italian Society of Chemistry (SCI)

10:30

**Claudio Luchinat**, Center of Magnetic Resonance (CERM), Florence, Italy

Metabolomics by NMR: achievements and perspectives
11:00

**Luisa Mannina**, University of Rome "Sapienza", Rome, Italy

NMR-based metabolomics in food science

### 11:30 Coffee break

12:00

**Roberto Gobetto**, University of Turin, Turin, Italy

Two Case Studies in the Application of <sup>1</sup>H NMR in Food and Health Protection: Authentication of Italian Hazelnut and Early Detection of the Cytomegalovirus Infection

12:30

**Cristina Airoldi**, University of Milan Bicocca, Milan, Italy

NMR-based identification of bioactive compounds in edible plants
13:00

**Alberto Ceccon,** Laimburg Research Centre, Bozen, Italy

Improved detection and quantification of cyclopropane fatty acids (CPFAs) by <sup>1</sup>H NMR spectroscopy using a combination of homonuclear decoupling with double irradiation methods

13:30 Light lunch

14:30

Claudia Napoli, Bruker, Milan, Italy Nutritional health by NMR based metabolic profiling

15:00

lain Day, Jeol (UK), Welwyn Garden City-London, UK

qNMR with JASON: What is SMILEQ and how can it help your workflow?
15:30

**Matthias Weber,** European Directorate for the Quality of Medicines & HealthCare (EDQM), Strasbourg, France

The Use of qNMR for the Characterisation of European Pharmacopoeia Reference Standards

### 16:00 Coffee break

16:30

**Sandra Weber**, Chemischen und Veterinäruntersuchungsämter (CVUA), Karlsruhe, Germany

Validation and standardization of NMR methods

17:00

Vito Gallo, Polytechnic University of Bari

Validation of qNMR and non-targeted NMR methods: towards the collective NMR analysis

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**Round table** – Future Actions in collaborative NMR analysis

Collaborative analysis represents an important aspect of the scientific community, enabling researchers to share data, expertise, and resources. This has led to new discoveries, better understanding of complex systems, and improved reproducibility of results. However, challenges exist in collaborative NMR analysis, such as standardization of data acquisition and processing, data sharing and archiving, and communication among collaborators. This round table will feature speakers discussing possible actions to achieve collaborative NMR analysis, emphasizing the importance of standards and best practices.

