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# Portals for the WeNMR Community

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The WeNMR (http://www.wenmr.eu) project is an EU-funded international effort to streamline and automate structure determination from Nuclear Magnetic Resonance (NMR) and small angle X-ray scattering (SAXS) data. Conventionally calculation of structure requires the use of various software, considerable user expertise and vast computational resources. To facilitate the use of NMR spectroscopy in life sciences the eNMR/WeNMR consortium has set out to provide protocolized services through easy-to-use web interfaces, while still retaining sufficient flexibility to handle more specific requests. Thus far, a number of programs often used in Structural Biology have been made available through portals, including HADDOCK, XPLOR-NIH, CYANA, CS-ROSETTA, MARS, MDDNMR and now AMBER and GROMACS. We will present a few of the web-portals and demonstrate that the designed interfaces are as easy as possible for new users who often have limited computational experience, while still providing advanced users with more control over the calculation parameters. The implementation of these services, in particular the distribution of calculations to the Grid, involves a novel mechanism for submission and job handling that is independent of the type of job being run. With currently 330 registered users from all over the world, WeNMR has become the largest Virtual Organization (VO) in life sciences.

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