



SEVENTH FRAMEWORK
PROGRAMME

Research Infrastructures

Deliverable 3.2.1

Periodic report on the use of wiki and surveys



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Project coordinator name, title:	Prof. Alexandre M.J.J. Bonvin
Organization:	Utrecht University, The Netherlands
Tel:	+31 30 2533859
Fax:	+31 30 2537623
E-mail:	a.m.j.j.bonvin@uu.nl
Project website address:	www.wenmr.eu

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Section 1: Summary of Deliverable

Background

User community outreach is an important determinant of the success of the Virtual Research Community (VRC) of WeNMR. It is important that users incorporate WeNMR into their working practice, can find relevant information and get actively involved by suggesting improvements and participating in mailing lists. Users can come from different disciplines and they can have different background and different levels of expertise.

Therefore, the WeNMR Wiki should target such differ levels of user expertise. The Wiki pages serve to spread good practice from the consortium partners and from active users to others within the community. A core set of documents is being created to by the consortium partners, but also external VRC members are invited to actively contribute and to provide feedback to the developers. This organized approach to the Wiki should encourage active user participation and lead to a lively Virtual Research Community.

To monitor the usage of the VRC, a user survey was created. This survey allows us to explore the needs and problems of the user by giving them the opportunity to write feedback about the tools and overall organization in WeNMR. Similar modes of interaction with the WeNMR community will also be used to get feedback on other project aspects, like for example the industry participation and interest in WeNMR.

Goal

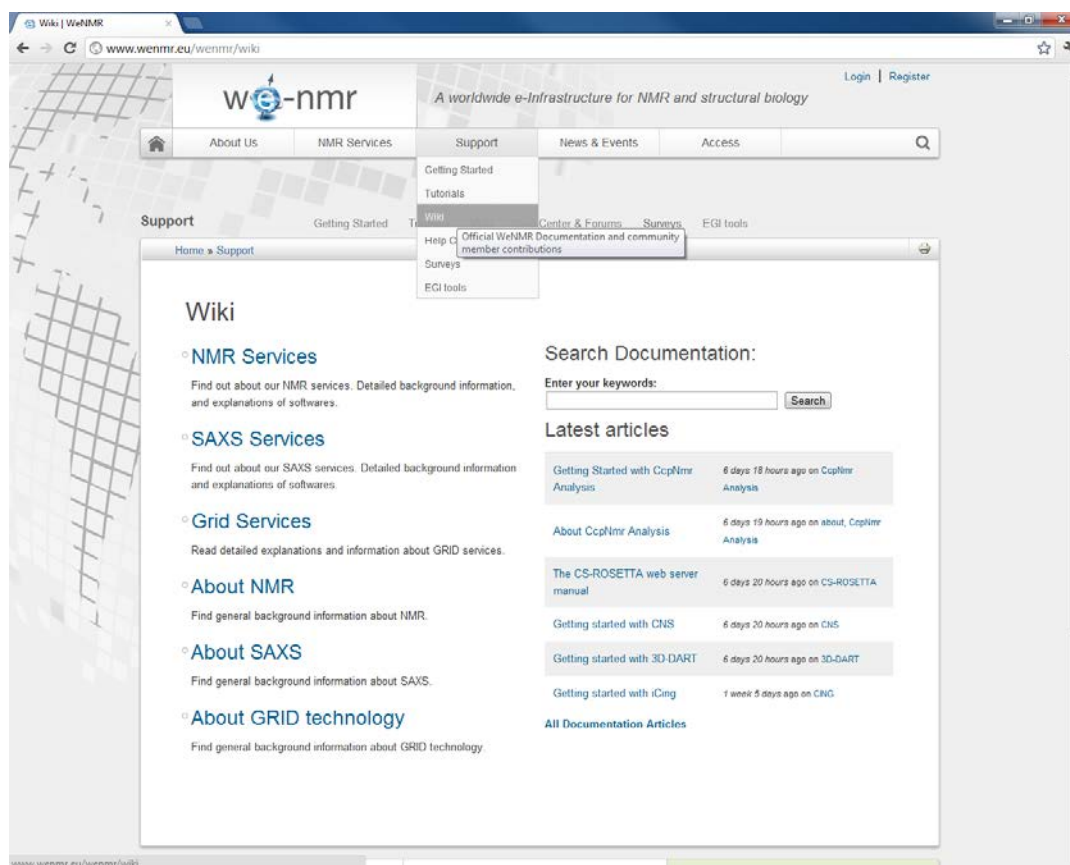
The goal of this Deliverable is to monitor the current usage of the Wiki pages and to evaluate the results obtained in the user survey.

Section 2: Wiki, Getting Started and Tutorial usage

Summary

Originally, the WeNMR Wiki was meant as a mechanism by which users of the VRC would be able to contribute themselves to the documentation available on the WeNMR VRC, in addition to the official documentation. However, user contributions have been only limited so far and this dual setup caused documentation to be spread out of the various parts of the WeNMR VRC. Therefore, it was discussed at a consortium meeting in Cambridge, that the official documentation (the “Getting started” documents and the “Tutorials”) could be merged with the Wiki. In that way, information will be less scattered throughout the website and documentation as well as support will be easier for users to find. In addition, because some content already is available, the threshold for contribution by users to this Wiki might be lowered. Note that at this time users have not yet been actively encouraged to contribute to the wiki.

Currently, the “Getting started” documentation is merged into the Wiki, but the “Tutorials” documentation is still separate. To monitor the usage of the different pages of the WeNMR VRC, we analyzed the total number of views for each of these pages. Although that number is not a direct indicator for the number of users reading those pages, it does provide a clear picture of which pages are been read the most.



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Figure: Entry point of the now combined Wiki and documentation resources of the WeNMR VRC.

Analysis of usage of Wiki / Getting Started pages

The combined Wiki and Getting Started section contains a total of 63 pages, which have seen a total of almost 16.000 views. The top 10 of the currently most viewed pages:

Page title	Views
3D-DART User Manual	891
VO registration troubleshooting	752
The WeNMR web Portals for Structural Biology	625
Getting started with AMBER	576
perusal option: save your job output before reaching walltime	565
3D-DART Example Gallery	454
Introduction to Biomolecular NMR spectroscopy and WeNMR	431
Getting started with MDD NMR	420
About 3D-DART	409
Getting started with CYANA	396

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 the most important introductory pages for people who are starting to use the WeNMR VRC, like the general introduction to WeNMR, the overview of web portals and the Grid registration troubleshooting page. In addition, the list contains documentation and Getting Started pages for some of the web portals, of which especially the “*Getting started with AMBER*” page is remarkable, as this is a web portal that was only added to the WeNMR VRC last year and thus clearly seems to serve an important need of the WeNMR user community, something that is also shown by its usage statistics.

home >> AMPS-NMR

AMPS-NMR
(including paramagnetic restraints plugin)
WeNMR GRID-enabled web portal

WeNMR home NMR services SAXS services WeNMR Support Center

WELCOME TO AMPS-NMR WEB PORTAL PROFILE >>

Supported browser:

AMBER-BASED PORTAL SERVER FOR NMR STRUCTURES (AMPS-NMR)

Amber (acronym to Assisted Model Building with Energy Refinement) is a suite of programs that allow users to perform molecular dynamics (MD) simulations on biological systems. This web portal makes available the entire functionality of AMBER, in particular (but not only) using NMR-derived information as restraints for MD.

we-nmr
e-infrastructure

: Access to AMPS-NMR :

Username:

Password:

Figure: The AMBER (AMPS-NMR) web portal.

Analysis of usage of Tutorial pages

The Tutorial section contains a total of 51 pages, which have seen a total of over 14.000 views. The top 10 of the currently most viewed pages:

Page title	Views
MaxOCC usecase	1537
HADDOCK web server tutorial	984
Xplor-NIH use case with a User Interface	641
Generating the Necessary Restraint Files for running HADDOCK Manually	617
Quick gLite Middleware Deployment HOW-TO for WeNMR	616
Structure refinement using Restrained Molecular Dynamics (RMD) with the AMBER package	589
Xplor-NIH calculation with paramagnetic restraints using the web portal	490
Using and contributing to the WeNMR VRC	486
How to Prepare PDB Files for Running HADDOCK Manually	475
CYANA 3.0 Use Case Examples	463

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.

The top viewed tutorials are those corresponding to the MaxOCC, HADDOCK and XPLOR-NIH and AMBER (AMPS-NMR) portals, which is not surprising as these portals are all among the top portals that have the most number of active users or generate the most number of grid jobs (as was presented in Deliverable 1.5, the 1st period report) and thus seem to be very popular among the WeNMR community. A very popular portal that is not in the list above is the CS-ROSETTA portal, but the first Tutorial for CS-ROSETTA was only added to the WeNMR VRC about one week ago (see supplementary information 2), explaining why it has not yet seen as many views as the other tutorials.

A very promising observation is the high ranking of the tutorial on “Using and contributing to the WeNMR VRC”, which seems to indicate that quite some of the VRC users are at showing an interest in actively contributing to the community, something that was also reflected in the analysis of the user survey (see below).

Section 4: User survey

Summary

To be able to monitor the needs and issues of users and other stakeholders when using the WeNMR VRC and services, several continuously running surveys are in place on the WeNMR website, which also have been advertised among relevant communities. Currently, three different surveys are in place, one dedicated for concerns regarding the security of the Grid usage, one directed at Industry, and one general user survey, on which we already reported in a previous report outside the standard set of deliverables.

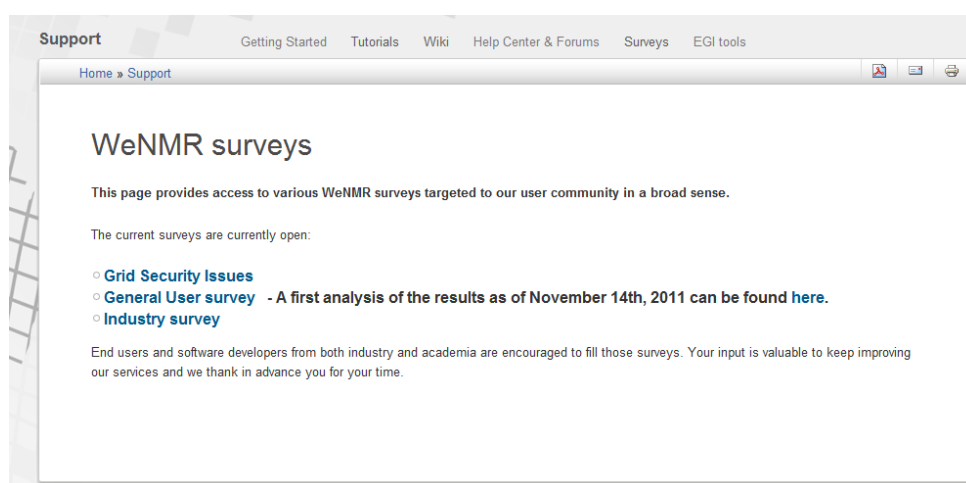


Figure: The surveys on the WeNMR website.

Key user survey results

The results from the user survey (full result available here: <http://www.wenmr.eu/wenmr/wenmr-user-survey-2011>) indicated that approximately 60% of the people using the VRC are based in Europe, with the remaining 40% being located mainly in the Americas and Australasia. Interestingly, over 60% of the respondents also indicated that they have used grid computing either via web-portals or a user interface, showing that there seems to be no real burden for users to engage in grid computing. Nevertheless, several people did indicate they used the [WeNMR site tutorials and use-cases](#) to successfully use the WeNMR tools, showing the clear need for the availability of proper documentation on using the grid. Promisingly, quite a few users also indicated that they had an interest in actively contributing to the WeNMR VRC.

Other surveys

The results from the other two surveys have not been analyzed in detail yet, but both have been advertised broadly in the relevant communities, which has led to a reasonable number of responses, especially in the survey targeted towards industry, with which we aim to get a better view of the potential industrial structural biology user community and to understand their concerns and security requirements about using the WeNMR grid platform.

Supplementary information 1: Wiki / Getting Started page usage

This is the full list of usage of all Getting Started and Wiki pages, as of March 13, 2013. The current status is available at: <http://www.wenmr.eu/wenmr/all-documentation-articles>

Page Title	Categories	Created	Last editing activity	Views
3D-DART User Manual	3D-DART	3/14/2011 20:19	6 days 20 hours ago	891
VO registration troubleshooting	enmr.eu VO, grid, personal certificate, Registration, web browser	3/16/2011 14:20	51 weeks 5 days ago	752
The WeNMR web Portals for Structural Biology	NMR Services, Grid Services	7/20/2011 12:03	33 weeks 5 days ago	625
Getting started with AMBER	Amber	7/20/2011 11:17	1 week 6 days ago	576
perusal option: save your job output before reaching walltime	gLite, gLite, jdl, perusal, walltime	7/20/2011 13:08	18 weeks 6 days ago	565
3D-DART Example Gallery	3D-DART	3/14/2011 21:42	52 weeks 12 hours ago	454
Introduction to Biomolecular NMR spectroscopy and WeNMR	About NMR	7/20/2011 11:36	33 weeks 5 days ago	431
Getting started with MDD NMR	MDD	7/20/2011 9:54	33 weeks 5 days ago	420
About 3D-DART	3D-DART	2/25/2011 15:19	2 weeks 1 hour ago	409
Getting started with CYANA	CYANA	7/20/2011 9:32	29 weeks 3 days ago	396
Getting started with HADDOCK	HADDOCK	7/20/2011 9:15	33 weeks 5 days ago	380
Getting started with CS-ROSETTA	CS-ROSETTA	7/20/2011 9:36	33 weeks 5 days ago	375
Testing accessibility of all SE from all CE (for grid admin)	gLite, grid admin SE CE	5/4/2011 18:17	44 weeks 5 days ago	374
Getting started with UNIO	UNIO	7/20/2011 11:20	33 weeks 5 days ago	370
Getting started with CcpNmr format converter	FormatConverter	7/20/2011 11:14	33 weeks 5 days ago	348
Getting started with MARS	MARS	7/20/2011 9:48	33 weeks 5 days ago	332
Usefull link for GRID related work (mainly for site admin)	Grid Services, accounting, admin, grid, monitoring	10/6/2011 17:33	21 weeks 5 days ago	327
Counting the WeNMR members per country.	gLite, grid vo WeNMR user member country user list	5/4/2011 20:36	44 weeks 5 days ago	300
Getting started with TALOS+	Talos	7/20/2011 9:51	33 weeks 5 days ago	297
About HADDOCK	complex, DNA, docking, HADDOCK, ligand, Nucleic acid, protein, RNA	2/21/2011 15:34	52 weeks 2 hours ago	291
eToken with Xen (grid admin)	gLite, Xen etoken	5/13/2011 16:57	5 weeks 3 days ago	291
About CING	CING	3/7/2011 15:42	1 week 5 days ago	279

Page Title	Categories	Created	Last editing activity	Views
About FormatConverter	conversion, format, FormatConverter, NMR	7/13/2011 8:21	34 weeks 6 days ago	267
jobs - user friendly utility to manage the users jobs	gLite	8/23/2011 18:19	28 weeks 5 days ago	260
Grid deployment scripts (for site admin)	deployment, gLite, gLite, site-admin, software	8/2/2011 11:12	31 weeks 6 days ago	258
CheckGRID - Utility to test and publish GRID resources (for site admin)	gLite	8/23/2011 17:51	28 weeks 5 days ago	253
JobControl - utility to manage multi jobs submission (for site admin)	gLite	8/23/2011 18:09	28 weeks 5 days ago	253
Ab initio shape determination by simulated annealing using a single phase dummy atom model	ab initio, DAMMIN, Dammin	7/22/2011 12:50	33 weeks 3 days ago	246
The EGI services API wiki page	Grid Services, documentation, EGI, gLite	8/23/2011 10:39	28 weeks 6 days ago	243
About CS-Rosetta	chemical shifts, CS-ROSETTA, NMR, structure calculations	7/13/2011 8:16	34 weeks 6 days ago	242
About Antechamber	AMBER, Antechamber, Organic molecules	7/13/2011 8:36	34 weeks 4 days ago	236
About MaxOCC	Maximum Occurrence of a conformer, MaxOCC, NMR, SAXS	7/13/2011 8:38	34 weeks 4 days ago	236
Things to do to "add" a new grid site admin	Grid Services, site admin	10/7/2011 12:06	22 weeks 3 days ago	232
Grid User Interfaces	Grid Services	7/7/2011 7:52	35 weeks 5 days ago	222
Ensemble Optimization Method	EOM, Eom, GAJOE, RANCH	7/22/2011 12:32	33 weeks 3 days ago	220
About AutoAssign	assignment, AutoAssign, automated, chemical shifts, NMR, resonance	7/13/2011 8:07	34 weeks 6 days ago	216
Getting started with XPLOR-NIH	Xplor-NIH	7/20/2011 9:17	33 weeks 6 days ago	215
Modelling of multisubunit complexes	rigid body modelling, SASREF, Sasref	7/22/2011 12:59	33 weeks 3 days ago	215
About AMBER	Amber, Force Fields, Molecular Dynamics, Refinement	7/12/2011 16:06	15 weeks 18 hours ago	213
About Talos	dihedral angle prediction, protein, secondary chemical shifts, Talos, Talos	7/12/2011 16:13	34 weeks 6 days ago	213
Small angle X-ray scattering	About SAXS, complexes, nucleic acids, proteins, SAXS, solution scattering	7/22/2011 12:10	33 weeks 3 days ago	205
About Xplor-NIH	Molecular Dynamics, Monte Carlo, NMR restraints, structure calculation, Xplor-NIH	7/15/2011 7:51	33 weeks 3 days ago	202
About CNS	CNS, NMR, structure calculation, X-ray	7/13/2011 8:11	34 weeks 6 days ago	200
Ab initio shape determination by simulated annealing using a multiphase dummy atom model	ab initio, MONSA, Monsa	7/22/2011 12:55	33 weeks 3 days ago	200
Automated grid submission and polling daemons	About GRID technology, gLite	11/2/2011 10:14	18 weeks 5 days ago	198
Getting started with GROMACS	GROMACS	12/7/2011 15:47	13 weeks 5 days ago	193
About UNIO	automated assignment, NMR, resonance, structu	7/13/2011 8:28	34 weeks 6 days ago	192

Page Title	Categories	Created	Last editing activity	Views
	re calculation, UNIO			
About MARS	automated assignment, chemical shifts, MARS, NMR, resonance	7/13/2011 8:24	34 weeks 6 days ago	168
Evaluation of the solution scattering from macromolecules with known atomic structure and fitting to experimental data	CRY SOL, Crysol	7/22/2011 12:41	33 weeks 3 days ago	167
Automatic test of enmr.eu jobs on all supporting CEs.	enmr.eu, gLite, grid, jobs, site admin,test	2/2/2012 12:39	5 weeks 4 days ago	81
Getting started with iCing	CING	2/29/2012 18:03	1 week 5 days ago	48
RCI documentation	flexibility, protein, RCI, RCI	2/24/2012 0:04	2 weeks 4 days ago	44
About CS23D	chemical shift, CS23D, CS23D, protein,structure	2/23/2012 22:16	2 weeks 4 days ago	40
About RCI (Random Coil Index)	flexibility, protein, Random Coil Index, RCI, RCI	2/23/2012 23:54	2 weeks 4 days ago	36
ResProx documentation	equivalent resolution, resprox, ResProx	2/27/2012 21:45	2 weeks 12 hours ago	36
The CS-ROSETTA web server manual	CS-ROSETTA	3/6/2012 13:32	5 days 3 min ago	36
About GeNMR	chemical shifts, GeNMR, GeNMR, NOEs,protein, structure	2/23/2012 23:13	2 weeks 4 days ago	35
About CcpNmr Analysis	about, CcpNmr Analysis	3/6/2012 15:02	6 days 18 hours ago	32
CS23D documentation	chemical shift, CS23D, CS23D, protein,structure	2/23/2012 22:43	2 weeks 56 min ago	30
About ResProx	equivalent resolution, protein, ResProx,structure	2/24/2012 22:00	2 weeks 3 days ago	30
Getting Started with CcpNmr Analysis	CcpNmr Analysis	3/6/2012 15:24	6 days 18 hours ago	29
GeNMR documentation	generation, GeNMR, GeNMR, structure	2/23/2012 23:33	2 weeks 4 days ago	25
Getting started with 3D-DART	3D-DART	3/6/2012 13:22	6 days 20 hours ago	24
Getting started with CNS	CNS	3/6/2012 13:28	6 days 20 hours ago	22

Supplementary information 2: Tutorial page usage

This is the full list of usage of all Getting Started and Wiki pages, as of March 13, 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
MaxOCC usecase	MaxOCC	3/18/2011 15:02	41 weeks 4 days ago	1537
HADDOCK web server tutorial	HADDOCK	3/8/2011 8:57	1 year 5 days ago	984
Xplor-NIH use case with a User Interface	paramagnetic restraints, paramagnetism, structure calculation, UI, Xplor-NIH	3/18/2011 17:00	29 weeks 3 days ago	641
Generating the Necessary Restraint Files for running HADDOCK Manually	HADDOCK	3/18/2011 14:01	51 weeks 4 days ago	617
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 20:26	5 days 23 hours ago	616
Structure refinement using Restrained Molecular Dynamics (RMD) with the AMBER package	Amber, AMBER, Molecular Dynamics, Refinement, RMD, structure calculations	3/11/2011 11:43	36 weeks 1 day ago	589
Xplor-NIH calculation with paramagnetic restraints using the web portal	paramagnetic restraints, paramagnetism, structure calculation, web browser, Xplor-NIH, Xplor-NIH	3/18/2011 16:46	39 weeks 1 day ago	490
Using and contributing to the WeNMR VRC	General Tutorials	10/26/2011 8:13	9 weeks 5 hours ago	486
How to Prepare PDB Files for Running HADDOCK Manually	HADDOCK, manual Haddock, protein docking	3/11/2011 11:25	51 weeks 4 days ago	475
CYANA 3.0 Use Case Examples	CYANA	3/10/2011 15:39	52 weeks 23 hours ago	463
GROMACS use case example for calculations on the GRID	example, grid submission, GROMACS, gromacs, Molecular Dynamics, use case	3/10/2011 15:16	1 year 3 days ago	451
Restrained Molecular Dynamics (RMD) refinement of structures including RDC's	Amber, Molecular Dynamics, RDC, Refinement, RMD, structure calculations	6/28/2011 14:16	34 weeks 4 days ago	447
A Case Study: Preparing Input Files for a Manual HADDOCK Run	HADDOCK	3/18/2011 14:04	51 weeks 4 days ago	434
Quick gLite HOW-TO for WeNMR users	CA, certificate, enmr.eu VO, GRID Tutorials, jdl, job submission, proxy, UI	3/14/2011 15:58	12 weeks 3 days ago	394
Gromacs on the GRID	grid submission, GROMACS, gromacs, Molecular Dynamics, tutorial	3/10/2011 18:09	48 weeks 1 day ago	383
CNS use case example for running on the Grid	CNS, CNS, grid submission, Refinement, structure calculations	3/9/2011 9:15	1 year 5 days ago	368

MDDNMR Use Case Examples	MDD	3/14/2011 16:37	52 weeks 22 hours ago	341
MDDNMR webportal server tutorial	MDD	3/10/2011 16:37	1 year 18 min ago	331
CYANA wiki tutorials	CYANA	3/8/2011 11:34	1 year 6 days ago	301
MARS Use Case Example	MARS	3/14/2011 16:10	50 weeks 6 days ago	291
CYANA demos	CYANA	3/8/2011 12:30	1 year 6 days ago	285
MDD-NMR Job Submission Demo	MDD	3/8/2011 12:34	1 year 6 days ago	282
PROSA 6.4 Use Case Example	PROSA	3/14/2011 16:25	52 weeks 22 hours ago	278
NUSSAMPLER Use Case Example	MDD	3/14/2011 16:43	52 weeks 22 hours ago	262
Restrained Molecular Dynamics (RMD) refinement of structures including Disulfide bond	Amber	9/19/2011 15:39	25 weeks 22 hours ago	249
Video tutorials - Contributing content	General Tutorials	1/10/2012 9:36	9 weeks 5 hours ago	240
Maximum Occurrence calculations with the MaxOcc web portal	Maximum Occurrence, MaxOCC,PCS, RDC, SAXS	8/19/2011 17:12	29 weeks 3 days ago	235
VO registration troubleshooting	certificate, GRID Tutorials, SSL error, TLS, voms, X.509	3/14/2011 18:03	51 weeks 5 days ago	208
GARANT 2.0 Use Case Example	GARANT	3/14/2011 15:41	52 weeks 23 hours ago	201
MAPPER 2.0 Use Case Example	MAPPER	3/14/2011 16:29	52 weeks 22 hours ago	193
INFIT 2.0 Use Case Example	INFIT	3/14/2011 15:31	52 weeks 23 hours ago	189
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 11:41	12 weeks 3 hours ago	161
How to use the NRG-CING website.	CING	11/7/2011 12:05	18 weeks 1 day ago	143
CcpNmr Analysis 2.1.5 course: Triple resonance based protein NMR assignment - video tutorials	CcpNmr Analysis	2/27/2012 13:41	6 days 5 hours ago	97
3D-DART user manual	3D-DART	3/3/2012 5:29	1 week 1 hour ago	33
CS-ROSETTA use case example: UVRC	CS-ROSETTA	3/3/2012 6:56	1 week 3 days ago	33
Modelling DNA from a base-pair step parameter file	3D-DART	3/3/2012 5:56	5 days 3 hours ago	32
CcpNmr Analysis Structure Course from CCPN	CcpNmr Analysis, tutorial	3/6/2012 14:44	1 week 27 min ago	28
CNS online tutorials (version 1.3)	CNS	3/3/2012 6:34	1 week 3 days ago	28
Modelling a smooth 60 degrees bend in a 20 nucleotide BDNA, but of different directions	3D-DART	3/3/2012 5:53	5 days 3 hours ago	26
Modelling DNA using local bend angle definitions	3D-DART	3/3/2012 5:55	5 days 3 hours ago	26
HADDOCK portal - easy interface use case	HADDOCK	3/3/2012 5:20	1 week 3 days ago	26

CcpNmr Analysis Beginners' Course from CCPN	CcpNmr Analysis,tutorial	3/6/2012 14:57	1 week 21 min ago	25
Modelling a smooth 60 degrees bend in a 20 nucleotide BDNA	3D-DART	3/3/2012 5:49	5 days 3 hours ago	25
HADDOCK portal - guru interface use case	HADDOCK	3/3/2012 5:24	1 week 3 days ago	23
Protein NMR - A Practical Guide	CcpNmr Analysis,tutorial	3/6/2012 14:40	1 week 38 min ago	23
Running other CNS scripts on the Grid	CNS	3/3/2012 6:24	1 week 3 days ago	22
CcpNmr Analysis Solid State Course from CCPN	CcpNmr Analysis,tutorial	3/6/2012 14:49	1 week 29 min ago	21
Modelling a localized 30 degrees bend in in a 20 nucleotide BDNA sequence	3D-DART	3/3/2012 5:51	5 days 3 hours ago	21
CNS online tutorials (version 1.2)	CNS	3/3/2012 6:33	1 week 3 days ago	20