

Motivation - the need for networking

The scientific community has reaffirmed that NMR, as an invaluable tool not only for the investigation of the structure and dynamics of biomolecules, but also for their functional characterization, is an integral part of on-going efforts in disciplines such as structural biology and molecular systems biology. Progressing into research in the next decade, it may be time for a cooperative effort as we work towards tackling increasingly more complicated problems. By jointly identifying the frontiers in science and technology, and in the knowledge and expertise that will be required to explore them, we strive to advance research faster and further, adding more challenging problems at a higher level of complexity than has previously been possible. The impact of the NMR scientific community as a whole on pushing the current limits of scientific disciplines critically depends on how well the NMR community is organized and structured. The synergistic involvement of national, regional, and other major facilities is necessary for the progress of the biological sciences, for ensuring that the reality of NMR services and research infrastructures can live up to their promise, and for the personal scientific success of all members of the community.

A meeting entitled "Networking in Bio-NMR" was held on January 5, 2008 in Florence, Italy for representatives of regional bio-NMR facilities as they address their modes of interaction in the face of the new challenges posed to NMR by their users. The meeting was organized within the framework of the Coordination Action NMR-Life (www.postgenomicnmr.net), an EC funded project to promote the networking and coordination of NMR research. This action aims to foster cross-fertilization among scientific areas of interest, to contribute to the development and dissemination of common good practices and methodological approaches, to encourage the transfer of knowledge among different research teams, thereby enhancing the spread of innovative methods and tools, and to identify bottlenecks and possible breakthroughs in the field of biological NMR, among other goals. While these are specific tenets upon which the CA NMR-Life is built, they are also themes important for and common to the larger NMR community.

Specifically, we want each regional/national facility to guide the researchers belonging to its scientific/geographical domain so that they can perform the measurements of interest not only locally, but also at the most appropriate instrument, wherever located, so that they may exploit the competences available there, and receive assistance in planning for NMR-specific project aspects. The participants in this meeting are convinced that encouraging further collaboration in the bio-NMR area will make the entirety of European research projects in the field more productive, and will allow the community to tackle greater scientific challenges. Such an increase in collaborative research will be extremely beneficial for the role and importance of NMR in the entire Life Sciences arena.

A key point that has been highlighted during discussions within the Coordination Action NMR-Life is that interaction among the above-mentioned players is crucial for the thorough and timely dissemination of the best experimental and computational practices as soon as they become available. This objective is common to the three actions described above, and enhances their impact on the scientific panorama. Under the umbrella of the CA, we want to establish a network of European, national, regional, and other major NMR facilities with the aim of optimizing research activities within the three major European actions. This network will rely on the active participation of each facility to assist individual researchers in bio-NMR with solving prominent scientific challenges and trying to tackle important biological problems that single researchers/facilities cannot afford individually.

Meeting and discussions

The meeting involved 35 experts, who as representatives of European NMR infrastructures were invited to share their suggestions on how to improve the network among them. The first session addressed the EU-NMR Integrated Infrastructure Initiative (I3), under which part of this network is currently active. One point of discussion was related to new forms of integration between the national and transnational facilities. The second session was devoted to the upcoming eNMR initiative (grid for computing in bio-NMR), under which networking also plays an important role - users of the facilities were asked to give suggestions on what platforms they would like to see and how they foresee the workflow. The third session focused on the INSTRUCT infrastructure, which is in the preparatory phase – discussions were held on how to define the organization of the bio-NMR community with respect to the infrastructure. It is believed that the synergistic interaction between these three actions will enhance the visibility of the entire

scientific community. These sessions were followed by a general discussion, to identify pathways toward the most efficient and effective involvement of national, regional, and other major NMR facilities.

EU-NMR – Integrated Infrastructure Initiative

Within the I3, funds for networking will be used to make each laboratory aware of the potentialities of all the others. Seed money for researchers at regional and national facilities to encourage the implementation of new, advanced experimental methods may also be provided, to foster the exchange of best practices within the network. It can be foreseen that future developments in I3 projects will be in the directions of, for example, offering sample preparation and labeling schemes as part of the access, networking with regional/national infrastructures to broaden the users' base and to provide pre-screening of users' needs, and expanding the offer of service to life science projects in agriculture and food science. It was suggested that the I3 should continue to focus on encouraging users in emerging applications at the forefront of systems biology as they appear where NMR measurements have a particularly high value. Ideas for future applications have been presented.

eNMR – grid for computing in bio-NMR

In the context of eNMR, the network will allow the partners to obtain the training and information required to profitably access and use the most advanced computational tools within a grid-based calculation platform. The eNMR initiative also offers to the scientists in bio-NMR the possibility to have their programs of choice run on the grid, with great enhancement of their performances and maintainance of the most current improvements in each calculation protocol defined by the needs of the community.

In the discussion, the potential advantages of adopting the CCPN data model have been highlighted. It has been pointed out that this would enable easier handling not only of present-day programs, but would also make inclusion of new programs or of updated versions of the present programs relatively straightforward. Whereas the eNMR platform aims at being as inclusive as possible, it is made clear that a preference should and will be given to open-source programs. It has been suggested that the eNMR partnership makes available a repository for such sources. In the future, if the project is successful, it could exert pressure on developer teams to make their sources available.

Users would welcome the implementation of “recommended” computational protocols within eNMR for common tasks such as structure calculation or the characterization of protein-protein adducts. These protocols will be endowed with appropriate documentation and tutorials. It has been pointed out that the impact of eNMR will not be mainly linked to the increased computational power that it can provide but to the enhanced interoperability of programs, to the ease of running and comparing different protocols, and also to the possibility of making innovative or complex tools promptly available to the community. In this way, the use of computational tools will be made lighter for users.

INSTRUCT – Integrated Structural Biology Infrastructure

INSTRUCT will be another major player in European systems biology. When this infrastructure will be fully operational, users will have the chance to design and carry out complete projects in the field of systems biology, including sample preparation, X-ray crystallography, electron microscopy, and of course, bio-NMR. The present network will encourage partners with relevant problems to benefit from INSTRUCT.

INSTRUCT is a science-driven Infrastructure and not technique-driven. Its goals will be to exploit the 3D structures of macromolecular assemblies to help model functional processes with a systems biology perspective and to predict the outcomes in the systems (cells, tissues, organisms, etc.) at the molecular level. These goals will be achieved through an integrated pool of approaches and the corresponding instrumentation to integrate structural information at different resolution levels and with temporal dimension within a systems description.

The Infrastructure will be nationally funded. Every government that has agreed on the ESFRI Roadmap and on INSTRUCT should provide money for the National Group to contribute and to access to INSTRUCT. All the participants in this meeting were invited to contact their national governments to establish their involvement in INSTRUCT. The participants were informed of the

developments of the preparatory phase of INSTRUCT and its organization into 15 working groups. The next action will be the establishment of the participation of NMR scientists in the appropriate working groups, not limited to those directly related to NMR.

Conclusion

European NMR facilities can achieve close and lasting interactions through their involvement in providing access to users, in pursuing technological innovation, in the various aspects of spreading good practices, and in optimizing the workflows associated with activities such as protein structure determination and validation, modeling of intermolecular complexes, etc. Only if we attain a high level of interaction and integration will we be able to guarantee that European NMR facilities will continue to implement and maintain the best available practices beyond the duration of any of the funded actions (most notably the present CA) mentioned in this document. This is crucial to sustain the European excellence in the field of bio-NMR.

Participants in the meeting

Daniel Abergel	<i>Ecole Normale Supérieure de Paris</i>
Lucia Banci	<i>CERM Magnetic Resonance Center</i>
Ivano Bertini	<i>CERM Magnetic Resonance Center</i>
Rolf Boelens	<i>Universiteit Utrecht</i>
Iain Campbell	<i>University of Oxford</i>
Alex Dikij	<i>Norwegian U. of Science and Technology</i>
Lyndon Emsley	<i>Centre National de la Recherche Scientifique</i>
Christian Griesinger	<i>Max Planck Ges. zur Ford. der Wiss.</i>
Peter Guentert	<i>J.W. Goethe Universität</i>
Ulrich Gunther	<i>University of Birmingham</i>
Juri Jarvet	<i>Nat'l Inst. of Chemical Physics and Biophysics, Estonia</i>
Goran Karlsson	<i>Göteborg University</i>
Robert Konrat	<i>University of Vienna</i>
Katalin Kover	<i>University of Debrecen</i>
Ernest Laue	<i>University of Cambridge</i>
Claudio Luchinat	<i>CERM Magnetic Resonance Center</i>
Beat Meier	<i>Laboratory for Physical Chemistry, Switzerland</i>
Henriette Molinari	<i>University of Verona</i>
Jose Moura	<i>Instituto de Tecnologia Química e Biológica</i>
Hartmut Oschkinat	<i>Forschungsinstitut für Mol. Pharm. im Forsch.</i>
Janez Plavec	<i>National Institute of Chemistry, Slovenia</i>
Miquel Pons	<i>Parc Científica de Barcelona</i>
Flemming Poulsen	<i>University of Copenhagen</i>
Angelo Ripamonti	<i>Bruker</i>
Antonio Rosato	<i>CERM Magnetic Resonance Center</i>
Ago Samoson	<i>Nat'l Inst. of Chemical Physics and Biophysics, Estonia</i>
Michael Sattler	<i>GSF – Nat'l Res. Center for Env. and Health</i>
Harald Schwalbe	<i>J.W. Goethe Universität</i>
Vladimir Sklenar	<i>Masaryk University</i>
Georgios Spyroulias	<i>University of Patras</i>
Miguel Teixeira	<i>Instituto de Tecnologia Química e Biológica</i>
Henk Van As	<i>Wageningen University</i>