



SEVENTH FRAMEWORK
PROGRAMME

Research Infrastructures

Deliverable 3.2.2

Periodic report on the use of wiki and surveys



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Section 1: Summary of Deliverable

Summary

At the start of the project, it was envisaged that user involvement in the VRC could be significant part of developing the WeNMR community. As has been reported in the periodic reports and at the WeNMR review meetings, however, the involvement of users in the VRC and the contribution of documentation to the website by users has been very limited. This has led to a paradigm shift in how the documentation for the available tools and services should be provided and an effort has been made by the WeNMR partners over the last period to provide tutorials and documentation for as much of the services as possible.

In this deliverable, an overview of the currently available documentation on the WeNMR site is presented, as well as the user and stakeholder surveys that were held.

Section 2: Wiki, Getting Started and Tutorial usage

Summary

As explained in March 2012 in Deliverable 3.2.1, one of the efforts made to make the information on the WeNMR website more accessible to users was to bring all documentation pages together in the “Wiki” section of the website. That merger was completed just before the delivery of Deliverable 3.2.1 and while the menu structure of the website still allows separate browsing of these sections, they are all part of the same system, are interlinked often and therefore now provide a much more homogenous user experience.

Interestingly, this merger has been accompanied by an significant increase in page views (see below), concomitant with a continued increase in WeNMR users as has been reported in the period report over period 2.

All in all, it is clear that the “Tutorials” as well as the “Getting started” pages on the WeNMR website are an important aspect of the WeNMR service, as they provide starting points for new users and references for usage by more experienced WeNMR users.

In the near future, the website will be moved to the Drupal 7 content management system, With that new website, the Tutorials, Documentation, but also the Help Desk and other sections of the website will be further integrated, such that all relevant information is available directly from the services page, making it easier to browse and which thus should further enhance the usage experience of the WeNMR website.

Analysis of usage of documentation pages

The documentation pages (the combined Wiki and Getting Started sections) contain a total of 73 (compared to 63 in March 2012) pages, which have seen a total of over 52.000 views (compared to 16.000 views in March 2012). The top 10 of the currently most viewed pages:

Page title	Views
The WeNMR web Portals for Structural Biology	1,762
3D-DART User Manual	1,631
VO registration troubleshooting	1,631
Getting started with CcpNmr format converter	1,570
Getting started with AMBER	1,450
Getting started with MDD NMR	1,414
HADDOCK scriptorium - chemical shift scoring	1,406
Getting started with HADDOCK	1,351
Introduction to Biomolecular NMR spectroscopy and WeNMR	1,293
Getting started with CYANA	1,292

A table with the views of all pages in this section of the VRC can be found in the supplementary information 1 at the end of this deliverable.

This set of most viewed pages contains important information about how the VRC is used by its visitors. The fact that the two main introductory pages on the VRC are among the most viewed pages (including the top one), seem to show that new users are visiting those pages first to get an introduction to the project. The other pages largely correspond to the getting started pages of the most used web portals of the VRC.

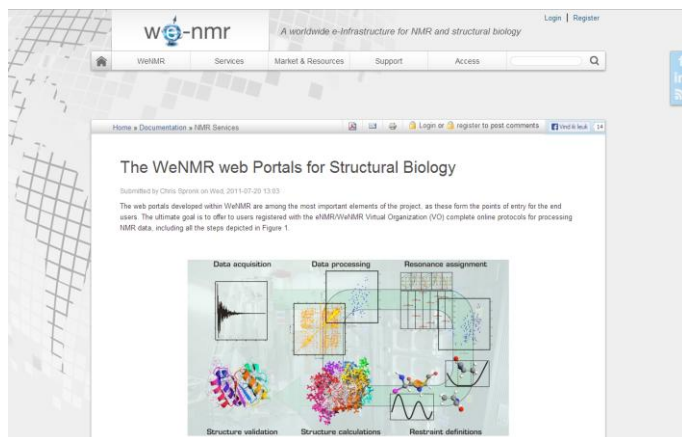


Figure: The WeNMR web Portals for Structural Biology page.

Analysis of usage of Tutorial pages

The Tutorial section contains a total of 60 pages (compared to 51 in March 2012), which have seen a total of over 42.000 views (compared to 14.000 views in March 2012). The top 10 of the currently most viewed pages:

Page title	Views
MD simulations using the GROMACS web server	3099
HADDOCK web server tutorial	2399
CS-ROSETTA web server tutorial	2084
MaxOCC usecase	1798
Generating the Necessary Restraint Files for running HADDOCK Manually	1606
Using and contributing to the WeNMR VRC	1365
Quick gLite Middleware Deployment HOW-TO for WeNMR	1323
Structure refinement using Restrained Molecular Dynamics (RMD) with the AMBER package	1175
Xplor-NIH use case with a User Interface	1046
Restrained Molecular Dynamics (RMD) refinement of structures including RDC's	1023

A table with the views of all pages in this section of the VRC can be found in the supplementary information 2 at the end of this deliverable.

Among the top viewed tutorials are those corresponding to the top portals that have the most number of active users or generate the most number of grid jobs (as was presented in the 1st and 2nd periodic reports) and thus seem to be very popular among the WeNMR community.

As expected the list now includes the tutorial for the CS-ROSETTA, which was added about a year ago and which, due to the high popularity of the web portal is already ranking as the third most viewed tutorial in the list, despite having been added later to the VRC than most others (see also D3.2.1).

Section 3: Surveys

Summary

To be able to monitor the needs and issues of users and other stakeholders when using the WeNMR VRC and services, there have been three surveys, one dedicated for concerns regarding the security of the Grid usage, one directed at Industry, and one general user survey.

The results of the user survey were mentioned already in D3.2.1 and are also available on the WeNMR website (<http://www.wenmr.eu/wenmr/wenmr-user-survey-2011>).

As was also reported to the EU in a letter about the lack of interest from industry in WeNMR products, on May 1st, 2013, WeNMR targeted the industrial structural biology user community with survey to collect more feedback, but the final number of responses was relatively poor (despite initially receiving some responses as reported in D3.2.1) and indicative for the general lack of interest from industry the project has seen.

The same was true for the survey on security of the Grid usage, which also had an emphasis on industrial usage, where we envisaged security to be one of the main issues. Remarkably, the responses we did receive indicated that the current security measures in place (so-called hydra encryption services), together with the provision of a simple method for secure access, would largely satisfy security concerns of potential industrial users.

Supplementary information 1: Wiki / Getting Started page usage

This is the full list of usage of all Getting Started and Wiki pages, as of May 15, 2013. The current status is available at: <http://www.wenmr.eu/wenmr/all-documentation-articles>

Page Title	Categories	Created	Last editing activity	Views
The WeNMR web Portals for Structural Biology	NMR Services, Grid Services	7/20/2011 13:03	1 year 43 weeks ago	1,762
3D-DART User Manual	3D-DART	3/14/2011 21:19	1 year 10 weeks ago	1,631
VO registration troubleshooting	enmr.eu VO, grid, personal certificate, Registration, web browser	3/16/2011 15:20	8 weeks 5 days ago	1,631
Getting started with CcpNmr format converter	FormatConverter	7/20/2011 12:14	1 year 6 weeks ago	1,570
Getting started with AMBER	Amber	7/20/2011 12:17	1 year 11 weeks ago	1,450
Getting started with MDD NMR	MDD	7/20/2011 10:54	1 year 43 weeks ago	1,414
HADDOCK scriptorium - chemical shift scoring	analysis, chemical shifts, Haddock, HADDOCK, scoring	6/6/2012 14:20	12 weeks 6 hours ago	1,406
Getting started with HADDOCK	HADDOCK	7/20/2011 10:15	1 year 43 weeks ago	1,351
Introduction to Biomolecular NMR spectroscopy and WeNMR	About NMR	7/20/2011 12:36	1 year 43 weeks ago	1,293
Getting started with CYANA	CYANA	7/20/2011 10:32	1 year 38 weeks ago	1,292
Getting started with GROMACS	GROMACS	12/7/2011 16:47	6 weeks 3 days ago	1,279
Getting started with CS-ROSETTA	CS-ROSETTA	7/20/2011 10:36	48 weeks 5 hours ago	1,226
perusal option: save your job output before reaching walltime	gLite, gLite, jdl, perusal, walltime	7/20/2011 14:08	1 year 28 weeks ago	1,202
Getting started with 3D-DART	3D-DART	3/6/2012 14:22	1 year 10 weeks ago	1,135
3D-DART Example Gallery	3D-DART	3/14/2011 22:42	2 years 9 weeks ago	1,130
Usefull link for GRID related work (mainly for site admin)	Grid Services, accounting, admin, grid, monitoring	10/6/2011 18:33	1 year 31 weeks ago	1,040
Getting started with UNIO	UNIO	7/20/2011 12:20	1 year 43 weeks ago	1,020
Getting started with TALOS+	Talos	7/20/2011 10:51	1 year 43 weeks ago	913
Automated grid submission and polling daemons	About GRID technology, gLite	11/2/2011 11:14	1 year 28 weeks ago	888
Getting started with XPLOR-NIH	Xplor-NIH	7/20/2011 10:17	1 year 43 weeks ago	862
Getting started with MARS	MARS	7/20/2011 10:48	1 year 43 weeks ago	857
Testing accessibility of all SE from all CE (for grid admin)	gLite, grid admin SE CE	5/4/2011 19:17	2 years 1 week ago	765

Page Title	Categories	Created	Last editing activity	Views
eToken with Xen (grid admin)	gLite, Xen etoken	5/13/2011 17:57	1 year 14 weeks ago	750
Ensemble Optimization Method	EOM, Eom, GAJOE, RANCH	7/22/2011 13:32	1 year 42 weeks ago	684
About CING	CING	3/7/2011 16:42	1 year 11 weeks ago	676
Things to do to "add" a new grid site admin	Grid Services, site admin	10/7/2011 13:06	1 year 31 weeks ago	670
Getting Started with CcpNmr Analysis	CcpNmr Analysis	3/6/2012 16:24	1 year 1 week ago	669
About HADDOCK	complex, DNA, docking, HADDOCK,ligand, Nucleic acid, protein, RNA	2/21/2011 16:34	2 years 9 weeks ago	645
Useful interface predictors for HADDOCK	Haddock, HADDOCK, interface predictors	6/11/2012 9:13	22 weeks 2 days ago	643
About 3D-DART	3D-DART	2/25/2011 16:19	1 year 11 weeks ago	638
Counting the WeNMR members per country.	gLite, grid vo WeNMR user member country user list	5/4/2011 21:36	2 years 1 week ago	633
The EGI services API wiki page	Grid Services, documentation, EGI, gLite	8/23/2011 11:39	1 year 38 weeks ago	633
Grid deployment scripts (for site admin)	deployment, gLite, gLite, site-admin,software	8/2/2011 12:12	1 year 41 weeks ago	616
About FormatConverter	conversion, format, FormatConverter, NMR	7/13/2011 9:21	1 year 6 weeks ago	608
Getting started with iCing	CING	2/29/2012 19:03	1 year 11 weeks ago	606
jobs - user friendly utility to manage the users jobs	gLite	8/23/2011 19:19	13 weeks 23 hours ago	605
CheckGRID - Utility to test and publish GRID resources (for site admin)	gLite	8/23/2011 18:51	1 year 38 weeks ago	591
About Talos	dihedral angle prediction, protein,secondary chemical shifts, Talos, Talos	7/12/2011 17:13	1 year 44 weeks ago	579
Getting started with CNS	CNS	3/6/2012 14:28	1 year 10 weeks ago	573
The CS-ROSETTA web server manual	CS-ROSETTA	3/6/2012 14:32	1 year 10 weeks ago	573
About CS-Rosetta	chemical shifts, CS-ROSETTA, NMR,structure calculations	7/13/2011 9:16	1 year 44 weeks ago	571
JobControl - utility to manage multi jobs submission (for site admin)	gLite	8/23/2011 19:09	1 year 38 weeks ago	568
About CcpNmr Analysis	about, CcpNmr Analysis	3/6/2012 16:02	1 year 1 week ago	560
Ab initio shape determination by simulated annealing using a single phase dummy atom model	ab initio, DAMMIN, Dammin	7/22/2011 13:50	1 year 42 weeks ago	549
Getting started with FANDAS	FANDAS	5/31/2012 12:54	50 weeks 1 day ago	542
FANDAS web server documentation	FANDAS	4/25/2012 10:28	1 year 3 weeks ago	537
Grid User Interfaces	Grid Services	7/7/2011 8:52	1 year 45 weeks ago	512
HADDOCK scriptorium - geometrical properties of a molecule	HADDOCK	5/31/2012 15:33	49 weeks 2 days ago	508

Page Title	Categories	Created	Last editing activity	Views
About CNS	CNS, NMR, structure calculation, X-ray	7/13/2011 9:11	1 year 44 weeks ago	493
About Xplor-NIH	Molecular Dynamics, Monte Carlo, NMR restraints, structure calculation, Xplor-NIH	7/15/2011 8:51	1 year 42 weeks ago	488
out GeNMR	chemical shifts, GeNMR, GeNMR,NOEs, protein, s structure	2/24/2012 0:13	1 year 11 weeks ago	488
Small angle X-ray scattering	About SAXS, complexes, nucleic acids, proteins, SAXS, solution scattering	7/22/2011 13:10	1 year 42 weeks ago	486
About Antechamber	AMBER, Antechamber, Organic molecules	7/13/2011 9:36	1 year 43 weeks ago	477
Automatic test of enmr.eu jobs on all supporting CEs.	enmr.eu, gLite, grid, jobs, site admin,test	2/2/2012 13:39	1 year 15 weeks ago	471
Modelling of multisubunit complexes	rigid body modelling, SASREF,Sasref	7/22/2011 13:59	1 year 42 weeks ago	466
About AMBER	Amber, Force Fields, Molecular Dynamics, Refinement	7/12/2011 17:06	1 year 24 weeks ago	465
Ab initio shape determination by simulated annealing using a multiphase dummy atom model	ab initio, MONSA, Monsa	7/22/2011 13:55	1 year 42 weeks ago	462
About MaxOCC	Maximum Occurrence of a conformer,MaxOCC, NMR, SAXS	7/13/2011 9:38	1 year 43 weeks ago	455
About AutoAssign	assignment, AutoAssign, automated,chemical shifts, NMR, resonance	7/13/2011 9:07	1 year 44 weeks ago	454
Evaluation of the solution scattering from macromolecules with known atomic structure and fitting to experimental data	CRY SOL, Crysol	7/22/2011 13:41	1 year 42 weeks ago	426
About MARS	automated assignment, chemical shifts, MARS, NMR, resonance	7/13/2011 9:24	1 year 44 weeks ago	415
ResProx documentation	equivalent resolution, resprox,ResProx	2/27/2012 22:45	1 year 11 weeks ago	397
About UNIO	automated assignment, NMR,resonance, structure calculation,UNIO	7/13/2011 9:28	1 year 44 weeks ago	397
FCC Clustering	clustering, contacts, HADDOCK,protein complex	10/13/2012 9:32	30 weeks 6 days ago	390
About RCI (Random Coil Index)	flexibility, protein, Random Coil Index,RCI, RCI	2/24/2012 0:54	1 year 11 weeks ago	371
RCI documentation	flexibility, protein, RCI, RCI	2/24/2012 1:04	1 year 11 weeks ago	303
About CS23D	chemical shift, CS23D, CS23D,protein, structure	2/23/2012 23:16	1 year 11 weeks ago	301
About ResProx	equivalent resolution, protein,ResProx, structure	2/24/2012 23:00	1 year 11 weeks ago	300
CS23D documentation	chemical shift, CS23D, CS23D,protein, structure	2/23/2012 23:43	1 year 11 weeks ago	266
GeNMR documentation	generation, GeNMR, GeNMR,structure	2/24/2012 0:33	1 year 11 weeks ago	215
HADDOCK Scriptorium - Producing restraints for gapped structures	Chain Break, CNS, docking, Gap,Haddock, HADDOCK, Python, TBL File	3/17/2013 16:32	8 weeks 4 days ago	158
PDB Cleaner - Web resource to 'clean' PDB files before HADDOCKing	docking, Haddock, HADDOCK, PDB Cleaner, PDB file	3/20/2013 4:36	8 weeks 2 days ago	153

Supplementary information 2: Tutorial page usage

This is the full list of usage of all Getting Started and Wiki pages, as of May 15, 2013. The current status is available at: <http://www.wenmr.eu/wenmr/tutorials-and-use-cases/all-wenmr-tutorials>

Page Title	Categories	Created	Last editing activity	Views
MD simulations using the GROMACS web server	GROMACS	4/10/2012 12:32	1 year 5 weeks ago	3099
HADDOCK web server tutorial	HADDOCK	3/8/2011 9:57	2 years 10 weeks ago	2399
CS-ROSETTA web server tutorial	chemical shifts, CS-ROSETTA, CS-Rosetta, structure calculations, Talos, WeNMR	4/20/2012 11:45	1 year 3 weeks ago	2084
MaxOCC usecase	MaxOCC	3/18/2011 16:02	1 year 51 weeks ago	1798
Generating the Necessary Restraint Files for running HADDOCK Manually	HADDOCK	3/18/2011 15:01	2 years 8 weeks ago	1606
Using and contributing to the WeNMR VRC	General Tutorials	10/26/2011 9:13	1 year 18 weeks ago	1365
Quick gLite Middleware Deployment HOW-TO for WeNMR	BDII, CE, certificate, configuration, D GAS, gLite, GRID Tutorials, HLR, jdl, job submission, release, sensor, service, v oms, X.509, yaim	3/14/2011 21:26	3 weeks 3 days ago	1323
Structure refinement using Restrained Molecular Dynamics (RMD) with the AMBER package	Amber, AMBER, Molecular Dynamics, Refinement, RMD, structure calculations	3/11/2011 12:43	1 year 45 weeks ago	1175
Xplor-NIH use case with a User Interface	paramagnetic restraints, paramagnetism, structure calculation, UI, Xplor-NIH	3/18/2011 18:00	1 year 38 weeks ago	1046
Restrained Molecular Dynamics (RMD) refinement of structures including RDC's	Amber, Molecular Dynamics, RDC, Refinement, RMD, structure calculations	6/28/2011 15:16	1 year 43 weeks ago	1023
Quick gLite HOW-TO for WeNMR users	CA, certificate, enmr.eu VO, GRID Tutorials, jdl, job submission, proxy, UI	3/14/2011 16:58	3 weeks 6 days ago	995
A Case Study: Preparing Input Files for a Manual HADDOCK Run	HADDOCK	3/18/2011 15:04	2 years 8 weeks ago	993
How to Prepare PDB Files for Running HADDOCK Manually	HADDOCK, manual Haddock, protein docking	3/11/2011 12:25	2 years 8 weeks ago	982
Xplor-NIH calculation with paramagnetic restraints using the web portal	paramagnetic restraints, paramagnetism, structure calculation, web browser, Xplor-NIH, Xplor-NIH	3/18/2011 17:46	1 year 48 weeks ago	980
GROMACS command line use case example for calculations on the GRID	example, grid submission, GROMACS, gromacs, Molecular Dynamics, use case	3/10/2011 16:16	1 year 4 weeks ago	966
CYANA 3.0 Use Case Examples	CYANA	3/10/2011 16:39	2 years 9 weeks ago	912
CNS use case example for running on the	CNS, CNS, grid	3/9/2011	2 years 10 weeks ago	835

Page Title	Categories	Created	Last editing activity	Views
Grid	submission, Refinement, structure calculations	10:15		
MDDNMR webportal server tutorial	MDD	3/10/2011 17:37	2 years 9 weeks ago	830
Gromacs on the GRID	grid submission, GROMACS, gromacs, Molecular Dynamics, tutorial	3/10/2011 19:09	2 years 5 weeks ago	823
Restrained Molecular Dynamics (RMD) refinement of structures including Disulfide bond	Amber	9/19/2011 16:39	1 year 34 weeks ago	715
How to use the WeNMR Talos+ webserver	backbone dihedral angles, chemical shifts, restraints, Talos, Talos+	4/19/2012 11:54	1 year 3 weeks ago	697
MDDNMR Use Case Examples	MDD	3/14/2011 17:37	2 years 9 weeks ago	651
Maximum Occurrence calculations with the MaxOcc web portal	Maximum Occurrence, MaxOCC,PCS, RDC, SAXS	8/19/2011 18:12	1 year 38 weeks ago	626
Video tutorials - Contributing content	General Tutorials	1/10/2012 10:36	1 year 18 weeks ago	623
AnisoFIT webserver tutorial	AnisoFIT	5/10/2012 18:27	1 year 5 days ago	621
CYANA wiki tutorials	CYANA	3/8/2011 12:34	2 years 10 weeks ago	611
PROSA 6.4 Use Case Example	PROSA	3/14/2011 17:25	2 years 9 weeks ago	603
MARS Use Case Example	MARS	3/14/2011 17:10	2 years 8 weeks ago	601
CYANA demos	CYANA	3/8/2011 13:30	2 years 10 weeks ago	590
Develop a charge distribution and automatically generate input force field parameters for most organic molecules.	Antechamber, Charge distribution, Force Fields, Organic molecules	12/20/2011 12:41	1 year 21 weeks ago	547
HADDOCK portal - easy interface use case	HADDOCK	3/3/2012 6:20	1 year 10 weeks ago	542
MDD-NMR Job Submission Demo	MDD	3/8/2011 13:34	2 years 10 weeks ago	521
NUSSAMPLER Use Case Example	MDD	3/14/2011 17:43	2 years 9 weeks ago	504
VO registration troubleshooting	certificate, GRID Tutorials, SSL error, TLS, voms, X.509	3/14/2011 19:03	2 years 8 weeks ago	499
INFIT 2.0 Use Case Example	INFIT	3/14/2011 16:31	2 years 9 weeks ago	466
CcpNmr Analysis Beginners' Course from CCPN	CcpNmr Analysis, tutorial	3/6/2012 15:57	1 year 10 weeks ago	431
HADDOCK portal - guru interface use case	HADDOCK	3/3/2012 6:24	4 weeks 25 min ago	428
Almost	Almost	5/10/2012 18:09	1 year 3 days ago	427
Converting NmrView to XEASY - with test data	FormatConverter	4/6/2012 17:24	1 year 3 weeks ago	419
GARANT 2.0 Use Case Example	GARANT	3/14/2011 16:41	2 years 9 weeks ago	405
MAPPER 2.0 Use Case Example	MAPPER	3/14/2011 17:29	2 years 9 weeks ago	403

Page Title	Categories	Created	Last editing activity	Views
How to use the NRG-CING website.	CING	11/7/2011 13:05	1 year 6 weeks ago	403
CS-ROSETTA webportal use case example: UVRC	CS-ROSETTA	3/3/2012 7:56	1 year 3 weeks ago	385
FormatConverter walk-through	FormatConverter	4/5/2012 14:32	1 year 6 weeks ago	382
Video tutorial - CYANA to CCPN project	FormatConverter	4/5/2012 16:00	1 year 6 weeks ago	370
CcpNmr Analysis Structure Course from CCPN	CcpNmr Analysis, tutorial	3/6/2012 15:44	1 year 10 weeks ago	367
CNS online tutorials (version 1.3)	CNS	3/3/2012 7:34	1 year 10 weeks ago	327
Modelling DNA from a base-pair step parameter file	3D-DART	3/3/2012 6:56	1 year 10 weeks ago	325
Exporting from existing CCPN project	FormatConverter	4/5/2012 14:52	1 year 6 weeks ago	305
CcpNmr Analysis Solid State Course from CCPN	CcpNmr Analysis, tutorial	3/6/2012 15:49	1 year 10 weeks ago	295
How to use the CING report.	CING	4/5/2012 11:05	1 year 4 weeks ago	293
Modelling DNA using local bend angle definitions	3D-DART	3/3/2012 6:55	1 year 10 weeks ago	288
Modelling a localized 30 degrees bend in in a 20 nucleotide BDNA sequence	3D-DART	3/3/2012 6:51	1 year 10 weeks ago	263
Protein NMR - A Practical Guide	CcpNmr Analysis,tutorial	3/6/2012 15:40	1 year 10 weeks ago	260
Modelling a smooth 60 degrees bend in a 20 nucleotide BDNA	3D-DART	3/3/2012 6:49	1 year 10 weeks ago	259
CNS online tutorials (version 1.2)	CNS	3/3/2012 7:33	1 year 10 weeks ago	250
Running other CNS scripts on the Grid	CNS	3/3/2012 7:24	1 year 10 weeks ago	247
Modelling a smooth 60 degrees bend in a 20 nucleotide BDNA, but of different directions	3D-DART	3/3/2012 6:53	1 year 10 weeks ago	230
3D-DART user manual	3D-DART	3/3/2012 6:29	1 year 10 weeks ago	164