SEVENTH FRAMEWORK PROGRAMME

Research Infrastructures

Deliverable 6.2

Report on standard protocols and tutorials

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Section 1: Summary of Deliverable

Background

The WeNMR Virtual Research Community website forms the central point of access for the users, developers and contributors that are targeted by the WeNMR project. One of the core sources of information to be provided is a set of standard protocols and tutorials, that will help users of the various portals get started with a good basic understanding of the usage of the tools that they need for doing their research.

Goal

Our goal has been to provide at least one standard protocol per WeNMR service that is being offered from the site by WeNMR partners. A standard protocol is defined as the combination of a tutorial for running GRID calculations with parameter settings for a common case, accompanied with test data. In addition, partners aim to provide additional tutorials, to cover a wide range of situations that users may encounter in practice. In addition to the tutorials and standard protocols provided by WeNMR partners, we encourage and strongly support external contributors of service portals and software to add their tutorials and documentation to the WeNMR site.

Summary

At the end of Month 18 of the project, a total of 24 webportals are up and running, of which 17 are provided by WeNMR partners. 14 of the 17 WeNMR provided portals have at least one tutorial and test data set provided. The total number of tutorials and test data sets for these 14 portals is 43 and 36 (including 20 command line grid use cases), respectively. In addition, other tutorials, test data and command line use cases have been provided for NMR tools that are not (yet) available as service portals, but which provide additional useful information and resources to users of and members of the VRC. The total of tutorials is now over 50, and a total of 41 sets of test data and use cases.

None of the portals provided by external partners so far have tutorials or test data sets associated. However, as these are voluntary contributions, it cannot be demanded of these partners to provide these tutorials. Given their positive attitude towards the project we do expect though that these partners will start providing tutorials and test data in the future.

In summary, WeNMR is well on the way to provide a good foundation for community members to use the WeNMR services effectively.

Section 2: Tutorials and Standard protocols

Detailed tables

Below we have detailed the currently available tutorials and available test data in tables describing the tutorials for service portals contributed by WeNMR partners (Table 1), tutorials for other WeNMR tools (Table 2), and tutorials for portals and tools contributed by external partners (Table 3).

Table 1: Tutorials and test data for WeNMR portals.

Service Portal	*Tutorials*	*Grid command line use cases*	*Test data sets**	*Getting started*	*WIKI*
3D-DART	5	0	5	✓	4
CNS	4	2	2	✓	2
CS-ROSETTA	1	1	1	✓	3
GROMACS	3	1	5	✓	1
HADDOCK	6	0	0	✓	2
Talos	1	1	1	✓	2
Amber	3	0	2	✓	2
AnisoFIT	1	0	1		0
Antechamber	1	0	1		1
Xplor-NIH	2	1	1	✓	2
MaxOCC	2	1	1		1
CYANA	3	6	6	✓	1
MARS	1	1	1	✓	2
MDD	4	6	7	✓	1
UPLABEL	0	0	0		0
CING	2	0	1	✓	2
FormatConverter	4	0	1	✓	2
Total	43	20	36	13	28

*Including grid command line use cases

Table 2: Tutorials and test data for other WeNMR tools.

Tool	*Tutorials*	*Grid command line use cases*	*Test data sets**	*Getting started*	*WIKI*
ALMOST	0	1	1		0
FANDAS	0	0	0	✓	0
GARANT	1	1	1		0
INFIT	1	1	1		0
MAPPER	1	1	1		0
PROSA	1	1	1		0
CcpNmr Analysis	5	n.a.	0	✓	2
Total	9	5	5	2	2

*Including grid command line use cases

Table 3: Tutorials and test data for portals and tools contributed by external partners.

Service Portal	*Tutorials*	*Grid command line use cases*	*Test data sets**	*Getting started*	*WIKI*
PREDITOR	0	0	0		0
RCI	0	0	0		2
SHIFTX2	0	0	0		0
Auto Assign	0	0	0		1
ASDP	0	0	0		1
RPF	0	0	0		0
DisMeta	0	0	0		0
UNIO	0	0	0	✓	2
GeNMR	0	0	0		2
PROSESS	0	0	0		0
ResProx	0	0	0		1
CS23D	0	0	0		2
Total	0	0	0	1	11

*Including grid command line use cases. Shaded in grey are tools that are not yet available as service portals.

Conclusion

The number of webportals and tutorials with test data and grid command line use cases keeps growing, and will increase further with the growing number of portals. Hereby we aim to lay a solid and attractive basis for community members to find information, get practical expertise and to contribute and share their own materials with the WeNMR community. Several external groups have already started adding their portals to the WeNMR site (Herrmann, Lyon, France; Montelione, Rutgers, USA; Wishart, Edmonton, Canada), and we will encourage and support them to start adding tutorials and test data as well.

Finally, the ultimate assessment of the quality of the WeNMR tutorials and test data must come from the feedback of users. Therefore, we recently added the possibility for users and visitors of the website to rate content on its usefulness. However, at this moment we have not received any meaningful statistics or feedback on the quality and usefulness of our tutorials and protocols from community members, and it is too early to make any statements on this part.