# CISUP – University of Pisa Bruker Avance NEO 500 solid state NMR spectrometer: 2022 activity report

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### Laboratory users

The following persons have been enabled by CISUP to operate on the spectrometer:

Marco Geppi (associate professor, DCCI-UniPI, lab head and responsible of the spectrometer)

Silvia Borsacchi (ICCOM-CNR researcher)

Lucia Calucci (ICCOM-CNR researcher)

Elisa Carignani (post-doc, DCCI-UniPI, then ICCOM-CNR researcher)

Claudia Forte (ICCOM-CNR researcher)

Francesca Martini (RTDA, DCCI-UniPI)

Francesca Nardelli (post-doc, DCCI-UniPI)

Silvia Pizzanelli (ICCOM-CNR researcher)

The technical service concerning the refill of cryogenic liquids (nitrogen and helium) is guaranteed by DCCI.

An expert technician able to follow the every-day tasks and perform experiments would be strictly necessary, but such a person is not present at the moment. The recruitment of a person with a strong background in solid state NMR is necessary and strongly requested to improve the efficiency of the activities connected with this spectrometer.

## Days worked

The total spectrometer working time in 2022 was 193 days over a maximum of 237. Only working days (from Monday to Friday) were taken into account here, but usually the spectrometer ran experiments even during the weekends without operators or with operators handling the experiments remotely from home.

Unfortunately the spectrometer did not operate for a total of 44 working days:

- The 3<sup>rd</sup> January for works at the electric network at DCCI;
- The 14<sup>th</sup> January for yearly maintenance of air-drying columns of the spectrometer;
- From 14<sup>th</sup> to 17<sup>th</sup> February for a problem with spinning rotors on the 1.3 mm CPMAS probe;
- from 5<sup>th</sup> May to 1<sup>th</sup> June due to a problem with the hard disk of the EPU component of the console, which took some weeks to be identified and then solved by the Bruker technicians.
- The 6<sup>th</sup> June for installation and set-up of the new EPU hard disk.
- From 23<sup>rd</sup> August to 2<sup>nd</sup> September for unavailability of operators due to simultaneous institutional duties and/or season holidays.
- From 19<sup>th</sup> to 30<sup>th</sup> September for a combination of problems to console and probes, which were solved after a visit to Bruker in Milan.

The following activities have been carried out (the percentages refer to the effective working+maintanance days):

Set-up operations and developments: 18 days (9.3 %)

Maintenance done by operators: 3 days (1.6 %) "In house" research activity: 48 days (24.9 %)

Free CNR research activity: 48 days (24.9 %)

Paid activity for UNIPI/CNR customers: 74 days (38.4 %) Paid activity for external institutions: 2 days (1.0 %)

#### **Incomes** and costs

In 2022 incomes arose mainly from activity to UNIPI and CNR researchers (14365  $\in$ ), and in a small fraction to other institutions (1000  $\in$ ), for **a total of 15365**  $\in$ .

Part of the incomes, due to bureaucratic difficulties, were acquired in the form of acquisition of consumables for the spectrometer (rotors, caps, and related small accessories) for a total of  $5465 \in$ . The other incomes (9900  $\in$ ) were directly paid to CISUP and were already collected or are in the process of being collected.

On the other side, the maintenance costs of the spectrometer were kept to a very low level since in the contract for the acquisition of the spectrometer from Bruker a 3-year warranty of the newly acquired components was included, covering most technical services. It must be noted that this agreement was re-negotiated in 2020 with Bruker, obtaining a 2-month extension of the warranty period. The updated warranty deadlines are the following:

• Ascend 500 magnet; new RF components upgrading CNR console; BCU II; MASIII; CPMAS 1.3mm probe: 5/2/2023

CPMAS 2.5mm probe: 3/9/2023CPMAS 4mm probe: 26/4/2023

• CPMAS 3.2mm low-gamma probe: 31/8/2023

• HRMAS 4mm probe: 3/9/2023

Several breakages (especially of probes) were solved by repairs within the warranty.

The costs (IVA included) were relative to:

- cryogenic liquids (nitrogen and helium) for ordinary maintenance of the superconducting magnet: 4544.81 €
- substitution of the EPU hard disk (out of warranty): 1464.00 €
- purchase of a sample used as a NMR reference: 100.16 €
- acquisition of consumables (rotors, caps and related small accessories): 5465.00 € (expenses directly done by customers)

#### for a total of **11573.97** €

Therefore the SSNMR spectrometer produced this semester a **net income of 3791.03** €. This, added with the 2021 net income (5926.94 €), produced a **total net income from the beginning of the activities of 9717.97 €.**