Deliverable D5.9

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Project Acronym:	West-Life	
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Contributing partners:	1 – STFC, 2 – NKI, 3 – EMBL, 5 – CSIC, 6 – CIRMMP, 7 – Instruct, 8 – UU, 10 - INFN	

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1 Executive summary

Support is a fundamental requirement of the West-Life VRE. Documentation and support material both improve the user experience of software-based services such as those provided through the West-Life VRE, and feed back into improvements in the quality of the software. Both of these improvements have consequent impacts on user satisfaction, user outcome from the service, and the penetration of the service within the structural biology community and beyond.

Within West-Life, the support available is organised into a help desk. Users accessing the help desk can quickly and simply access the support they require for any West-Life tool/service from a single location.

The help desk has been evolving throughout the West-Life project to integrate new features such as a search of support material. The help desk has also expanded to add support for the new tools/services developed and added to the West-Life catalogue.

This deliverable is an update on the activities of the help desk. Following from the initial report on the activities of the help desk, this deliverable provides an updated list of all support material available for West-Life portals and documents the new pages, new features and changes to the West-Life website which develop and improve the help desk. A recent user survey suggests that users are generally satisfied with the ease of use of West-Life tools/services which may be attributable to the quality and availability of support through the help desk.

The sustainability of the help desk and support materials for individual tools and services is considered and a plan for the sustainability of the help materials is put forward to explain how user support will continue beyond the West-Life project.

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

The West-Life project provides a Virtual Research Environment (VRE) for structural biology. The VRE combines a range of computational tools and services in the areas of NMR, SAXS, X-Ray crystallography and Cryo-Electron Microscopy. The West-Life website provides a single access point for these services. Correspondingly the West-Life help desk provides a single access point for support across the catalogue of West-Life tools and services.

Since the publication of West-Life deliverable D5.4 “Report on the activities of the help desk”, there have been a number of developments and improvements to the support resources available and to their organisation in the help desk. This deliverable aims to showcase these new developments and provides evidence from user feedback that the West-Life portal tools are easy to use. Finally, the deliverable addresses the future sustainability of help materials beyond the West-Life project.

3.2 Documentation and knowledge bases

3.2.1 Existing support and knowledge base for scientific users

Support for users of structural biology tools and services provided in the West-Life VRE is crucial for the maximisation of uptake of use of the services, and optimisation of the outcome of the service for users. Support can take the form of online materials including documentation, FAQ, tutorials and demos both in text or video form to inform the user about the service and how it can be used, or direct contact with developers or other users of the service through email contact, forums and mailing lists to address specific questions when they arise.

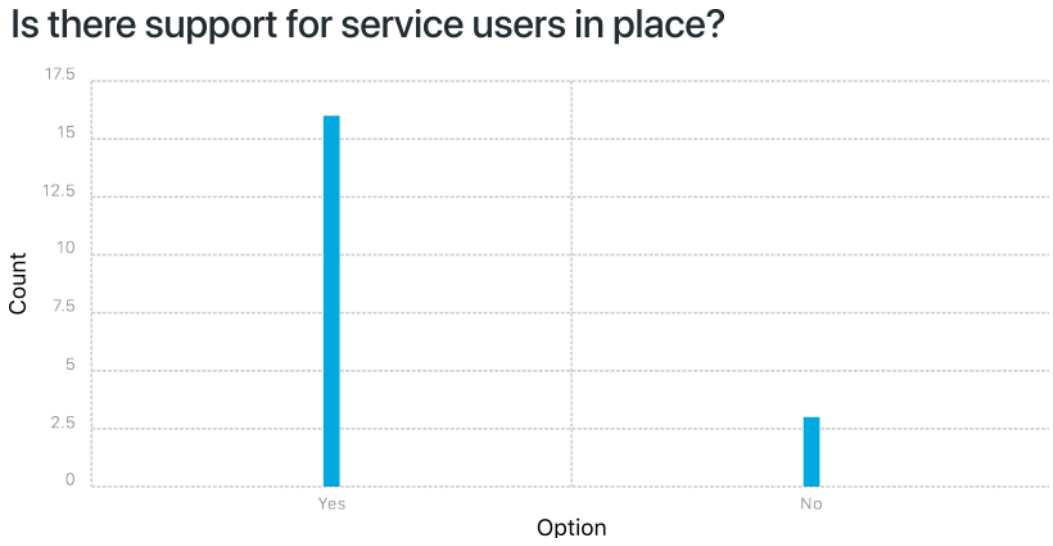

Figure 1: Responses from West-Life Sustainability questionnaire for the question "Is there support in place for service users?". Responses showed that from the 19 West-Life services which responded to the survey, 84% provided support to service users.

As many of the tools and services integrated as part of the West-Life project already have well-established and well-used support material (see Figure 1), an ongoing activity has been to collect as much information as possible about the plethora of support available for these tools and to provide a comprehensive list of support for West-Life tools on the West-Life website. Table 1 is an updated and extended version of the table in West-Life deliverable D5.4 and provides current information on the type of support available for each tool/service, the location of the support, and in some cases information on the frequency of update of the material and metrics of usage of the material.

Tool/Service	Partner	Support type	Support location	Frequency	Usage metrics
3DBIONOTES	P5 - CSIC	Tutorial/ Documentation	3dbionotes.cnb.csic.es/ws/help	Updated when new functionality is available	
AMPS-NMR	P6 - CERM	Email enquiries	py-enmr.cerm.unifi.it/feedback/index?type=amps-nmr	On demand	
ARIA	P7 - Instruct	Telephone enquiries	+44 (0)1865 988639	On demand	
		Email enquiries	aria@structuralbiology.eu	On demand	400-600 enquiries resolved per year
		Documentation	www.structuralbiology.eu/help		1600 page views
ARP/wARP	P3 - EMBL	Contact after job failure		After job failure	100 per year
		Email enquiries	www.embl-hamburg.de/arp-cgi-bin/Emailsender7.6.pl	On demand	
		FAQ	arpwarp.embl-hamburg.de/faq/		
		Tutorial/ Documentation	www.embl-hamburg.de/ARP/	Updated at each software release	
Auto-Rickshaw	P3 - EMBL	Contact after job failure		After job failure	150 per year
		Email enquiries	www.embl-hamburg.de/Auto-Rickshaw/contact.htm	On demand	
		FAQ	www.embl-hamburg.de/Auto-Rickshaw/faq.htm		
CCD	P2 - NKI	Contact after job failure		After job failure	
		Email enquiries	proteinccd@gmail.com	On demand	
		FAQ	xtal.nki.nl/ccd/help	Updated if specific questions arise to warrant such an update	300 page views
		Documentation	xtal.nki.nl/ccd/help		
CCP4 (all portals)	P1 - STFC	Mailing list	www.jiscmail.ac.uk/cgi-bin/webadmin?A0=ccp4bb		
		Email enquiries	ccp4@ccp4.ac.uk		Enquiries received weekly
		Tutorial/ Documentation	www.ccp4.ac.uk/docs.php		
CS-ROSETTA	P8 - UU	Email enquiries	cs-rosetta@bonvinlab.org		

		FAQ	milou.science.uu.nl/enmr/services/CS-ROSETTA3/csr-tutorial.html#faq		
		Tutorial/ Documentation	milou.science.uu.nl/enmr/services/CS-ROSETTA3/csr-tutorial.html		
DipCheck	P3 - EMBL	Email enquiries	cluster.embl-hamburg.de/cgi-bin/dipcheck/dipcheck.cgi?page=contact	On demand	
		Documentation	cluster.embl-hamburg.de/cgi-bin/dipcheck/dipcheck.cgi?page=help		
DisVis	P8 - UU	Forum	ask.bioexcel.eu/c/disvis		6 posts 3000 total views
		Tutorial	www.bonvinlab.org/education/disvis-webserver/		
		Documentation	milou.science.uu.nl/cgi/services/DISVIS/disvis/help		
		Webinar	youtu.be/uxpG339UFJM		
FANTEN	P6 - CERM	Documentation	fanten-enmr.cerm.unifi.it:8080/manual/FANTEN_manual.pdf		
GROMACS	P8 - UU	Email enquiries	m4.van.dijk@vu.nl		
		Documentation	haddock.science.uu.nl/enmr/services/GROMACS/usage.php		
HADDOCK	P8 - UU	Forum	ask.bioexcel.eu/c/haddock		9000 views per month
		Email enquiries	haddock.support@gmail.com	On demand	
		Tutorials	www.wenmr.eu/tutorials/#haddock		
		Documentation	www.bonvinlab.org/software/haddock2.2/manual/	Updated at each software release	
		Demo	www.youtube.com/watch?v=5eS8BAOJ6es		
		Webinar	www.youtube.com/watch?v=kcTwts7_Wuc&feature=youtu.be		
MetalPDB	P6 - CERM	Email enquiries	metalweb.cerm.unifi.it/help/contact/	On demand	
PDB-REDO	P2 - NKI	Contact after job failure		After job failure	
		Email enquiries	pdbredo@gmail.com	On demand	175 per year
		FAQ	pdb-redo.eu/faq.html	Updated when new questions arise	
PowerFit	P8 - UU	Forum	ask.bioexcel.eu/c/powerfit		5 posts 2750 total views

		Tutorials	www.bonvinlab.org/education/powerfit-webserver/		
		Documentation	milou.science.uu.nl/cgi/services/POWERFIT/powerfit/help		
		Webinar	www.youtube.com/watch?v=uxpG339UFJM&feature=youtu.be		
Scipion	P5 - CSIC	Mailing list	sourceforge.net/p/scipion/mailman/scipion-users/		
		Email enquiries	github.com/I2PC/scipion/wiki/Contact-Us		Around 300 emails
		Slack channels (for EM facilities and developers)	https://scipion.slack.com		
		Tutorials	www.youtube.com/user/BiocompWebs		Video views: 48, 28 and 48.
		Documentation	github.com/I2PC/scipion/wiki		
SpotON	P8 - UU	Forum	ask.bioexcel.eu/c/spoton		
		Email enquiries	spoton.csbserver@gmail.com		
		Documentation	milou.science.uu.nl/cgi/services/SPOTON/spoton/help		
ViCi	P3 - EMBL	Email enquiries	victor@embl-hamburg.de	On demand	
		Documentation	www.embl-hamburg.de/vici	Additional documentation provided registration	
Virtual Folder	P1 - STFC	Documentation	h2020-westlife-eu.gitbook.io/virtual-folder-docs/virtual-folder	Updated at each software release	
XREC/FREC	P3 - EMBL	Email enquiries	victor@embl-hamburg.de	On demand	
		Documentation	www.embl-hamburg.de/XREC/		

Table 1: Support systems for tools and services enabled through West-Life portal

The types of support available can be broadly categorised into contact (email enquiries, telephone enquiries, mailing lists, forums, contact after job failure), and support material (FAQ, tutorials, documentation, webinars, demos). In many portals, both contact and support material are present. The type of support material available is adapted for the specific needs of the user community. For example HADDOCK has a large user base, and can therefore utilise the expertise of the user community with the tool in an online forum to provide support, and developers can respond to forum posts when required. Some other tools such ARP/wARP, CCD and PDB-REDO are able to provide pro-active support for example when a user submitted job fails, the user is contacted by email. These tools also provide email addresses/web contact forms for the users to

get in touch directly with the developers. This type of support is more appropriate for services that have a smaller support requirement from their respective user base.

3.3 Support enabled through West-Life Portal

The West-Life portal provides a comprehensive catalogue of tutorials 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.

The help desk provided through the West-Life portal is an amalgamation of all of the tutorials, documentation, support forums and other support material available for West-Life tools.

3.3.1 Locating support materials through the West-Life website

The help material provided for each portal is accessible from many different routes, to ensure that users easily find the help material that they require, whichever pages they are approaching from. In the main West-Life toolbar menu the third item is “Support”. It appears adjacent to the Services item showing its importance in the work of West-Life, and its close relationship with the services. With this close relationship in mind, the Support menu has been re-organised to mirror the Services menu, with support submenu items matching those in the services menu to further ease the navigation of the users to the appropriate support page (see Figure 2).

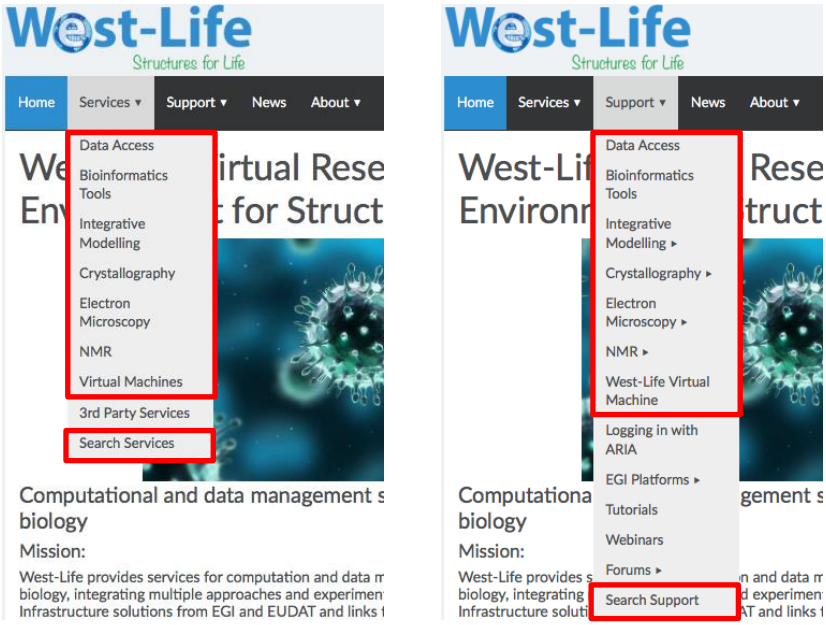

Figure 2: Services menu (left) and Support menu (right) are named and ordered to match each other to ease navigation.

Clicking on "Support" directs the user to a landing page about.west-life.eu/network/west-life/documentation welcoming them to the West-Life documentation and providing links to documentation pages internal to the West-Life website in a side panel for easy navigation. A table of support locations similar to that presented in Table 1 can be found at the bottom of the page. This table is a new feature, added after D5.4. Having this resource available makes it easy for users who access a range of tools through the West-Life VRE to be able to access a corresponding range of support for the tools in a single, centralised location.

Within the "Support" submenu there are pages grouping support material by thematic area e.g. "Integrative Modelling" or "NMR" which reflect the groupings in the Services menu; and pages grouping support material by support type: Tutorials, Webinars, Forums (see Figure 3). These pages list and link to all support material in that grouping, for example a page showing all the Webinar-type support material is provided at about.west-life.eu/network/west-life/support/webinars. This page has embedded videos of the webinars, and by clicking the "More…" link at the bottom of the page, users are directed to the WeNMR/West-Life YouTube channel where they can find more videos, playlists and relevant Featured channels.

The forums page about.west-life.eu/network/west-life/forums contains an table with the contact type support material from Table 1. Email contact is shown as a "Contact Developers button".

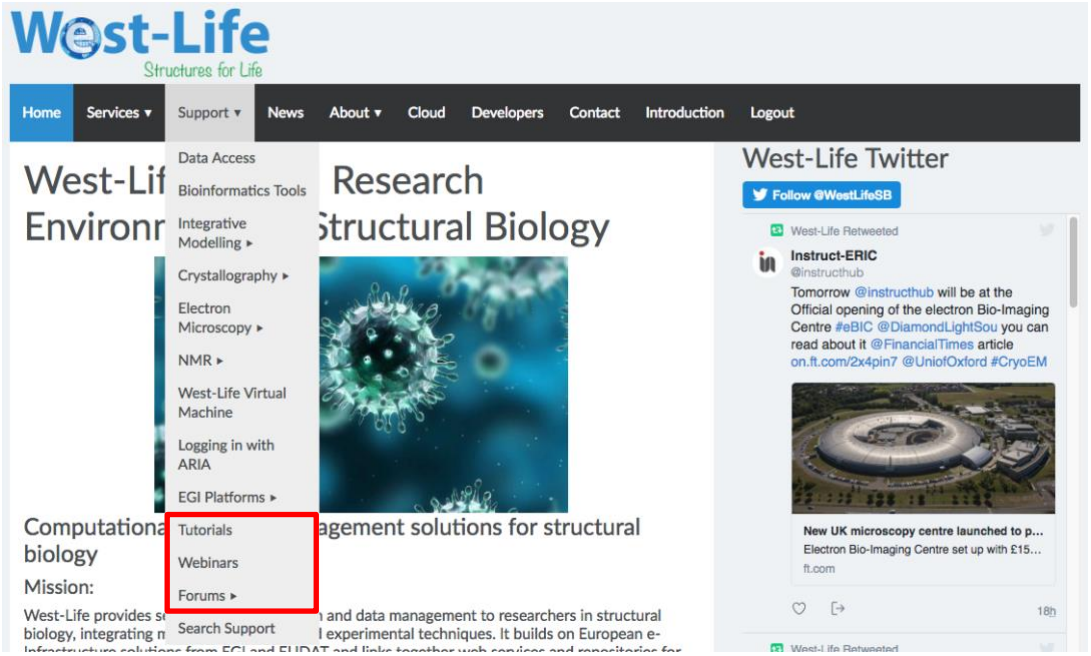

Figure 3: Support Menu in West-Life websites highlighting links to pages with consolidated lists of a particular type of support material (e.g. Tutorials).

3.3.2 Introduction to West-Life

A new introduction page added to the West-Life website about.west-life.eu/network/west-life/introduction provides a concise page with key information for new users. Distinct from the homepage and the "About" pages (which provide more detailed information about the project, its partners, its aims and its outputs), the introduction page firstly gives a single sentence summary of the project, then the page is split into three sections according to the three target stakeholder groups: Life scientists, Advanced users and Portal developers. Within each section, there is a link to a single relevant internal page for that particular audience where they can find more information and links targeted to them. The addition of this Introduction page makes it easier for users to locate the support that they need within the West-Life website.

3.3.3 Search functionality

ELIXIR Registry

The ELIXIR registry provides a catalogue of computational tools and data repositories in the life sciences. Many resources of use to the West-Life user community (primarily structural biologists, and scientific software developers) can be found in the ELIXIR registry, even those which are not currently supported by West-Life itself. As a result, to assist West-Life users in finding tools of

interest to them, a toolbox search of ELIXIR registry is now provided on the West-Life website at about.west-life.eu/network/west-life/toolbox or by clicking “Search Services” at the bottom of the Services menu.

Search of structural biology support sites

There are a number of valuable resources available on West-Life affiliated websites (e.g. the support pages of individual West-Life tools) which provide support for the structural biology community. To increase the ease of locating relevant results to this community, the West-Life website provides a federated Google search of these relevant forums and archives at about.west-life.eu/network/west-life/search-support or by clicking “Search Support” at the bottom of the Support menu. When a user performs a search for a term of interest for example “fitting” using the federated search, a number of highly relevant results appear. Had the user performed the search using a generic search, very few of the results would have any relevance to structural biology (see Figure 4).

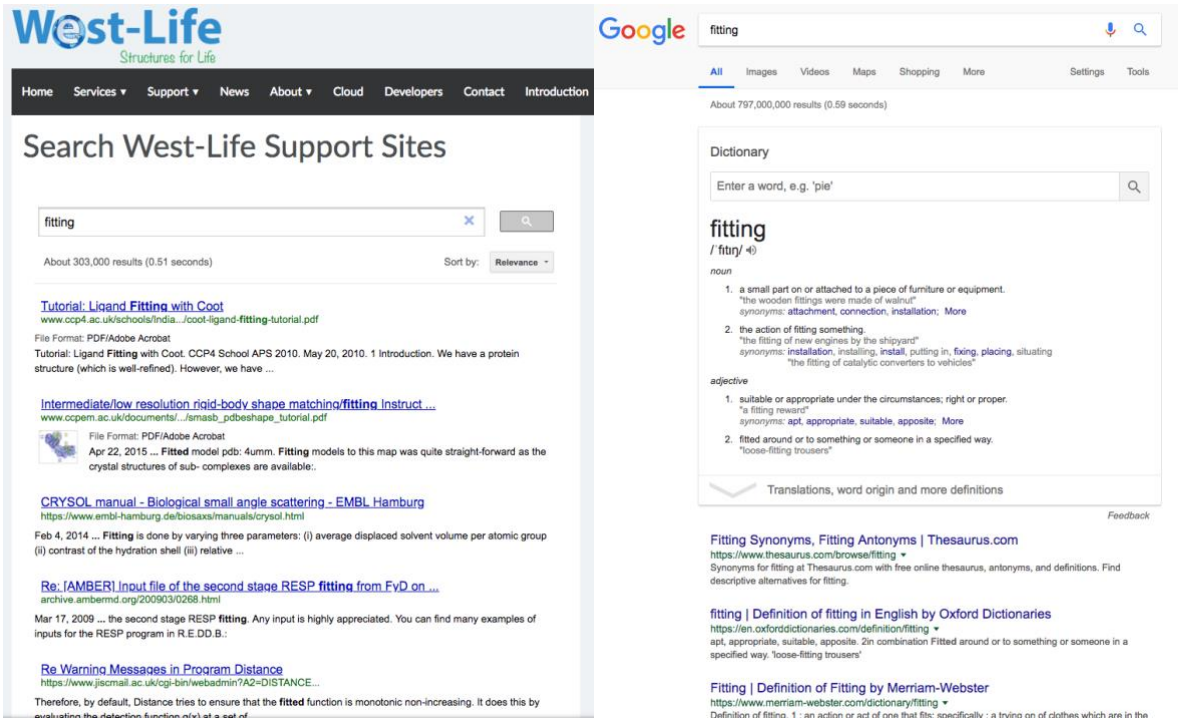

Figure 4: Comparison of federated search provided on West-Life website (left) to standard search (right) for search term “fitting”. The federated search of specific West-Life sites provides results more relevant to structural biology.

The sites currently searched are: www.embl-hamburg.de/, ask.bioexcel.eu, xtal.nki.nl/ccd/help, sourceforge.net/p/scipion/mailman/scipion-users, www.ebi.ac.uk/pdbe/, www.jiscmail.ac.uk/,

twitter.com/WestLifeSB, www.ccpem.ac.uk, about.west-life.eu/network/west-life, pdb-redo.eu, and www.youtube.com/user/WeNMRchannel.

3.3.5 Support for developers

West-Life aims to promote the development of new, cutting-edge structural biology software and resources. As a result, the pathway to creating a structural biology portal should be as easy as possible and this requires dedicated support for the portal developers themselves, not just for the end users of the portals. To achieve this there is a dedicated developers page on the West-Life website at about.west-life.eu/network/west-life/developer-help, accessible from a new main menu link. On this page there are:

- Links to the West-Life Wiki on how to implement the Single Sign On (SSO) with ARIA.
- Links to documentation on how to make your portal compatible with the West-Life virtual folder, a single point of access for cloud and local file storage for use with structural biology tools.
- Link to the DIRAC project documentation. DIRAC is a workload management service provided by EGI which manages access of users to compute services.
- Link to a page on best practices for web services.
- Contact form link to contact the West-Life team.

3.3.6 Grid and cloud infrastructure support

Developers of West-Life application portals that execute computing jobs on the underlining EGI HTC or Federated Cloud infrastructures can leverage the Global Grid User Support (GGUS) system (https://ggus.eu/) for any issue related to grid or cloud services supporting the enmr.eu VO. Since the beginning of the project, 86 support requests have been addressed, mainly related to misconfiguration of grid sites, authentication with X509 certificates, authorization issues with VOMS server, DIRAC access and EGI accounting system.

3.3.7 Cloud deployment

A page on cloud deployment has been added to the West-Life website, accessible via a main menu link or via about.west-life.eu/network/west-life/cloud. This page details how to deploy the West-Life services locally or on the cloud using Amazon Web Services or EGI Federated Cloud.

3.3.8 Publications

Publications are now displayed on the West-Life website page about.west-life.eu/network/west-life/outreach/Publications using the OpenAIRE javascript widget www.openaire.eu/components/com_openaire/js/widget.js for publications associated with the West-Life project. Publications are a form of support created by the scientific community, for the scientific community. Publications from the West-Life project are key resources for West-Life users as they demonstrate contexts in which West-Life tools/services have been used to answer scientific questions, or showcase and publicise new tools/services or extensions and improvements to existing tools/services.

3.4 User feedback on support material

Through June – July 2018 a user feedback survey was displayed as a pop-up across the West-Life website and the pages of individual tools. The survey aimed to collect feedback on the West-Life services available. To encourage responses from as many users as possible the survey was kept brief. Questions asked were “Which West-Life tool were you using?”, “Which route(s) do you use to access this tool?”, “On a scale of 1-5 how easy to use was the tool?”, “How satisfied were you with the outcome after using the tool?”. There was also a final text field for free comments about the tool. Although users were not explicitly asked about the help material, some insights can be gained from the question rating ease of use of the tools. Results from this question are shown in Figure 5. Responses showed generally high scores for ease of use of the tools with a mean score of 4.35 for possible scores in the range of 1-5. Ease of use is determined by both the tool interface itself, and by the support material available so such a high score indicates that the support material available is of sufficient scope and quality to satisfy the users in most cases. Some comments received in the free text field also related to the help material. Three comments related specifically to help material and are shown in Table 2. Two of these comments were about the tool HADDOCK, and one about the tool SpotON. The comments about the HADDOCK tool praised the tutorials provided. The comment about SpotON suggests an improvement for the help material in providing an FAQ on how to solve common error messages. This feedback will be used to improve support material.

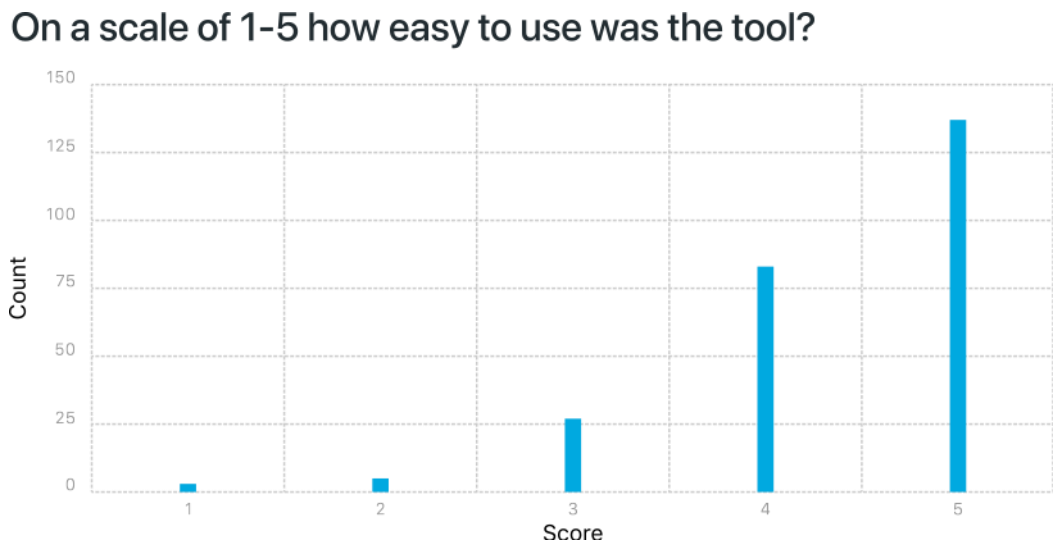

Figure 5: Responses from West-Life User Survey for the question "On a scale of 1-5 how easy to use was the tool?". 255 responses were received covering users of 22 different tools. The mean score for ease of use was 4.35/5.

Comment	Tool
Extremely good explanations and tutorials. The team responds to any questions quickly.	HADDOCK
It was a little difficult at first to use because it kept giving me errors without any clear reason for it not working. I discovered later (through looking at the tutorial page!) that haddock doesn't like any water molecules or metals AND that both the sequences needed different numbering. So there is a learning curve there, but once I figured it out it was super easy to use. Thanks so much for providing such an excellent tool!	HADDOCK
In some cases the tool fails, in my experience mostly when calculating the SASA features. It would be great if the developers could have a FAQ or guide where they explain the most common error messages and how to fix them (for the SASA error, I'm guessing that some manual edit of the input PDB file is required, to account for missing residues or duplicated side chains?).	SpotON

Table 2: West-Life User Survey free text comments relating to support material.

3.5 Sustainability of the support provided through West-Life Portal

The sustainability of the West-Life project is presented in deliverable D1.5, however when considering the sustainability of the project and the services it provides, one must also consider the sustainability of the support resources. As software evolves through new releases documentation can become updated and need refreshing. Where support is provided through direct contact with developers, the sustainability of this support must be carefully considered as staff members move between institutions.

The decision has been made that the individual West-Life partners will continue to maintain their tools/services in-house and Instruct-ERIC (P7) will oversee the transition of the links to West-Life services and help desk to its own website in the short term, subject to future review of the services by the Instruct-ERIC Executive Committee to ensure their continued relevance and quality. Instruct-ERIC is a distributed European structural biology research infrastructure which provides access to high-end structural biology equipment and expertise to its user community. The software resources which have been integrated and developed through the West-Life VRE will provide additional scientific value to Instruct users as part of an expanded catalogue of computational services. Instruct-ERIC will regularly review and update the links to support material for the former West-Life services and ensure that they are up to date in cooperation and communication with the West-Life partners providing these services, with many of which Instruct-ERIC has strong relationships pre-dating and continuing beyond the West-Life project. The WeNMR/West-Life YouTube channel where some tutorial videos are uploaded will be maintained by UU (P8).

Further, the support forums for HADDOCK, DISVIS, POWERFIT and SpotON, operated by the BioExcel Center of Excellence project (bioexcel.eu) are insured to keep working for at least three years since BioExcel2 has been funded. Considering the heavy use of those forums (especially for HADDOCK), this is expected to be maintained well beyond those three additional years.

As the tools/services are to be maintained by the partners themselves, so too are the support materials provided for these tools. The partners are best placed in terms of knowledge and experience to be able to maintain the support material and keep it current and have a vested interest in keeping their software and support resources updated.

The West-Life partners can, therefore, be confident that support for West-Life services will continue to be available to users beyond the end of the project.