

# we-nmr

## A worldwide e-Infrastructure for NMR and structural biology

### ! Introduction

Structural biology and life sciences in general, and NMR and SAXS in particular, have always been associated with advanced computing. The current challenges in the post-genomic era call for virtual research platforms that provide the worldwide research community with both user-friendly tools, platforms for data analysis and exchange, and an underlying e-Infrastructure.

### Virtual Community

WeNMR groups different research teams into a worldwide Virtual Research Community (VRC). The VRC represents the largest Virtual Organizations (VO) in the life sciences and the first one officially recognized by the EGI. To serve its various communities, from the general public to experienced users and software developers, WeNMR operates a VRC portal, [www.wenmr.eu](http://www.wenmr.eu), that offers a variety of services, information channels and communication tools.

### Science in the cloud

The WeNMR Virtual Research Community provides a variety of services such as:

- Documentation services: tutorials, use cases, wikis
- Support services: help center, forums
- Consulting services: workshops, technology transfer
- Communication services: blogs, forums, video conferencing

Visit the VRC @ <http://www.wenmr.eu>



#### Processing MDD NMR

#### Connecting GRIDS

Connect with: Asian, South-African, South-American (GISELA) and North-American GRID initiatives in close contact with existing EC projects (like CHAIN) and EGI and PRACE initiatives.

#### Workflow Format Converter CcpNMR Analysis

#### Analysis TALOS+ AnisoFIT ShiftX2

#### Assignment Auto Assign MARS UNIO

#### Structure Calculation CS-ROSETTA CYANA UNIO Xplor-NIH

#### Molecular Dynamics AMBER GROMACS Antechamber

#### Molecular Modelling 3D-DART HADDOCK

#### Statistics

As of November 2011

- Largest VO in Life Sciences
- >350 VO registered users
- 40 Countries
- >25 Sites
- >35000 CPU Cores
- >65 TB Storage

### Collaborations

As a recognized Virtual Research Organization, WeNMR is tightly interacting with the EGI and various other related European projects, such as the European Middleware Initiative, eScienceTalk, Erina+, Gisela, EUMED Grid, SBGrid, EMI and CHAIN, in order to facilitate and support its operation and continuing expansion.

### WeNMR Objectives

- Develop a sustainable, user-friendly science gateway for the NMR and SAXS communities.
- Establish a VRC and support adoption of e-Infrastructures by a wide range of flanking disciplines within the Life Sciences.
- Provide support to software developers, users and other e-Infrastructure projects in a knowledge and training centre.
- Extend the eNMR Grid infrastructure to interoperate with other worldwide Grid initiatives.

### How to benefit?

- Sign up for a free account at the WeNMR Virtual Research Community and benefit from:
  - A portal to exchange ideas, read documentation, follow tutorials, request support and contribute to various forums
- To perform calculations on the GRID using the web-based applications you must request a GRID certificate
- For more information visit: [www.wenmr.eu](http://www.wenmr.eu)