



SEVENTH FRAMEWORK
PROGRAMME

Research Infrastructures

Deliverable 3.3.1

Reports on Conferences attended and presentations / demos given



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Section 1: Summary of Deliverable

Background

Disseminating the results of the WeNMR project as well as the possibilities that the WeNMR VRC offers to scientists worldwide is one of the key goals of WeNMR, and is the topic of Workpackage 3. The “Dissemination and Outreach” workpackage targets several distinct groups of stakeholders, including the e-Science community, the WeNMR community, the broader structural biology, life sciences, and bioinformatics communities and the general public (Tasks 3.1 through 3.4). Because a dedicated report will be generated on the “participation in international e-Science conferences and workshops” (Deliverable 3.4, due in month 21), this report will focus on outreach activities to the WeNMR, structural biology, life sciences, and bioinformatics communities as well as the general public that were performed by all partners (Tasks 3.2 through 3.4) in the first 15 months of the project.

Goal

The goal of the WeNMR outreach activities are “to foster the adoption and use of e-Infrastructure on a global scale by supporting a wide range of flanking disciplines within the life sciences” (quote from original proposal). We work towards that goal by introducing our results and services to new user bases and to obtain user feedback on possible improvements to our services from existing users (Objectives 3.1 through 3.3).

Summary

The project results and services have been presented at a large number of structural biology workshops and conferences worldwide. The metrics of success final goals and the items achieved at the one-year milestone have been summarized in the first year's report. The report shows that the numbers are well underway to achieve full compliance with the project goals. In summary, the final goal is well within our reach.

Highlight

- A general public YouTube movie introducing the role of NMR and SAXS as structural biology techniques for studying molecules linked to diseases has been produced (available on the WeNMR web site (<http://www.wenmr.eu/wenmr/wenmr-demo-egi-user-forum-vilnius-2011>) or [here](#) on YouTube).

Section 2: Conferences attended and presentations / demos given

Outreach to the WeNMR community

Over the first period several workshops and courses were organized, specifically targeting the WeNMR community as well as interested scientists from the broader structural biology community.

Together with the [Bio-NMR](#) consortium a **workshop „Introduction to biological solid state NMR“** was organized aiming at giving the trainee basic knowledge to solid-state NMR spectroscopy in relation to structure determination of solid proteins. (28 March 2011)

Also co-sponsored by the Bio-NMR consortium, a 4-day **workshop “Acquisition and processing of sparsely sampled NMR data“** was organized, providing an introduction to applications of sparse sampling and Fourier Transformation processing in biomolecular NMR (27 April 2011).

Partner SpronkNMR hosted the **Advanced course: Protein NMR Structure Calculation and Validation** twice (May 17 - 19, 2011 and Februari 6 - 10, Vilnius, Lithuania). Partners BMRZ & RUN were also teaching at this course. The course was attended by students from Europe and the USA.

The BCBR Partner gave a talk and presented a poster at the Gordon [Conference on Computational Aspects of Biomolecular NMR](#) in Lucca (Barga), Italy (May 22 - 27, 2011) titled "Structural biology on the GRID: the tale of the WeNMR virtual research community". This conference represents a perfect medium to reach software developer in the NMR field. Several developer groups indicated interest in WeNMR, both to benefit from the Grid infrastructure, but also to give more exposure to their software as the WeNMR portal is becoming very well recognized internationally. A direct result of this conference was the addition of the new web portal to the WeNMR portal: [Shift2X](#) for the prediction of NMR chemical shifts from 3D structures.

A joint **NMR and SAXS WeNMR workshop** was held in Florence on May 27th, 2011. The workshop was scheduled right after the Gordon NMR conference on computational aspects of biomolecular NMR taking place in Il Ciocco, Italy (22 - 27 May 2011), and was thus attended by several delegates of the Gordon conference. The leaders of the major groups developing software for the joint SAXS-NMR applications from both the NMR field and the SAXS field were represented at the workshop, such that all the main novel approaches were covered. The talks were given by scientists from the Netherlands, Germany, Italy, Denmark, France and USA. Of all people attending the workshop, 16 (45%) were affiliated with WeNMR and 19 (55%) were from other research institutes in Europe, India and the USA.

In addition to the planned access to the ATSAS program suite from Hamburg (as a part of the WeNMR activity), interest has been expressed to provide grid portals for the Dadimodo software of J. Perez (Eur Biophys J, 2007, 37:95–104) and M. Sattler's implementation in CNS

(Gabel F, J Biomol NMR. 2008 41:199-208). A detailed description of the workshop was provided in [Deliverable 3.1](#).

On July 12 - 13, 2011 a **WeNMR developers workshop** was held in Utrecht. At this workshop a series of topics has been discussed, *Web services and end-user platform, The VRC web platform, Grid submission and monitoring tools, Centralized user administration/registration system, Harmonization / "branding" of web portals and new web server developments*. A representative of the EGI was present in the person of Dr. N. Ferreira from the user support team. Most effort was put into a discussion on harmonizing aspects of the multitude of web portals. This workshop essentially defined the Web services roadmap (Milestone 4) and was also highlighted in an [EGI blog](#) and available also from the WeNMR site [here](#).

WeNMR (partners BMRZ, BCBR and SpronkNMR) organized a **2-days workshop „NMR applications on the Grid“** in Frankfurt am Main on August 19-20 2011, connected to the EUROMARconference. The workshop gave an introduction, overview and practical training on how to use some of the widely used and state-of-the-art biomolecular NMR applications that are available on the Grid. The participants were first introduced to the WeNMR Grid and the principles of NMR structure calculations in general, followed by a tour along the BMRZ NMR spectrometer facility. The participants were made aware of all the possibilities within the Virtual Research Community (VRC), support, forums, and the WeNMR help centre. The workshop topics covered lectures and practicals about hyper dimensional processing with MDD-NMR, protein backbone resonance assignment with MARS, torsion angle prediction using TALOS+, structure calculation using CYANA and macromolecular docking and structure modelling with HADDOCK and 3D-DART. The covered software packages are integrated in WeNMR web portals and the practicals gave a comprehensive hands-on approach on how to use those, as well as how to analyze the results.

Partner UCAM co-organized the 3rd CCPN/EUconference "**NMR: Solids, Solutions and Samples**" that was held at the ITQB venue in Oerias, near Lisbon, Portugal from 28 - 30 September 2011.

Partner SpronkNMR, in collaboration with and sponsored by the Bio-NMR consortium, organized a Bio-NMR **Workshop: Protein NMR data processing and analysis** that was held in Vilnius on 4 - 7 October 2011.

On October 18, 2011, partner SpronkNMR launched an easy to access common [NMR marketplace](#) and world resources map. The marketplace allows members of the worldwide NMR community to list, advertise and search information about Events, Jobs, Products, Services and Training.

The Utrecht, Florence and Frankfurt partners all attended the [Bio-NMR meeting](#) on November 10 - 11, 2011 in Berlin. Presentations were given among others around HADDOCK, UNIO and CYANA, illustrating some of the capabilities of the WeNMR portals.

In summary, the project has been presented at a large number of NMR meetings, but also at

other conferences and (co-)organized a large number of workshops. An easy to access common NMR marketplace and a world resources map have been launched.

Outreach to the broader structural biology, life sciences and bioinformatics communities

To advertise the WeNMR project and its tools to the broader structural biology community, the project has undertaken the activities underlined in the following.

A phone conference with the [SBGrid](#) in the US took place in January to setup a collaboration plan. As a direct result, WeNMR was invited to give a presentation at the OSG meeting hosted by SBGrid in Boston to discuss further collaboration.

The project was represented at the following structural biology meetings:

- The **Bio-NMR and EAST-NMR Annual User Meeting** on January 24 - 27, 2011 in Brno, Czech Republic
- The **Midlands Biophysics Network**, Warrick, United Kingdom, April 2011
- **IWSG-Life** (June 2011, London, UK)
- **CCPN/EU conference** (September 2011, Oerias, Portugal)
- **Gordon Conference on Computational Aspects of Biomolecular NMR** (May 2011, Lucca, Italy)
- **14th European Conference on the Spectroscopy of Biological Molecules**, Coimbra, (August 2011, Portugal)
- **Structural Bioinformatics meets Structural Biology**, Dutch Cancer Institute, (September 2011, Netherlands)
- **German annual Bruker Biospin User Meeting** (8-9 November, 2011, Ettlingen, Germany)

In addition, the following targeted workshops and courses were (co-)organized by the consortium:

- WeNMR co-sponsored the **EMBO global exchange lecture course** on "[Structural and Biophysical Methods for Biological Macromolecules in solution](#)" hold at the Institute of High Energy Physics (IHEP) in Beijing, China, from April 28th until May 5th. Lectures covered NMR and bioinformatics, presenting the WeNMR project and its web portal. The course was followed by more than 47 participants. Next to the lectures, hands-on computer sessions were organized during which the HADDOCK WeNMR web portal was demonstrated. The course was followed by a one-day scientific symposium.
- Dr. Bonvin visited Taiwan where he gave a **one-day workshop on May 2nd at the National Tsing Hua University** with more than 50 participants. This workshop, co-organized by Dr. Shang-Te Hsu from the National Tsing Hua University, consisted of both lectures and computer practicals, again demonstrating the use of the WeNMR web portals with a focus on HADDOCK. During this visit, a meeting with Dr. Simon Lin and his team from the Academia Sinica Grid Computing Centre (ASGC) in Taipei took place. As a result, the ASGC grid side is now officially supporting WeNMR. A roadmap for further extension of the WeNMR services in Taiwan and Asia was discussed, including the

possible future addition of a Taiwanese partner to the WeNMR consortium.

- Dr. Bonvin has been invited to give keynote lecture at the **International Symposium on Grids and Clouds (ISGC) 2012** that took place at Academia Sinica in Taipei, from 26 February to 2 March 2012 (See also the GridTalk interview on [YouTube](#)). A **satellite WeNMR workshop** on protein-DNA modelling was organized in collaboration from Dr. Shang-Te Hsu, now at Academia Sinica.
- Partner Nijmegen has participated in the [EGI user virtualisation workshop](#) (May 12 - 13, 2011 Science Park Amsterdam). The outcome of this meeting has been reported to the WeNMR partners at the WeNMR internal workshop in Utrecht, July 12. The meeting in Amsterdam was particularly important to Partner Nijmegen for fostering international contacts.
- Partner BCBR has been teaching a **three days workshop in Istanbul** (20 - 22 June 2011) around the grid-enabled software HADDOCK. It is an information-driven docking software for the modelling of biomolecular complexes which is made available to end users the user-friendly and grid-enabled HADDOCK portal within WeNMR (see [here](#)). This workshop was highlighted in a blog posted to the EGI blog site and available also from the WeNMR site [here](#).
- At the **practical EMBO course** "Structure, dynamics and function of biomacromolecules by solution NMR" (Juli 29 - August 5, 2011 in Munich-Garching, Germany), an tutorial "introduction to WeNMR grid computing" was presented by the BMRZ partner.
- The Utrecht and Frankfurt partners attend the "**Protein Structure Determination in Industry**" meeting on November 14 - 16, 2011 in Goteborg, which offered a unique opportunity to meet with industry partners (see also WP2 sustainability). WeNMR sponsored this meeting. A detail report of this meeting has been already provided (WeNMR-M-NA-6-9-PSDI-report).
- Partner SpronkNMR started to hold the Beginners course: [Python Programming for Structural Bioinformatics](#). On November 29-30 2011, in Vilnius, Lithuania, a test course was held for a small audience and a first full version of the course was held on Februari 2-3, 2012.
- Partner Nijmegen explained the concepts of WeNMR at the **Elixir meeting** for interoperability and Grid and Cloud computing in Amsterdam at December 7-10 2011.

A flyer was developed to attract new users to the facilities and services offered under WeNMR. This flyer was distributed broadly by all WeNMR partners, within their network by direct mailing, at e-Science events (like at the recent EGI User Forum in Vilnius) and at the more general structural biology and life science meetings they have attended. The Nijmegen partner distributed WeNMR flyers at the Benelux Bioinformatics Conference (BBC) in Luxembourg on December 12-13, 2011. The WeNMR project was also highlighted in a plenary lecture. A total of 600 copies have already been distributed and another 1,000 copies of an updated version of this flyer have been ordered for future advertizing opportunities.

In summary, in the first year conferences and workshops have been the most important outreach vehicle towards the broader life-science, bioinformatics, and structural biology

communities, and several such activities have successfully taken place.

Outreach to the general public

Because outreach to the general public will be most useful when some results of the project can be presented, activities in this area until now have been limited. We expect our efforts in this field to intensify once WeNMR is more widely known in the e-Science and structural biology communities. Nevertheless, we have started with some activities towards the general public. For example:

- A **movie** was created for presentation at the EGI User Forum in Vilnius. It provides a general introduction to the role of NMR and SAXS as structural biology techniques for studying molecules linked to diseases. The movie is available from the WeNMR web site [here](http://www.wenmr.eu/wenmr/wenmr-demo-egi-user-forum-vilnius-2011) (<http://www.wenmr.eu/wenmr/wenmr-demo-egi-user-forum-vilnius-2011>)
- A **WeNMR Facebook account** (handle: [WeNMR](#)) and [Linkedin Group](#) were set up and the first posts have been made. Links to those are now available from the WeNMR web page. The Facebook account automatically displays the WeNMR blogs. Further, all pages of the WeNMR website now contain a “I like it” link for users to express their support to WeNMR. Since its creation early 2012, the LinkedIn group has grown to more than 100 members, and this without much advertisement.
- WeNMR features in an **EGI-sponsored movie** about Grid computing that has been released during the ISCG2012 in Taipei. The movie is available from the WeNMR web site at <http://www.wenmr.eu/wenmr/stories-grid-cone-snail-and-search-powerful-new-anaesthetics> and from YouTube [here](#).
- On the English **Wikipedia**, a page has been made about [WeNMR](#) with the project details for the general public and within two weeks became one of the top hits for a Google search for “WeNMR”.