

The present deliverable summarizes the dissemination activities that were aimed at spreading the achievements of e-NMR carried out during the second project year (from 01/11/2008 till 31/10/2009).

The activities targeting mainly the bio-NMR community are separated from those targeting mainly the e-Science community. Activities targeting broader communities, such as that of Structural Biology, are in the third section. Synergies and commonalities are discussed in the fourth section.

1. Activities toward the bio-NMR community

The table below lists the activities relevant for this section

Date	Title/subject of meeting	Location	# of attendees	Website address
14 th – 18 th December 2008	Magnetic Resonance in the Life Sciences: What's New (Closing meeting of NMR-Life)	Montecatini Terme (IT)	120	www.cerm.unifi.it/home/other/montecatini.html
26 th – 29 th January 2009	Annual meeting of the users of EU-NMR	Autrans (FR)	165	www.eunmr.eu/third_annual_meeting/eunmr2009/Presentation.html
15 th -20 th Feb. 2009	Keystone meeting on Frontiers of NMR in Biology	Santa Fe (NM, USA)	Ca. 300	www.keystonesymposia.org
8 th -13 th March 2009	XXI ^{ème} Conférence du GERM	Frejus (FR)	80	thibault.charpentier.free.fr/spip.php?article166
15-17 th June 2009	Joint East-NMR / eNMR conference	Florence (IT)	70	www.cerm.unifi.it/home/other/StructuringEuropeanNMR.html
5 th – 10 th July 2009	Italian Chemical Society conference	Sorrento (IT)	250	http://www.sci2009.org/congress_infos_in_english.php
22-24 th July, 2009	Collaborative Computing Project for the NMR community (CCPN) conference	Ambleside (UK)	150	www.ccpn.ac.uk
21-24 th Sept, 2009	GDCh meeting on Magnetic Resonance in Chemistry and Materials Research	Dresden (DE)	600	-

With the exception of the presentation at the Keystone meeting on “Frontiers of NMR in Biology”, the above meetings targeted mainly the European community of bio-NMR users. The NMR-Life coordination action worked during Framework Programme 6 to operate a network of NMR laboratories active in the fields of structural biology and structural genomics, promoting in particular dissemination of best practices and exchange of knowledge also through exchanges of personnel. This provided a “transversal” audience of European bio-NMRists to which the initial implementation of the e-NMR web portal was interactively

demonstrated. At the same time the meeting provided an occasion to instruct potential eNMR users on the procedures that should be followed in order to *i)* obtain personal certificates and *ii)* register with the e-NMR VO. This was done by installing a booth that was active throughout the meeting. There is a significant need to provide this kind of information to scientists in the field of NMR spectroscopy, as GRID computing, and the associated operational procedures, are essentially unprecedented in the field.

The above initiative was received so well by the audience, leading also to extensive discussions between project staff and various players in the field, that it was decided to replicate it in a similar format also at the Annual meeting of the users of the EU-NMR Research Infrastructures. Here the audience was composed by European researchers that had exploited the services of the RIs to obtain experimental NMR information for their own research projects. The attendees were thus familiar with but not necessarily expert in the uses of NMR instrumentation as well as of the corresponding experimental data. It therefore provided an audience that would be likely impressed by the availability of the integrated, streamlined tools provided by e-NMR. Also on this occasion, a booth to inform the participants on how to obtain personal certificates and register with the e-NMR VO was installed.

Similarly, the presentation at the CCPN conference in July targeted an audience of researchers already quite familiar with NMR, and additionally having some interest in the computational aspects of NMR spectroscopy.

Participation at the Keystone meeting on “Frontiers of NMR in Biology” allowed dissemination of e-NMR results to an international audience. This together with some of the initiatives described in the third section, allowed e-NMR to extend its user base by including a small but significant number of American users. The events in Frejus (FR), Sorrento (IT) and Dresden (D) promoted e-NMR activities and results mainly at the level of the respective national communities of chemists and NMR spectroscopists.

The Joint East-NMR / eNMR conference of June 2009, provided a venue to target the users of the Research Infrastructures that are involved in the EAST-NMR project, another transnational access initiative similar to EU-NMR, but with a distinct focus on New Member States. This occasion was exploited to pursue a double objective: *i)* to raise the awareness of bio-NMRists regarding the possibilities offered by GRID computing in general and, more

specifically, in the Life Sciences (this was done thanks to the participation of two distinguished scientists from the e-Science community, Dr. Matyska and Dr. Breton); *ii*) to organize a training event for both e-NMR registered users and potential new users, introducing them to both the basics of GRID computing and the use of the redesigned e-NMR web portal, featuring a significantly broader range of applications than the initial version presented in December-January. The training sessions were attended to the full capacity of the two computer rooms that were available in the building, and resulted in a very good visibility of the practical achievements that e-NMR afforded.

Finally, e-NMR has also been promoted at various institutions/laboratories focusing on the application of bio-NMR experimental techniques, on the occasion of seminars and lectures to students.

2. Activities toward the e-Science community

The table below lists the activities relevant for this section

Date	Title/subject of meeting	Location	# of attendees	Website address
2 nd -6 th March, 2009	4 th EGEE User Forum/OGF 25 and OGF Europe's 2nd International Event Search	Catania (IT)	615	egee-uf4.eu-egee.org
7 th -8 th May 2009	Research Connection 2009	Prague (CZ)	2000	ec.europa.eu/research/conferences/2009/rtid-2009
10-15 th May 2009	Biomed Grid School	Varenna (IT)	35	www.biomedgrid.it
21-25 th Sept, 2009	EGEE'09 Conference "Enabling Grids for E-sciencE '09"	Barcelona (ES)	600	egee09.eu-egee.com

The above events constitute occasions to demonstrate the achievements of the eNMR project to an audience that was primarily focused onto e-Science applications. In particular, the e-NMR contribution at the 4th EGEE User Forum constituted of a live demonstration that was a *début* for the project in the e-Science arena, after the demonstrations held in December and January to primarily NMR audiences. Instead, the meeting in Catania was primarily attended by GRID facility managers, developers and users from a various scientific fields, including life sciences, representing both potential users of the e-NMR platform and

potential collaborators. The demo of the e-NMR portal was awarded '[Best demonstration of an application](#)' with the following motivation: "it represented a unique and important application, was adopted to grid very fast, had a clear development strategy and most importantly brought new resources to the grid". A short video of the presentation is [available](#). This constituted the project milestone M1.2: "Demonstration of e-NMR at e-Science event". Following on this event, a publication was submitted to a special issue of the Journal of Grid Computing.

Live demonstrations were also given at the Research Connection 2009 and at the EGEE'09 Conference "Enabling Grids for E-science'09". For the latter occasion in particular, new presentation materials were developed, and shown at a booth that the e-NMR project maintained throughout the conference. The presentation included [showing a newly developed video on the project](#), also available [at higher resolution](#). The e-NMR project delivered also a lecture at a bioinformatics session in the meeting. Finally, the EGEE'09 conference additionally provided a further opportunity to discuss about the Life Sciences SSC and to include e-NMR in the current relevant draft proposal.

The Biomedgrid school in Varenna provided a completely different environment with respect to the aforementioned events, in that this is a small-scale event involving only people closely working on Life science and biomedical applications that are Grid-based. This event provided a venue for close interactions and exchanges of experience among people with different backgrounds but with an interest in related problems and often facing similar hurdles (e.g., web-based services, workflow management, etc.).

3. Activities toward broader communities

Date	Title/subject of meeting	Location	# of attendees	Website address
2 nd – 3 rd March 2009	Annual retreat of the North East Structural Genomics project	Princeton (NJ, USA)	80	www.nesg.org
4 th – 6 th March 2009	2009 NIGMS Workshop: Enabling Technologies for Structural Biology	Bethesda (MD, USA)	180	www.blsm meetings.net/2009workshop_enablingtechnologies/
13 th May 2009	4th International Symposium on Enabling Technologies for Proteomics	Vancouver (CA)	200	www.etpsymposium.com

The activities described in this section constitute efforts in the direction of targeting the broader Structural Biology community or neighboring communities such as those in Structural Genomics or in Proteomics. They additionally target an international audience by reaching out to researchers oversea. The first two events in particular created an interest within the North American scientific community that triggered initial contacts with the SBGrid initiative, ultimately leading to an agreement allowing US users to obtain personal certificates and register with the enmr.eu VO. Contacts with the NESG Structural Genomics initiative were also very useful in the context of the workshop for the assessment of the state-of-art in automated protein structure determination, by allowing the participants to get access to two complete datasets for protein structures not yet released in the public domain.

4. Synergies among the activities

The various dissemination activities described in the preceding sections constitute a portfolio of complementary, synergistic initiatives. By alternating presentations and demos at events targeting the NMR and the e-Science communities, the project obtains feedback on the different aspects that most relevant and/or more strongly perceived within each community, which ultimately can lead to developments that are quite innovative for the other or both communities. In other words, the new developments that are stimulated by interaction with NMR researchers motivate the project staff to explore solutions that are new or innovatively adapted from the point of view of the e-Science community. Viceversa, solutions learnt from and discussions held with scientists active in the e-Science community provide innovative design for services to be provided to enmr.eu users. We believe that in the medium term this will provide significant advances toward the development and adoption of common strategies for the provision of services, especially in the case of web based services.

The activities targeting broader communities than those “central” to the project lay the basis for further expanding the impact of the project and in particular the uptake of the technologies and approaches developed in the context of e-NMR. They also provide means for a geographical expansion of the user base of e-NMR beyond Europe.