SEVENTH FRAMEWORK PROGRAMME

Research Infrastructures

Deliverable 6.4

Report on standard protocols and tutorials

Grant Agreement number:	RI-261572
Project acronym:	WeNMR
Project title:	WeNMR, A worldwide e-Infrastructure for NMR and structural biology
Deliverable type and status	Report – Public
Due Date	May 1st, 2013
Delivery Date	May 2nd, 2013
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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 30 of the project, a total of 28 NMR specific web portals are up and running, of which 19 are provided by WeNMR partners. 15 of the 19 WeNMR provided portals have at least one tutorial and test data set provided. For these 15 portals, a total of 43 tutorials and 36 data sets (including 19 command line grid use cases) are available. 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 grand total of tutorials is now 52, and 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, a large number of NMR specific portals of WeNMR are up and running, and the inclusion of SAXS portals in the near future will further increase the number of portals and attract a broader structural biology community to use the WeNMR services.

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). Please note that the all the portals are NMR specific portals. SAXS portals will be included in the last part of the project.

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	✓	8
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
FANDAS	0	0	0	✓	0
sedNMR	0	0	0		0
Total	43	20	36	13	34

*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	1	1	1		0
GARANT	1	1	1		0
INFIT	1	1	1		0
MAPPER	1	1	1		0
PROSA	1	1	1		0
CcpNmr Analysis	4	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		0
RPF	0	0	0		0
DisMeta	0	0	0		0
UNIO	0	0	0	✓	2
UNIO ShiftInspector	0	0	0		0
GeNMR	0	0	0		2
PROSESS	0	0	0		0
ResProx	0	0	0		2
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 web portals and tutorials with test data and grid command line use cases has further grown compared to the last reporting period, albeit at much lower speed than during the initial phase of the project (as expected). Several external groups have added their portals to the WeNMR site (Herrmann, Lyon, France; Montelione, Rutgers, USA; Wishart, Edmonton, Canada), and we will further encourage and support them and others to add more portals, tutorials and test data.

During the last period of the project the SAXS portals, tutorials and use cases will be made available to the WeNMR structural biology community.

Finally, WeNMR ran a very successful and well-attended workshop at ISCG2013 in Tapei, Taiwan. The lectures were recorded and we are in the process of making those recordings suited for publication on the WeNMR web site. This will add video material to our standard protocol offering.