





e-nmr  e-NMR Annual Meeting  
Padova, 4 November 2008 

**WP1**  
**Monitoring, Standardisation and Outreach**

CIRMMP

[www.e-nmr.eu](http://www.e-nmr.eu)

e-NMR (RI-213010) is funded by the European Commission under the Research Infrastructure Programme



e-nmr  **Outline** 

- WP1 Mandate
- Tasks
- Milestones & Deliverables
- Conclusions

[www.e-nmr.eu](http://www.e-nmr.eu)

e-NMR (RI-213010) is funded by the European Commission under the Research Infrastructure Programme

2



e-nmr  **WP1 Mandate** 

- **Objective 1 (O1.1):** "Organization of a community-wide critical assessment of NMR computational approaches"
- **Objective 2 (O2.1):** "Study, design and adoption of policies accepted by all the partners, regarding the shared use of e-NMR. Policies will be discussed at relevant international e-science forums"
- **Objective 3 (O3.1):** "establish adequate support and dissemination mechanisms for the e-NMR infrastructure, provide training and promote the dissemination of good computational practices in bio-NMR"

[www.e-nmr.eu](http://www.e-nmr.eu)

e-NMR (RI-213010) is funded by the European Commission under the Research Infrastructure Programme

3

e-nmr  **WP1 Mandate- Measures of success** 

- **Measures of success:**
  1. Number and periodicity of assessment events
  2. Connections with other e-science projects
  3. Number of spreading and training activities

[www.e-nmr.eu](http://www.e-nmr.eu)

e-NMR (RI-213010) is funded by the European Commission under the Research Infrastructure Programme

4

e-nmr **WP1 tasks**

- Start date: PM0
- Duration: 36 Months
- WP leader: CIRMMMP
- Tasks:
  - **T1.1** Assessment of the state-of-the art in computational aspects of bio-NMR and establishment of software, protocols and data storage standards
  - **T1.2** Establish tight connections between e-science and bio-NMR communities
  - **T1.3** Spreading and training, both within the partnership and within the bio-NMR user community

Part.	BMZ	CIRMMMP	BCBR	INFN
PMs	12	14+2	12+6	18

[www.e-nmr.eu](http://www.e-nmr.eu)

e-NMR (RI-213010) is funded by the European Commission under the Research Infrastructure Programme

e-nmr **T1.1: Assessment of the state-of-the art**

- The first assessment event will take place in Florence, May 2009
- The following research teams will be involved (divided by topic)
  - **Automated structure calculations**
    - NOE-based**  
Guentert  
Herrmann  
Montelione  
Nilges
    - Chemical shift-based**  
Bax  
Vendruscolo  
Wishart
    - Other**  
Linás/Laue (NOE, CLOUDS)  
Blackledge (rdc)  
Zweckstetter (rdc)
  - Automated resonance assignment**  
Guentert  
Herrmann  
Laue  
Montelione  
Zweckstetter

[www.e-nmr.eu](http://www.e-nmr.eu)

e-NMR (RI-213010) is funded by the European Commission under the Research Infrastructure Programme

e-nmr **T1.1: Assessment of the state-of-the art**

- The groups will be provided with common data sets (NMR spectra) for the evaluations of performance
- The data sets will be provided by the NMR partners from published data
- A web-based data warehouse has been developed to facilitate exchange of the above data (D1.1)

[www.e-nmr.eu](http://www.e-nmr.eu)


e-NMR (RI-213010) is funded by the European Commission under the Research Infrastructure Programme

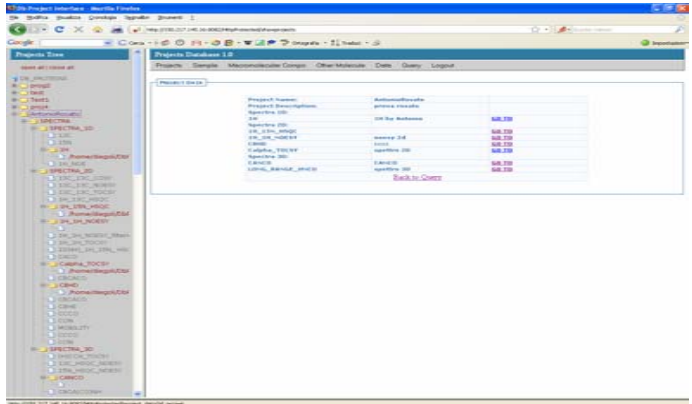
e-nmr **D1.1: e-NMR database model**

Public document describing the model @ [www.enmr.eu](http://www.enmr.eu)  
Compatible with available data sets

[www.e-nmr.eu](http://www.e-nmr.eu)

e-NMR (RI-213010) is funded by the European Commission under the Research Infrastructure Programme


e-nmr **D1.1: e-NMR database interface** 

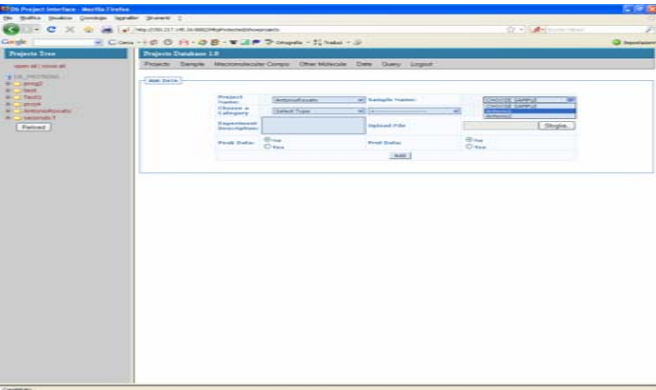


[www.e-nmr.eu](http://www.e-nmr.eu)

e-NMR (RI-213010) is funded by the European Commission under the Research Infrastructure Programme

9


e-nmr **D1.1: e-NMR database interface** 

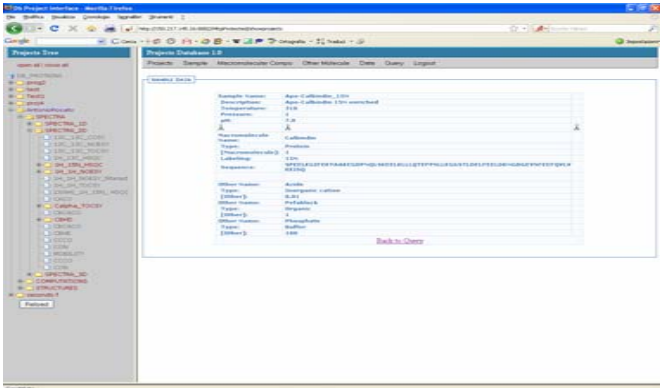


[www.e-nmr.eu](http://www.e-nmr.eu)

e-NMR (RI-213010) is funded by the European Commission under the Research Infrastructure Programme

10


e-nmr **D1.1: e-NMR database interface** 



[www.e-nmr.eu](http://www.e-nmr.eu)

e-NMR (RI-213010) is funded by the European Commission under the Research Infrastructure Programme

11


e-nmr **T1.2: Establish tight connections between e-science and bio-NMR communities** 

- **October 2008**
  - Signed Memorandum of Understanding with the Belief-II project
    - Presence at eConcertation events
    - Collaboration to the Digital Library (DL)
    - Contribution to the e-Infrastructures News Magazine

[www.e-nmr.eu](http://www.e-nmr.eu)

e-NMR (RI-213010) is funded by the European Commission under the Research Infrastructure Programme


12

e-nmr **T1.2: Establish tight connections between e-science and bio-NMR communities** 

- Close contacts are in place with various bio-NMR oriented European projects
  - NMR-Life (Coordination Action)
  - EU-NMR (Integrated Infrastructure Initiative)
    - eNMR presentation at the annual users' meeting
  - Extend-NMR (STREP)

[www.e-nmr.eu](http://www.e-nmr.eu)

e-NMR (RI-213010) is funded by the European Commission under the Research Infrastructure Programme 13


e-nmr **T1.3: Spreading and training, both within the partnership and within the bio-NMR user community** 

*Some recent examples of spreading activities*

- Joint NMR-Life and Extend-NMR meeting "New approaches to biomolecular structure determination" Hubertusstock, Berlin, October 27-29, 2008
- Presentation at BMRB, September 2008
- "Live" demonstration at the NMR-Life satellite meeting of the 23rd ICMRBS, August 24, 2008
- EMBO course "Multidimensional NMR in Structural Biology". Il Ciocco, Castelvecchio Pascoli, Italy, August 3-8, 2008

[www.e-nmr.eu](http://www.e-nmr.eu)

e-NMR (RI-213010) is funded by the European Commission under the Research Infrastructure Programme 14


e-nmr **T1.3: Spreading and training, both within the partnership and within the bio-NMR user community** 

*Partnership training activities*

- The first e-NMR gLite Training for grid administrators was held in Firenze, 17-18/1/2008. A theoretical presentation of the various gLite grid elements was followed by the practical deployment of remote CEs at BMRZ and BCBR sites.
- INFN co-organised the Biomed Grid School in Varenna, Italy, 12-16/5/2008.
- A meeting for e-NMR software development was held in Firenze, 14-15/4/2008. The first software packages were deployed at all sites.
- INFN is organising in Trieste, Italy, a Training for Grid Site Administrators, 24-28/11/2008, and a Training for Grid Application Developers, 29-12/12/2008, registrations are open until 10th of October at the above links.

[www.e-nmr.eu](http://www.e-nmr.eu)

e-NMR (RI-213010) is funded by the European Commission under the Research Infrastructure Programme 15

e-nmr **Milestones** 

- **M1.1: First assessment of the state-of-the-art (M 15) – public report**

[www.e-nmr.eu](http://www.e-nmr.eu)

e-NMR (RI-213010) is funded by the European Commission under the Research Infrastructure Programme 16



- **D1.1 e-NMR database model (month 9)**
- **D1.2 Test data sets: complete sets of raw and interpreted NMR data made for software development and testing (month 15)**
- **D1.3 Assessment of state-of-the-art: first workshop for assessing the state-of-the art in computational aspects of bio-NMR (month 18)**
- **D1.4 Assessment of state-of-the-art: second workshop for assessing the state-of-the art in computational aspects of bio-NMR (month 30)**
- **D1.5 Training of bio-NMR users: training sessions for bio-NMR users at the yearly meeting of the EU-NMR large facility and global evaluation of all training activities performed (month 33)**

[www.e-nmr.eu](http://www.e-nmr.eu)



- The partners have been trained on both site administration issues and software deployment specifically for the eNMR project. Newly enrolled units receive training on the occasion of events organized by INFN.
- Contacts with other projects in the field of bio-NMR as well as in the field of eScience have been made and formalized
- The project database model has been defined and an interface to the data warehouse is available
- The organization of the first assessment event is under way

[www.e-nmr.eu](http://www.e-nmr.eu)