CERM
Centro Risonanze Magnetiche
FIRENZE

CIRMMP
FIRENZE

SCIENTIFIC ANNUAL REPORT

2025

UNIVERSITÀ DEGLI STUDI FIRENZE

Contents

Foreword

In 2025, CERM/CIRMMP further consolidated its role as a leading international infrastructure for Life Sciences. The year was characterized by intense research activity, technological development, and international collaboration.

Scientific output remained strong, with numerous publications in high-impact journals addressing key topics in biomolecular NMR. This is evidenced by the substantial number of peer-reviewed publications (67) and their high scientific impact (mean impact factor of 7). Structural and cellular biology dominate the landscape of topics, but material science, new NMR methods and metabolomics are also well represented. The various research areas feature in more detail in the Research Activities section of this report.

Scientific excellence continues to represent one of the main strengths of the centre, constantly attracting users from the international scientific community and fostering long-term collaborations. Users of the infrastructure benefit not only from access to state-of-the-art NMR facilities but also from the high level of scientific expertise available at the centre, enabling complex data to be properly analysed and translated into impactful scientific results.

During the year, the role of CERM/CIRMMP within the European Research Infrastructure landscape was further reinforced. CERM/CIRMMP is the Italian centre (Instruct-IT) of Instruct-ERIC, a European Strategy Forum on Research Infrastructures (ESFRI) Landmark. The key role of the Italian centre within Instruct-ERIC was strongly reaffirmed thanks to our involvement in most Instruct-ERIC activities, with a leading role in the Council and in the Executive Committee, as well as in the support to training, internationalization, access, and data management.

The activities of CERM/CIRMMP related to Instruct-ERIC were framed also within several projects (page 7), aimed at creating platforms for access provision tackling cancer research, infectious disease outbreak, and effects of exposure to artificial materials, respectively.

At the national level, the activities of Instruct-ITALIA, the national consortium of facilities providing access to national users in structural biology, continued to expand, providing Italian researchers with coordinated access to complementary structural biology technologies, including NMR spectroscopy, cryo-electron microscopy, optical microscopy, and X-ray techniques.

Support from the National Recovery and Resilience Plan has also continued to strengthen research infrastructures in Italy. In particular, CERM/CIRMMP benefited from the ITACA.SB project, which aims to further develop the Italian centre of Instruct-ERIC and expand national facilities for structural biology research, ensuring high-level services for both national and international users. Training and knowledge dissemination also represented a central component of the infrastructure mission. Among the main initiatives, the international Summer School *"Exploiting heteronuclei at their best: novel probes for biomolecular NMR"*, held in September 2025 within the framework of

the ITACA.SB project, brought together young researchers from different countries for advanced training in heteronuclear NMR methodologies.

In addition to its scientific activities, the centre also strengthened its commitment to environmental sustainability. Six high field magnets are equipped with Bruker Smart Nitrogen Liquefier (BSNL) units, which drastically reduce the need of liquid N_2 refills of these magnets, while two nitrogen generators produce gaseous N_2 for the NMR instruments and the biotechnology labs. In 2025, a 40 kW-peak photovoltaic system was installed on the roof of the CERM building, enabling the generation of renewable energy directly on site. It is estimated that the photovoltaic plant will contribute to cover the annual electricity demand of the helium pumping system used to maintain the NMR magnets at cryogenic temperatures. This initiative represents an important step toward reducing the environmental footprint of the facility and promoting the use of green energy in large-scale scientific infrastructures.

As in previous years, the University of Florence (CERM) and CIRMMP have contributed to supporting the operational and personnel costs associated with our infrastructure. Also in 2025, the Italian Ministry of University and Research (MUR) confirmed its support to the Italian Centre of Instruct-ERIC within the International Action of the FOE funding. In addition, in 2025, the NRRP project ITACA.SB made a further investment of 2,182,194 € in the infrastructure: 1,790,809 € were allocated to the purchase of scientific instrumentation and technological systems, while 391,385 € were dedicated to covering the costs of personnel assigned to the infrastructure, as well as to supporting in-house training and research activities.

In 2025, besides the faculty staff, the body of researchers included 29 PhD students, 13 postdoctoral scientists, and 11 graduate students, as well as 16 between non-permanent and permanent technical and research staff.

We want to thank all the people that contributed to make CERM/CIRMMP what it is today, and who continue to drive it forward, and all the Institutions that provided their support.

Introduction

CERM is the Centre for Magnetic Resonance of the University of Florence. It operates in synergy and collaboration with the Interuniversity Consortium for Magnetic Resonance of MetalloProteins (CIRMMP) which includes three Italian Universities: Florence, Siena, and Bologna. CERM/CIRMMP is an infrastructure with a particular focus on structural biology and specialization in NMR spectroscopy and relaxometry, bioinformatics, molecular and cellular biology, novel drug and vaccine design, and metabolomics. Nevertheless, it is open towards interfaces with other research fields, for example new material and biomaterial developments, contrast agents and MRI techniques, and computing technology.

Being a leading laboratory at both national and international level, CERM/CIRMMP receives funding from competitive project calls from the Tuscan Regional Government, the Italian Ministry of Higher Education and Research (MUR), the Italian Ministry of Health, and the European Commission (EC), as well as from private institutions.

The core technology at CERM/CIRMMP is NMR spectroscopy, and the onsite instrumentation is among the most advanced in the world. Since 1994 a European transnational access service, funded by EC, flanked the service provision at national level, that was already active since 1990. With its long-term expertise in access provision, CERM/CIRMMP actively stimulates interactions between private industry and public research institutions such as Universities, National Research Council (CNR) Institutes, and European counterparts, promoting synergistic activities such as collaborations and services to SMEs.

Who We Are

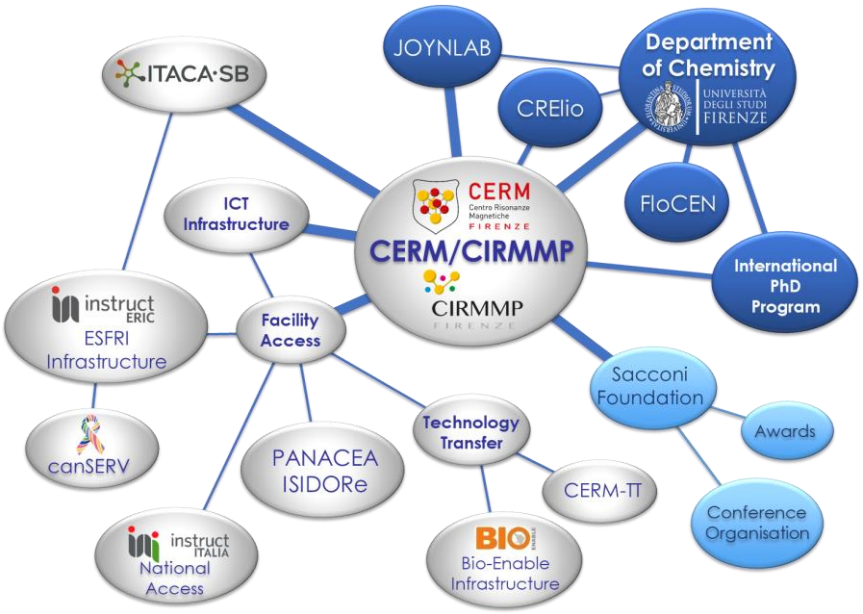
CERM/CIRMMP, besides being the Italian Centre of Instruct-ERIC, is also included in the MUR "Roadmap Italiana delle Infrastrutture di Ricerca di interesse Pan-Europeo". In parallel, CERM/CIRMMP is also the core centre of the Instruct-ITALIA network, an infrastructure to promote and foster an integrated approach at the national level providing access to X-ray crystallography, NMR, Cryo-EM, as well as protein expression and crystallization. Instruct-ITALIA has started its activity in early 2020, promoting a more effective interaction within Italian structural biologists, as well as supporting access to the facilities of its national network. Since 2023, CERM has been operating as an independent University Service Centre.

Under the Next Generation EU scheme, Italy is receiving resources (NRRP Program) and, through this scheme, CERM/CIRMMP scientists participated in several projects. Remarkably, CERM/CIRMMP is leading a consortium with a few CNR laboratories in Italy within the project ITACA.SB, which allocated significant resources (9.4 M€) to reinforce the Italian Center of Instruct-ERIC.

CERM/CIRMMP is an e-infrastructure, participating in a European GRID-based platform, providing access to user-friendly platforms and CPU/GPU resources for a broad range of services for structural biology. These services leverage technologies created in the context of EOSC (European Open Science Cloud) development initiatives and are made available through the EOSC Hub (for example, https://www.wenmr.eu/services/).

CERM/CIRMMP has also developed a centre for research and technology transfer: CERM TT, funded by the Tuscany Region. Finally, CERM/CIRMMP is coordinating the activities of Bio-Enable, a distributed Infrastructure promoting technology transfer to industry and funded by the Regional Government of Tuscany in the frame of POR FESR 2014-2020.

CERM/CIRMMP is inside the "Campus Sesto" site (formerly known as "Polo Scientifico") of the University of Florence in Sesto Fiorentino, an area just west of the city of Florence. The campus borders Florence International Airport and yet is a mere 30 minutes from the centre of Florence, world renowned cradle of renaissance art and culture.



CERM/CIRMMP labs

The CERM/CIRMMP building covers an area of 3000 square meters hosting several laboratories, offices, and common rooms. The hallmark of the Centre is the impressive collection of NMR spectrometers which feature the largest magnetic field range in the world (up to 1.2 GHz - installed in early 2020, the first commercial instrument in the world at this field) and ranks it among the best equipped laboratories in the world. The NMR labs are flanked by molecular and cellular biology laboratories that are optimized for NMR sample production. A complete list of the instruments available at CERM/CIRMMP is reported at page 11. In addition to the main building, a further 500 square meters in adjacent buildings are available to CERM scientists: laboratories at the Department of Chemistry Ugo Schiff and at Genexpress; X-rays facilities; Helium liquefier. www.cerm.unifi.it

Instruct-ERIC

CERM/CIRMMP is an Instruct-ERIC Centre. Instruct-ERIC is the European research infrastructure in integrated structural biology, making cutting-edge technologies and high-end methods in a palette of tools for structural characterization available to users.

Structural biology is one of the key approaches that contribute to the understanding of the molecular and cellular functions. The main experimental technologies are complementary and increasingly link detailed atomic structure with cellular context. Structural biology is currently in the middle of a revolution enabled by significant advances in various technologies (direct electron detectors in EM, advances in synchrotron sources and detectors, XFELs, ultra-high field NMR, super-resolution cryo-light microscopy, AI-driven prediction of protein structures).

Instruct-ERIC buildups on a number of Centres featuring the most advanced structural biology instrumentation and top-level expertise in the various methods. Instruct-ERIC offers a **single point of access** to both multiple techniques integrated at one Centre or over various Centres, or to some Centres specialized in specific techniques. www.instruct-eric.eu

Instruct-ITALIA is the Italian network of facilities for Integrated Structural Biology. It consists of a core of research institutions and large centres that have a proven track record in structural biology and in service and expertise provision to users. Instruct-ITALIA aims to serve as a national consortium covering all main areas of structural biology research within Italy. https://www.cerm.unifi.it/instruct-it/

The Infrastructure

CERM TT

The CERM TT Competence Centre dedicated to Ivano Bertini, one of the founders of CERM, was established in response to the request of the Tuscany Region to make available to the industries and production companies in Tuscany centres of technology transfer, innovation clusters with advanced equipment and skills to boost the economic growth of the region.

CERM TT strengthens and optimizes the services offered by CERM/CIRMMP to the industry of the area: NMR instrumentation and advanced computing, a molecular biology laboratory for the production of proteins, scientific expertise and excellence, together with the maximum protection of industrial IP. CERM TT provides analytical services and research and development (R&D) for companies. Specifically, it offers the following services:

- screening of drug candidates and provision of drug-target interaction studies.
- smart design of drugs.
- analysis of pharmaceutical formulations.

https://www.unifi.it/it/ricerca-e-innovazione/innovazione/collaborazioni-strategiche/centri-di-competenza-e-associazioni-lo

Bio-Enable

BIO-ENABLE is a "distributed research infrastructure" led by CERM/CIRMMP and includes a few other Centres in Tuscany. BIO-ENABLE provides access to equipment and expertise to support industrial research and innovation. Tuscan companies operating in fields ranging from pharmaceuticals to biotechnology, from vaccines to biomaterials, from food to nanotechnology, can exploit the services of BIO-ENABLE in the development of their activities to be competitive at the international level.

CERM leads the BIO-ENABLE consortium composed by:

- Magnetic Resonance Centre (CERM/CIRMMP, coordinator)
- Institute of Neurosciences of the CNR – Pisa;
- BioRobotics Institute of Sant'Anna School of Advanced Studies - Pisa;
- Department of Medical Biotechnologies – University of Siena.

BIO-ENABLE can provide support at various levels and through different types of contracts: from simple access to instrumentation to specific types of advice, help and assistance to industrial research. BIO-ENABLE guarantees total confidentiality of the data collected at the various platforms, both during the analysis and in the management and archiving of the data.

www.bio-enable.it

Funded projects

In addition to the individual research projects of CERM/CIRMMP members, CERM/CIRMMP cooperates at the international level with several universities, research institutions, and private industries with which it is involved in numerous research projects funded by the European Commission. Projects ongoing during 2025 are:

EOSC Data Commons - HORIZON-INFRA-2024-EOSC-01 Grant agreement n. 101188179 * 01/04/2025 - 21/03/2028)

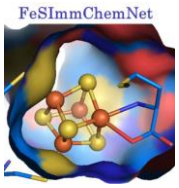
W-BioCat - Heavy metal enzymes for sustainable industrial biocatalysis. (HORIZON-EIC-2023-PATHFINDEROPEN-01 grant agreement n. 101129798 - 1/02/2024 - 31/01/2028)

MR LATVIA - Development of Magnetic Resonance in Latvia (HORIZON-WIDERA-2023-ACCESS-02 Grant agreement n. 101160091 - 01/09/2024 - 31/08/2027)

Fragment-Screen: From fragments to high affinity binders interfacing integrated structural biology, medicinal chemistry and artificial intelligence (HORIZON-INFRA-2022-TECH-01 grant agreement n. 101094131 - 01/01/2023 - 31/01/2027)

FC-RELAX NMR relaxometry for biomedicine and advanced materials. A multidisciplinary doctoral network for field-cycling NMR relaxometry. (HORIZON-MSCA-DN-2021 grant agreement: 101072758 - 01/03/2023-28/02/2027)

FHERITALE Food, Health and Environment Research Infrastructures to Tackle Emerging Priorities (HORIZON-INFRA-2023-DEV-01 Grant agreement ID: 101131588 01/01/2024 - 31/12/2026)



FeSImmChemNet - Iron-sulphur (FeS) clusters: from chemistry to immunology (Cost Action CA21115 19/09/2022 - 18/09/2026)

PANACEA "A Pan-European Solid-State NMR Infrastructure for Chemistry-Enabling Access" (H2020-INFRAIA-2018-2020 grant agreement n. 101008500 - 01/09/2021-31/08/2026)

The Infrastructure

ITACA.SB: Potentiating the Italian Capacity for Structural Biology Services in Instruct-ERIC National Recovery and Resilience Plan Strengthening and creation of Research Infrastructures – Mission 4 – Investment line 3.1 (Project code: IR_0000009 - 01/11/2022 - 30/04/2026)

HIRES-MULTIDYN "Multiscale Dynamics with Ultrafast High-Resolution Relaxometry" (H2020-FETOPEN-2018-2020 grant agreement n. 8996830 - 01/10/2020-30/09/2025)

ISIDORe Integrated Services for Infectious Disease Outbreak Research (HORIZON-RIA grant agreement n. 101046133 - 01/02/2022 - 31/07/2025)

Remote NMR (R-NMR): Moving NMR infrastructures to remote access capabilities (HORIZON-CSA grant agreement n. 101058595 - 01/07/202 2- 30/06/2025)

ITN "GLYTUNES – A multidisciplinary training network for the bioinspired development of glycomimetics tuning the Siglec-Sialoglycan axis" (H2020-MSCA-ITN-2020 grant agreement n. 956758 - 01/03/2021 - 28/02/2025)

NRRP and CERM/CIRMMP

The CERM/CIRMMP Infrastructure is also strongly involved in the National Recovery and Resilience Plan (NRRP), funded by NextGeneration EU, and participates in several projects either directly as infrastructure or through the involvement of its researchers. Specifically, ITACA.SB is an infrastructure project empowering the Structural Biology services offered by Instruct-IT (https://www.itaca-sb.it/).

ITACA.SB: Potentiating the Italian Capacity for Structural Biology Services in Instruct-ERIC

The activities of the ITACA.SB project aim at fostering the excellence of NMR services of the Italian Centre of Instruct-ERIC, empowering and integrating the service capacity for protein production and biophysical characterization, potentiating data management, and computational tools available for widening the exploitation of structural biology technologies. Furthermore, ITACA.SB promotes a reduction of the environmental impact of NMR structural biology activities at Instruct-IT. Finally, ITACA.SB promotes outreach and networking to build a strong Italian SB community.

National Recovery and Resilience Plan

Call MUR 3264/2021 – M4/C2/L3.1.1

Applicant: Consiglio Nazionale delle Ricerche (CNR)

Co-Applicant: Università degli Studi di Firenze

Starting date: 01.11.2022

Project Duration: 30 months

Total amount: 17.977.617,89€ (40% of funds to South Italy infrastructures)

CERM@UniFi: 9.388.657,28€
CNR: 8.588.960,61€

Research Facilities involved in ITACA.SB: CERM/CIRMMP (Florence), IC: Institute of Crystallography (Bari, Caserta, Catania), IBPM: Institute of Molecular Biology and Pathology (Rome), ICB: Institute of Biomolecular Chemistry (Catania), IPCB: Institute for Polymers and Composite (Catania).

Staff: In 2025, the ITACA.SB project has expanded the CERM staff by recruiting two fixed-term scientists, one dedicated to NMR instrumentation and the other to follow the project's communication activities.

Instrumentation upgrade: In 2025, a novel cryogenically cooled probehead allowing $^{1}H/^{19}F$, ^{13}C, and ^{15}N experiments has been installed on one of the 700 MHz instruments. This probehead, in addition to the increased sensitivity for proton detection, features a cold amplifier for all the other nuclei, enabling high-sensitivity heteronuclear experiments, including ^{19}F NMR spectra.

The Infrastructure

Publications: In 2025, ITACA.SB has been acknowledged in 30 peer-reviewed publications. An up-to-date list of publications is available at https://www.itaca-sb.it

SUMMARY OF NRRP PROJECTS WITH CERM/CIRMMP STAFF INVOLVED			
PROJECT			**Research Activities**
RI – ITACA.SB	Banci, Pierattelli, Turano, Felli, Fragai, Ravera, Rosato, Cerofolini, Schiavina, Allegrozzi, Del Conte, Gonnelli	Potentiating the Italian Capacity for Structural Biology Services in Instruct-ERIC	pg. 20-30
CN3 - SPOKE 5	Pierattelli, Fragai	Inflammatory and infectious diseases	pg. 20, 21, 24
THE - SPOKE 4	Banci, Cantini, Del Conte, Gonnelli	Nanotechnologies for diagnosis and therapy	pg. 20, 23, 26
THE - SPOKE 6	Rosato	Precision Medicine & Personalized Healthcare	pg. 27
THE - SPOKE 7	Ciofi Baffoni, Piccioli	Innovating Translational Medicine	pg. 25, 28
THE - SPOKE 8	Pierattelli, Felli, Parigi, Allegrozzi	Biotechnologies and imaging in neuroscience	pg. 24, 29
PE8 - SPOKE 2	Tenori, Vignoli	Improving the understanding of the biology of ageing	pg. 31
PE12 - SPOKE 6	Felli	Mechanisms of neuronal cell degeneration and drug dependent reversal	pg. 24

Solution and Solid-State NMR Spectrometers

All NMR instruments at CERM are state-of-the-art, digital spectrometers equipped with a variety of cryo-probes, as well as with specific probes covering a broad range of frequencies and of observable nuclei. In addition to the standard pulse sequences for spectroscopic, structural, dynamical, and functional characterization, tailored pulse sequences for structural determination of high molecular weight proteins, intrinsically disordered proteins and paramagnetic systems are implemented. Furthermore, protocols and pulse sequences tailored for in-cell NMR experiments are also implemented, including two flow NMR bioreactor units that can fit any 5-mm probe and preserve cell viability for prolonged NMR acquisitions, up to ~3 days and allow to follow cellular processes over time. Pulse sequences and experiment setup for the detection and characterization of paramagnetic systems have been pioneered at CERM for decades. Solid-state MAS probes cover almost all the presently achievable MAS frequencies, for both biological and inorganic material characterization. A prototype shuttle system for high-resolution relaxometry measurements at 700 MHz, part of the HIRES-MULTIDYN research activities, allows for nuclear spin relaxation measurements at fields as low as 47 mT (~2 MHz ^{1}H Larmor frequency) by moving the sample inside the stray field of the magnet, while providing high resolution readout through high field detection.

In 2025, a new 5-mm TCI (^{1}H&^{19}F/^{13}C/^{15}N) Cryoprobe has been installed at 1.2 GHz. This probe has been co-developed with Bruker as part of the consortium activities of the EC-funded FragmentScreen project and is the first of this kind to be developed for ultrahigh magnetic fields. In addition to the triple resonance channels for biomolecular applications, this probe allows tuning the ^{1}H coil to for ^{19}F acquisition. This probe offers unmatched resolution and sensitivity for the analysis of small fluorinated compounds and will allow a vast range of applications towards the screening of fluorinated fragments or drugs. A second TCI (^{1}H&^{19}F/^{13}C/^{15}N) probe of the same kind has been installed at 700 MHz. Together with the existing QCI-F probe at 600 MHz, these instruments allow a wide range of applications of ^{19}F NMR at very different magnetic fields.

Instrumentation

B_0 Field (T)	^{1}H Larmor Frequency (Bore)	Probe heads
28.2	1.2$^{\#}$ GHz (NB 54 mm)	TCI Cryo 5 mm solution (^{1}H/^{13}C/^{15}N with ^{2}H decoupling) TCI Cryo 3 mm solution (^{1}H/^{13}C/^{15}N with ^{2}H decoupling) TXO Cryo 5 mm solution (^{1}H/^{13}C/^{15}N with ^{2}H decoupling) PI HR RT 3 mm solution ^{1}H/^{13}C/^{15}N/ with ^{2}H decoupling) 0.7 mm CP MAS ^{1}H/^{13}C/^{15}N
22.3	950*$^{\#}$ MHz (NB 54 mm)	TCI Cryo 5 mm solution (^{1}H/^{13}C/^{15}N with ^{2}H decoupling)
21.1	900$^{\#}$ MHz (NB 54 mm)	2x TCI Cryo 5 mm solution (^{1}H/^{13}C/^{15}N with ^{2}H decoupling) TXI RT 5 mm solution (^{1}H/^{13}C/^{15}N with ^{2}H decoupling)
20.0	850 MHz (WB 89 mm)	3.2 mm CP MAS DVT ^{15}N/^{13}C/^{1}H 1.3 mm CP MAS ^{1}H-^{19}F/BB/^{15}N 0.7 mm CP MAS ^{1}H/^{13}C/^{15}N
18.8	800 MHz (NB 54 mm)	TXI RT 5 mm solution (^{1}H/^{13}C/^{15}N with ^{2}H decoupling) QXI RT 5 mm solution (^{1}H/^{13}C/^{15}N/^{31}P with ^{2}H decoupling) ^{1}H-Selective High Power RT (prototype) 3.2 mm CP MAS DVT Low-E ^{15}N/^{13}C/^{1}H 1.3 mm CP MAS ^{1}H-^{19}F/BB-X/BB-Y 1.3 mm CP MAS ^{1}H/^{13}C/^{15}N

Instrumentation

16.4	700* # MHz (NB 54 mm)	TCI Cryo 5 mm solution (^{1}H&^{19}F/^{13}C/^{15}N with ^{2}H decoupling) TXI RT 5 mm solution (^{1}H/^{13}C/^{15}N with ^{2}H decoupling)
16.4	700# MHz (NB 54 mm)	TXO Cryo 5 mm solution (^{13}C/^{15}N/^{1}H with ^{2}H decoupling) TXO RT 5 mm solution (^{13}C/^{15}N/^{1}H with ^{2}H decoupling) TXI RT 5 mm solution (^{1}H/^{13}C/^{15}N with ^{2}H decoupling)
16.4	700 MHz (WB 89 mm)	3.2 mm CP MAS ^{15}N/^{13}C/^{1}H 4.0 mm CP MAS ^{15}N/^{13}C/^{1}H DIFF-DR-BB/^{1}H&^{19}F-D-Z-5mm
14.1	600 MHz (NB 54 mm)	2 x TXI RT 5 mm solution (^{1}H/^{13}C/^{15}N with ^{2}H decoupling) HR-MAS 4.0mm (^{1}H/^{13}C/^{15}N with ^{2}H decoupling) ^{1}H - Selective High Power RT, 5 mm solution ^{1}H - Selective RT, 5 mm solution BBI RT 5 mm solution BBO RT 5 mm solution BBO RT 10 mm solution / BB RT -Low-γ -10 mm solution
14.1	600** MHz (NB 54 mm)	TXI RT 5 mm solution (^{1}H/^{13}C/^{15}N with ^{2}H decoupling)
14.1	600# MHz (NB 54 mm)	QCI-F Cryo 5mm solution (^{1}H/^{19}F/^{13}C/^{15}N)
11.7	500 MHz (NB 54 mm)	QCI-P Cryo 5 mm solution(^{1}H/^{13}C/^{31}P/^{15}N) TCI Cryo 5 mm solution(^{1}H/^{13}C/^{15}N) TXI RT 5 mm solution (^{1}H/^{13}C/^{15}N) TBO RT 5 mm solution (^{1}H/^{31}P/BB) BBI RT 5 mm solution
9.4	400* MHz (NB 54 mm)	BBO RT 5 mm solution BBI RT 5 mm solution (^{1}H/BB) BBI RT 3 mm solution (^{1}H/BB) ^{1}H-Selective High Power 5 mm solution
0.33-1.25	Pulsed EPR	X and Q Band cavities, X (9.43 GHz), Q-Band (35 GHz), ENDOR Module for Q-Band
0.00024-1	Fast Field Cycling Relaxometer	0.01-40 MHz 10 mm solution tubes

* With sample changer.

** Standardized for metabolomics: equipped with the SampleJet robotic and refrigerated charger, along with dedicated routines for the analysis of biofluids through the Bruker IVDr platform.

Bruker Smart Nitrogen Liquefier (BSNL) to reliquefy nitrogen from the NMR magnet

Biological and Biophysical Facilities and Services

X-ray Crystallography

CERM/CIRMMP is equipped with standard crystallization facilities and with an automated nano-dispensing device (Mosquito, TTP Labtech). Furthermore, it has full access to the Interdepartmental Crystallography Centre of the University of Florence (CRIST, https://www.crist.unifi.it), equipped, among other instruments, with two sealed-tube diffractometers. The most recent one is a Bruker D8 Venture with double microsource (Cu and Mo) bearing a Photon III Pixel Array detector and the older one is an Xcalibur PX Ultra (Oxford Diffraction) equipped with a 165 mm CCD detector for routine in-house data collections. Both diffractometers are equipped with a liquid nitrogen cryosystem. Regular access to synchrotron beam time slots in European facilities is also available.

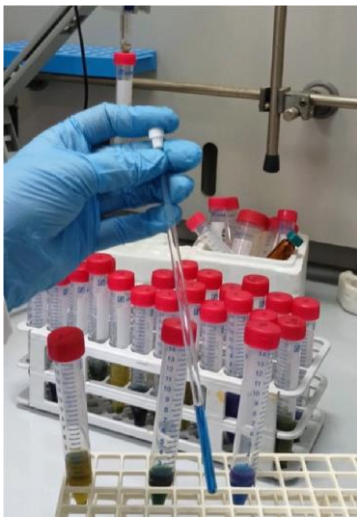
Molecular and Cellular Biology

CERM/CIRMMP is equipped with state-of-the-art facilities for gene cloning and protein expression and purification. Large scale protein expression in prokaryotes and yeast is available through the use of fermenters. Different isotope labelling schemes, including specific labelling schemes oriented to NMR characterization, can be achieved using auxotrophic strains. Fully equipped facilities for protein purification are available, including last-generation instruments for streamlined purification (ÄKTA chromatography system, including two newly installed ÄKTA Pure and ÄKTA Go machines) and equipment for protein purification. A dedicated modern glove box, equipped for protein purification and reconstitution in anaerobic environment is also available as support for the biomolecular Lab.

A mammalian expression lab for in-cell NMR is equipped with a CO_2 incubator, two laminar flow hoods, a brightfield microscope, a Nikon Eclipse Ts2RFL Optical Microscope, and a Guava Easycyte 5 HT flow cytometer.

Instrumentation

EPR



A Bruker ELEXYS E580 spectrometer allows operating in continuous wave at X-band (9.8 GHz) and in pulsed mode at Q-band (34 GHz). The spectrometer is equipped with a newly installed a DICE-II Pulse ENDOR System E560D-P-RF for spectroscopic characterization of the molecular and electronic structure of paramagnetic species.

Multi Angle/Dynamic Light Scattering

A new Dawn-18 system (SEC-MALS complete with HPLC DLS and FFF) instrument for measurements on batch samples or on in-flow samples (FPLC coupling) has been installed, which allows for high-sensitivity measurements of proteins, polymers and nanoparticles to determine sample polydispersity, molar mass, size, conformation, and interactions.

Isothermal Calorimetry (ITC)

A new Isothermal Titration Calorimeter (MicroCal PEAQ-ITC) to measure thermodynamical parameters in micro-samples has been installed. The instrument is fully equipped for studying protein-ligand and protein-protein thermodynamical parameters.

Optical Spectroscopy

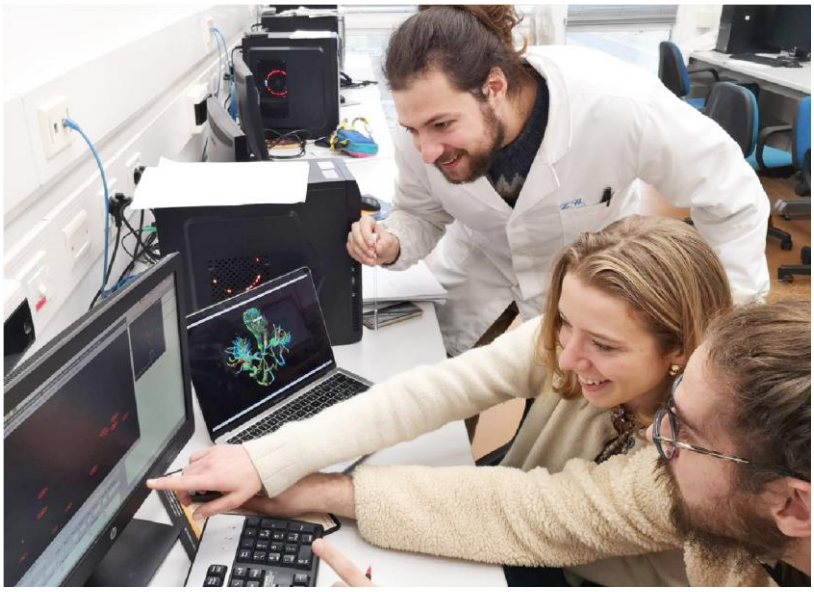
Absorption/Fluorescence Spectrophotometer (newly installed Varian Cary Eclipse Spectrophotometer) operating from 1000 to 200 nm, *Circular Dichroism* (CD) spectrometer operating from 1200 to 200 nm (Near-IR, Visible, UV) to derive information on the proteins secondary structure or protein-metal interaction, and newly installed SFM-4000 stopped-flow spectrophotometer are available in the infrastructure.

Computational Structural Biology Tools

CERM/CIRMMP provides integrated databases and software for genome browsing, the analysis and prediction of metal bindings, NMR-based macromolecular structure calculations with/without paramagnetic restraints, investigation of protein complexes. Access to programs for NMR data processing and structural calculations is also provided via web.

Electronic infrastructure (e-infrastructure)

The grid and cloud-based services of CERM/CIRMMP are part of the WeNMR thematic services (https://www.egi.eu/case-study/wenmr/), which have been developed throughout a variety of collaborative European projects involving the European Grid Infrastructure and other partners. At present this collaboration is funded via the EOSC Data Commons initiative (https://www.eosc-data-commons.eu/).



Services for structural biology are indeed a crucial component of technological development ongoing in the context of the European Open Science Cloud (EOSC). The standardized data processing and deposition frameworks previously established within EOSC-Life enable our structural biology workflows to be deposited in public repositories and be reused also by other NMR centres on their own computing infrastructure. The WeNMR thematic services provide application-level services specific to different cases in Structural Biology, with special focus on NMR-based tools. The user community served by the WeNMR services encompasses over 14000 registered users over the years from nearly 100 different countries. Among recently added services, there are pipelines for data analysis in fragment screening campaigns, which will be exploited in conjunction with EOSC services and other European projects.

The available hardware at CERM/CIRMMP comprises two clusters with 80 and 1024 CPU-cores respectively, a cluster with 16 Nvidia L40 GPU cards and 256 CPU Cores, and two NAS storage units with 120 TB each.

Instruct-ERIC ESFRI Infrastructure – European and National NMR Research Infrastructure

CERM/CIRMMP is a key centre for application and development of NMR spectroscopy within Instruct-ERIC, an ESFRI infrastructure operative since 2012.

Instruct-ERIC provides access to unique instrumentation in a variety of different structural techniques (see page 5). This approach allows for a description of biological cells at the molecular level, in order to understand how living organisms function in normal and pathological conditions and to design drugs and vaccines. Currently, dedicated access routes are available for research tackling cancer and infectious diseases through the canSERV and ISIDORe projects, respectively. Access to Instruct-ERIC represents a unique opportunity for researchers, across national and European levels to enhance the impact of their work and bolster their overall innovation capacity.

The project PANACEA (https://panacea-nmr.eu/), started in 2021, is funded by the HORIZON2020 program to offer European researchers access to advanced Solid-State NMR instruments for the investigation of chemical and pharmaceutical solid compounds, as well as organic and inorganic materials. The platform is open to scientists and industrial partners with or without previous experience in solid-state NMR.

CERM/CIRMMP continues to provide access to its instrumentation to all national users as well as European and international researchers where alternative routes are unavailable, provided their research project matches quality criteria in terms of scientific interest, excellence and feasibility.

In all cases, access is granted on the basis of peer-review of the received proposals, and after a feasibility check by the staff scientists of CERM/CIRMMP. Technical assistance is provided for the acquisition of the data. Scientific collaborations are welcome but not required. The uniqueness of access provision at CERM/CIRMMP infrastructure lies in the wide number of available NMR instruments, the variety of the NMR equipment (probes, automatic sample changers, …) and the exceptional expertise of the scientific and technical stuff, which represents an ideal environment for NMR research, especially in the field of structural and functional characterization of biological systems.

Molecular biology and cellular biology labs are also strategic for the users' needs to prepare and/or optimize a large variety of samples for structural characterization, together with other biophysical equipment for EPR, CD, UV-vis, stopped-flow measurements, manual and automated crystallization facilities and X-ray diffractometry. Users can also access other university facilities

National and Transnational Access

available in the campus, such as those for cryo-electron microscopy (FloCEN), mass spectrometry, Raman resonance, and non-linear spectroscopies.

During 2025 we recorded 541 days of external access to the NMR spectrometers. A more detailed analysis shows that 340 days of NMR access were provided to academic users via Instruct-ERIC, Instruct-ITALIA, and PANACEA, 120 days through formal collaborations, while 81 days were provided to industry users as services.

Beside NMR access provision, the infrastructure also provided access to protein production services via Instruct-ERIC and to other structural biology techniques via Instruct-ITALIA.

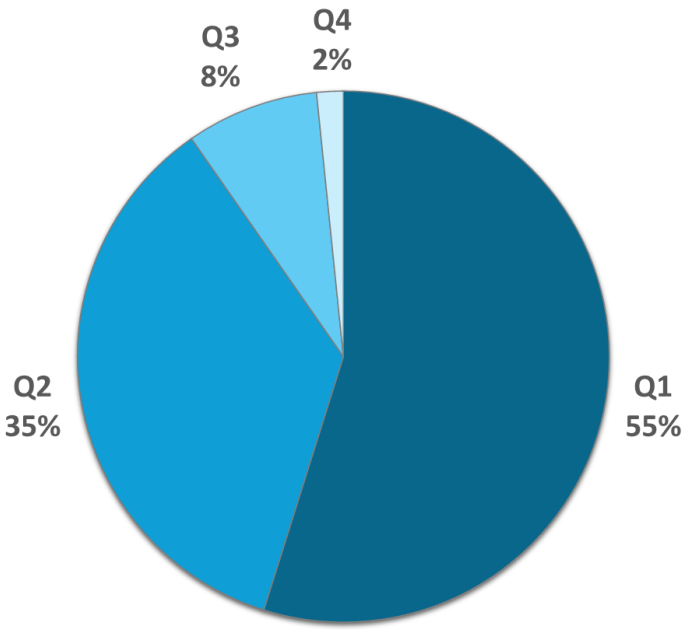
Worth to mention the implementation of a platform for the management of NMR access (https://amp.cerm.unifi.it/) improving data findability and experiment reproducibility and, thanks to new in-house LIMS, track of all the experiments performed and allows long-term data storage.

Scientific Output 2025

During 2025, several research projects have been carried out at CERM, either as an extension of the activities of previous years or as new projects. Most of these projects receive specific funding from national and/or European organizations.

While NMR remains the core technology at CERM/CIRMMP, research over the years has progressively expanded to new applications, integrating NMR with a range of complementary techniques. This approach reflects the principles of integrated structural biology, which underlie the Instruct-ERIC consortium.

Current research at CERM/CIRMMP spans a broad spectrum of applications, from NMR studies of proteins in vitro and in intact cells, to bioinformatics and computational methods; from paramagnetic NMR spectroscopy and relaxometry to the development of novel MRI contrast agents; from investigating proteins and peptides as drugs or therapeutic targets to the development of metal-based drugs; and from metabolomics and biomedical applications to advanced solid-state NMR techniques for material characterization.

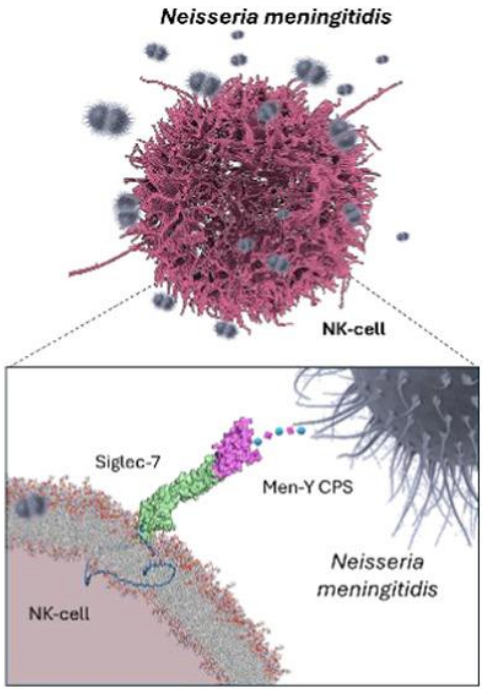


During 2025 we published 67 papers in international peer-reviewed journals, with several publications on high-impact journals. Our publications have an average journal impact factor (JIF) of 6.9, with 50% of the publications on journals with JIF higher than 5. Notably, 55% of papers have been published in journals ranked in the first JIF quartile of their subject areas (Q1). A complete list of publications is available at page 43.

Structural Biology for Immunology

A cutting-edge research activity aimed at understanding molecular interactions between pathogens and the host immune system has been carried out at CERM/CIRMMP, with the ultimate goal of developing innovative therapeutic and prophylactic strategies. A central research theme is the structural and molecular characterization of bacterial and viral components, including surface proteins, polysaccharides, and glycoconjugates. By combining techniques such as NMR spectroscopy, structural biology, and biophysical analysis, the researchers have contributed to elucidate how these molecules mediate virulence, host recognition, and immune evasion.[1-2] Another major focus has been the design and development of next-generation vaccines and immunotherapies. The groups worked on glycoconjugate vaccines, GMMA (Generalized Modules for Membrane Antigens)-based platforms, and tumor-associated carbohydrate antigens, aiming to elicit targeted and protective immune responses against both infectious agents and cancer.[3] These approaches are complemented by efforts to develop monoclonal antibodies capable of neutralizing highly resistant pathogens, including pandrug-resistant bacterial strains.[4]

CERM/CIRMMP laboratory integrates chemistry, biology, and medicine to address urgent global health challenges, including antimicrobial resistance, emerging infectious diseases, and cancer, with a strong emphasis on translational impact and vaccine innovation. The research activity has leaded to the development of new monoclonal antibodies and vaccine models.



Siglecs, sialic acid-binding immunoglobulin-like lectins, are key immune cell receptors that recognize sialic acid residues on cell surfaces.

The laboratory is also active in the field of glycoscience and biomimetic systems, contributing to design synthetic receptors and glycan mimetics to probe and interfere with biologically relevant interactions, such as viral entry mechanisms (e.g., SARS-CoV-2 glycan recognition). This work bridges fundamental chemistry with antiviral strategy development.[5] In addition, the researchers have developed and applied advanced analytical methodologies, particularly NMR-based approaches, for the rapid and accurate characterization of complex biomolecules and pharmaceutical formulations, including lipid components in vaccines and drug delivery systems.[6]

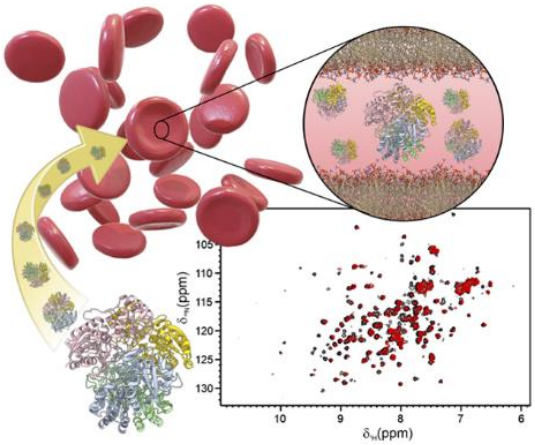
1) C. Di Carluccio *et al.* ***JACS. Au***. 2025, 5, 2257–2269. 2) V. Monaci *et al.* ***Protein Sci.*** 2025, 34 (11). 3) E. Pesce *et al.* ***npj Vaccines*** 2025, 10 (1). 4) E. Roscioli *et al.* ***Nature*** 2025, 646, 1204–1213. 5) C. Santambrogio *et al.* ***ChemBioChem*** 2025, 26 (7). 6) F. Currò *et al.* ***ACS Omega*** 2025, 10 (44), 53586–53595.

Proteins as drugs and drug targets

Proteins are important pharmaceutical targets, and an increasing number of drugs are proteins. Studying protein structure of the protein targets and their interactions with partners is crucial for finding new drugs and developing potential treatments. Protein-based and ligand-based NMR assays are also routinely applied to identify and validate the binding of drug candidates to their target.

The development of new drugs is a fundamental research topic at CERM/CIRMMP.

In the development of biotherapeutics the use of an effective delivery system is crucial for ensuring its efficacy. To this aim, whole erythrocytes (RBCs) have been applied in preclinical studies to deliver biological therapeutics. However, characterization of such complex systems poses challenges that complicate their development and optimization. To this end, the researchers at CERM have implemented NMR spectroscopy to monitor the preservation of the high order structure of encapsulated proteins in RBC, as well as their concentration, providing a tool to assist in formulation design, development, and manufacturing.[1] Protein–polysaccharide interactions underlie both the process of immune evasion by cancer cells and bacterial colonization, mediated by the binding of sugars, overexpressed on the surface of cancer or bacteria cells, with receptors (like Siglec-7) on immune system cells. Researchers at CERM have combined structural biology techniques, including NMR, biophysical, and computational methods, to provide insights about the binding of Siglec-7 both to GD3 and Gb3 saccadic derivatives and Fusobacterium nucleatum lipopolysaccharides O-Antigen, occasionally linked to systemic diseases, including colorectal cancer. Understanding of these interactions could contribute to elucidate molecular mechanisms of cancer immune evasion and facilitate the development of therapeutic strategies.[2,3] Targeting protein-nucleic acids interaction has been a topic of research at CERM. A multidisciplinary approach was applied to provide insights into the structural and energetic aspects of the recognition of G-quadruplex DNA by KHSRP protein.[4] Finally, a continuous flow protocol was undertaken for the generation of new metallo-β-lactamases inhibitors.[5]



NMR provides a rapid assessment of structural preservation and a semi-quantitative evaluation of the concentration of therapeutic proteins encapsulated within RBCs.

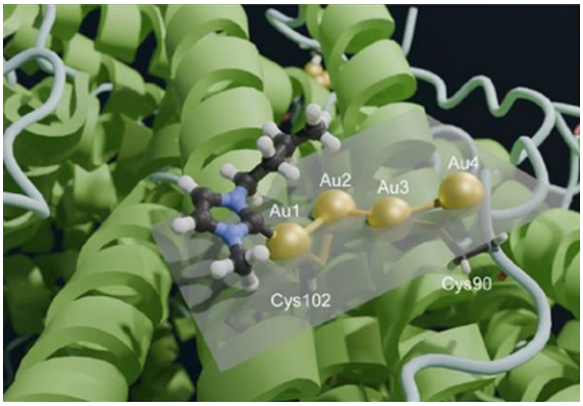
L. Padilla-Cortés, *et al.* ***J. Am. Chem. Soc***. 2025, 147, 26379–26388. 2) C. Di Carluccio, *et al.* ***Adv Sci (Weinh)*** 2025, 12, e2415782. 3) C. Di Carluccio, *et al.* ***JACS Au*** 2025, 5, 5367–5380. 4) P. Russomanno, *et al.* ***Adv Sci (Weinh)*** 2025, 12, 2410086. 5) A. I. Alfano, *et al.* ***J. Med. Chem.*** 2025, 68, 17236–17257.

Metal-based drugs: metabolomic alterations and ferritin-mediated delivery

Gold metal-based compounds show promise as experimental anticancer drugs due to their ability to alter cancer cell metabolism. Their effectiveness appears to depend on the type of gold ligands and their oxidation state. To analyze metabolic changes in A2780 ovarian cancer cells, we developed a method that combines pathway enrichment and metabolite clustering analysis. We created a genome-scale metabolic model to better understand the effects of key compounds like auranofin (AF), aurothiomalate (AuTM) and gold-carbenes (Au(NHC)Cl and An(NHC)$_2$). This model predicts how each gold compound affects metabolism and reveals common changes, offering insights into their mechanisms and potential uses in therapy.

Computational approaches were developed to enable an informative comparison of the effects induced by a panel of cytotoxic gold compounds in A2780 ovarian cancer cells. The suitability of human H ferritin as a nanocarrier for metallo-drugs was further investigated by examining the binding of a gold(I) carbene to the protein surface in a pocket, defined by two surface-exposed cysteines, that is highly selective for gold(I) compounds. ^{19}F NMR of ferritin incorporating a fluorinated tryptophan adjacent to this pocket, was proposed as a probe for monitoring the binding and release of these metallo-drugs.

The structure of the adduct between Au(NHC)Cl and human H ferritin (HuHf) was solved by cryo-EM at 1.51 Å resolution. It shows a novel tetranuclear gold(I) cluster, located in a surface pocket of each subunit where it is bound to C90 and C102, with short inter-metal distances diagnostic of the occurrence of aurophilic interactions.[3]



Structure of the tetranuclear gold cluster bound to C90/C102 of HuHf.[3]

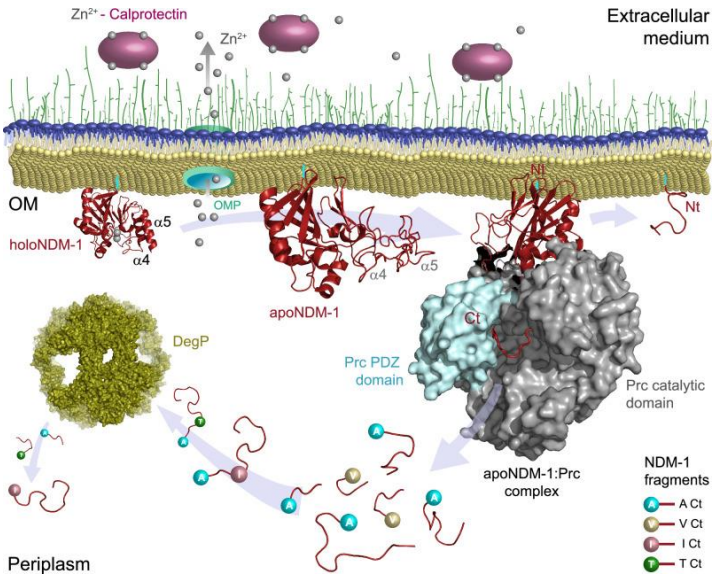
This structure, together with the MD models derived for AF and AuTM, was used to interpret the ^{19}F NMR chemical shift signatures for each compound in terms of site-specific interactions at the cysteine dyad (C90/C102).[4] HuHf is instead not suitable as a carrier for Pt(II) drugs: oxaliplatin indeed exhibited a complete loss of anti-cancer activity when bound to HuHf, probably because binding to ferritin severely disrupts the normal intracellular trafficking of Pt, making it unable to reach nuclear DNA.[5]

1) V. Ghini et al. ***J. Proteome Res.*** 2025, 24, 813-823. 2) W. Vieri et al. ***NPJ Syst. Biol. Appl.*** 2025, 11, 83. 3) L. Cosottini et al. ***Angew. Chem. Int. Ed.*** 2025, 64, e202503778. 4) V. Ghini et al. ***Mater. Adv.*** 2025,6, 6337-6344 5) V. Vitali et al. ***J. Inorg. Biochem.*** 2025, 273, 113019.

In-cell NMR in Bacteria and Human Cells

At CERM, novel in-cell NMR methods are developed that provide physiologically relevant insights on proteins in living bacteria and human cells. In bacteria, the periplasmic degradation mechanism of a metallo-β-lactamase was elucidated. In human cells, an inducible protein expression system was developed to allow in-cell NMR in synchronized human cells and 3D cultures, while ^{19}F competition binding in-cell NMR provided a qualitative ranking of novel carbonic anhydrase inhibitors.

In-cell NMR spectroscopy provides unique details on the structure, dynamics and function of macromolecules inside living cells. The highly physiologically relevant data obtained can complement the characterization carried out in vitro, providing structural and functional insights in the native cellular environment. CERM has a long-standing experience in developing and applying in-cell NMR approaches to study proteins both in bacteria and human cells. The bacterial periplasm is essential for bacterial survival and is critically involved in antibiotic resistance. Through in-cell NMR, we investigated the mechanism of periplasmic quality control of the zinc-dependent New Delhi Metallo-β-lactamase 1 (NDM-1), disclosing a sequential degradation process involving two proteases: the first, Prc, targets NDM-1 at the membrane, while the second, DegP, further degrades the released products.[1] In human cells, we reported a methodology to allow high-level inducible protein expression, enabling NMR studies in synchronized cells and in spheroids (3D tissue models).[2] Furthermore, a recently developed ^{19}F in-cell ligand-observe NMR approach was applied to monitor drug binding to soluble intracellular targets. A novel series of fluorinated ligands was designed as potential inhibitors of carbonic anhydrase (CA) cytosolic isoforms, each incorporating a trifluoromethyl group for NMR detection with high sensitivity. In-cell ^{19}F NMR allowed assessing target engagement towards each intracellular CA isoform, while competition binding provided qualitative affinity rankings toward each isoform, which critical for selecting promising inhibitors in pre-clinical stages of drug development.[3]



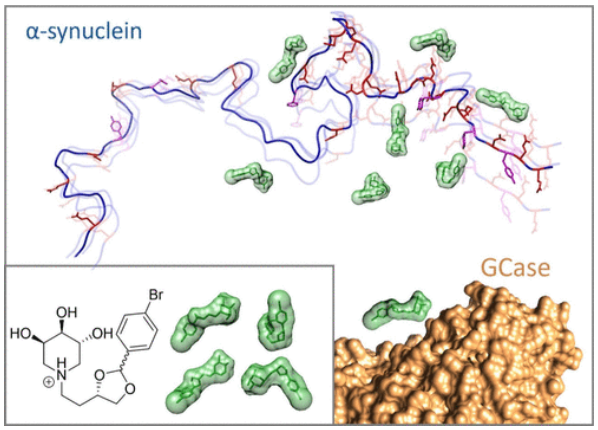
The molecular events elicited by Zn(II) deprivation and destabilization of NDM-1 at the inner leaflet of the bacterial outer membrane (OM).

1) González, L. J.; Hita, F. J.; Pontoriero, L.; Pierattelli, R.; Binolfi, A.; Vila, A. J. ***Nat. Commun.*** 2025, 16, 8366. 2) Ryneš, J.; Ištvánková, E.; Dzurov Krafcikova, M.; Luchinat, E.; Barbieri, L.; Banci, L.; Kamarytova, K.; Loja, T.; Fafílek, B.; Rico-Llanos, G.; Krejčí, P.; Macůrek, L.; Foldynova-Trantirkova, S.; Trantírek, L. ***Commun. Biolog.*** 2025, 8, 194. 3) Costantino, A.; Barbieri, L.; Giovannuzzi, S.; Nocentini, A.; Supuran, C. T.; Raitelaitis, M.; Nordlund, P.; Banci, L.; Luchinat, E. ***J. Med. Chem.*** 2025, 68, 23363–23374.

Intrinsically Disordered Proteins

Advanced NMR methodologies, including ^{15}N-detected experiments and optimal control pulses, enable high-resolution characterization of intrinsically disordered and multidomain proteins. Studies on the SARS-CoV-2 nucleocapsid protein show how structural heterogeneity regulates interactions with nucleic acid-like and polyanions molecules. Parallel work on neurodegeneration reveals interactions with different ligands and insights on how post-translational modifications modulate aggregation.

Development and application of advanced NMR methodologies are fundamental to investigate structurally complex and dynamic biomolecular systems such as multidomain and intrinsically disordered proteins (IDPs). For this reason, particular focus has been given to novel ^{15}N-detected approaches, including TROSY-based strategies[1] and optimal control pulses[2], which significantly improve sensitivity and resolution at high magnetic fields. These developments expand the available NMR toolkit, enhancing spectral quality under challenging conditions[3]. These and other tools have been applied to biologically relevant systems, particularly the SARS-CoV-2 nucleocapsid protein. Detailed studies dissect its multidomain organization[4], internal dynamics, and interactions with polyanions such as heparin[5]. The results reveal how structural heterogeneity and transient contacts regulate binding and functional adaptability. Complementary work introduces a peptide–PNA chimera[6] designed to target this protein, demonstrating the potential of hybrid molecules in modulating viral protein interactions. Beyond viral systems, we have focussed on proteins related to neurodegeneration. Investigations on α-synuclein[7] and tau[8] highlight how various partners or post-translational modifications are able to interfere with IDPs or to modulate their amyloid formation. At a broader level, integrative NMR approaches link structural features to functional outcomes. In-cell NMR studies were carried out to obtain atomic resolved information on a periplasmic protein[9]. Finally, contributions to database development enhance accessibility of IDPs, supporting a wider scientific community[10].



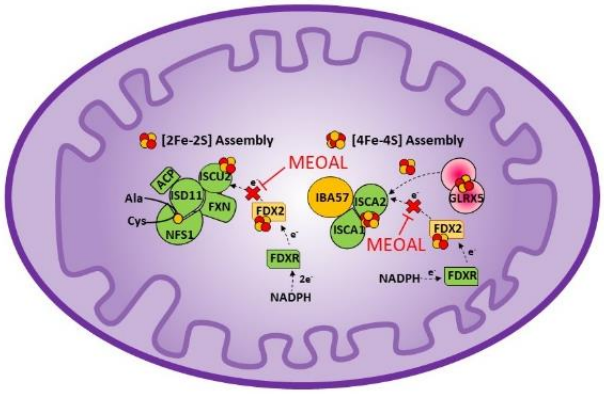
IDPs are often considered as undruggable. However, small molecules interacting with α-synuclein were recently identified and shown to act as chemical chaperones by NMR.

1) M. A. Rodella, et al., ***J. Magn. Reson.*** 2025, 381, 107972. 3) L. Bracaglia, et al., ***J. Am. Chem. Soc.*** 2025, 147, 13146–13157. 4) T. Bolognesi, et al., Prog. ***Nucl. Magn. Reson. Spectrosc.*** 2025, 148–149, 101577. 5) T. Bolognesi, et al., ***J. Mol. Biol.*** 2025, 437, 169437. 6) A. S. Tino, et al., ***Angew. Chem. Int. Ed.*** 2025, 64, e202420134. 7) G. Tagliaferro, et al., ***ACS Chem. Neurosci.*** 2025, 16, 1251–1257. 8) G. Viola, et al., ***Proc. Natl. Acad. Sci. U.S.A.*** 2025, 122, e2425831122. 9) L. J. González, et al., Nat. Commun. 2025, 16, 62340. 10) M. V. Nugnes, et al., ***Nucleic Acids Res***. 2025, 54, D383–D392.

Iron-sulfur protein biogenesis and related human diseases

CERM continues to pioneer the investigation of the molecular mechanisms of iron-sulfur protein biogenesis by applying a solution NMR-based approach. These studies provide a rationale for the pathogenicity of a novel mutation in FDX2, a protein essential for the biosynthesis of mitochondrial [2Fe–2S] and [4Fe–4S] clusters and implicated in the pathogenesis of MEOAL, a rare autosomal recessive mitochondrial neuromuscular disorder.

Over the past decade, structural insights into iron-sulfur (Fe/S) protein biogenesis have become increasingly important for understanding the mechanistic complexity of mitochondrial and cytosolic Fe/S cluster maturation machineries. In this regard, solution NMR has had a significant impact, owing to its ability to monitor transient protein-protein interactions, which are widespread in pathways involved in Fe/S cluster biosynthesis and transfer.[1] These studies are crucial for unravelling the molecular determinants of rare human disorders associated to "Fe/S diseases". In this respect, we focused our attention on an Fe/S protein (FDX2) that has recently been shown to be involved in a rare autosomal recessive neuromuscular disorder (MEOAL). In a recent study,[1] we have characterized a pediatric patient with a novel homozygous mutation in FDX2, i.e., c.200+4 A>G. We found that this mutation results in an altered protein, which is present at low levels in patient's cells. Biological and NMR-based structural data showed that any potential alteration found in MEOAL patient cells carrying the c.200+4 A>G mutation in FDX2 is likely due to the decrease of the FDX2 protein levels rather than to a structural alteration of the mature protein. Collectively, our findings highlight the crucial role of solution NMR spectroscopy in characterizing the first Italian patient with this severe mitochondrial disease and in elucidating the pathogenesis of this MEOAL case. These results provide a foundation for the development of targeted therapeutic strategies.



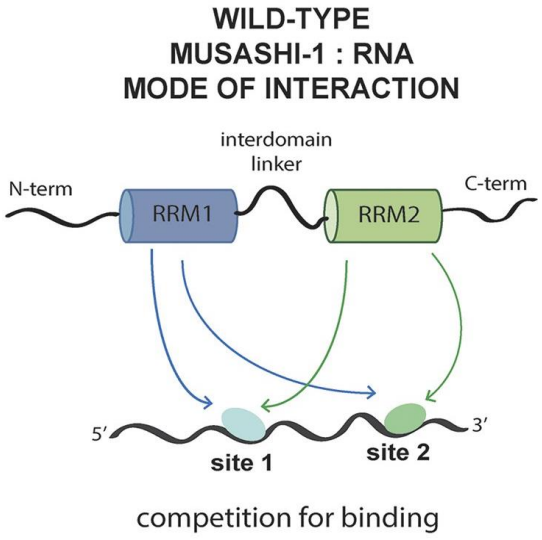
FDX2 is part of an electron transfer chain consisting of NADPH and FDXR driving the biosynthesis of [2Fe-2S] on ISCU2 protein and [4Fe-4S] clusters on ISCA1-ISCA2-IBA57 complex. To date there are gaps in our understanding of how FDX2 pathogenic mutations impact mitochondrial pathophysiology in MEOAL patients.

1) D. Doni, D. Grifagni, F. Cavion, B. Buchignani, R. Battini, E. Baschiera, M.A. Desbats, R. Pasquariello, G. Covello, E. De Pascale, A. Boarolo, I. Cestonaro, D. Badocco, P. Pastore, G. Sartori, O. Stehling, R. Lill, F.M. Santorelli, L. Salviati L, S. Ciofi-Baffoni, P. Costantini, **Cell Death Dis.** 2025, 17, 59.

The Role of NMR in Integrative Structural Biology

The research activity of researchers at CERM/CIRMMP lies within the field of the integrated structural biology, with a focus on the use of NMR for the characterization of structure, dynamics, and function of biomolecules relevant to both cellular and prebiotic contexts. One research line has investigated protein–RNA interactions, with particular emphasis on the molecular recognition mechanisms of Musashi-1, enabling the rational design of protein and RNA variants for in vitro and in vivo applications.[1] In parallel, the structural dynamics of the metal-binding proteins CIB2 was explored, revealing remarkable conformational flexibility and heterogeneous calcium and magnesium coordination, key features for their biological function.[2]

At CERM/CIRMMP, solution NMR is employed within integrated structural biology studies to investigate the structure, dynamics, and function of biomolecules. Combined with complementary biophysical methods, it enables deeper insights into protein–RNA recognition, metal-binding proteins, prebiotic systems, proteostasis, and protein modifications, revealing key structure–function relationships.



The analyse of the binding of Musashi-1 with single-stranded and structured RNA ligands allowed the design of protein and RNA variants for in vitro and in vivo applications

Another study investigated the origin of life, showing that prebiotic metallopeptides exhibit enhanced resistance to ultraviolet radiation, thus suggesting a potential selective role of metal ions in early evolutionary processes.[3] In the context of cellular proteostasis, the role of folding pathways and chaperone-like systems is also examined, as exemplified by studies on MIA40 and TRIAP1, which elucidate mechanisms that overcome conformational constraints during protein maturation.[4] Finally, high-resolution structural investigations of model proteins, such as chemically modified lysozyme, provide insights into the subtle structural effects induced by post-translational or chemical modifications.[5] Overall, these studies combine advanced experimental approaches to elucidate structure–dynamics–function relationships in complex biological systems.

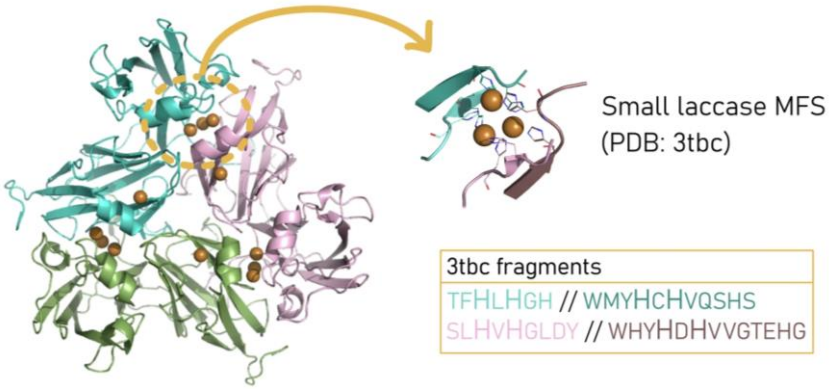
1) A. Pérez-Ràfols *et al.* ***Nucleic Acids Res***. 2025, *53* (15). 2) G. Olivieri *et al.* ***Int. J. Biol. Macromol.*** 2025, *286*. 3) D. Rossetto *et al.* ***Chem. Sci.*** 2025, *16* (25), 11246–11254. 4) J. Pujols *et al.* ***J. Biol. Chem.*** 2025, *301* (3). 5) J. M. da Silva *et al.* ***Acta Crystallogr. Sect. F Struct. Biol. Commun.*** 2025, *81* (Pt 2), 41–46.

Computing for Integrative Structural Biology

CERM is committed to the development and application of innovative computational methods for the prediction and analysis of metal-binding sites. A new approach enables the de novo design of minimal functional sites, such as biomimetic peptides capable of replicating complex enzymatic catalysis.

The field of inorganic biochemistry has undergone a profound transformation over the last two decades, evolving from a primarily experimental discipline into a science where bioinformatics and computational modelling serve as indispensable pillars. Institutions such as the Magnetic Resonance Center (CERM) in Florence have been at the forefront of this revolution[1,2]. The synergy between predictive tools and AI opens new perspectives for bioinformatic research on metalloproteins. In a recent study, we evaluated the effectiveness of computational tools in predicting zinc-binding sites in protein structures[3]. Another line of activity has focused on *de novo* biomimetic design. The goal is no longer just to observe nature, but to replicate its efficiency through synthetic catalysts that combine the selectivity of enzymes with the robustness of industrial materials. A landmark example of this is the design of the H4pep peptide. By applying the concept of the Minimal Functional Site to the design of metal-binding peptides, we successfully reduced the immense complexity of the laccase enzyme—specifically its trinuclear copper site—into a sequence of just eight amino acids. When bound to Cu^{2+}, this short peptide self-assembles into a complex with a β-sheet secondary structure capable of O_2 reduction[4].

We have also developed tools for the crystal field analysis, in view of the application to refining the structure of metal binding sites,[5] as well as user friendly tools for extracting data from NMR spectra.[6,7]



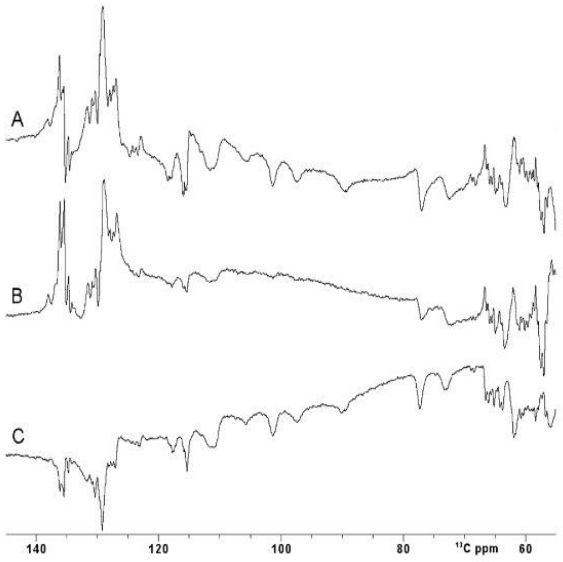
Pipeline for H4pep peptide design

1) C. Andreini, ***JIB.*** 2025, 266, 112854. 2) M.K. Maximillian K Osterberg et all. ***ACS Chem. Biol.*** 20(11), 2808-2826 3) C. Ciofalo, V. Laveglia, C. Andreini, A. Rosato, ***J. Chem. Info. Mod.*** 2025, 65(10), 5205-5215. 4) C. Spallacci, M. Chino, A. Rosato, O. Maglio, P. Huang, L. D'Amario, A. Lombardi, C. Andreini, M.H. Cheah ***Comm. Chem.*** 2025, 8(1), 7336–7336. 5) L. Fiorucci, E. Ravera, **J. Comput. Chem.** 2025, 46 (6), 6) Fiorucci, L.; Bruno, F.; Ricci, M.; Cicone, A.; Ravera, E. **Magn. Reson. Chem.** 2025, 63 (9), 737–747. 7) Fiorucci, L.; Bruno, F.; Querci, L.; Kubrak, A.; Bindi, J.; Rodić, N.; Licciardi, G.; Luchinat, E.; Parigi, G.; Piccioli, M.; Ravera, E. **Magn. Reson. Chem**. 2025, 63 (8), 628–654.

NMR of Paramagnetic Systems

The combination of paramagnetic NMR and density functional theory data provides evidence of the way unpaired electron density map is at the origin of the inequivalence of the two iron(III) ferredoxin centers. An electron spin density transfer is observed between cluster inorganic sulphide ions and aliphatic carbon atoms, occurring via a C–H---S–Fe^{3+} interaction. An extended assignment of ^{1}H, ^{13}C, and ^{15}N nuclei allows to estimate the magnetic exchange coupling constant between the two Fe^{3+} ions of the $[Fe_2S_2]^{2+}$ cluster of 386 cm–1. The approach developed here can be extended to other iron–sulfur proteins. [1] At ultra-high magnetic fields, the selectivity and efficiency of inversion pulses needs to be addressed. This is peculiarly relevant in paramagnetic systems, in which relaxation phenomena occurring during the pulse cannot be ignored nor neglected. Within this frame, optimal control pulses (OC pulses) have been, for the first time, applied to paramagnetic systems in a ^{13}C superWEFT experiment. The application to paramagnetic signals of Optimal Control Pulses has been successfully tested. OC pulses are much more efficient with respect to the phase- and amplitude-modulated ones routinely used at lower fields while providing bandwidth excitation profiles that are sufficient to meet the need to cover up to an 80 ppm spectral region. [2]

Density functional data, relaxation-based NMR assignments and tailored NMR experiments can be used to analyse NMR data at ultra-high magnetic field in order to provide advances in the understanding of electron delocalization and field-dependent shifts



Comparison between ^{13}C IR experiment performed with different inversion π pulses on oxidized $[Fe_2S_2]$ FDX2. (A) A rectangular (Squa.100) pulse, (B) shaped (Q3.1000) pulse and(C) optimal control (SURBOP180) pulse.

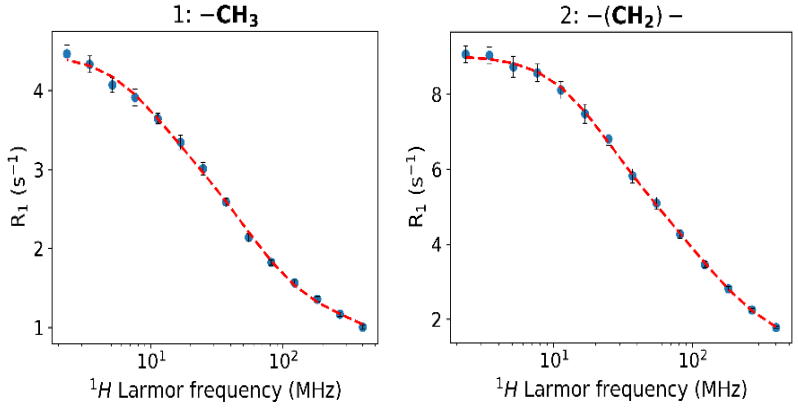
We have also contributed to the development of a quantum chemical approach to the determination of the field dependence of hyperfine shifts.[3]

1) Querci, L.; Fiorucci, L.; Grifagni, D.; Costantini, P.; Ravera, E.; Ciofi-Baffoni, S.; Piccioli, M. Shedding Light on the Electron Delocalization Pathway at the [Fe2S2]2+ Cluster of FDX2. **Inorg. Chem.** 2025, 64 (13), 6698–6712. 2) Querci, L.; Burgassi, L.; Ciofi-Baffoni, S.; Schiavina, M.; Piccioli, M. Optimized 13C Relaxation-Filtered Nuclear Magnetic Resonance: Harnessing Optimal Control Pulses and Ultra-High Magnetic Fields for Metalloprotein Structural Elucidation. **Int. J. Mol. Sci.** 2025, 26 (8). 3) Lang, L.; Fiorucci, L.; Parigi, G.; Luchinat, C.; Ravera, E. Theory of Field-Dependent NMR Shifts in Paramagnetic Molecules. **J. Chem. Theory Comput**. 2025, 21 (11), 5642–5660. .

Field-Cycling and High-Resolution Relaxometry

Fast field-cycling relaxometry (0.01–40 MHz) and high-resolution measurements acquired using a sample shuttle system installed on a 600 MHz spectrometer[1] were performed to determine the dynamics of individual hydrogen atoms in olive oil. The analysis of the relaxation profiles revealed their mobility, occurring on a wide range of timescales (from microseconds to tens of picoseconds), and their relative weights, providing insights on the different dynamics of molecular groups.[2] Fast field-cycling relaxometry was also applied for the characterization of candidate MRI contrast agents of improved efficacy. These molecules, containing paramagnetic metals like Gd^{3+}, increase the relaxation rates in such a way to generate brighter MRI signals and thus to enhance the sensitivity of the technique. Relaxometry measurements can provide mechanistic information about these paramagnetic complexes, their hydration and dynamics.[3-5] A gadolinium-based disulphide homodimer has been incorporated into a lipoic acid-based hydrogel for potential applications in tracking internal injuries. The measurements indicate a relaxation enhancement attributed to a significant increase in the reorientation correlation time of the complex.[4] Manganese-doped ferrite nanoparticles were also characterized as potential temperature–sensitive exogenous MRI contrast agents at low magnetic fields for non-invasive MRI thermometry.[5]

Field-cycling relaxometry is an extremely informative tool for investigating molecular dynamics. By probing the magnetic field dependence of nuclear relaxation rates across nearly four orders of magnitude, this technique provides direct access to spectral density functions and thus to the correlation times of the underlying dynamic processes. Relaxometry is extensively employed to characterize the efficacy and mode of function of MRI contrast agents.



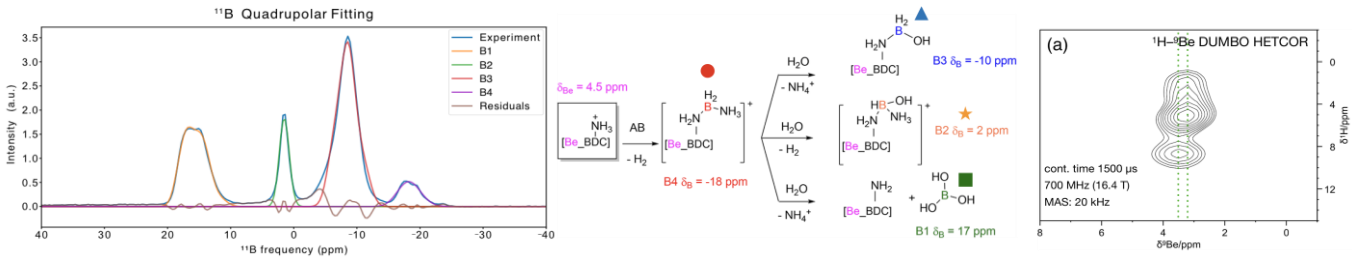
Field dependence of the relaxation rates observed for methyl protons and for -CH_2- protons of olive oil.[1]

1) J.A. Villanueva-Garibay et al. ***Magnetic Resonance*** 2025, 6, 229–241. 2) G. Licciardi, L. Fiorucci, J.A. Villanueva-Garibay, O. Stenström, E. Ravera, F. Ferrage, C. Luchinat, G. Parigi, ***J. Mol. Liq.*** 2025, 437, 128538. 3) A. Kubrak, R. Pejanovic, K. Kamau, D. Kruk, F. Ferrage, G. Parigi, ***Phys. Chem. Chem. Phys.*** 2025, 27, 1756–1771. 4) A. Brotherton, B. Phillips-Sorich, N. DomNwachukwu, M. Bailey, A. Patel, C. Luchinat, G. Parigi, T.J. Meade, ***ACS Appl. Bio Mater.*** 2025, 8, 5903–5911. 5) S.D. Oberdick et al. ***ACS Appl. Nano Mater.*** 2025, 8, 18424−18433..

Solid-state NMR for Materials

Solid state NMR (ssNMR) is a powerful technique for the characterization of materials, this because it allows one to obtain structural and dynamical information at atomic level independently on the aggregation phase of the investigated system either we investigate a crystalline system or an amorphous or composite material. Here ssNMR is applied to investigation of materials for hydrogen storage, introducing new Metal Organics Frameworks (MOF) suitable for hydrogen incorporation.

The the development of hydrogen economy is strongly limited by the problems related to hydrogen storage. Metal Organic Frameworks (MOF) are versatile materials that can be used to sizably incorporate hydrogen at low temperature (77 K), but with much less efficiency at room temperature. In collaboration with the ICCOM-CNR, we have developed new MOF designed to incorporate ammonia borane ($BH_3{\cdot}NH_3$, AB) in a nano-confinement strategy. This makes it possible to reversibly bind hydrogen in stable boron hydride species that release back hydrogen by warming them at mild temperatures. Solid-state NMR is the method to choose for investigating these systems and it is more and more applied to characterize advanced materials[1] as in the case of bioinspired materials[2] or in material related to the energetic transition[3,4]. We prepared zirconium based MOF with a UiO-67 structure but endowed with bis-pyridyl or bis-thiazole dicarboxylate ligands, loading it with AB or with hydrazine bis-borane molecules (AB@MOF and HBB@MOF). ssNMR revealed that these molecules interact with the metallic node and the MOF linker, significantly reducing to 50°C the hydrogen release temperature.[3] A new lightweight MOF was also developed, with a beryllium metallic node and ammino-terephthalic linker in MOF-5 like structure, and we loaded it with AB. The multi nuclear ssNMR analysis, involving either the analysis of the quadrupolar lineshape in ^{11}B and ^{9}Be spectra, and the 1D and 2D ^{1}H, ^{13}C and ^{15}N spectra made it possible to obtain an accurate description of the fate of the incorporated AB, unravelling the formation of several boron hydride species that plays a role in the hydrogen release.[4]



The analysis of the quadrupolar ^{11}B and ^{9}Be ssNMR, together with ^{1}H, ^{13}C, ^{15}N, allowed us to describe the boron hydride species in AB@MOF.

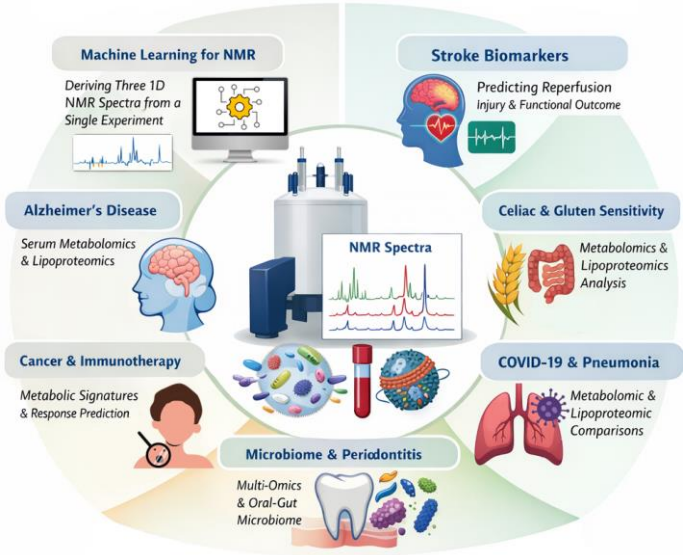
1) Coulon, R.*; et al.* ***Solid State Nucl. Magn. Reson.*** 2025, *140, 102048*. 2) Lanuza, J.*; et al.* ***Inorganics*** 2025, *13*, 206. 3) Provinciali, G.; Consoli, N.A.*; et al.* ***ACS Appl. Ener. Mat.*** 2025, *8*, 16891–16903. 4) Provinciali, G.; Consoli, N.A.*; et al.* ***J. Phys. Chem. C*** *2025, 129, 6094–6108*.

Metabolomics in Biomedicine

NMR-based metabolomics at CERM spans a broad range of activities. In 2025, the research focus was oriented to both methodological developments and clinical applications.

Two methodological contributions highlight ongoing efforts to improve the efficiency and robustness of NMR data acquisition and analysis. In particular, a machine-learning approach was developed to derive three one-dimensional NMR spectra (CPMG, Diffusion-edited, JRES projections) from a single 1D NOESY experiment, significantly increasing throughput for large metabolomics studies[1]. In parallel, the open-source Python package pyIHM was introduced to implement the Indirect Hard Modelling approach, enabling robust quantification of metabolites in complex mixtures and supporting reproducible computational workflows[2].

Metabolomics provides a comprehensive, dynamic, and accurate picture of a cellular model, a biofluid, an organ, or an organism at the molecular level. Consequently, it is an invaluable tool to obtain information on the underlying biochemistry of diseases, to diagnose and to prognosticate pathological conditions.



NMR-based metabolomics activities in 2025

NMR metabolomics was also applied to a wide range of clinical research questions. Blood serum metabolic profiles integrated with circulating inflammatory biomarkers were used to predict reperfusion injury and functional outcomes after ischemic stroke[3]. Serum metabolomic and lipoproteomic analyses were used to study metabolic alterations associated with Alzheimer's disease prognosis[4] and to discriminate between celiac disease and non-celiac gluten sensitivity[5]. The metabolic signatures associated with response to immunotherapy in melanoma patients was identified[6]. Significant overlap was instead reported for the plasma profiles of COVID-19 patients and patients with other forms of pneumonia[7]. Furthermore, metabolomics and lipoproteomics were integrated with the microbiota analysis to investigate the systemic effects of periodontitis and periodontal therapy on both oral and gut microbial communities[8]. Overall, these studies demonstrate the versatility of NMR spectroscopy as a platform for high-throughput metabolomics with the aim of translational biomedical research.

1) Vignoli, A.; et al. ***Nat Commun*** 2025, 16 (1), 10159. 2) Bruno, F.; et al. pyIHM: Indirect Hard Modeling, in Python. ***Analytical Chemistry*** 2025, 97 (8), 4598–4605. 3) Vignoli, A.; et al. ***Journal of Translational Medicine*** 2025, 23 (1). 4) Vignoli, A.; et al. ***Journal of Translational Medicine*** 2025, 23 (1). 5) Vignoli, A.; et al. ***Clinical Nutrition*** 2025, 45, 31–35. 6) De Summa, S.; et al. ***Front Immunol*** 2025, 16, 1536710. 7) Ghini, V.; et al. ***Scientific Reports*** 2025, 15 (1). 8) Baima, G.; et al. Multi-Omics Signatures of Periodontitis and Periodontal Therapy on the Oral and Gut Microbiome. ***J Periodontal Res*** 2025, 60 (12), 1237–1253.

Metabolomics of Foods, Plant and Animals

In 2025, our research activities focused on the application of NMR-based metabolomics to characterize and compare the metabolic profiles of a variety of biological matrices, including plant-derived products, dairy foods, and animal biofluids.

Metabolomics has become an important approach for investigating the biochemical composition of foods, plants, and animal systems. NMR spectroscopy enables robust and high-throughput metabolic profiling of complex biological matrices, supporting studies on composition, quality, authenticity, and biochemical variability across diverse biological products.

NMR metabolomics was applied to extra virgin olive oils to investigate quality attributes and compositional variability. By combining NMR spectra with machine learning models, several chemical and sensory parameters were predicted and oils were successfully classified according to cultivar and harvest year[1].

A major research line focused on milk and milk-derived products, as well as plant-based alternatives. NMR metabolomics was applied to plant-based beverages (soy, almond, coconut, rice, and oat) and compared with cow and goat milk, revealing distinct markers that allowed discrimination among beverage and milk categories[2]. The same approach was used to investigate compositional differences among human milk, cow milk, goat milk, and commercial infant and toddler formulas. The analysis revealed clear metabolic distinctions between human milk and other mammalian milks, while formulas showed a more homogeneous composition but remained metabolically distinct from human milk[3]. NMR spectroscopy was also applied to compare whey and whey protein concentrate (WPC-80), highlighting metabolic changes introduced by industrial processing and providing insights into the nutritional and functional properties of whey-derived ingredients[4].

Applications in 2025 of NMR-based metabolomics in food, dairy, and veterinary systems.

Finally, NMR metabolomics was applied to dog serum to investigate metabolic alterations associated with canine parvovirus infection, revealing differences in metabolites related to energy and lipid metabolism[5].

Overall, these studies highlight the versatility of NMR-based metabolomics as a platform for the characterization of complex biological matrices across food, plant, and animal systems.

1) Meoni, G.; et al. ***Comput. Struct. Biotechnol. J*** 2025, 27, 135-1369. 2) Meoni, G.; et al. ***J. Dairy Sci.*** 2025, 108 (6), 5675-5695. 3) Meoni, G.; et al. ***Metabolites*** 2025, 15 (9). 4) Sousa, I.; et al. ***Metabolites*** 2025, 15 (12). 5) Başoğlu, A.; et al. ***Vet. Ital.*** 2025, 61 (1).

Collaborations with Industries

CERM/CIRMMP has a long tradition in collaborations with industries: from simply providing access and service to its instrumentation, to establishing a more collaborative activity in research projects or to the participation as partners in international project calls. This number does not include the access provided to industrial partners through collaborative projects.

We warmly thank the following companies for stimulating interactions:

Bracco

Bruker BioSpin

Dompé Pharmaceutica

Glaxo Smith Kline

Giotto Biotech

Merck

Menarini

Infineum

Stelar

Extra Byte

Latus Pet

Collaborations

Maven Health

Evonik

Resonate Bio

A special acknowledgment to
Gruppo SAPIO
official supplier of all the cryogenic gases
of CERM/CIRMMP

Florence Center for Electron Nanoscopy (FloCEN)

FloCEN (https://www.flocen.unifi.it/index.) is a laboratory located at the Department of Chemistry of the University of Florence, which houses state-of-the-art equipment for Cryo-Electron Microscopy (Cryo-EM), which includes a ThermoFisher Transmission Electron cryo-Microscope Glacios at 200-kV (also equipped with a Falcon III direction electron detector), a ThermoFisher Vitrobot Mark IV for specimen preparation, and a PELCO easiGlow™ Discharge Cleaning System (optimized for cleaning TEM grids). Furthermore, FloCEN has a low humidity room and a shielding system to keep the microscope free from electromagnetic interference, thus guaranteeing a very stable environment. FloCEN was established thanks to the funding provided by MUR (grant Dipartimento di Eccellenza 2018-2022), with an important co-financing with the MUR International Action of FOE dedicated to the Italian centre of Instruct-ERIC. Cryo-EM and NMR are complementary techniques, providing insights into biomolecular structures at different resolutions and under diverse conditions.

Recombinant Proteins JOYNLAB

The “Recombinant Proteins JOYNLAB” is a joint laboratory established between CERM, the Department of Chemistry (DICUS) “Ugo Schiff”, and Giotto Biotech S.r.l. (https://www.giottobiotech.com/). JOYNLAB, through various activities including the execution of shared research and development projects, aims to achieve scientific and applied objectives in the development and study of:

- Recombinant proteins in both natural and isotopically enriched forms;
- Methodologies for the metabolomic analysis of biofluids;
- Reference standards for NMR in solution and solid state;
- Organic compounds of pharmaceutical and industrial interest.

In 2025, JOYNLAB is actively involved in several ongoing projects. These include the European MSCA project ENSCC, which started in 2024 and under which a PhD student was hired and enrolled in the PhD program in Structural Biology in November 2024. In addition, JOYNLAB continues its participation in two projects started in 2024: the Tuscany regional project EMILE and the Marie-Curie Staff Exchange Project McGEA ("Metallo-enzymes and Cells for Green Environmental Alternatives," Call HORIZON-MSCA-2023-SE-01 – Action HORIZON-TMA-MSCA-SE, No. 101183014).

Other Institutions

CRElio

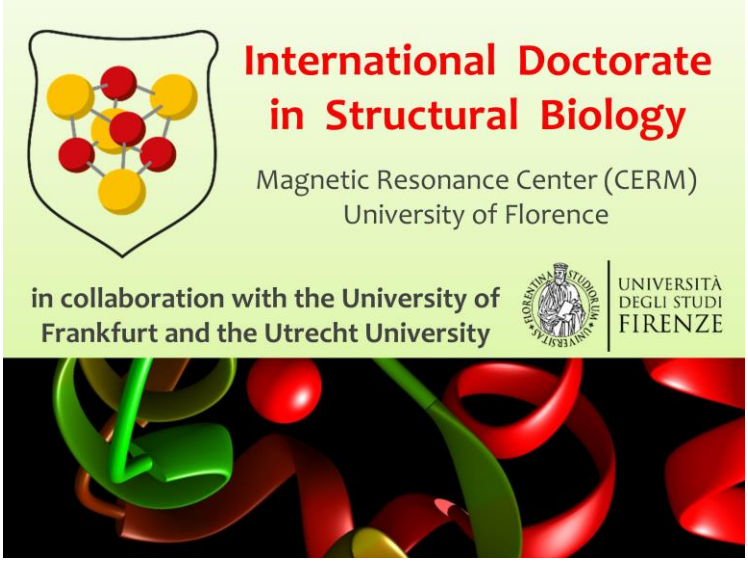
CRElio is the Service Centre of the University of Florence dedicated to the recovery and liquefaction of helium gas. Helium is a scarce and non-renewable resource. The extraction of helium is energy-intensive and has a non-negligible environmental impact. Therefore, the recovery and liquefaction of helium are important to ensure a stable and sustainable supply of this resource to support the needs of scientific applications. Liquid helium plays a crucial role in NMR spectroscopy by providing the necessary cooling for superconducting magnets. CERM joins CRElio together with a series of University Departments and other structures. For its activities, CERM is the main supplier of He gas to CRElio and the main user of liquefied He. This partnership with CRElio allows CERM to obtain a good share of the helium needed for refilling its NMR instruments in a sustainable manner. In 2024-2025, as part of ITACA.SB project, the CRElio liquefaction centre was upgraded by replacing the compressor cooling system and installing an additional high-pressure compressor, increasing liquid helium production capacity while reducing gas losses and energy consumption.

Fondazione Sacconi

The Luigi Sacconi Foundation (https://www.cerm.unifi.it/fondazione-luigi-sacconi) was established in 1996 to honour the memory of Prof. Luigi Sacconi, who was a prominent figure in Chemistry and founder of the General and Inorganic Chemistry School in Florence where many international scientists have been educated. The Luigi Sacconi Foundation has its register office at CERM and members of CERM/CIRMMP are part of the Foundation's Board of Directors. The aim of the Foundation is to promote scientific research in the molecular sciences at the local, national, and international levels. Particular attention is devoted to chemistry and its implications and applications in the fields of health, quality of life, the environment, energy, and technological and industrial development. To this end, the Luigi Sacconi Foundation collects documents and publications, promotes awards, seminars, courses, and meetings, as well as other activities supporting the exchange of scientific knowledge, and subsidizes the activity of Italian and foreign researchers. On the occasion of the *50th Congress of the Inorganic Chemistry Division of the Italian Chemical Society*, held in Naples from September 9 to 12, 2025, the *Sacconi Medal 2025* was awarded to Dr. Geneviève Blondin, Research Director at CNRS (France). The recipient was selected jointly by the Board of Directors of the Foundation and the Executive Council of the Inorganic Chemistry Division of the Italian Chemical Society. The *"Luigi Sacconi Memorial Lecture in Chemistry" 2025* was delivered by Prof. Rinaldo Poli, Laboratoire de Chimie de Coordination, Toulouse, France. The title of the lecture was: "Combining Precision Polymer Synthesis and Coordination Chemistry for Innovative Aqueous Biphasic Catalysis". The Foundation also collaborated in organizing the *third edition of IMPP-3 (Italian Meeting on Porphyrins and Phthalocyanines)*, held from June 25 to 27, 2025, at the University of Milan.

International Doctorate in Structural Biology

The **International PhD course in Structural Biology** is a research doctorate of the *University of Florence*, administered by the Department of Chemistry and hosted at CERM, that runs in collaboration with the *Frankfurt and Utrecht Universities*. The scientific fields cover most of the molecular aspects of life sciences.



The main objective of the International PhD course in Structural Biology is the training of research doctors at the forefront of the knowledge in modern methodologies in molecular and structural biology, biotechnology and systems biology. It provides both theoretical and hands-on training in structural techniques applied to biological macromolecules in solution and in the crystalline state, as well as in non-crystalline materials such as fibrils or amyloid, and to biological macromolecules in their cellular environment. It also provides state-of-the-art training in molecular biology for the expression of isotope-enriched recombinant proteins and specifically those for NMR studies. Finally, it offers top level ICT training thanks to the well-established expertise and the exploitation of the e-infrastructure. Bioinformatics, biostatistics and NMR-metabolomics training is offered as well.

The scientific themes covered by the PhD course are:

1. **NMR spectroscopy** (in solution and in the solid state) and X-ray crystallography aimed at studying structure, function and dynamics in biological macromolecules and protein-protein adducts;
2. **Molecular and cellular biology techniques** for the production of proteins, DNA and bacterial and prokaryotic cell growth;
3. **Drug and vaccine development**, through rational design techniques and structural characterization of biological drugs;

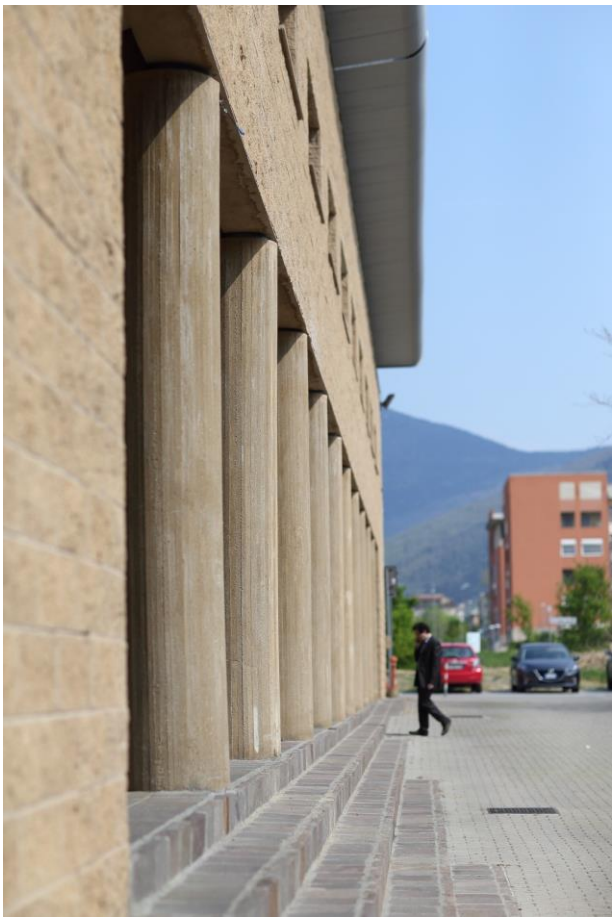
4. **Bioinformatics** to understand the structure-function relationship in biomolecules and in particular in metalloproteins through the large-scale analysis of databases;

5. **In-cell NMR** studies, by which molecular pathways and cell import-export mechanisms are investigated;

6. **Metabolomics** studies, in which the individual metabolic fingerprints are related to disease states and fingerprints are utilized to provide early diagnosis or even identification of pre-disease states.

The added value of this PhD course is in the development of a *transnational educational project,* able to form PhDs at the forefront regarding the scientific formation, knowledge and development of research and technology, capable of considering multi-disciplinary, transnational cooperation and mobility as primary needs, and to evaluate collaborative projects as a requirement for high quality research. The doctoral program also relies on Faculty members who, in addition to scientists from CERM, include professors from the Universities of Frankfurt, Utrecht, Madrid and Lyon, all top places for structural biology.

Full-time attendance is mandatory, as is commitment to research activities. In addition to seminars and courses, students are asked to provide research seminars as a basic tool for their own training. Every PhD student is encouraged to liaise with foreign universities and take part in teaching and research training as well as internships abroad. Post-Doctorate



Post-Doctorate

CERM/CIRMMP hosts several post-doctoral researchers. Some of them are former PhD students who remain at CERM after the end of the PhD, others come from all over the world for performing research projects and being trained in the methodologies in which CERM/CIRMMP excels. There are also several short- or long-term visitors coming from Italian and foreign universities.

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Prof. Edoardo Saccenti (Wageningen University & Research)

Prof. Alejandro Vila (Instituto de Biologia Molecular y Celular de Rosario, Argentina)

List of Publications

SCIENTIFIC ARTICLES

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Meetings and Conferences

"Building connections through the exchange of ideas and practices in NMR"

September 5th 2025

A MR Latvia satellite event to the Summer School “Exploiting heteronuclei at their best: novel probes for biomolecular NMR”

CERM

Summer School “Exploiting heteronuclei at their best: novel probes for biomolecular NMR”

1-4 September 2025

CERM

Seminars Held at CERM

FHERITALE Webinar
Innovation Through Access: FHERITALE and the JRC Nanobiotechnology Laboratory
Tuesday, December 16th 2025, 11:00-11:45 CET

Instruct-ERIC Webinar series
Structure Meets Function
Webinar 42
Tuesday, December 2nd 2025, 11:00-12:00 CET

Alexandre M.J.J Bonvin
Professor of Computational Structural Biology, Utrecht University, Faculty of Science, Bijvoet Centre
The Netherlands
"Solving 3D puzzles of biomolecular interactions by physics- and AI-based integrative modelling"
Friday, November 13th 2025, 17:30

Prof. Jose-Maria Carazo
Spanish National Center for Biotechnology, CNB-CSIC, Universidad Autonoma de Madrid, Spain

"Exploring macromolecular conformational landscapes with cryoEM"
Friday, November 21st 2025, 14:30

Prof. Yann Ferrand
Université de Bordeaux, CNRS CBMN, France
"Engineering Aromatic Oligoamide Capsules: A Dual Role in Molecular Recognition and Catalysis"
Wednesday, October 22nd 2025, 16:00

Prof. Francesco G. Gervasio
Geneve University, Switzerland
"Beyond the Fold: Simulating Protein Dynamics and Function in the AI Era"
Wednesday, October 15th 2025, 12:30

Prof. Sebastian Hiller
Biozentrum, University of Basel, Switzerland
"The dynamic chaperone network in the endoplasmic reticulum"
Tuesday, June 10th 2025, 14:30

Dr. Alessandro Piai
Senior Research Investigator, IRBM, Italy
"Accelerating Drug Discovery via NMR: Practical Applications for Impactful Results"
Thursday May 22nd 2025, 14:30

ITACA.SB Webinar
March 12th 2025, 15:00-16:00
Challenging metalloproteins
Chair: **Lucia Banci** (University of Florence, Italy)
Speaker 1: **Nick Le Brun** (University of East Anglia, UK)
Title: "Iron-sulfur cluster proteins as sensor-regulators of environmental change"
Speaker 2: **Francesca Camponeschi** (University of Florence, Italy)
Title: "Integrated approaches to unravel the complex(iti)es of Iron-Sulfur protein biogenesis"

Carlos G. Acevedo-Rocha
The Novo Nordisk Foundation Center of Biosustainability, Lyngby, Denmark
"ProteusAI: An Open-Source and User-Friendly Platform for Machine Learning-Guided Protein Design and Engineering"
March 7th 2025, 14:30-15:30

Dr. Catherine Goodman
Senior Associate Publisher, American Chemical Society

Meetings and Events Organized by CERM

"Getting away from the bench: behind the scenes of scholarly publishing"
Friday March 7th 2025, 12.45-13.30

Prof. Peter-Leon Hagedoorn
Delft University of Technology
"EPR for Biocatalysis"
March 6th 2025, 16:30-17:15

ITACA.SB Webinar
February 12th 2025, 15.00-16.00
Computational approaches
Chair: **Antonio Rosato** (University of Florence, Italy)
Speaker 1: **Robbie Joosten** (Netherlands Cancer Institute, The Netherlands)
Title: "PDB-REDO et al.: online resources for your structural biology research"
Speaker 2: **Paolo Carloni** (Forschungszentrum Jülich GmbH, Germany)
Title: “In silico drug design in the exascale era: a perspective from Juelich”

ITACA.SB Webinar
January 15th 2025, 15.00-16.00
Macromolecular complexes
Chair: **Roberta Pierattelli** (University of Florence, Italy)
Speaker 1: **Francesco Berti** (GSK Vaccines, Siena, Italy)
Title: “Recent advancements in the glycoconjugate vaccines field”
Speaker 2: **Linda Cerofolini** (University of Florence, Italy)
Title: "Selectivity in target recognition by full-length clinically approved monoclonal antibodies"

Group Meetings

Friday, December 12th, 2025 at **2:30 pm**
Prof. Mario Piccioli - Leonardo Querci
"Probing domain-linker-domain dynamics using paramagnetic lanthanides"
CERM Conference room

Friday, December 5th, 2025 at 1:00 pm
Prof. Marco Fragai - Sara Callozzo
"Integrated structural characterization of two pathological mutants of human Transthyretin"
CERM Conference room

Friday, November 28th, 2025 at 1:00 pm
Prof. Giacomo Parigi - Jlenia Bindi
"Characterizing molecular interaction and dynamics through high-resolution relaxometry"
CERM Conference room

Friday, November 7th, 2025 at 1:00 pm
Prof. Giacomo Parigi - Madalina Ranga
"Pure proton-exchange based relaxation agent for MRI applications"
Online: meet.google.com/sho-yrst-hvc

Friday, October 31st, 2025 at 1:00 pm
Prof. Paola Turano - Stefano Zineddu
"Combinatorial synthesis for the discovery of novel metalloantibiotics"
CERM Conference room

Friday, October 10th, 2025 at 1:00 pm
Prof. Antonio Rosato - Giulio Tassini
"Antibody-antigen binding characterization for the rational development of an *in vitro* potency assay for a *Strep A* vaccine"
CERM Conference room

Friday, October 3rd, 2025 at 1:00 pm
Prof. Marco Fragai - Siyu Lin
"Expression and NMR characterization of labelled p-domains of emerging norovirus"
CERM Conference room

Meetings and Events Organized by CERM

Friday, September 26th, 2025 at 1:00 pm
Prof. Marco Fragai - Bianca Susini
"Expression and characterization of proteins involved in neurodegenerative diseases"
CERM Conference room

Friday, September 19th, 2025 at 1:00 pm
Prof. Giacomo Parigi - Adam Kubrak
"Metabolites and macromolecules in blood serum – what does high-resolution-relaxometry reveal about their mobility and interactions?"
CERM Conference room

Friday, September 12th, 2025 at 1:00 pm
Prof. Lucia Banci - Martina Masini
"BOLA2 and GLRX3: key players in human cytosolic [4Fe-4S] cluster assembly"
CERM Conference room

Friday, July 4th, 2025 at 1:00 pm
Prof. Roberta Pierattelli - Tessa Bolognesi
"An NMR workflow for RNA–ligand studies"
CERM Conference room

Friday, June 27th, 2025 at 1:00 pm
Prof. Antonio Rosato - Cosimo Ciofalo
"A benchmark for the assessment of tools for the prediction of metalloproteins"
CERM Conference room

Friday, June 20th, 2025 at 1:00 pm
Prof. Lucia Banci - Rosanna Cuccaro
"Human Glutaredoxin 3: multiple domains for a unique function"
CERM Conference room

Friday, June 13th, 2025 at 1:00 pm
Prof. Roberta Pierattelli - Maria Anna Rodella
"Seedless in practice: a GRAPE-derived tool for testing optimal control pulse performance"
CERM Conference room

Friday, June 6th, 2025 at 1:00 pm
Prof. Cristina Nativi - Andrea Baldi
"Targeting BambL and LecA with glycomimetics: assessing complex stability and lectin bridging using computational tools: A dual-target approach against polymicrobial infections."

Meetings and Events Organized by CERM

CERM Conference room

Friday, May 30th, 2025 at 1:00 pm
Prof. Marco Fragai - Ricardo Pereira
"Functionalization of PD-1 mutant with immunomodulator self-assembling peptide"
CERM Conference room

Friday, May 23rd, 2025 at 1:00 pm
Prof. Cristina Nativi - Ileana Žeravica
"Design, synthesis, and characterization of human milk oligosaccharide analogues as NoV ligands"
CERM Conference room

Friday, May 16th, 2025 at 1:00 pm
Prof. Simone Ciofi Baffoni - Gabriele Olivieri
"Human monoclonal antibodies against Shigella (ShiMabs), for therapy and vaccine acceleration. Antibody discovery and epitope mapping of different protein antigens"
CERM Conference room

Friday, May 9th, 2025 at 1:00 pm
Prof. Roberta Pierattelli - Silvia Oliveti
"Tracing structure, function, and modulation of intrinsically disordered regions"
CERM Conference room

Friday, April 18th, 2025 at 1:00 pm
Prof. Marco Fragai - Francesco Currò
"Advanced structural and morphological characterization by NMR technologies of different biomolecules and biotechnological systems"
CERM Conference room

Friday, April 11th, 2025 at 1:00 pm
Prof. Roberta Pierattelli - Caterina Lippi
"Integrated approach to study the druggability of structurally heterogeneous proteins involved in the onset of pathologies of various origins"
CERM Conference room

Friday, April 4th, 2025 at 1:00 pm
Prof. Antonio Rosato - Chiara La Guidara
"Studying the interaction between the SARS-CoV-2 main protease NSP5 and novel PROTAC molecules: one step closer to the ternary complex"
CERM Conference room

Meetings and Events Organized by CERM

Friday, March 28th, 2025 at 1:00 pm
Prof. Cristina Nativi and Paula Gonzalez
"Development of saccharide analogues for protein functionalization and as ligands for binding studies with CBMs. Multivalent presentation of CBMs"
CERM Conference room

Friday, March 21st, 2025 at 1:00 pm
Prof. Paola Turano and Giorgio Di Paco
"Ferritin as a carrier for anticancer drugs"
CERM Conference room

Friday, March 14th, 2025 at 1:00 pm
Prof. Marco Fragai and Francesco Currò
"Advanced structural and morphological characterization by NMR technologies of different biomolecules and biotechnological systems"
CERM Conference room

Friday, February 28th, 2025 at 1:00 pm
Prof. Enrico Luchinat and Love Elizabeth Afolayan
"Characterization of ligand binding to a membrane protein by in-cell NMR spectroscopy"
CERM Conference room

Friday, February 14th, 2025 at 1:00 pm
Prof. Francesca Cantini and Alessia De Santis
"Application of cellular approaches to characterize NEET proteins in different cancer cell lines"
CERM Conference room

Friday, February 7th, 2025 at 1:00 pm
Prof. Marco Fragai and Rebecca Calamandrei
"Targeting the PD-1/PD-L1 axis: structural biology by NMR for developing and characterizing nanotheranostics"
CERM Conference room

Friday, January 31st, 2025 at 1:00 pm
Prof. Lucia Banci and Azzurra Costantino
"A bioreactor: overcoming challenges in ligand-target competition binding with ^{19}F in-cell NMR"
CERM Conference room

Friday, January 24th, 2025 at 1:00 pm

Meetings and Events Organized by CERM

Prof. Lucia Banci and Martina Rosati

"Improving in-cell NMR: inducible stably transfected cell lines and spheroids to achieve more endogenous-like conditions in in-vitro protein studies"

CERM Conference room

Friday, January 10th, 2025 at 1:00 pm

Prof. Roberta Pierattelli and Lorenzo Bracaglia

"Structurally heterogeneous proteins studied by relaxation-edited NMR experiments"

CERM Conference room

Funding Institutions

Acknowledgements

University of Florence

Italian Ministry of University and Research

European Commission

Tuscany Regional Government

Fondazione Cassa di Risparmio di Firenze

Italian National Research Council

Italian National Institute of Health

National Institutes of Health

Cariplo Foundation

Funding Institutions

Italian Association for Cancer Research

National Recovery and Resilience Plan (NRRP)

Italian Ministry of Agriculture

Italian Ministry of Health

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