Deliverable 1.5

Training of bio-NMR users

INFRA-2007-1.2.2 - Deployment of eInfrastructures for scientific communities

Grant agreement for: **Combination of Collaborative projects & Coordination and support actions**

Proposal/Contract no.: 213010 – **e-nmr**

Project full title: Deploying and unifying the NMR e-Infrastructure in System Biology

Project coordinator: Prof. Dr. Harald Schwalbe

Project website: http://www.enmr.eu/

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Introduction

In addition to outreach activities to the bio-NMR community (and beyond), which are described in deliverables D1.7 (month 24) and D1.8 (month 36), the planning of the e-NMR project included the provision of specific training events aimed at making bio-NMR users not only aware of but also able to use the tools provided by e-NMR.

Specifically, the training events that have been organized focused on two main themes:

a. the use of the e-NMR portal
b. what is the grid and what are electronic certificates

Point b has been of particular importance because grid infrastructures and their mechanisms of function are generally not known to the majority of the users of the European bio-NMR facilities, who typically have a chemist/biochemist/biologist background. In addition, bio-NMRists are typically unfamiliar with electronic certificates, which are not required for the use of the overwhelming majority of the web-based services that are available to the community.

In order to be able to successfully convince the community that the e-NMR services would represent a leap forward in their routine practice, the training events were scheduled in the second half of the project. This allowed the e-NMR portal to be developed and tested thoroughly, with the main aim of making the users' experience as seamless as possible, while guaranteeing high computational efficiency and a very flexible approach to the use of the various programs in order to satisfy both novice and advanced users. At the time of preparation of this report, three main events have taken place already and a fourth has been scheduled (Table 1).

Title/subject of the event	Date	Location	Attendance	Web site
Joint East-NMR / eNMR conference	15th-17th June 2009	Florence (IT)	70	www.cerm.unifi.it/home/other/StructuringEuropeanNMR.html
NMR Software Workshop	4th–5th November 2009	Hinxton (UK)	22	http://www.ebi.ac.uk/pdbe/docs/NMR/workshop200911/main.html
NMR structure calculation - GRID applications and integrated tools	7th-11th June 2010	Vilnius (LT)	10	http://training.spronknmr.eu/index.php?mact=Workshops,cntnt01,frontend_category_items,0&cntnt01category_id=1&cntnt01returnid=68

Title/subject of the event	Date	Location	Attendance	Web site
NMR structure calculation - GRID applications and integrated tools	4th-8th October 2010	Vilnius (LT)	n.a.	http://training.spronknmr.eu/index.php?mact=Workshops,cntnt01,frontend_category_items,0&cntnt01category_id=1&cntnt01returnid=68

Table 1. e-NMR training events. The attendance does not include project partners/collaborators.

Several actions of Table 1 have been organized in conjunction with other European initiatives such as EC-funded RTD or Transnational access projects, in order to help to reach a wider audience. In addition to the aforementioned specific events, other meetings provided occasions for training of the users, including the annual meetings of the users of the bio-NMR facilities and other large NMR meetings. In these occasions, a booth has been installed to provide a venue for potential as well as current e-NMR users to interact with the e-NMR staff and explore the services of the project's web portal. The meetings where e-NMR have been presented are reported in deliverables D1.7 and D1.8.

The initiatives of Table 1 are described in some detail in the sections below.

Joint East-NMR / eNMR conference (Florence, June 2009)

The Joint East-NMR / eNMR conference of June 2009 provided a venue to target the users of the bio-NMR Infrastructures providing access within the EAST-NMR project; the latter is a transnational access initiative with a distinct focus on New Member States. The meeting also involved also the participation of two distinguished scientists from the e-Science community, Dr. Matyska and Dr. Breton.

Three training sessions were organized, making use of two separate computer rooms at the University of Florence. Each training session involved six to eight trainers in two separate computer rooms, to ensure a sufficiently high trainers:trainees ratio (1:4-6) as well as the availability of a computer to each trainee. Each trainee received information on using the grid and using the eNMR portal in two different sessions, and was allowed a third session to solve possible doubts. Users were also allowed to submit example data to the portal and run calculations. This was the first training event that was built around the current uniform design

of the e-NMR portal, whereas previous demonstrations involved non-standardized web servers independently developed by the various partners.

NMR Software Workshop (Hinxton, November 2009)

This event was organized together with the CCPN annual meeting, and focused especially on British users, even though it was open to participants from all countries. CCPN is an initiative for the bio-NMR community based in the United Kingdom and was involved in the EC-funded project Extend-NMR, which has developed innovative software programs for NMR data analysis. The organization of the workshop was curated by the PDBe, which is one of the founding members of the world wide PDB. The aim of the training event was to give to NMR users hands-on experience with various NMR software tools. The attendance to the workshop comprised 22 participants, which the organizers unanimously judged to be a very good number to allow close interactions between the teachers and the trainees.

In order to start developing a model in which users' training could generate revenues to the project, a small fee was asked to the participants. The main result of the fee was practically to select only participants that were truly interested in the workshop. It is to be noted that whereas for the e-NMR project this was only the second training event organized, CCPN had already a long tradition of organizing workshops for their users (including potential new users). A survey among the participants carried out at the end of the workshop highlighted that the event had been very well received and that the participants had a very high perception of the usefulness of the e-NMR portal for their research (with nearly 90% of the participants stating that they were most likely or sure to make use of the eNMR portal in the future, and 70% of the participants either having or being in the process of getting a Grid certificate). Opportunities for improvement of the presentations were also indicated. The results of the survey are appended to this document.

NMR structure calculation - GRID applications and integrated tools (Vilnius, June 2010)

This workshop has been organized by the e-NMR consortium with additional contributions from Extend-NMR and CCPN as an advanced workshop on biomolecular structure calculations. The main goal of the workshop was to introduce participants into widely applied and state-of-the-art structure calculation techniques and software packages. The topics and

softwares covered provide the tools for the majority of computational biomolecular NMR applications, such as structure calculation, refinement and validation, as well as macromolecular docking. Most of the covered software packages are currently available from the e-NMR portal, or are in the process of being integrated in it.

The program of the workshop has been designed carefully, with a practical and comprehensive approach that introduce and train participants in the various topics. Further, a logical order of topics is used that can be commonly applied in real NMR research projects. In summary, the program covers:

- Introduction to the eNMR Grid
- Introduction to protein structure determination
- Visualization and analysis of protein NMR spectra and structures: ***CcpNmr Analysis***
- Structure calculation: ***CYANA; TALOS+; CS-ROSETTA***
- Structure refinement: ***Yasara; AMBER***
- Structure validation: ***CING***
- Macromolecular docking: ***HADDOCK***
- Integrated tools: ***Extend-NMR***

Note that the topic “Visualization and analysis of protein NMR spectra and structures” is not comprised in the portfolio of planned e-NMR applications as it involves extensive real-time interactions with the user in a complex graphics environment. Each of the topics was presented by highly skilled lecturers that are either authors of the softwares or directly connected to the development thereof. For optimal knowledge transfer combinations are used of lectures, live demos, video demos and well worked out exercises that were designed to prepare the participants to apply their knowledge in practice to their own projects.

The workshop, already in its current form, can be of great value for the structural biology community. There is a great need in the community for high level practical training in applied methods, and this is what the workshop is designed for. Unique features of the workshop are the well-worked out and streamlined program, the professional training environment, which has been outsourced to a small company, the practical handles for participants’ projects and the constant updating and improving of the program to include new softwares and updates thereof. In addition, the organization of the workshop in the Lithuania will aid in promoting

structural biology and NMR in the New Member States of the EU, which are goals of upcoming EU projects (BioNMR, WeNMR).
The workshop has been designed to be the first of a series of workshops, of which a second one will be held within the lifetime of the -NMR project, while further events will take place within the FP7 WeNMR project (with a planned 2 times per year availability).
A survey has been carried out at the end of the workshop, whose results are appended to this documents.

Final remarks

The achievements described in the above sections clearly indicate that the training activities of the e-NMR project towards the bio-NMR community have been growing significantly since their inception. This is true both of the quality of the organization of the activities themselves and of level and comprehensiveness of the topics tackled (including the training materials made available to the participants). In parallel, the growth of the services provided through the e-NMR portal has allowed new aspects of the typical workflow of an NMR lab to be included in the training. As a result, the impact on the attendees is generally extremely positive, thus boosting the positive perception of the e-NMR activities within the community.
In addition, the e-NMR partnership has worked to develop a model of training workshop that can be provided in the future on a fee basis. It appears that the workshop series held in Vilnius, organized by the SpronkNMR subcontractor, have the potential indeed fulfill this aim, which could constitute a reasonable means to generate revenues to sustain e-NMR in the future.

Annex 1.

The joint e-NMR/CCPN workshop was organised by the PDBe on the 4th and 5th of November 2009 to give NMR users hands-on experience with NMR software developed as part of several European based projects: e-NMR, the Collaborative Computational Project for NMR (CCPN) and Extend-NMR. These projects are aimed at making software more accessible for the user, especially those who do not have the computational (or human) resources to run demanding software locally.

The registration information page is available from:

http://www.ebi.ac.uk/training/workshops/nmr_041109.html

A post-workshop resource web page is also available:

http://www.ebi.ac.uk/pdbe/docs/NMR/workshop200911/main.html

The participants.

Figure 1 shows the current position of the respondents. In addition there are 2 Masters level students that replied. In total 18 out of the 22 workshop participants responded.

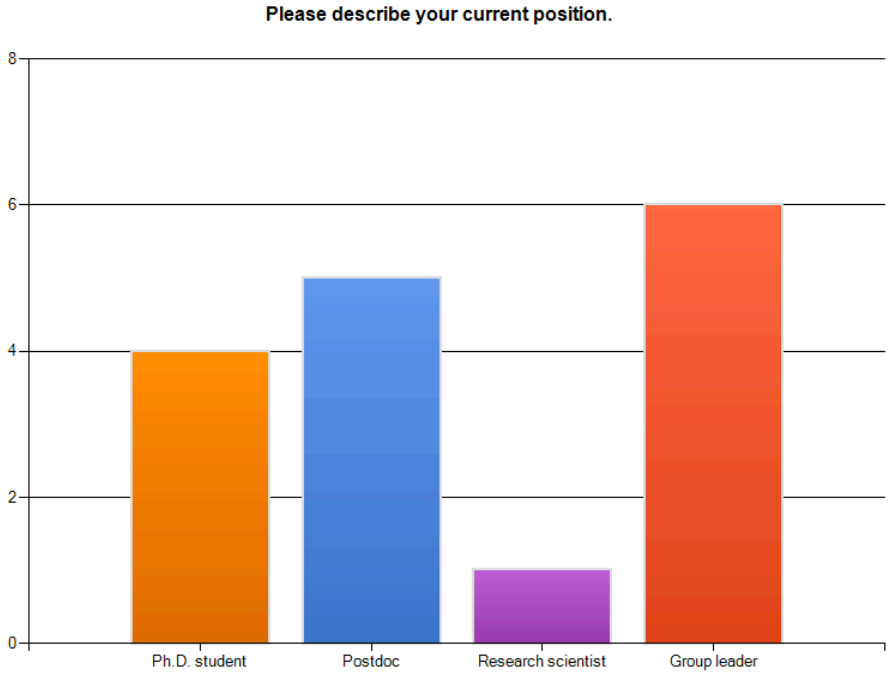

Figure 1: Current position of participants

Figure 2 shows the knowledge level of the participants in the areas of Experimental NMR, Computational NMR and General computer use.

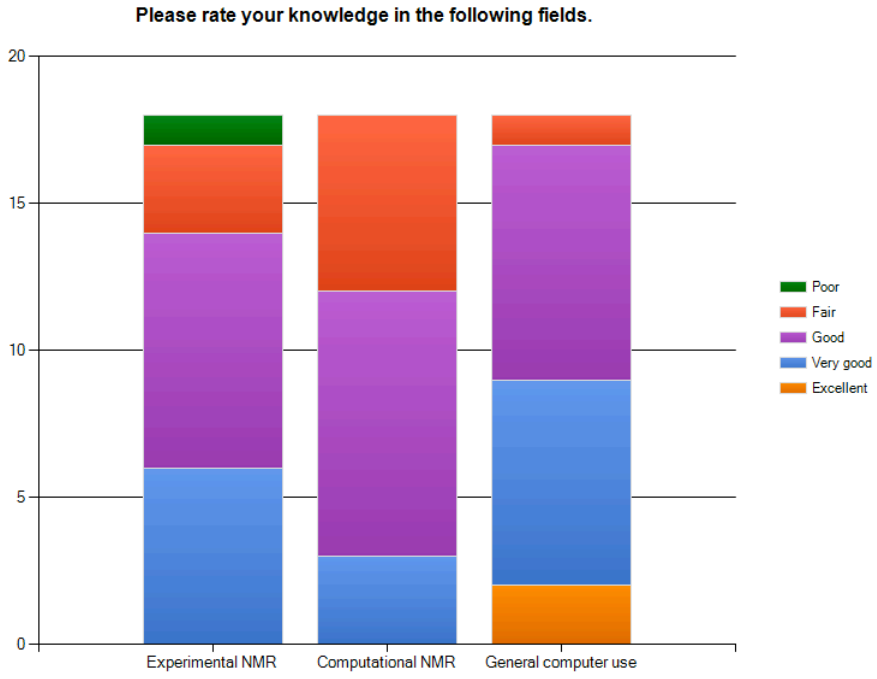

Figure 2: Knowledge level of participants in three key areas.

Overall the participants thus already had a Ph.D. and had good knowledge of NMR and computers.

The e-NMR project

The first day of the workshop started with a workshop introduction, followed by an introduction to the e-NMR project and demonstrations of the e-NMR web portals. Figure 3 shows how the participants assessed the presentations of this first workshop day, Figure 4 how they rated the demonstrators and materials presented.

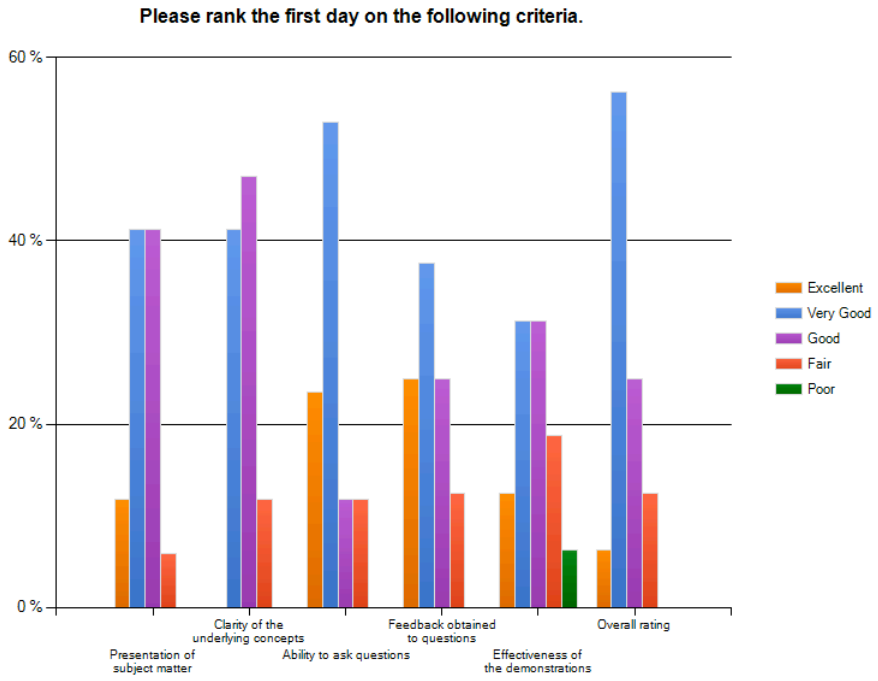

Figure 3: Participant assessment of first day.

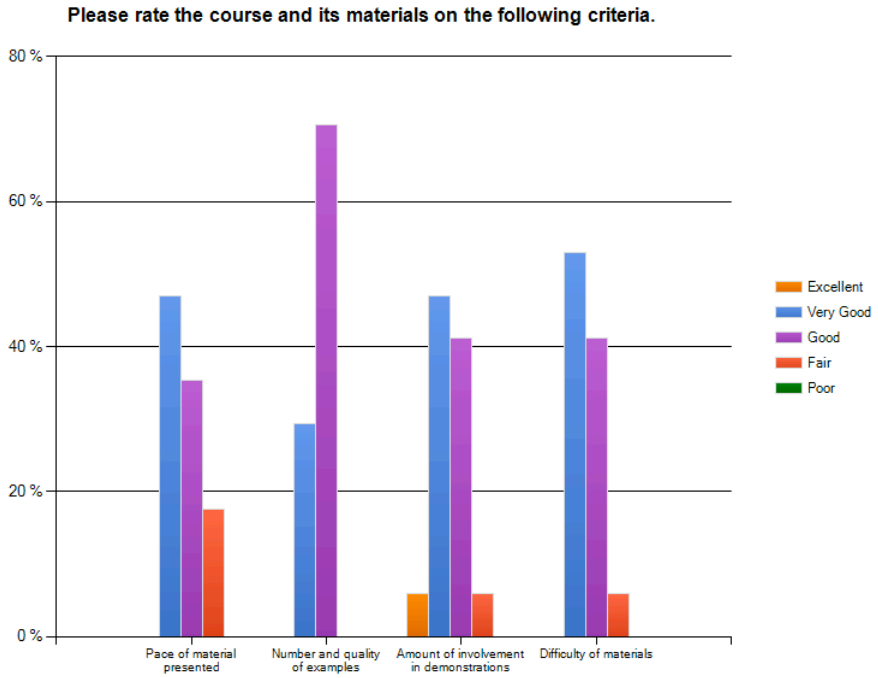

Figure 4: Participant assessment of workshop material on the first day.

Overall, the participants thus thought the presentations and material to be good to very good, with especially the ability to ask questions and the feedback obtained ranked high. The effectiveness of the demonstrations and the pace of the material was ranked lower. The participants were also asked whether they felt like they learned how to use the tools, and whether they are planning to use them in the future (Figure 5).

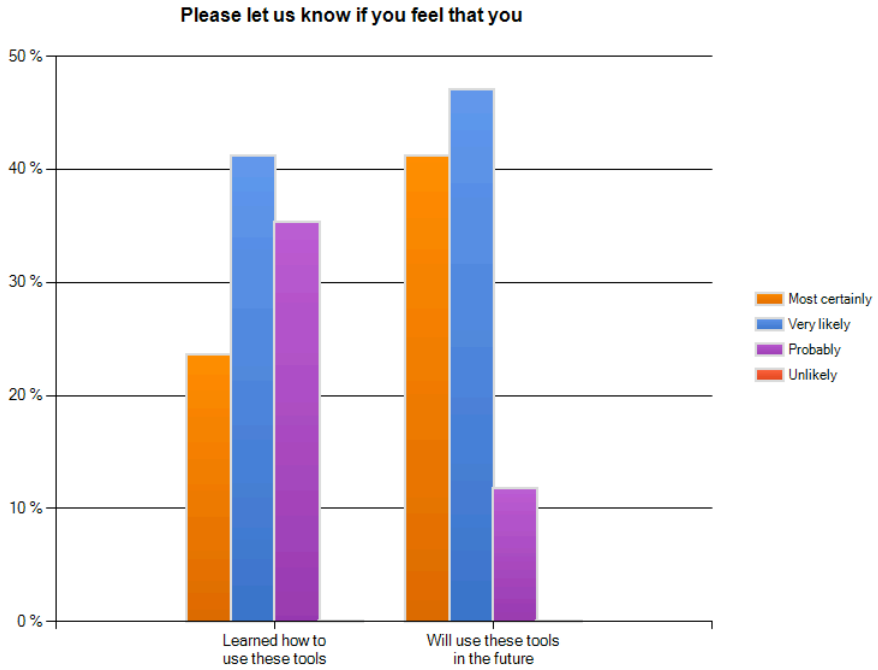

Figure 5: Participant assessment of workshop tool elucidation, and future prospect for tool usage.

The participants were thus mostly convinced that the e-NMR tools will be useful for them, and that they learnedhow to use them. Finally, there was an option to leave open text comments about this day. The full results are available in appendix I. In summary, the software specific comments were (in brackets the number of participants that made a specific point, also note that these comments were compiled from the day-specific open questions only):

CYANA	Practical part too fast (2)
	Not clear whether tutor knew learners were able to follow (1)
FormatConverter	One of better ones of the day (1)
HADDOCK	One of better ones of the day (1)
	Software covered twice, was plenty on first day, merge in the future (3)
MDD	Practical part too fast (1)
	Not clear whether tutor knew learners were able to follow (1)
XPLOR-NIH	Difficult to follow, no audience participation (2)
	Pseudocontacts too specialist (1)

Annex 2.NMR structure calculation - GRID applications and integrated tools

The workshop „NMR structure calculation - GRID applications and integrated tools“ is a workshop organized and sponsored by the e-NMR consortium with additional support from Extend-NMR.
The workshop covers theory and practical aspects of state of the art NMR structure calculation techniques that are currently employed on the e-NMR webportal. The participants will first be introduced to the eNMR GRID, followed by introductions and practical applications of programs such as CYANA, CING, HADDOCK and CcpNmr Analysis. Several computationally intensive procedures will be run on the eNMR GRID. In addition, the workshop includes an introduction to the integrated software pipeline Extend-NMR.

Vilnius, June 7-11, 2010

Lecturers & Trainers:

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Ezgi Karaca	ezzgikaraca@gmail.com
Chris Spronk	chris@spronknmr.eu

Survey results

1. The workshop.

The e-NMR / CCPN workshop was organised by Spronk NMR Consultancy on June 7-11, 2010 to give NMR users hands-on experience with NMR software developed as part of the e-NMR project and the Collaborative Computational Project for NMR (CCPN). These projects are aimed at making software more accessible for the user, especially those who do not have the computational (or human) resources to run demanding software locally.

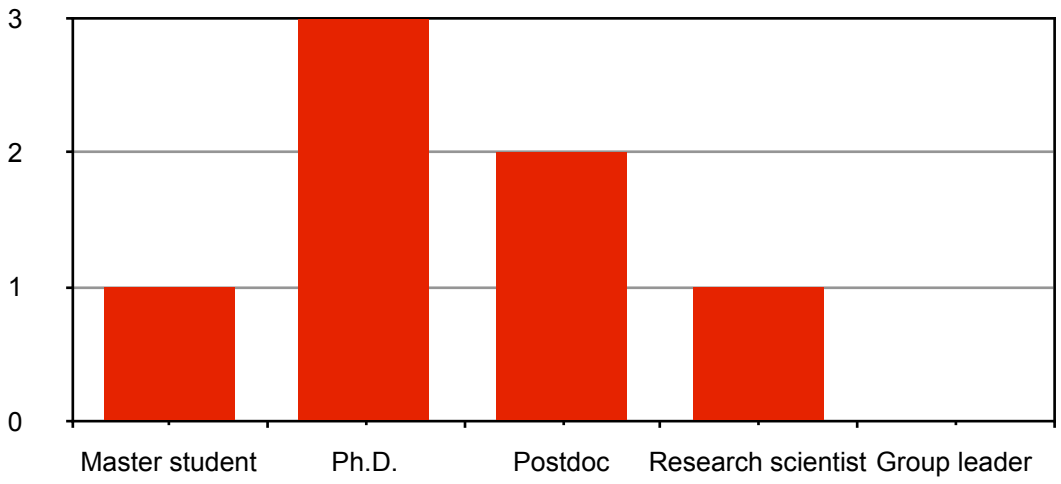
The registration information page is available from:

http://training.spronknmr.eu/index.php?mact=Workshops,cntnt01,frontend_category_items,0&cntnt01category_id=1&cntnt01returnid=68
and advertised on:
http://www.enmr.eu/eNMR-news-events

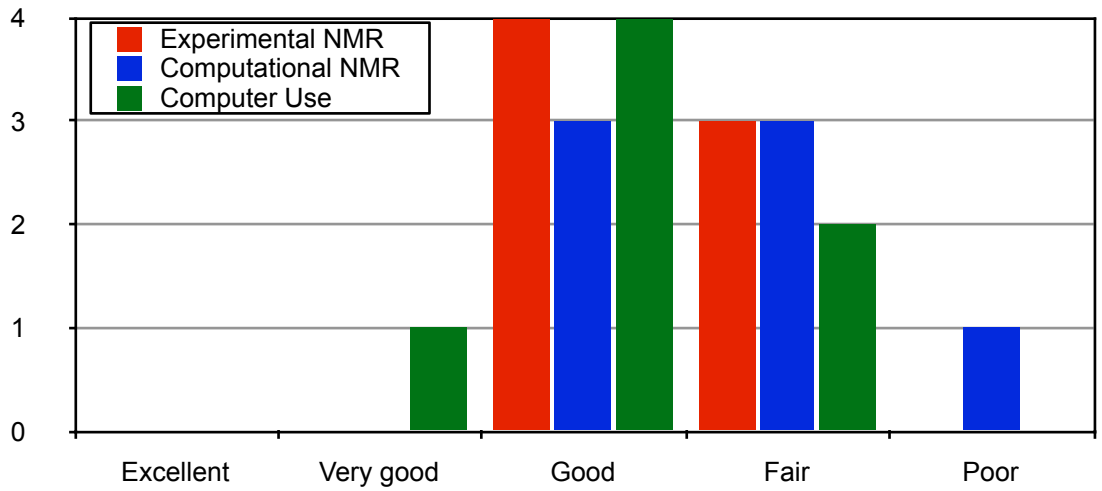
All participants were asked to fill in a survey at the end of the workshop.

2. Results of the survey.

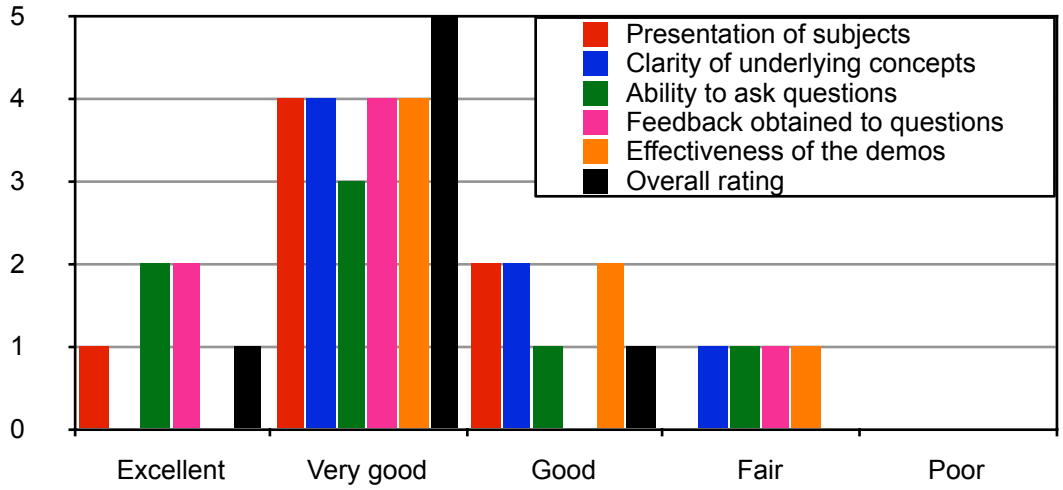
1. The figure below shows the current position of the workshop participants that responded (7 out of 10). Most of the participants were Ph.D. or Postdoc, there was one Master student and one participant came from industry.



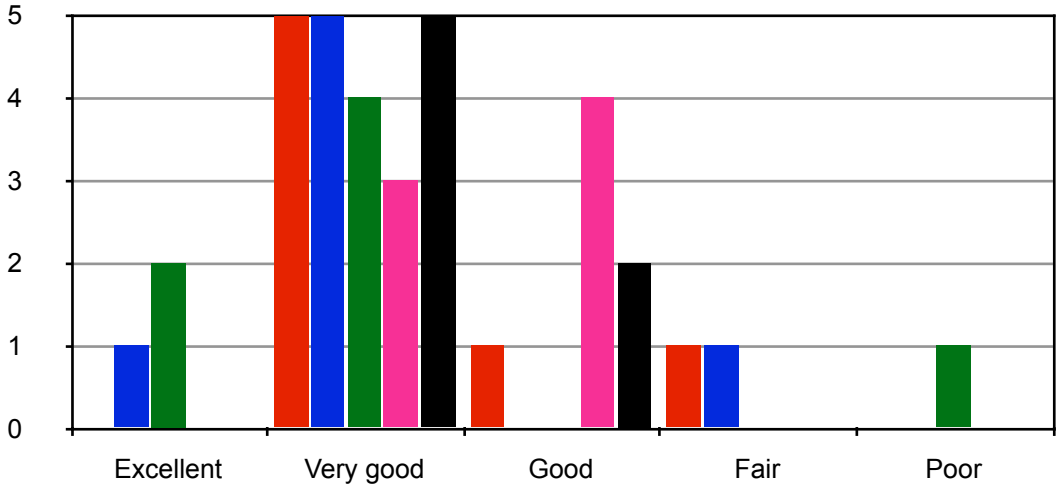
2. The participants were asked about the background knowledge level in the areas of experimental NMR, computational NMR and general computer use. Overall the pre-knowledge level of the participants was fairly good.



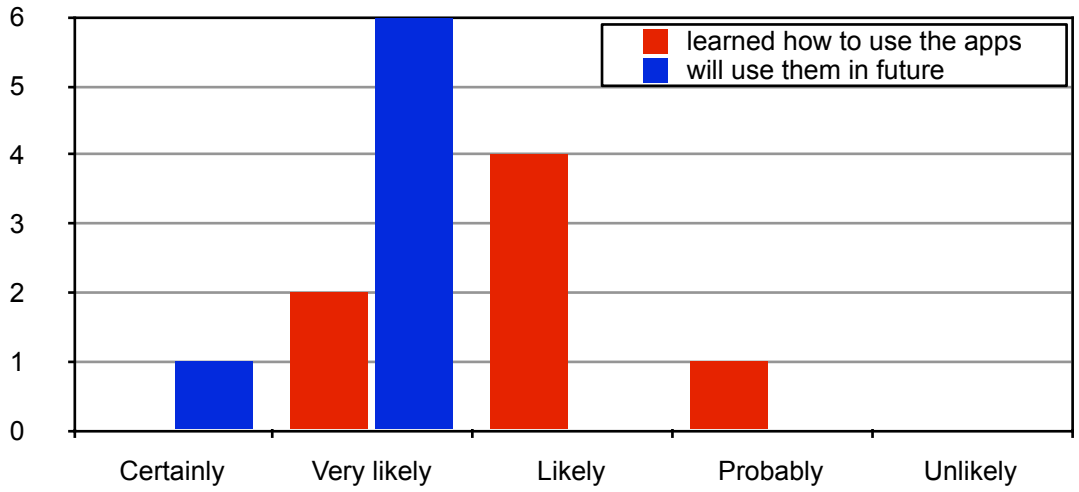
3. The perception of the workshop was evaluated; like the quality and clarity of the presentations and the concepts, as well as the ability to ask questions, the feedback, and the effectiveness of the demonstrations. Overall the perception of the workshop was evaluated to be very good by the participants.



4. Also the course material was rated. Overall the pace, number, quality and amount of involvement was evaluated very good. The difficulty level was generally rated good to very good.



5. It was asked if the participants felt that they learned how to use the presented applications and if they plan to use them in future. All participants were planning to use (some of) the presented applications in the future and had a good feeling about their knowledge of how to use the software after the workshop.



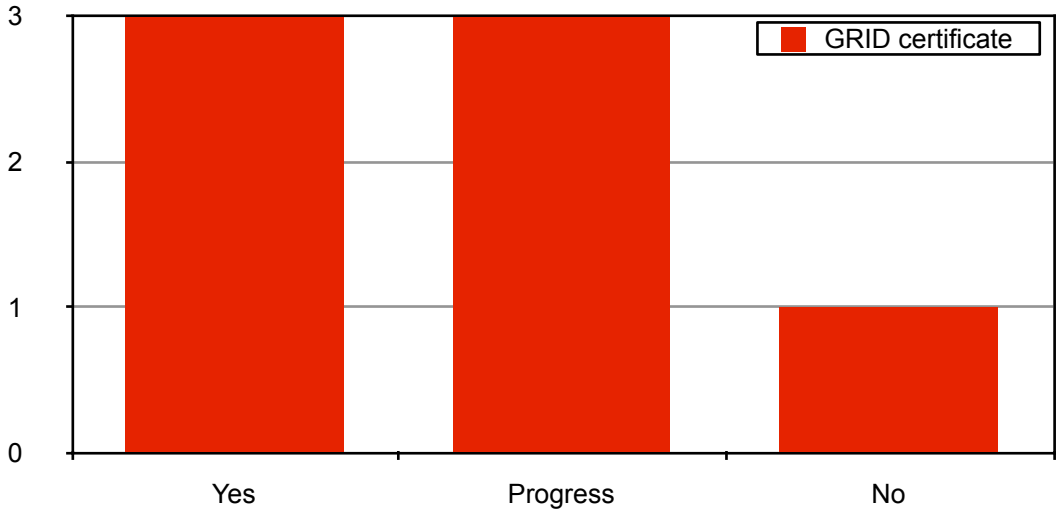
6. The participants were asked to write down their comments concerning the demonstrations. The collected and summarized answers:

- (1) Excellent that the outcome and results were shown and discussed after the practicals.
- (2) CING and HADDOCK were clear, interesting and stimulating, and logical about what should be done and seen as result. (1) Highly involved practicals helped very much in understanding the topics and how to use it (and awareness of problems).
- (1) CING was very detailed.
- (1) HADDOCK: good introduction, well design and covered quite a lot of interesting features.
- (2) CCPN analysis is fine and very well structured.
- CCPN clearly needs more than one day to get a grip on it.
- (1) Extend-NMR was less organized.
- (1) CYANA was very stimulating, but more details could be added (for example to modify restraint output to obtain better restraint lists).
- (1) Demo video's were very useful (should probably be made for more subjects).
- (1) Would have been useful to have the slides beforehand.

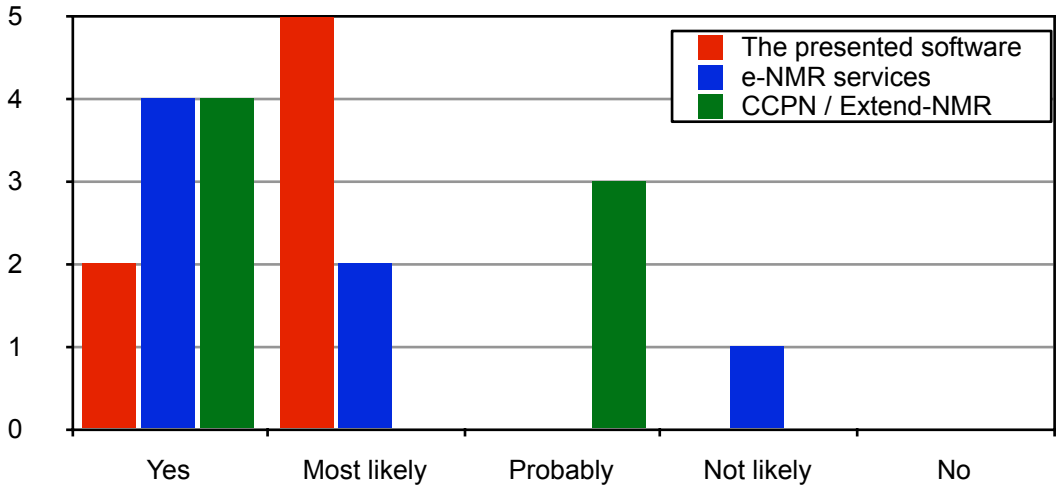
7. The participants were asked which software they already use:

- (3) CYANA
- (1) TALOS
- (4) CCPN
- (1) CING
- (1) HADDOCK
- (2) TALOS+
- (1) CS-Rosetta

8. There was much interest in obtaining GRID certificates for the e-NMR project and quite some participants already possessed one. One new certificate request was directly handled at the workshop.



9. The participants were asked for a second time if they expect to use the software in future. Many expect to use the e-NMR services (webportals) and most expect also to use the CCPN / Extend-NMR software (see question 7, also 4 people are already using the CCPN package), though quite some participants still have doubts.



10. What the participants liked most about the workshop:

- (3) Easy interaction and accessibility of all the experts who gave contributions like lectures and practicals during and after the course.
- (1) The cover of a broad introduction to the topic
- (1) Demonstrations, Practicals
- (1) Experts were teaching excellent (presentations on their subject)
- (1) Because of the small number of people, it was easier to ask questions

- (2) Some questions about using some programs were solved hands-on and in private conversation.

11. What the participants liked least about the workshop:

- (1) Large amount of information (especially for the ones unexperienced in the field)
- (1) Less information about dealing with incomplete assignment or improve restraint lists
- (1) Best time for brainstorming would be in winter (to cold to think about anything else, but the course) - Now it was too nice outside to be really concentrated.
- (2) Sometimes to many programs and to much input at once, maybe one week is too short time to get good practice in all the programs (like Yasara). (Might get too motivated with these many programs to start using them, but too little knowledge about the individual ones)
- (1) Not a fan of CCPN, but it was nice to see and learn some of the functions that has been impossible to find on my own.
- (1) Nothing!

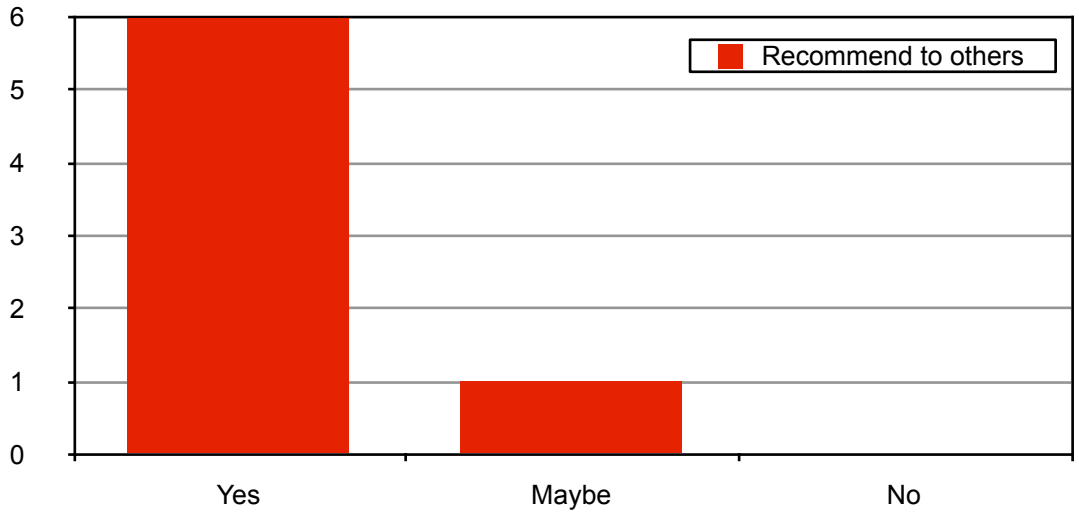
12. How the workshop could be improved:

- (1) Already well done and probably difficult to improve much.
- (2) A good idea not to increase (too much) the number of participants (although that would increase the number of people introduced to the grid, it may lower the level of accessibility to the experts)
- (3) Provide more information to the participants on topics, material and program beforehand that will be discussed in the course (so that not everything is new if you never used the program)
- (1) More linking between the topics and speakers
- (1) Encourage people to bring their own dataset.
- (1) Maybe to concentrate on fewer topics
- (1) Every topic should have a clear message and a manual specifically for this course (so not just practical notes and presentations; CING and CCPN analysis were close to ideal)

13. What did the participants think of the overall format of the workshop:

- (4) 5 days seems a good balance and was optimal for the intensive workshop (with practicals and expert talks) (too many expert talks would have been hard to keep concentrated)
- (1) More specialized courses and use of programs (the course content seems little broad, not enough time to go deep(er) into the different subjects)
- (1) Quality of the talks was very high; only the presentation on CCPN was a bit too fast and confusing; not always clear what was the point of the discussion.
- (1) A bit more time for private questions would be good (like on the 2nd part of friday)
- (1) More days to go in-depth.
- (1) Some programs might have needed more in-depth treatment (Yasara, CYANA).
- (1) Underline the important steps to remember.
- (1) Just nice for me.

14. It was asked if the participants would recommend the workshop to others. The large majority (6 out of 7 participants) answered 'yes'.



15. The accommodation was:

- (2) Perfect, Great
- (2) Very nice hotel, fine service, comfortable rooms
- (4) Fine, no complaints
- (1) A coffee after lunch would be nice before starting the lecture again
- (1) Choice of food was sometimes questionable