

CISUP - University of Pisa

Bruker Avance Neo 700 MHz solution-state NMR spectrometer: 2024-2025 activity report

Bruker Avance Neo 700 MHz solution-state NMR spectrometer was installed in June 2024. It has been operated since July 2024. Several technical/operative problems (instability of magnetic field, automatic insertion of sample tubes, temperature control of BBI probe, tuning error for MicroProbe, and shimming in apolar solvents) affected the real operativity of such instrumentation for the first 6 months (35%). The 1-year warranty (June 2025) was re-negotiated and extended to March 2026.

Laboratory rules

For the optimization of the instrumental time, the delivery of the sample and the execution of the NMR measurements will be agreed by email (federica.balzano@unipi.it) with Dr. Federica Balzano, who will include the reservation in the booking calendar.

Laboratory users

The persons habilitate by CISUP to operate on the spectrometer are:

Prof. Gloria Uccello Barretta (DCCI-UNIFI, lab head and responsible of the spectrometer)

Prof. Lorenzo Di Bari (DCCI-UNIFI, lab head and responsible of the spectrometer)

Dr. Federica Aiello (CNR-IPCF, researcher)

Dr. Federica Balzano (CISUP-UNIFI, technical personnel and super-user)

Refill of cryogenic liquids (nitrogen and helium) is guaranteed by DCCI.

1. Use of the Laboratory -2024

In 2024 (july -december) Avance Neo 700 MHz NMR laboratory has operated for 85 days (2040 hours) over a maximum of 120 working days (from Monday to Friday). Usually, the experiments can run in complete automated way during the week-ends as well.

The spectrometer did not operate for a total of 50 working days (42%) due to technical problems and/or Bruker technical assistance:

- from 1st to 22nd July for shimming problems
- from 19th to 23rd August for temperature control error of BBI probe; Bruker technical assistance (21-23 August) assessing the need of repairing BBI probe and changing to MicroProbe
- from 2nd to 10th September due to the blocking of automatic sample loading
- from 25th September to 7th October due to impossibility of tuning the MicroProbe
- from 8th to 9th October for Bruker technical assistance

- the 5th and 27th November for shimming problems
- from 4th to 5th December for Bruker technical assistance

The spectrometer time was employed for several types of activity (in parenthesis, the percentage calculated on the basis of the effective working days):

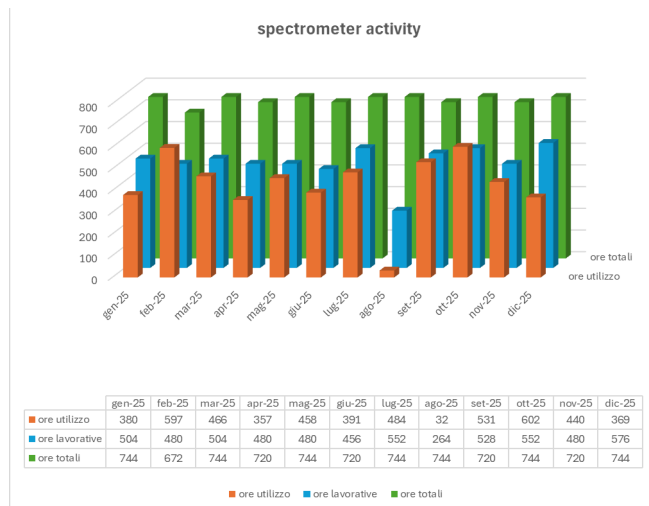
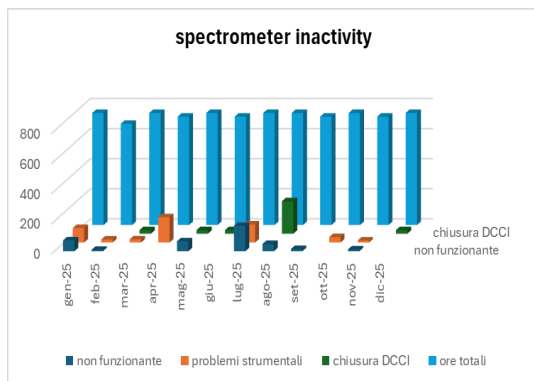
- Bruker training: 5 days (6%)
- Lab management, set-up operations, testing of pulse sequences, developments (done by the super-user): 28 days (33%)
- UNIFI users: 42 days (49%)
- External institution (CNR): 5 days (6%)
- Third-party users: 5 days (6%)

2. Use of the Laboratory -2025

In 2025 Avance Neo 700 MHz NMR laboratory has operated for 213 days (5107 hours, 88%) over a maximum of 241 working days (from Monday to Friday) with some technical problems (mainly instability of air and shims) for a total of about 13 days throughout the year. Usually, the experiments can run in complete automated way during the week-end as well (instrument working days 337).

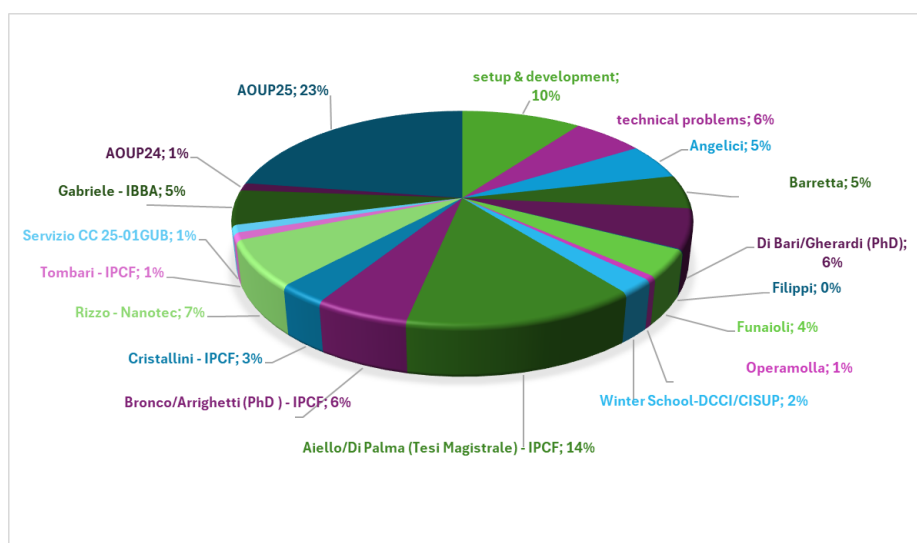
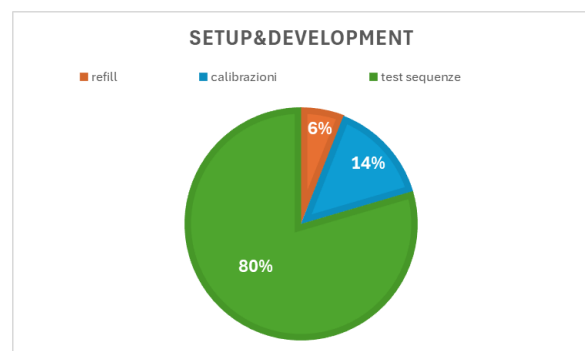
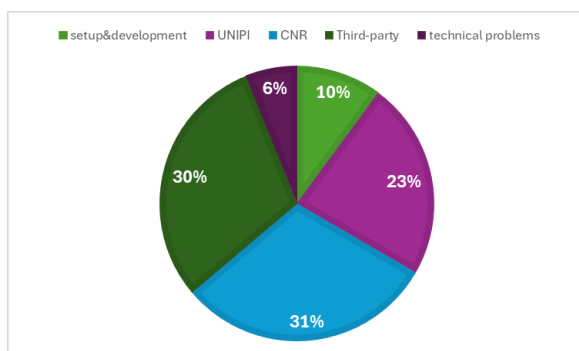
The spectrometer did not operate for a total of 25 working days (10%) due to maintenance, technical problems, Bruker technical assistance/training and/or DCCI closure:

- from 14th to 17th January for air conditioning system machine replacement
- from 14th to 16th March for weather alert
- from 1st to 3rd April due to Bruker technical assistance for changing probe (1H/19F BBI)
- on 2nd and 20th May for DCCI closure
- from 6th to 8th May for Bruker training on site
- from 16th to 18th May for electric cabin maintenance
- on 16th June for DCCI closure
- from 30th June to 2nd July for Bruker training on site
- from 25th to 26th August for maintenance of electrical systems
- on 24th December for DCCI closure



The spectrometer time was employed for several types of activity (in parenthesis, the percentage calculated on the basis of the effective working days):

- Lab management, set-up operations, testing of pulse sequences, developments (done by the super-user): 22 days (10%)
- UNIPI users: 50 days (23%)
- External institution (CNR): 67 days (31%)
- Third-party users: 65 days (30%)
- Technical problems: 13 days (6%)



3. Lab management

This activity, mostly supported by the super-user, includes routine activities (tests to verify the instrument performance and ensuring the supply of cryogenic liquids), and extraordinary activities connected with the functionality of the NMR spectrometer (probes, auto-sample, data storing, etc.), with the calibration of specific parameters for non-routine uses (quantitative calibration, temperature calibration, etc.), and with the development of particular pulse sequence/experiment.

4. Free-of-charge measurements

Free-of-charge measurements, programmed without interfering with the other NMR activities, include: preliminary experiments/tests on new protocols and pulse sequences that may be functional to future financed collaboration projects/third-party services/collaborations with UNIPI-researcher and researchers of other universities and/or research institutes; in-house measurements (compensate the time head of lab dedicate for third-party services and reports and the lab management); experiments performed in view of possible financed collaborations and projects.

5. Financed projects / collaborations.

Collaborations were carried out during the year, both with staff of UniPI and with external researchers.

The research projects that are benefitting of the service produced by the Avance Neo 700 MHz spectrometers are:

- PRIN2022, 3D-BIOSAME, A 3D BIOprinted SpinAl cord Model to reach functional meaningful and clinically translatable rEgeneration, 2022YY9AR2 (Dr. Federica Aiello)
- PNRR MISS4, COMP2, INV1.3 ON FOODS "Research and innovation network on food and nutrition Sustainability, Safety and Security – Working ON Foods", Cod. PE000000003 – Next Generation EU (Dr. Morena Gabriele)
- PNRR2023, BRAVEHEART, Realizzazione di un cerotto cardiaco bioartificiale a rilascio di farmaco per prevenire l'insufficienza cardiaca, PRR.AP015.154, PNRR-POC-2023-12378186 (Dr. Cristallini)
- PRIN2022, BIOSMARTFERT, BIOpolymers from agri-food waste digestates for SMART release bioFERTilisers, 20225WLFRR (Prof. Gloria Uccello Barretta)
- NANOFUN, Nanocellulose-based membranes for water purification with enhanced efficiency by chemical functionalization. Bilateral project (2023-2025) involving the Department of Chemistry and Industrial Chemistry of the University of Pisa (Italy) and the Council of Scientific and Industrial Research of Pretoria (South Africa), CUP I53C22003350001 (Prof. Alessandra Operamolla)
- PRIN 2022 PNRR - Large-area two-dimensional pentagonal PdSe₂ for novel gas sensing applications (2D-PentaSensing), P2022HT3FF (Dr. Rosanna Mastria, CNR NANOTEC).

6. Third-party measurements

There is a long-lasting agreement for NMR analyses on antitubercular drugs, active ingredients and galenics with the Azienda Ospedaliera Universitaria Pisana (AOUP) for 2024-2026.

Deltatech (October 2024).

LMPE (November 2024)

LMPE (March 2025)

Dr. Morena Gabriele (CNR-IBBA) (October 2025)

7. Education & Dissemination

Bruker Avance Neo 700 MHz NMR spectrometer was used for supporting 5 PhD projects at UniPI and UNISI and 1 Master Degree theses at UniPI:

Luca Gherardi (Stereochemistry of oligo-based therapeutics, Prof. Lorenzo di Bari, Demartis Salvatore (PPM Services SA, Switzerland), DSCM, DCCI-UNIFI, 38th cycle, 2022-2025)

Arrighetti Leonardo (Design of innovative materials based on renewable/biobased polymers and Made in Italy agrifood wastes as cutin from tomato and inorganic waste as marble sludge from Italian geoclusters, Dr. Simona Bronco and Prof. Valentina Domenici, DSCM, DCCI-UNIFI, 39th cycle, 2023-2026)

Dawid Rossino (Process design, development and shelf-life of innovative micro-nano structured polymeric products for biomedical applications, Dr. Caterina Cristallini and Dr. Maria Beatrice Coltelli, Corso di Dottorato in Ingegneria industriale, UNIFI, 40th cycle, 2024-2027)

Sara Corti (Dr. Isabella Pecorini, Prof. Renato Iannelli, Prof. Lorenzo Ferrari, Prof. Andrea Baccioli, Dottorato in ingegneria dell'energia, dei sistemi, del territorio e delle costruzioni, DESTEC-UNIFI, 40th cycle, 2024-2027)

Mario Calora (Hybrid Perovskite Material Development for Highly Efficient and Stable Tandem Solar Cells, Dr. Aurora Rizzo and Dr. Rosanna Mastria, Dottorato in Fisica e Nanoscienze-UNISalento, 38th cycle)

Paolo Di Palma (Analysis of honey samples and of their adulteration processes via solution NMR spectroscopy, Dr. Federica Aiello, aa 2025-2026)

Only partial cost was claimed for education and (no-profit) dissemination activities.

The Avance Neo 700 spectrometer was also employed for supporting the laboratory training of the CISUP Winter School "Advanced techniques for the analysis of novel materials strategic for sustainability transitions. 3 – BIODEGRADABLE POLYMERS" (9-13 February 2026).

8. Research Products

- Molinari, G.; Parlanti, P.; Passaglia, E.; Aiello, F.; Gemmi, M.; Lazzeri, A.; Righetti, M.C. Dependence of the crystal structure on the D-units amount in semi-crystalline poly(lactic acid). *International Journal of Biological Macromolecules* 2024, 281, 136296; doi: <https://doi.org/10.1016/j.ijbiomac.2024.136296>.

- Traldi, C.; Chiappini, V.; Chasseur, S.; Aiello, F.; Boido, M.; Tonda-Turo, C. 3D in vitro modeling of neural microenvironment through a multi-scaffold assembly approach. *Materials Today Bio* 2025, 33, 102086. doi: <https://doi.org/10.1016/j.mtbio.2025.102086>.
- Uccello Barretta, G.; Wenzel, T.; Balzano, F.; Aiello, F. Enantiomeric Purity Studied Using NMR, *Encyclopedia of Spectroscopy & Spectrometry*, 4e under review
- Castagnoli, A.; Pezzini, S.; Aiello, F.; De Monte, C.; Bronco, S.; Balzano, F.; Uccello Barretta, G.; Iannelli, R.; Pecorini, I. Polyhydroxyalkanoates production through Mixed Microbial Cultures: Generalized Additive Model and Network analysis of Process Drivers and Structural Insights, under preparation
- Gabriele, M.; Uccello Barretta, G.; Balzano, F.; Aiello, F. et al. Impact of thermal processing and simulated in vitro digestion on phytochemical content, nutritional profile, and biofunctional properties of fenugreek seeds, under preparation.
- Pezzini, S. BIOSMARTFERT: Advancing Sustainable Biofertilizers through Smart Release Technology, IPCF meeting 18-20 marzo 2025, Pisa, Italy
- Aiello, F. Characterization of derivatized biopolymers via solution NMR spectroscopy, IPCF meeting 18-20 marzo 2025, Pisa, Italy
- Aiello, F. Exploiting the tools of NMR spectroscopy for the analysis of derivatized biopolymers, European polymer Congress (EPF) 2025, 22-27 June 2025, Groningen, Netherlands
- Aiello, F. Characterization of derivatized biopolymers via solution NMR spectroscopy, 34th Annual Conference of European Society for Biomaterials (ESB 2025), September 7-11 2025, Torino, Italy
- Trouki, C. Molecular and physico-chemical characterization of multilayered PLGA/Gelatin-based patches incorporating Fmoc-diphenylalanine for myocardial repair, 34th Annual Conference of European Society for Biomaterials (ESB 2025), September 7-11 2025, Torino, Italy
- Rossino, D. Effect of an engineered interface on the mechanical, biodegradative and functional properties of a multi-layered cardiac patch, 34th Annual Conference of European Society for Biomaterials (ESB 2025), September 7-11 2025, Torino, Italy
- Aiello, F. NMR analysis of gelatin and investigation of its derivatization process, 34th Annual Conference of European Society for Biomaterials (ESB 2025), September 7-11 2025, Torino, Italy
- Gherardi, L.; Cupellini, L.; Demartis, S.; Viti, F.; McNulty, M.; Di Bari, L. Conformational freedom of single stranded oligonucleotides, TIDES 2025, May 11-14 2025, San Diego, USA
- Gherardi, L.; Cupellini, L.; Demartis, S.; Viti, F.; McNulty, M.; Di Bari, L. Conformational freedom of single stranded oligonucleotides, Chemistry for Future International Conference (CFF) 2025, July 7-9 2025, Pisa, Italy
- Francescato, G.; Bacq, V.; Angelici, G. Easy Access to Tetrahydro-[1,4]diazepino-indoles Through Intramolecular Cyclization, Chemistry for Future International Conference (CFF) 2025, July 7-9 2025, Pisa, Italy

9. Incomes and costs

The gas costs for 2024 and 2025 (9271 € + IVA), excluding the helium refill on September 3rd 2025 (about 3221 € +IVA), were covered by the lab heads, Prof. Gloria Uccello Barretta and Prof. Lorenzo Di Bari, which also covered the purchase of accessories for the NMR laboratory (precision balance, fume hood for sample preparation, consumables, NMR tubes and solvents) for a total of 28000 €.

The NMR laboratory income for 2024-2025 amounts to a total of 28750 €. This includes income from UNIFI users (10450 €), from external users (CNR, 8100 €) and from third-party users (10.200 € + IVA). The AOUP-2025 service will be cashed in the following year.