

## Building bridges between services and e-infrastructure in structural biology

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Structural biology deals with the characterization of the structural (atomic coordinates) and dynamic (fluctuation of atomic coordinates over time) properties of biological macromolecules and adducts thereof. Since 2010, the WeNMR project has implemented numerous web-based services to facilitate the use of advanced computational tools by researchers in the field, using the grid computational infrastructure provided by EGI [1]. These services have been further developed in subsequent initiatives, such as the MoBrain competence center within EGI-ENGAGE.

Currently, in the context of the West-Life Virtual Research Environment H2020 project [2], we have been working on the integration of different pre-existing services to enable the combined application of tools on the same given dataset. Here we will demonstrate how a user can exploit these integrated services without the need to download partial data, entirely via a browser interface. Examples involve the calculation of protein-protein complexes from nuclear magnetic resonance (NMR) data using the FANTEN web server, followed by the optimization of the initial model using HADDOCK and fitting structures into cryo-EM maps with the PowerFit web server using maps obtained from the Scipion web portal.

In addition, we will show the implementation of a cloud storage solution developed by the West-Life H2020 project [2], called VirtualFolder [3], which allows the user to connect to her/his account on for example B2DROP or on public clouds (e.g. Dropbox). In the future, this will allow users to access datasets acquired in different experimental facilities directly from the web interfaces of the services connected to West-Life.

1. Wassenaar TA, et al. WeNMR: Structural biology on the Grid. *J. Grid. Computing* 10:743-767, 2012
2. <https://www.west-life.eu/>
3. <https://portal.west-life.eu/virtualfolder/>

### Summary

Since 2010, the WeNMR project has implemented numerous web-based services to facilitate the use of advanced computational tools by researchers in structural biology, using the grid computational infrastructure provided by EGI. These services have been further developed in subsequent initiatives, such as the MoBrain competence center within EGI-ENGAGE. In the context of the West-Life Virtual Research Environment H2020 project, we have been working on the integration of different pre-existing services to enable their combined application to the same given dataset. For this purpose, we have built bridges between web portals and with storage infrastructure to allow users to exploit these services and access their data in an integrated manner entirely via a browser interface.

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