



SEVENTH FRAMEWORK
PROGRAMME

Research Infrastructures

Deliverable 1.2

Minutes of the kick-off meeting



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| Grant Agreement number: | RI-261572 |
| Project acronym: | WeNMR |
| Project title: | WeNMR, A worldwide e-Infrastructure for NMR and structural biology |
| Deliverable type and status | Report - Public |
| Due Date | January 1 st , 2011 |
| Delivery Date | M2 (December 9, 2010) |
| Project coordinator name, title: | Prof. Alexandre M.J.J. Bonvin |
| Organization: | Utrecht University, The Netherlands |
| Tel: | +31 30 2533859 |
| Fax: | +31 30 2537623 |
| E-mail: | a.m.j.j.bonvin@uu.nl |
| Project website address: | www.wenmr.eu |



WeNMR project kickoff meeting

Date: 18/19 November 2010

Location: University Museum, Utrecht, the Netherlands

People attending the meeting

Partner 01 (BCBR):

Alexandre Bonvin
Rolf Boelens
Reinout Raijmakers
Marc van Dijk
Christophe Schmitz

Partner 02 (BMRZ):

Harald Schwalbe
Peter Güntert
Henry Jonker

Partner 03 (CIRMMP):

Antonio Rosato
Claudia Andreini

Partner 04 (INFN):

Marco Verlato

Partner 05 (RUNMC):

Gert Vriend (first day only)
Geerten Vuister
Jurgen Doreleijers

Partner 06 (UCAM):

John Ionides
Ernest D. Laue
Rasmus Fogh

Partner 07 (EMBL):

Daniel Franke

Partner 08 (SPRONKNMR):

Chris Spronk

External

Steve Brewer (EGI, first day)
Hayo van Buuren (FP-Tools, second day)
Marnix van Berchum (UU library, second day)

Agenda of the meeting

Thursday, November 18, 2010

13:00 - 14:00 Lunch

14:00 - 14:20 Welcome and general introduction WeNMR - Prof. A.M.J.J. Bonvin, coordinator WeNMR

14:20 - 14:50 overview of eNMR achievements - Prof. H. Schwalbe, coordinator eNMR

14:50 - 16:10 Partner presentations (10 minutes per partner, emphasis on what each brings into the project)

16:10 - 16:30 Coffee/tea break

16:30 - 16:50 Presentation of networking WPs (WP2+WP3, by WP leaders)

16:50 - 17:20 Presentation of service WPs (WP4+WP5+WP6, by WP leaders)

17:20 - 17:30 Presentation of RTD WP7 by WP leaders

17:30 - 17:45 The EGI perspective on Virtual Research Communities - Steve Brewer, chief community officer EGI

17:45 - 18:00 General discussion

Friday, November 19, 2010

09:00 - 09:30 Presentation reporting tools (FP-Tools) - Hayo van Buuren

09:30 - 09:45 Presentation OpenAIRE - drs. Marnix vanBerchum - UU library (this is about openaccess publishing - OpenAIRE is an EU project)

09:45 - 10:15 Financial and management aspects

10:15 - 12:30 Discussion of timeline of first 6 months of WeNMR, plan of action

12:30 - 13:30: Lunch and closing

Minutes of the meeting

Thursday November 18, 2010

13.00: Opening and presentation of the agenda and global overview by project coordinator prof. dr. Alexandre Bonvin. He presented the main objectives and activities of WeNMR and how the project will be build on the previous eNMR initiative. The website of WeNMR was presented as well as the other things that have happened during the first 2 weeks, mainly in terms of organization and coordination.

14.24: Harold Schwalbe presented the eNMR project. He showed the organization as well as the results of eNMR. He showed a movie that was generated to present the eNMR project and explains the current GRID capacities of the groups involved and how this evolved during the course of the project. He presented detailed statistics of eNMR users and projects as well as GRID and tool reliability. He also showed the results of user surveys and interviews with users from academia and industry.

14.55: Presentation by the different partners, introducing themselves as well as their groups, what they are bringing to the consortium and what their plans in WeNMR are.

Partner 1 (Bonvin) presented the people involved in WeNMR in his group and in the coordination of the project as well as how access to the HADDOCK tool is currently supplied.

Partner 2 (Schwalbe) presented their two PIs involved in the project as well as very shortly their role as WP2 leader.

Partner 4 (Verlato) presented their institute, how it is linked to national and European GRID projects and what their role in the different WPs will be.

Partner 3 (Rosato) introduced the people in the institute in Florence that are involved in the project as well as their current involvement in the GRID and the fact that they are leader of the JRA workpackage.

Partner 5 (Vuister) introduced the two groups and the people of Nijmegen that will be part of WeNMR and which software they are now and in the future planning to transfer to GRID computing.

Partner 6 (Ionides) showed how they have been working towards data integration and conversion as well as GUI based user access to NMR analysis software.

Partner 7 (Franke) gave a short introduction into SAXS technology and the software used that will be implemented into the GRID as part of WeNMR. Finally, he introduced the people and the work that are bringing into the WeNMR project.

The last *partner 8* (Spronk) introduced the type of work his company does in training, consultancy and services in NMR and structure determination.

16.55: The leader of *WP2* (Schwalbe) presented the tasks, deliverables and milestones related to the “Sustainability of WeNMR”. Point of minor discussion is MS21/MS29, mainly with regard to which companies might be interested in supporting a sustainable WeNMR community.

The *WP3* leader (Vuister) presented the objectives and tasks that are related to “Dissemination and outreach” and reminds everybody that all partners are involved in this WP. It was suggested that T3.3 is partially done together with the BioNMR project and that T3.4 can be based on the current eScienceTalk project.

WP4 was presented by Rosato, who discussed the objectives of the WP on the “Operation and maintenance of the Grid” and its links to the rest of the WeNMR project, especially *WP5* and *WP6*.

The leader of *WP5* (Verlato) presented the timeline and tasks of the workpackage on “Worldwide Grid extension” with a focus on which potential worldwide partners (e.g. USA, South Africa, Latin America, India, China) the current Grid could be linked to. He showed that initial contact with Grid centers in Latin America and India had been established and received positively.

The “Virtual Research Community” *WP6* was presented by WP leader Spronk who focused on how the “support and expertise centre” will be organized and that input from all partners is required there. He presented a timeline on the milestones and deliverables and how these can contribute to the generation of the Virtual Research Community. Also here it was suggested that this could be connected to the BioNMR project and that at least every portal that will be a part of WeNMR will come with an online tutorial.

Finally, the representative of the JRA *WP7* (Franke) presented the research that will be done as part of WeNMR.

18.05: Steve Brewer (Chief Community Officer EGI) presented the European Grid Initiative (EGI), how it links to the National Grid Initiatives and the type of support it can lend to European collaborations such as WeNMR. He presented the way EGI handles their Virtual User Community. Finally, he emphasized the role of EGI in ESFRI and the fact that EGI is now also talking to SARA.

18.37: Closing remarks by Alexandre Bonvin.

Friday November 19, 2010

9.13: Hayo van Buuren of the company *FP-Tools* presented the online reporting tool that will be used for the reporting of the WeNMR project, called EU-xpert. He showed how the tool can be used to assign specific tasks of the reporting to certain users and how it will generate the final report for submission to the EU. He also introduced the financial reporting tool that will be used, EU-fin, which raised some questions on the flexibility of the tool and the support for the financial controllers who will be using the tool. Reinout Raijmakers explained that the management office of WeNMR will be the first contact point for questions and that he will collect contact details of the financial controllers involved and will contact them directly to explain the use of the system. He also indicated that he will distribute a proposal for the division of the budget of the different WPs, based on the requested number of PMs, because the EU-fin tool will require reporting of the costs per WP.

9.45: Marnix van Berchum (Utrecht University library) gave an overview of the current European initiatives and policies on Open Access (OA) and the OpenAIRE project in particular. WeNMR is part of the OA pilot of the EC, and OpenAIRE can assist with complying with the obligations of this pilot. He showed the goals of the OpenAIRE infrastructure where the (open access) publications of EU funded projects are collected and how they link other open access initiatives. He also showed what researchers have to do to comply with the OA pilot. He emphasized the importance of acknowledging the FP7 funding in any publication resulting from WeNMR.

10.10: Reinout Raijmakers discussed some *financial issues* regarding WeNMR, in particular related to the distribution of the budget over the WPs and remarked that 12'500.- euros in the money allocated for travelling in COORD are marked for general costs to cover workshops as described in the DoW. It is also emphasized that no equipment costs can be declared on this project and that all costs declared should be without value added tax (VAT).

10.37: The coordinator of the project introduced the *management structure* of the project to the GA, with Alexandre Bonvin (partner 1), Harald Schwalbe (partner 2), Marco Mazzucato (partner 4) and Ivano Bertini (partner 3) as the Management Committee. The GA approved the Management Committee. He also introduced Reinout Raijmakers (partner 1) as the contact for the project office. The GA approved of the project office. Finally, the signed CA and form A of the GA were distributed to each of the partners by the coordinator, achieving by this Deliverable 1.1.

11.00: Alexandre Bonvin started a discussion on the deliverables and milestones that have to be met during the first 6 months of the project (see below). The first deliverable (D1.1) has been met and two others (D1.2 and D1.3) are also close to be met.

MS1, a joint NMR-SAXS workshop, was suggested by partner 7 to be organized in Hamburg at the SAXS facility. This was positively received by the GA. It is agreed that the organization will have to be jointly between partner 7 and partner 6. Some discussion ensued on which people should be invited and what the focus should be. It was agreed that the focus should be on the

software and analysis. Partner 7 is asked to take the lead in organization this and to also contact the people of the upcoming Gordon Conference in Tuscany (22-27 May 2011) and see if the workshop could be linked to that instead with organization in Florence. Linking it to the Gordon Conference might make it easier to get speakers from the USA, who will also attend the Gordon Conference. If this option is not possible, organization in Hamburg is the alternative.

Partner 8 mentioned that *MS2 (WIKI operational)* and *MS3 (Initial version of the VRC web portal deployed)* will be delivered at the same time. Partner 6 mentioned that it is important that all web traffic is directed to the new WeNMR site, including the addresses of the previous eNMR website. From there, a link to the old pages will be supplied. It was discussed that the current CCPN wiki data has to be transferred to the new WeNMR wiki. Partner 8 is asked to research if there is a technical solution to do this, otherwise the data will have to be transferred manual by the individual partners.

For *MS4 (Web services roadmap defined)* it was discussed that the portal for the different services should be similar in terms of use, both in respect of looks and ease of use. Especially the login procedure was discussed, as a single username and password for all portals would be preferable for users, although this involves getting a GRID certificate for all users.

Partner 1 mentioned that in addition to these deliverables and milestones, two *workshops* have to be organized. It was suggested that one of the workshops should be organized as a satellite meeting to a technical forum. Because that might be not the right audience and the workshop might attracted few attendees then, partner 1 and partner 8 suggested that at the technical forum only an announcement (presentation in a VRC session) and display of WeNMR is done and two separate workshops are organized. Partner 1 suggested that one is held in Vilnius and one is linked to either a meeting in Frankfurt or the European CCPN meeting, as suggested by partner 6. Partner 2 mentioned that in 2012 one meeting is linked to an EAST-NMR meeting. Partner 1 emphasized that WeNMR should be represented at all of these meetings, with at least a presentation or a demo. Partner 2 mentioned that the quality of the workshops should be at the same level as the EMBL NMR workshops. It is agreed that the target number of participants in the workshops should be 20-24. It is also suggested that a specific topic for the workshops is chosen. Partner 8 indicated the intention to organize a workshop for 24 participants November 2011 in Vilnius, based on the eNMR workshops.

Partner 1 discussed the number of web portals that are available and that their number should be expanded as part of WeNMR, including both NMR and SAXS services. Partner 2 mentioned that the coordinator can make a list of suggested additions and partner 7 suggested that it would be good to also ask the users on the website what additions they would like to see added. Some suggestions were made on which current services might be implemented in the GRID (UNIO, ARIA, RECORD, MECHANA). The coordinator asked all partners to send suggestions and ask around, also in the other communities, for input.

Partner 5 asked if a *to-do list* can be added to the minutes. Partner 1 said it will be made and will be send as a separate document to all partners.

12.12: The meeting was closed by the coordinator, Alexandre Bonvin.

Timeline We-NMR Nov 1, 2010 – June 1, 2011

| Number | Name | WP | Lead beneficiary | Month | Date due | Comment | Current status |
|--------|--|----|------------------|-------|----------|---|---|
| D1.1 | Consortium Agreement | 1 | BCBR / NL | 1 | 1-dec-10 | O - CO | <input checked="" type="checkbox"/> Done, will be distributed at kickoff meeting. |
| D1.2 | Minutes of the kick-off meeting | 1 | BCBR / NL | 2 | 1-jan-11 | R - PU | |
| D1.3 | eNMR fact sheet defining the baseline for WeNMR | 1 | BCBR / NL | 2 | 1-jan-11 | R - PU | |
| D1.4.1 | Quarterly progress report (QR1) | 1 | BCBR / NL | 4 | 1-mrt-11 | R - PU | |
| D2.1 | Sustainability plan from local sites regarding Grid computational infrastructure | 2 | BMRZ / DE | 6 | 1-mei-11 | R - PU | |
| D4.1.1 | Periodic report on the operation of the GRID and of the WeNMR Gateway | 4 | CIRMMP / IT | 6 | 1-mei-11 | R - PU | |
| MS1 | Joint NMR-SAXS workshop | 3 | RUNMC / NL | 6 | 1-mei-11 | Programme on web portal and D3.1 | |
| MS2 | Wiki operational | 3 | RUNMC / NL | 6 | 1-mei-11 | Services available on web portal | |
| MS3 | Initial version of the VRC web portal deployed | 6 | SPRONKNMR / LI | 6 | 1-mei-11 | VRC available and accessible | |
| MS4 | Web services roadmap defined | 7 | EMBL / DE | 6 | 1-mei-11 | Access protocol description published on web portal | |
| D1.4.2 | Quarterly progress report (QR2) | 1 | BCBR / NL | 7 | 1-jun-11 | R - PU | |