

Deliverable D5.4

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1 Executive summary

Support for users and developers is an integral part of the project and its objectives, and is essential to promote take-up of services and monitor service quality.

The support to users provided through the West-Life portal combines tutorials, documentation and support forums which provide answers by experts/developers covering areas of NMR, SAXS, X-Ray crystallography, Cryo-Electron Microscopy and related integrative methods in structural biology. The West-Life portal also has a dedicated page on Webinar and Video Tutorials.

User support has long been an integral part of the services brought together in the West-Life VRE, and these services have well-established forums for user engagement. These support forums act as a repository of issues and solutions that is of help to future users. The West-Life web site provides navigation to these services and federated search of them.

New forums will also be provided, and we will move the forums from the old WeNMR site to the West-Life forum page.

2 Project objectives

With this deliverable, the project has reached or the deliverable has contributed to the following objectives:

No.	Objective	Yes	No
1	Provide analysis solutions for the different Structural Biology approaches		x
2	Provide automated pipelines to handle multi-technique datasets in an integrative manner		x
3	Provide integrated data management for single and multi-technique projects, based on existing e-infrastructure		x
4	Foster best practices, collaboration and training of end users	x	

3 Detailed report on the deliverable

3.1 Background

West-Life VRE is an integrated platform for providing access to structural biology computational tools and services. The web site provides the entry point for users, developers and all other stakeholders of the structural biology community, as well as members of the wider biomedical community who need to understand or analyse structural data. The web site integrates all already existing and operating services from various partners and existing virtual research communities like WeNMR and also includes new portals developed for West-Life. Support for users and developers is an integral part of the project and its objectives, and is essential to promote take-up of services and monitor service quality. The West-Life web site provides access to the extensive knowledge and support documentations provided by existing tools and services covering areas of NMR, SAXS, X-Ray crystallography, Cryo-Electron Microscopy and related integrative methods in structural biology.

3.2 Documentation and knowledge bases

West-Life users include scientists who access the services in order to manage, analyse and refine their data and developers whose use is to expand, monitor and troubleshoot the software tools and services technically. The diversity of users makes the help desk an important service for users and one which provides feedback on how the portal can be improved, maintained and further developed to meet current, emerging and future VRE needs.

3.2.1 Existing support and knowledge base for scientific users

User support has long been an integral part of the services brought together in the West-Life VRE, and these services have well-established forums for user engagement. For some of the new tools developed under West-Life, user support is most naturally provided through these existing forums. As part of West-Life, concerted efforts were made to collect information about the different service support locations. These are represented below.

Tool/Service	Partner	Support type	Support location
CCP4	1 STFC	Mailing list	https://www.jiscmail.ac.uk/CCP4BB
CCP-EM	1 STFC	Mailing list	https://www.jiscmail.ac.uk/CCPEM
CCD2	2 NKI AVL	Direct support upon request or job failure.	https://xtal.nki.nl/ccd/help
PDB_REDO	2 NKI AVL	Also CCP4 Mailing List	https://pdb-redo.eu/faq.html
ARP/wARP	3 EMBL		http://www.embl-hamburg.de/ARP/
Autorickshaw	3 EMBL		http://www.embl-hamburg.de/Auto-Rickshaw/intro.htm
Scipion	5 CSIC	Mailing list	https://sourceforge.net/p/scipion/mailman/scipion-users/
AMPS-NMR	6 CIRMMP	Direct support upon request or job failure; Online Forum	http://www.wenmr.eu/wenmr/help-center/nmr-services-issues/amber
UNIO	8 UU	Online Forum	http://www.wenmr.eu/wenmr/help-center/nmr-services-issues/unio
DisVis	8 UU	Online Forum	http://ask.bioexcel.eu/c/disvis
PowerFit	8 UU	Online Forum	http://ask.bioexcel.eu/c/powerfit
HADDOCK2.2	8 UU	Online Forum	http://ask.bioexcel.eu/c/haddock
CS-ROSETTA3	8 UU	Online Forum	http://www.wenmr.eu/wenmr/help-center/nmr-services-issues/cs-rosetta

Table 1: Support systems for existing/new tools and services enabled through West-Life

Not all our tools are supported by online forums/ mailing lists. Some tools/services are supported by direct contacts through email to the developers/scientists and some like PDB_REDO contact users when wrong data sets/incorrect information is supplied. The services that were developed and are maintained through WeNMR, like the GROMACS web portal, are supported through the WeNMR support forums <https://www.wenmr.eu/wenmr/support/help-center-forums>. These support forums also act as a repository of issues and solutions that is of help to future users. Within West-Life we will move the forums from the old WeNMR site to the West-Life forum page. Other external forums, like the Discourse forum for HADDOCK will remain as is since they are already widely used.

The support forums/ mailing lists/ email contacts are very well used and regularly serviced by developers and scientists from different partner institutions. The response times for queries are generally dependent on the availability of developers/scientists. In forums like the CCP4BB, the answers to queries are provided by fellow users from the community and issues with the software/service handled by developers. The advantage of this is the immediacy of a response and the benefit of experiences derived from other scientists with real scenarios, often providing valuable insights that have added value over and above a technical fix.

For e-Infrastructure related issues, the GGUS (<https://ggus.eu>) helpdesk provides support to the users of both grid or cloud infrastructures: users with appropriate Grid User Certificates can raise tickets and get support. GGUS also uses EGI AAI CheckIn service and West-Life users registered through ARIA Authentication will be able to use this service in the near future.

3.3 Support Forums enabled through the West-Life Web site

The West-Life web site provides a comprehensive catalogue of tutorials produced for different tools and services and extensive documentation on how to use the tools and services enabled through West-Life. There is also documentation for developers trying to integrate specific tools to their solutions. For example, the West-Life Virtual Folder can be integrated into partner portals, and has been already been integrated in the development version of Haddock. Documentation for these can be found from <https://h2020-westlife-eu.gitbooks.io/virtual-folder-docs/> which is accessible from the project support pages.

The support to users provided through the West-Life web site combines tutorials, documentation and support forums which provide answers by experts/developers. The West-Life web site also

has a dedicated page on Webinar and Video Tutorials (<http://about.west-life.eu/network/west-life/support/webinars>) and a WeNMR/West-Life YouTube channel (<https://www.youtube.com/user/WeNMRchannel>) building on the webinars/videos/tutorials from the WeNMR project. West-Life also provides support through its Twitter presence (<https://twitter.com/WestLifeSB>).

While the documentation, tutorials and help texts for West-Life have been set up and sustained through the West-Life contributing partners, a longer-term strategy to sustain these support services must be identified and preliminary ideas are set out below.

3.4 Sustainability of support provided through the West-Life Web site

While deliverable D1.5 will report on the sustainability of the whole project and its products, it is important to consider the sustainability of the support infrastructure. Maintaining the tutorials, support documentation and support forums will be critical to the sustainability of the services provided through West-Life.

The tutorials, webinars and documentation are provided by those partners who produced and maintain the tools and services. Recurrent or iterative changes and upgrades to the offerings, are therefore best handled by the originators who will also synchronise changes on the West-Life web site. As the West-Life web site aggregates tutorials and documentation from partner website pages, there will be minimal maintenance required. However, for any documentation added directly to the West-Life web site, the respective partners will regularly check the validity and update the text/links as required. The WeNMR/West-Life YouTube channel, where some tutorial videos are uploaded, will be maintained by Partner 8 (UU) hosting WeNMR.

The forums within the West-Life web site were set up by Partner 7 (Instruct) within the context of ARIA (<http://aria.structuralbiology.eu>), and will continue to be maintained beyond the term of the West-Life project. This ensures that the software underpinning the forums supporting user queries on different facilities provided through West-Life will remain supported. Instruct, as an ERIC and part of the European Strategy Forum for Research Infrastructures (ESFRI), has a broad membership, multi-national funding and many expert user-members. West-Life forums are available to and supported by these experts and this provides an element of sustainability for Structural Biology tools currently provided via West-Life. Discussions are underway to consider governance and financial models for these services to either become integrated into

Instruct or to be retained through some other host. Integration must take account of service quality, demand, technical integration with existing software and scientific impact. In some cases, where the West-Life forum provides links to separate and existing well-established forums/ mailing lists (e.g. CCP4bb), the existing in-house support systems will be kept unchanged.