



# A Worldwide e-Infrastructure for NMR and structural biology

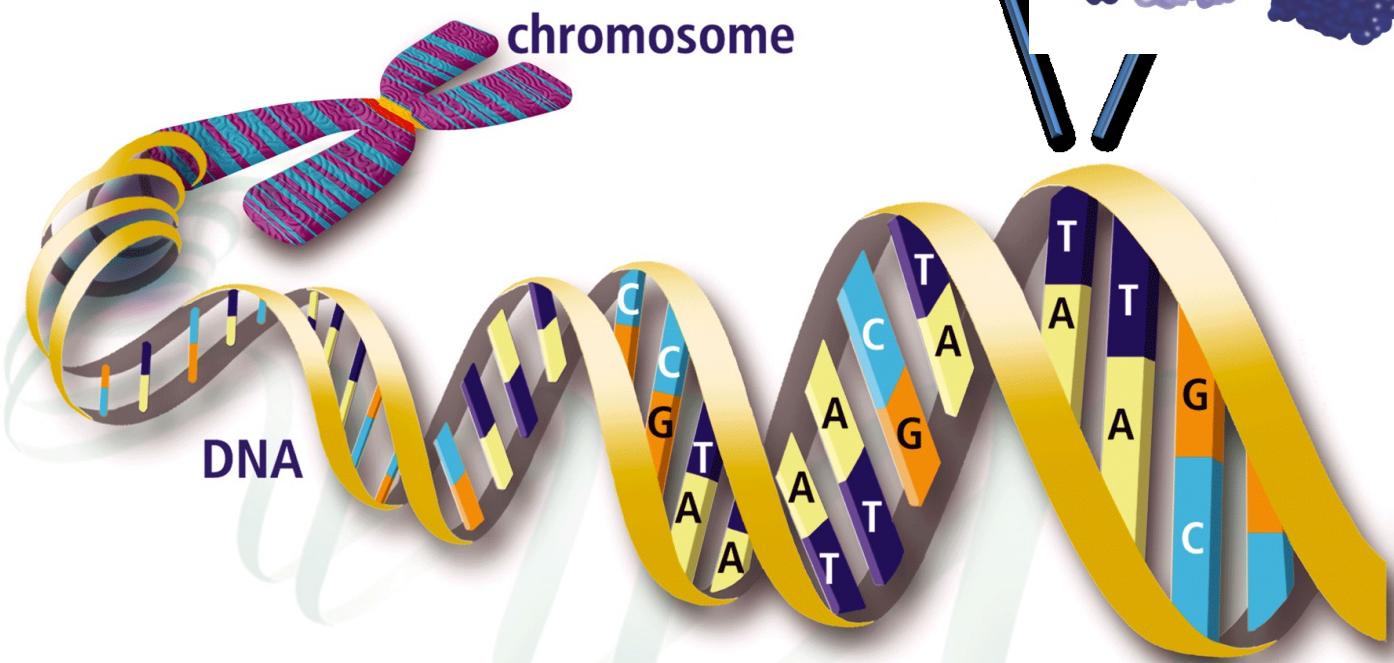
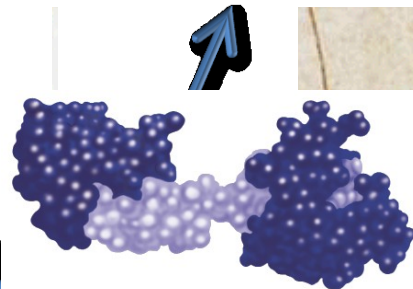
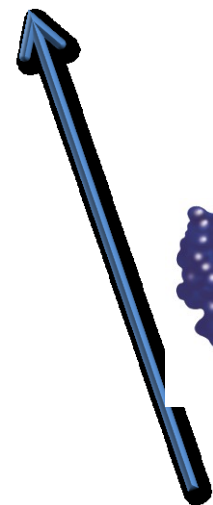
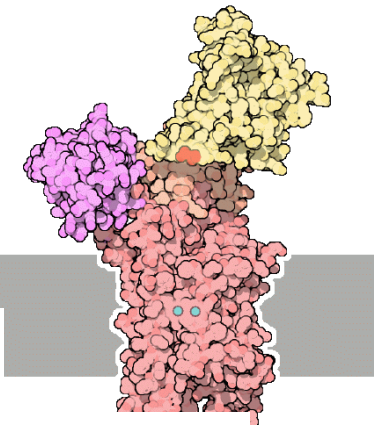
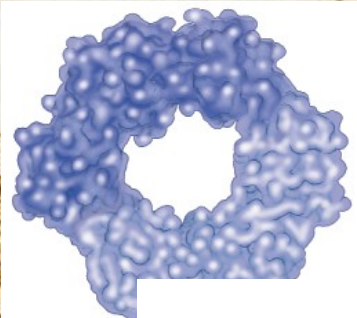
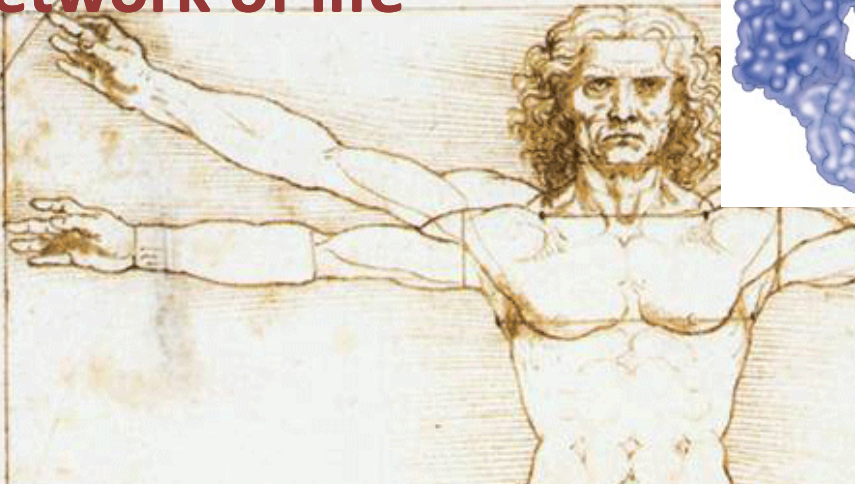
Contract n°: RI-261572  
Project type: CP-CSA  
Duration: 36 months  
Total budget: 2'434'000 €  
EC Funding: 2'150'000 €

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## Project participants:

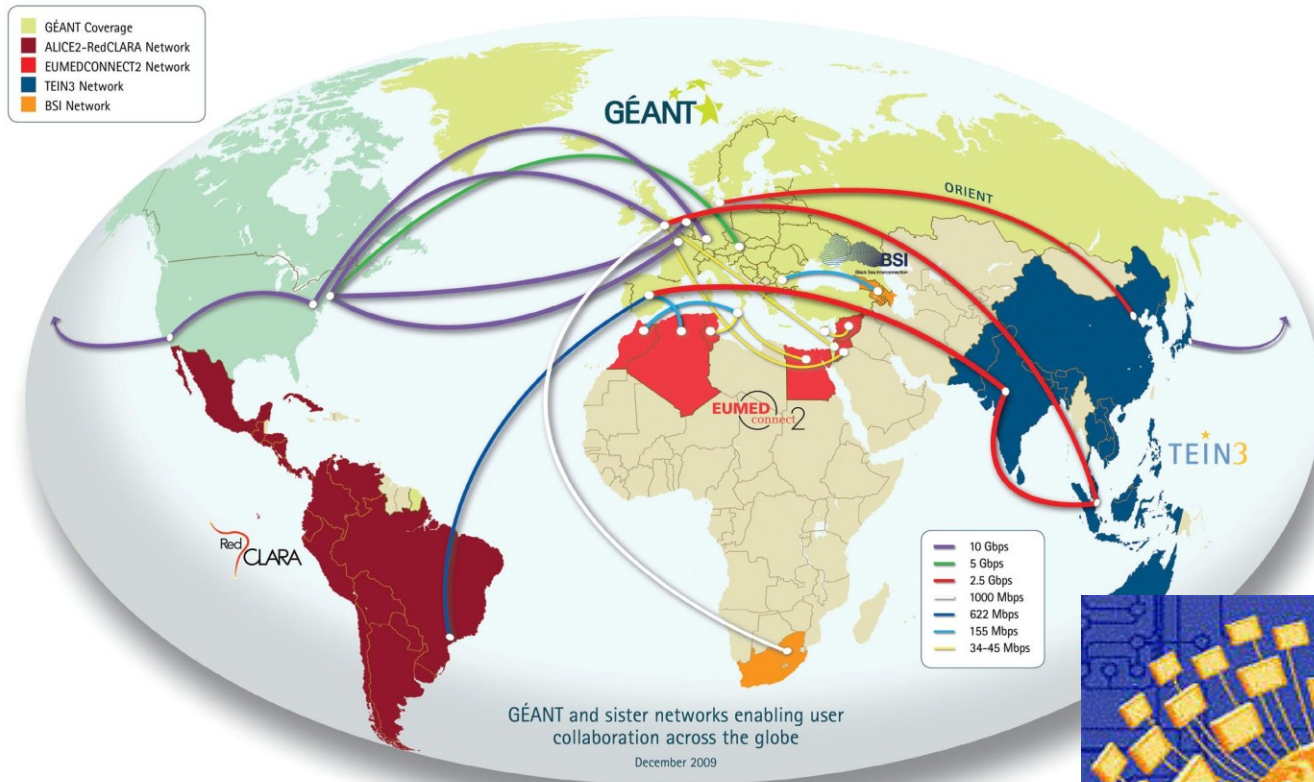
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# The molecular machines and network of life



# The network of science...

## GÉANT At the Heart of Global Research Networking



connect • communicate • collaborate

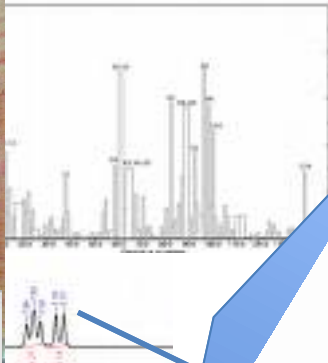


**GRID resources**

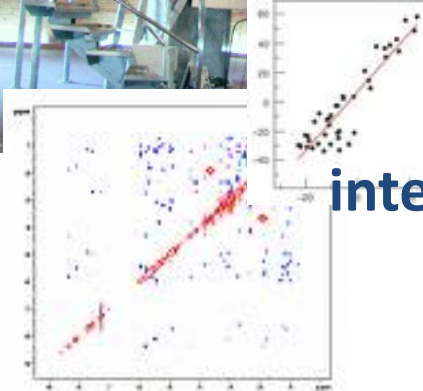


# Exploiting GRID resources in structural biology...

NMR data collection and processing



Data interpretation



SAXS data analysis

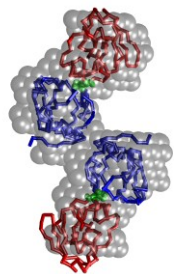
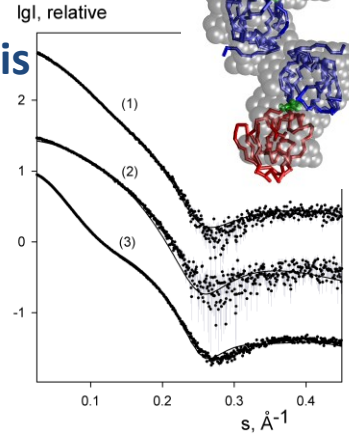


Table 2.3: Hydrogen Bonding (

| Donor | Acceptor | Pair    | Dist |
|-------|----------|---------|------|
| H1N   | -        | Val19 O |      |
| H2N   | -        | Val19 O |      |
| H3N   | -        | Leu21 O |      |
| H4N   | -        | Leu21 O |      |
| H5N   | -        | Leu21 O |      |
| H6N   | -        | Leu21 O |      |
| H7N   | -        | Val40 O |      |
| H8N   | -        | Val40 O |      |

| Residue | B-factor |
|---------|----------|
| 652     | -6.92    |
| 653     | -6.10    |
| 654     | -10.37   |
| 655     | -6.02    |
| 656     | -9.85    |
| 657     | -2.70    |
| 658     | -10.03   |
| 659     | -5.12    |
| 660     | -9.12    |

|      |   |
|------|---|
| 760  | 0 |
| 752  | 0 |
| 2257 | 0 |
| 2587 | 0 |
| 2257 | 0 |
| 2259 | 0 |
| 2587 | 0 |
| 2257 | 0 |
| 2259 | 0 |

Computations

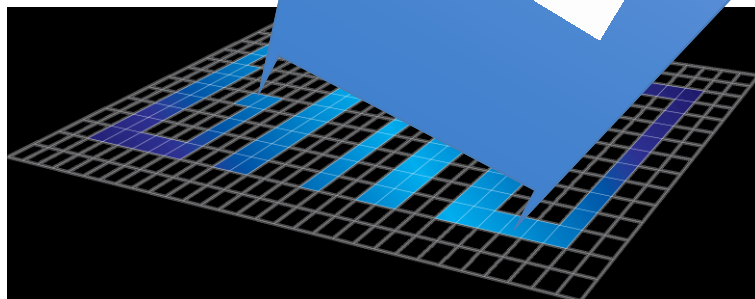


Molecular NMR

Structure, dynamics & interactions

→ impact on research and health:

- origin of disease
- design of new experiments
- drug design...



# wE-nmr **Main objectives**

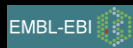
- Operate and further develop a user-friendly **e-Science gateway for the NMR and SAXS communities**
- Establish a **virtual research platform** for (interaction with) the user community
- **Provide support** to software developers, users and other e-Infrastructure projects
- **Foster the adoption and use of e-Infrastructure** in a wide range of flanking disciplines within the life sciences
- **Operate and consolidate the eNMR Grid infrastructure** and to extend it to interoperate with other **worldwide Grid initiatives**
- Develop a model to ensure **sustainability** of the project



## eNMR platform operational and well used!

- 2<sup>nd</sup> largest VO in the life sciences
- Over 225 registered users and growing
- >16000 CPUs
- >350 CPU years over the last 12 months
- 20% of Life Sciences on the Grid
- User-friendly access to e-Infrastructure via web portals

[www.enmr.eu](http://www.enmr.eu)







# User-friendly access to Grid resources via web portal



**e-NMR**  
NMR computational infrastructure

[Home](#)
[HADDOCK](#)
[Xplor-NIH](#)
[AMBER](#)
[CYANA](#)
[CS-ROSETTA](#)
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[eNMR-Grid](#)
[eNMR Wiki](#)

WELCOME TO THE E-NMR WEB PORTAL >>

PROFILE >>

e-NMR aims at deploying and unifying the NMR computational infrastructure in system biology, a project funded under the 7th framework program of the European Union (Contract no. 213010 - e-NMR).

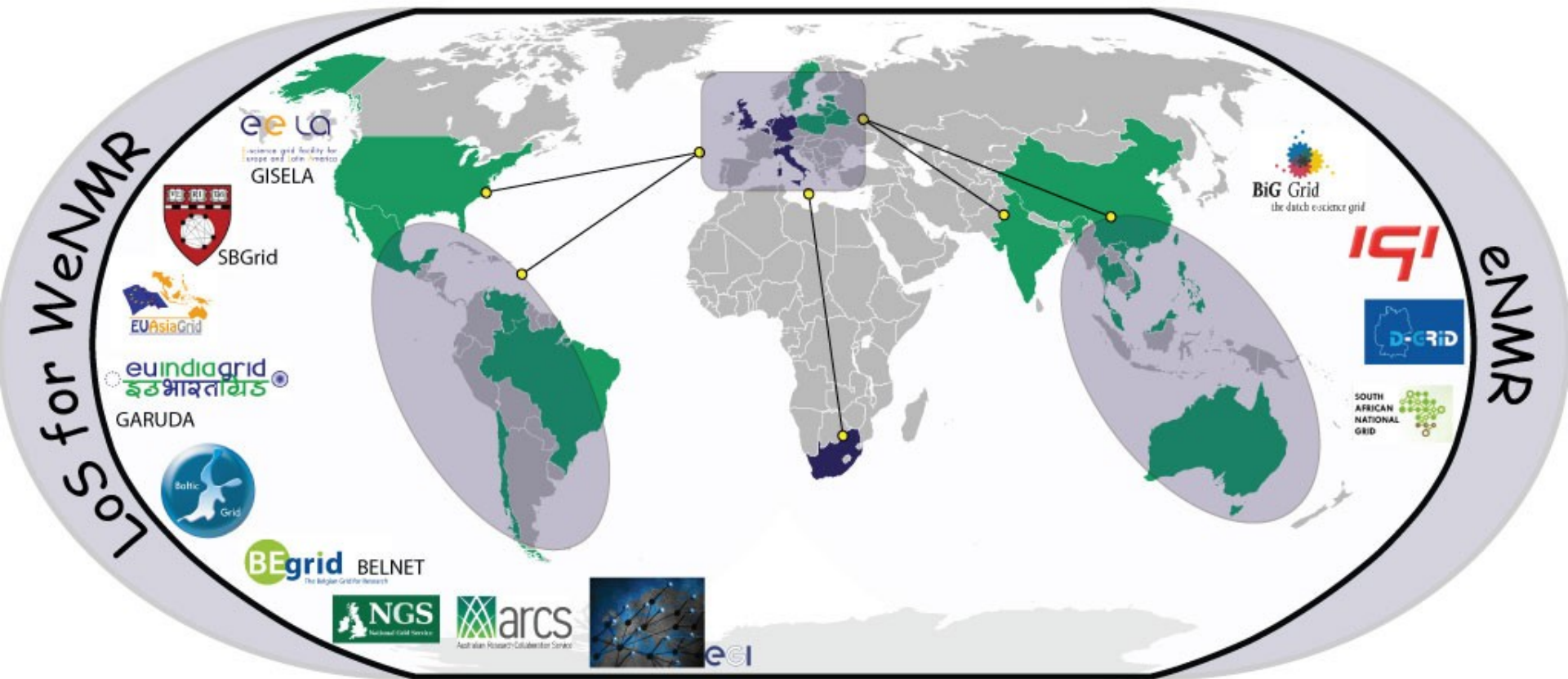
NMR plays an important role in life sciences (biomolecular NMR), and structural biology in particular, at both European and international levels. Our main objective is to optimize and extend the use of the NMR Research Infrastructures of EU-NMR through the implementation of an e-Infrastructure in order to provide the biomolecular NMR user community with a platform integrating and streamlining the computational approaches necessary for NMR data analysis and structural modelling (e-NMR).




<http://www.enmr.eu/webportal>



# A global virtual research community



we-nmr

