

## Rules of procedure of PANACEA

### Preamble

The purpose of these internal regulations is to specify the operating and access procedures to the Research Infrastructures (RI) of the European project PANACEA which are described down below, and whose purpose is to pool and optimize investments in, to open up access to solid-state NMR spectrometers to the European scientific, academic and industrial communities.

These internal regulations are provided to every user: it does not replace the internal regulations in force on each site, but supplements them.

### Title I – Partners

Platforms concerned:

	RMN	Scientific manager(s)	Local operator
<b>CNRS-LYON</b>	1 GHz 800 MHz DNP 500 MHz 400 MHz	Guido Pintacuda <a href="mailto:guido.pintacuda@ens-lyon.fr">guido.pintacuda@ens-lyon.fr</a> Anne Lesage <a href="mailto:anne.lesage@ens-lyon.fr">anne.lesage@ens-lyon.fr</a>	David Gajan <a href="mailto:david.gajan@ens-lyon.fr">david.gajan@ens-lyon.fr</a>
<b>CNRS-ORL</b>	850 MHz 750 MHz 200 MHz	Franck Fayon <a href="mailto:franck.fayon@cnrs-orleans.fr">franck.fayon@cnrs-orleans.fr</a>	Pierre Florian <a href="mailto:pierre.florian@cnrs-orleans.fr">pierre.florian@cnrs-orleans.fr</a>
<b>AU</b>	950 MHz 700 MHz	Thomas Vosegaard <a href="mailto:tv@chem.au.dk">tv@chem.au.dk</a>	Dennis W. Juhl <a href="mailto:dwj@chem.au.dk">dwj@chem.au.dk</a>
<b>CERM/CIRMMP</b>	1.2 GHz 850 MHz 800 MHz 700 MHz 600 MHz	Moreno Lelli <a href="mailto:moreno.elli@unifi.it">moreno.elli@unifi.it</a>	Massimo Lucci <a href="mailto:lucci@cerm.unifi.it">lucci@cerm.unifi.it</a> Linda Cerofolini <a href="mailto:cerofolini@cerm.unifi.it">cerofolini@cerm.unifi.it</a>
<b>RU</b>	850 MHz 600 MHz DNP	Akbey Umit <a href="mailto:U.Akbey@science.ru.nl">U.Akbey@science.ru.nl</a>	Ruud Aspers <a href="mailto:r.aspers@nmr.ru.nl">r.aspers@nmr.ru.nl</a>
<b>UAVR</b>	700MHz 400 MHz DNP	Luís Mafra <a href="mailto:lmafra@ua.pt">lmafra@ua.pt</a>	Mariana Sardo <a href="mailto:msardo@ua.pt">msardo@ua.pt</a>
<b>UGOT</b>	400 MHz	Göran Karlsson <a href="mailto:goran.karlsson@nmr.gu.se">goran.karlsson@nmr.gu.se</a>	Arthur Pinon <a href="mailto:arthur.pinon@gu.se">arthur.pinon@gu.se</a>
<b>UW</b>	1 GHz 850 MHz 700 MHz 600 MHz 300 MHz 100 MHz	Steven Brown <a href="mailto:s.p.brown@warwick.ac.uk">s.p.brown@warwick.ac.uk</a>	Anjali Menakath < <a href="mailto:A.Menakath.1@warwick.ac.uk">A.Menakath.1@warwick.ac.uk</a> >
<b>FSU</b>	1.5 GHz 600 MHz DNP	Lucio Frydman <a href="mailto:frydman@magnet.fsu.edu">frydman@magnet.fsu.edu</a>	Frederic Mentink-Vigier <a href="mailto:fmentink@magnet.fus.edu">fmentink@magnet.fus.edu</a>

## Title II – Method of project selection

### Article 1 – Project screening

The project submission interface allows a transparent, continuous, simple and rapid evaluation of the projects submitted by the users.

Reminder of the procedure:

Step 1: **Submission** of a project by a user on the PANACEA website; automatic email notifications to the user him /herself and to the local operator (or operational manager) and scientific manager of the platform. Before this step, the user has to create a login and a password.

Step 2a: If the user is **familiar or expert** with solid-state NMR, assessment of the feasibility of the project by the scientific manager and by the operational manager with regard to the NMR equipment available on the requested platform; the project can possibly be directly rejected if insufficiently documented.

Then, three options are possible:

- a) project accepted (and then sent for evaluation),
- b) project redirected to another RI platform,
- c) project refused

Automatic email notifications to at least 2 experts chosen from the list of the User Selection Panel by the operational manager and to the platform coordinator in the case of acceptance.

Step 2b: If the **user is unfamiliar** with solid-state NMR, he/she has the possibility to submit a short proposal which will be promptly examined (within 5 working days) by an internal panel made of local operators. This panel will decide which site will be best suited to host the project. The appropriate local operator will then help the user to prepare a full proposal in line with the scientific and technological expertise of his/her site.

Step 3: **Evaluation and validation** of the project by two experts from the User selection Panel (USP); automatic email notifications to the experts and to the user, when the project is accepted or rejected.

Step 4: The account created by the user makes it possible to securely provide a certain amount of information which will be accessible to the local operator, in particular the information necessary to prepare and schedule his/her travel and accommodation arrangement for the on-site visit. Once the experiments are performed, the local operator indicates the user experiment and visit days and dates in the interface and asks users to complete a satisfaction survey. The local operator is informed by an automatic email as soon as the user has completed the satisfaction survey.

## ***Article 2 – Evaluation of the project***

The procedure is the same for all the 8 TA sites and is implemented within the internet-based access management system.

The review procedure follows the principles of transparency, fairness and impartiality.

The reviewers of the USP select the projects according to the following pre-defined criteria: scientific merit, scientific feasibility, innovation and novelty of the expected results. The ranking is as follows:

Evaluation criteria for the external independent reviewers

- Scientific merit of the proposal (rank: weak: 0; outstanding: 10)
- Scientific feasibility of the proposal (rank: weak: 0; outstanding: 5)
- Demonstration of the need to use the infrastructure (rank: weak: 0; outstanding: 5)
- Novelty of the expected results (rank: weak: 0; outstanding: 10)
- Potential for academic or industrial innovation (rank: weak: 0; outstanding: 5)

Proposals with a total ranking of less than 20 out of 35 will be rejected.

Evaluation reports will be provided to the users for all projects, including for those that fail. These reports will provide constructive feedback that will help users to improve their projects. In a few cases, the site coordinator or local operator may decide to allocate the project to another RI (for example to direct the user to a facility better suited for solving his/her scientific challenge, or to a geographically nearer facility of equal expertise).

The whole review protocol is fully transparent, and is designed so as to ensure that PANACEA supports projects of any European chemist in multi-disciplinary areas, that users make a best use of its resources, and benefits from the highest level of services.

## ***Article 3 – Closure form and satisfaction survey***

A closure form is associated to each project, that includes a user satisfaction survey.

All the events related to a project are recorded in the management system and all corresponding information are used to evaluate the access activity.

## **Title III – Access modalities**

### ***Article 1 – Access conditions - generalities***

Access is provided to users working in a country other than the country where the spectrometer is located. Users are encouraged to favor, when possible, gender balance among the group of visiting scientists.

### ***Article 2 – Access fee***

Trans-national access to the eight research infrastructures is free of charge for researchers from academia, and limited to industrials that agree to disseminate the results they have generated within the integrated facility, with an exception for users

working for SMEs. For industrial IPR-sensitive projects, contract fees will be established in accordance with fully-justifiable full costs, that will be calculated according to harmonized and established guidelines.

### ***Article 3 – Duration of the work***

Typically, visits at the RIs will last from 1 day to 2 weeks of NMR instrument time. Time prior to the NMR measurements used for sample preparation, writing/adapting NMR pulse sequences and setting up the instrumentation is considered as access time. Once the experiments have been performed, the data are saved, processed, and reviewed for preliminary interpretation.

While some experienced users may come only for the initial stages of experimental set-up, new users not familiar with solid-state NMR spectroscopy are encouraged to stay not only for the entire measurement time but also have the possibility to extend their stay to gain experience on data handling and analysis.

### ***Article 4 – Integration into the scheduling of the local infrastructure***

The scheduling of external European users will take precedence over the allocation of NMR time dedicated to in-house research and to national users (for RIs that are providing access at a national level).

Projects from new users and/or from users coming from countries where high-level solid-state NMR infrastructure and expertise are not available will be scheduled with the highest priority.

The target delay between the approval of the project and the first spectrometer time slot proposed to the applicant is **less than a month** for new users and/or from users coming from countries where high-level solid-state NMR infrastructure and expertise are not available, and **less than one month and a half** for other categories of users. All the eight RIs have committed themselves to make all efforts to achieve these objectives.

### ***Article 5 – Degree of independence of the users***

During their visit, many users may wish to conduct their research fully with total independence. In this case, the technical and scientific staff of the RI are available to provide any kind of assistance as described below, but will not interfere, allowing the users to define the lines of their projects or to change their orientation.

Chemistry users without a solid-state NMR background, which are a special target of this project, will be closely guided, supervised and advised by the local technical and scientific staff.

Associating members of the RI to the exploitation of the results are left to the discretion of the users, and in any case, is not mandatory. In cases where the project presents a conflict of interest to current research activities of the selected site, the site coordinator will reject the project, and suggest to the user to resubmit his/her proposal to another site of the Infrastructure.

## **Article 6 – Personal data**

The management system allows the automatic gathering of statistics regarding the users (origin, expertise, level of training, gender, etc.), the application field of their research (discipline, NMR methods, instrumentation, etc.), the evaluation scores, the average access days per proposal, the balance of access between sites, the delays between the request for access and the access provision, the user satisfaction level.

Long-term follow-up statistics are also carried out to evaluate the outcomes of the access activity beyond the project duration. These statistics are compiled on a regular basis and are accessible in the annual reports on access activity that are published on the website of the Infrastructure.

## **Title IV – Organizational aspects**

### **Article 1 - Access to infrastructure**

An applicant (i.e. a user or a research team) can submit a proposal on the portal of the integrated PANACEA Infrastructure (a unique web portal for the eight infrastructures providing access) via an on-line application form, which will be automatically processed by an intranet-based management system: <https://dev.panacea-nmr.eu/access/submit-a-project>.

Unless otherwise specified, the presence of users at the spectrometers for the implementation of their experiments is from Monday to Friday, from 9 a.m. to 6 p.m. In all cases, the access to the access sites and the NMR equipment is done in accordance with the internal regulations applying at the site concerned.

At most of the sites, the users will have access to a given number of peripheral infrastructures (such as chemistry or biology wet labs, workshops, computer rooms for data processing, internet access, etc.).

Users are required to use these collective facilities with due respect for the host environment, ensuring that the equipment used is kept clean and tidy, and strictly complying with the internal regulations and safety rules in force on the site.

Visitors must immediately report to the local staff any problem encountered when using the on-site equipment.

### **Article 2 - Use of workstations and IT resources**

Users must neither install nor uninstall programs on the NMR spectrometer control stations made available. They are committed to not store any personal data on these workstations, except for files related to the acquisition of NMR data. They are also committed to not consult or manipulate the data stored on workstations that do not belong to them.

The connection of laptops to the computer network of the host site is subject to authorization by the site manager, who ensures proper compliance with the charter for the use of computer resources in force.

### ***Article 3 - Scientific and technical support***

The scientific and technical staff on site are prepared to provide any kind of support. At each site, the scientific coordinator designates the most expert and suitable research staff to perform and/or advise on the NMR experiments as well as on the processing and analysis of the data (the “local contact”).

Experimental support may also include computational assistance, for example on ab-initio calculation and prediction of NMR parameters by qualified theoretical research staff of the infrastructure.

### ***Article 4 - Logistic support***

Besides direct access to the equipment, the visiting scientists benefit from the office and lab infrastructure of the NMR facilities to make their research a success. Equipped offices (including computers, internet, printing facilities etc.) are provided to the users during their visit for data processing, analysis and communication. Available (commercial and locally developed) programs for solid-state NMR data processing, spectral simulation and fitting, along with training on how to use this software are provided. Furthermore, consumables (i.e. sample holders, dopants for DNP sample formulation) and laboratory space for sample conditioning (including glove boxes for charging the sample holders with air or moisture sensitive samples) are made available to the users.

The administrative/secretarial RI staff are available to assist users with the on-site arrangements (accommodation, local transportation) and with administrative issues. Accommodation for the users is organized in local hotels or in various ancillary on-campus facilities.

In order to encourage / facilitate the visits of parents having a young child, the consortium offers the possibility to fund the travel costs and the accommodation of user partner.

### ***Article 5 - Transfer and backup of data***

In case the user and the visiting scientists leave the access site before the end of the NMR experiments, the data are sent to them by the local staff of the host site within 48 hours after the end of the experiments.

Users are responsible for backing up and archiving their data. The data will be stored for at least a month on the workstation of the host site. Some platforms may have the ability to keep an archived copy of the data, if the user so desires. Inquire with the corresponding platform.

### ***Article 6 - Sending and returning samples***

Users are responsible for sending their samples to and from the host platform, and bear the costs thereof. In particular, shipments by courier (DHL, FEDEX, etc.) are paid by the users.

### ***Article 7 - NMR consumables***

Specific NMR consumables (such as rotors, inserts) related to the performance of their experiments are provided by the access site. Unless agreed in advance, they must be returned clean to the local staff at the end of the experiments. The provision of these consumables only concerns use on site: the host platforms do not loan or send consumables for external usage, before or after the visits.

## **Title V – Prevention, health and safety at work**

At each transnational access site, the Director the Research Infrastructure is responsible for the safety at work and is in charge of the application of the regulatory safety requirements in force.

The usual safety instructions, as well as any specific safety requirements in force at the access site, must be strictly followed by PANACEA visitors.

Due to the presence of strong magnetic fields, the access to the spectrometer rooms is not accessible to people bearing medical devices such as pacemakers, ferromagnetic surgical implants, etc. Access to the spectrometer rooms is not accessible to pregnant women. The list opposite is not exhaustive. In case of doubt, it is of the user's responsibility to consult a medical doctor before accessing the site.

The user and the visiting scientists are responsible for knowing the chemical and/or biological risks associated with the samples they bring to the site. They have the duty to inform the local staff on site about these specific risks and safety measures related to sample handling. In addition, they must ensure, before their visit that all the safety equipment necessary to handle and formulate securely their samples is available at the access site (such as fume hoods, glove boxes, etc.).

Access is prohibited for samples containing infectious or pathogenic agents requiring containment, or radioactive isotopes.

For any sample with a specific risk, the user will first contact the access platform and the local operator on site, who may ask his/her local safety staff about specific safety procedures.

Users and visitors will also ensure that they are informed and comply with the specific instructions of the access site in terms of waste disposal.

Any health or safety issue occurring during a visit at the access site should be immediately brought to the attention of the local operator and scientific manager of PANACEA.



## **Title VI – Valorization/dissemination of results**

The users are asked to acknowledge PANACEA when disseminating their results as follow: *“The authors acknowledge financial support from the European Union under the Horizon 2020 program within a contract for Integrating Activities for Starting Communities, contract number 101008500.”* They will also be asked to use the PANACEA logo when presenting the work carried out within the infrastructure.



## **Title VII – Modification of the rules of procedure**

These internal regulations only specify the general service provisions of PANACEA, they do not replace the internal regulations of each access sites.

The rules of procedures are established by the PANACEA Committee.  
The Project Coordinator of PANACEA can propose modifications that will have to be approved by the General Assembly.