

Structural biology applications within WeNMR

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WeNMR is both a three years project funded under the European Commission's 7th Framework Programme (e-Infrastructure RI-261571) and a Virtual Research Community supported by EGI. WeNMR aims at bringing together research teams in structural biology into a virtual research community at a worldwide level and provide them with a platform integrating and streamlining the computational approaches necessary for NMR and SAXS data analysis and structural modelling. The WeNMR Virtual Research Community (VRC) provides access to the services, a knowledge base, help center and various information and (social) communication channels. Access to the services is provided through easy-to-use web interfaces using the computational resources provided by the grid through the eNMR Virtual Organization (VO).

In this contribution, we will present an overview of the WeNMR services as well as of the WeNMR VRC implementation and features. A relatively detailed demonstration will be given of the portals available for NMR-based protein structure calculation and refinement with molecular dynamics.

References:

Wassenaar et al. (2012). WeNMR: Structural Biology on the Grid. *J. Grid. Comp.*, 10:743-767. DOI: 10.1007/s10723-012-9246-z

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Session Classification: Scaling up life sciences with grids and clouds - stories and recommendations