Deliverable D1.5

Project Title:	World-wide E-infrastructure for structural biology
Project Acronym:	West-Life
Grant agreement no.:	**675858**
Deliverable title:	Sustainability Report
WP No.	1
Lead Beneficiary:	7: Instruct
WP Title	Management
Contractual delivery date:	31 October 2018
Actual delivery date:	5th November 2018
WP leader:	1: STFC	1
Contributing partners:	Instruct – 7; NKI AVL – 2; EMBL – 3; MU – 4; CSIC – 5; CIRMMP – 6; UU – 8

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Contents

1   Executive summary

West-Life has worked with all stakeholders involved in the development, use and evaluation of services offered through the West-Life web-portal to identify and execute a sustainability solution for their future use. Information was gathered on the West-Life service provision, use by the structural biology community and the ability of ARIA (Instruct-ERIC) to adopt some or all services for continuity. Following this data capture, responses were evaluated and a plan formulated to provide solutions for each service.

A significant part of the plan was to migrate services which are not self-sustainable to the ARIA service platform and this was achieved on 26th September at a Hackathon, hosted at the Instruct Hub in the UK. Migration is now complete. The final service access route can be viewed at https://www.structuralbiology.eu/compute

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 solutions to ensure the long-term availability of software services developed through West-Life, beyond the life of the project**	Yes	
2	**Provide a mechanism for independence of the infrastructure from single providers or funding sources (where necessary)**	Yes	
3	**Provide a plan for integration with training programmes that include new software solutions for emerging use cases**	Yes	
4	**Provide a model which embeds e-infrastructure services in everyday research practise**	Yes	
5	**Provide a framework for the use of software services by industry**	Yes	

3   Detailed report on the deliverable

3.1   Introduction

As set out in the recent ESFRI Roadmap 2018: A Strategy Report on Research Infrastructures, Europe is developing a connected ecosystem of research and e-infrastructures that will form a unique resource for advanced research and interdisciplinary analysis of important and complex scientific problems[1]. Underpinned by the European Open Science Cloud (EOSC), access to e-infrastructure tools and services for data management will enable ever increasing interdisciplinarity which in turn will increase the impact of research, particularly enhancing societal and economic gains. Key to providing value to data-generating research infrastructures and to the research community in general is the long-term sustainability of the horizontal e-infrastructures which provide digital tools and services for data management and analysis.

The goals of e-infrastructure tools and services are:
- to offer state of the art and high-quality services;
- to meet user needs and enhance their research;
- to facilitate access to research results (data and metadata);
- to increase efficiency by providing fast secure services;
- to make e-infrastructure easily available through simple web-interfaces and where possible using single user authentication steps;
- to ensure services and tools are supported and updated to meet emerging scientific demand.

These expectations can only be met if the following requirements can be achieved:
- tools and services are maintained in the long term with sufficient funding and staff resources to ensure continuity of service;
- service provision is supported by specific training for new software and application of services to emerging scientific use cases;
- data security can be guaranteed;
- the value of tools and services is demonstrable (scientific relevance, ability to measure impact).

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[1] http://roadmap2018.esfri.eu/

3.2 Description of the work package task and the deliverable

3.2.1 Objectives

The West-Life Virtual Research Environment (VRE) includes multiple components handling data processing, data management, compute resources, infrastructure for authentication and authorisation, quality assurance and user help. The entry point to access is mainly through the portal at http://west-life.eu but many services are available via other routes, directly or via the European Open Science Cloud hub (EOSC-Hub) portal. Structural biologists are able to access services directly from individual host/developers which in many cases allows users additional integration tools. Techniques complementary to those provided through West-Life are available through a number of other infrastructure resources: Instruct provides technical infrastructure for structural techniques; data deposition is supported by a number of federated databases; access to structural techniques complementary to the Instruct catalogue are available through iNEXT for projects that advance translational research.

The West-Life website adds value by providing links to various tutorials which teach how to make best use of the services. Partner MU has committed to continue operating the West-Life SSO service.

In addition to providing a single portal to many services, West-Life has enabled significant improvements to existing web services for structure determination, including extending their application to different experimental data and expanding usability. New services have also been added to the West-Life catalogue, including SpotOn, 3DBionotes, Dipcheck and a new application of ARP/wARP Classic EM. A full description of the West-Life VRE is included in an article 'West-Life: a virtual research environment for structural biology' (J. Struct. Biol, 2018, submitted).

West-Life aims to support and extend a platform of interoperable data services that enable integrative research, wherever structural methods can contribute. Crucial to achieving this is to establish sustainability for the services that have been brought together within West-Life which means continuity of service underpinned by reliability, excellent user support and quality standards. so that continuity is not compromised and users continue to be supported.

At the West-Life 'All Partners' meeting (May 3-4th 2018) in Madrid, sustainability for West-Life tools and services beyond November 2018 (project end-date) was discussed with the Scientific Advisory Board members who provided guidance on measuring the impact of individual software tools, on the basis of the plan reported in D1.4, which was prepared during Report Period I. A set of Key Performance Indicators (KPIs) were proposed which could be used in assessing the case for maintaining services in the long term. Details of the KPIs are in Section 3.

Pathways to sustainability could then be considered based on the following options:
- continue providing the service from the originator/home institution if resources allow;
- adopt the service and integrate it into the Instruct catalogue of services via the Instruct web portal;
- seek a third-party institution/organisation to adopt and host the service;
- discontinue the service.

This report sets out the method used for assessing each infrastructure service and presents a plan for sustainability for West-Life legacy tools and services to maintain their value for the structural biology cross-disciplinary user communities.

3.2.2   Methods used to gather information and metrics on West-Life tools and services

The principle method for information capture was via questionnaires. The first established the properties of each of the West-Life services to determine whether the service.   The same assessment questionnaire was also completed for ARIA, access management software developed and maintained by Instruct-ERIC, to assess whether West-Life services could be sustained through ARIA in the future. Standards of reliability, maintenance, support and future-proofing were examined. The questionnaire was compiled and distributed in March 2018 and responses collated.

A second questionnaire, aimed at end-users of West-Life services, was displayed as a pop-up on the West-Life home page (https://about.west-life.eu) and on the pages of many individual West-Life services. This questionnaire provided information on the routes used by end-users to access the services developed/supported by West-Life, on the satisfaction of end-users on the outcome after using the tools, and on ease of use of the services. This user questionnaire provided a measure of value of the services to the user communities that they serve, where sufficient responses for that service exist (NB: Number of responses to the user survey per portal varied from 0 – 159 due to differences in the size of the user base and the prominence of the questionnaire pop-up on the service pages. Some services had too few responses to the user questionnaire to assess value).

A working group was nominated to follow up on the use of West-Life tools in the 6 month period to the end of the project in order to make recommendations for sustainability solutions for each service.

The summary responses are given below:

West-Life Sustainability Questionnaire: ARIA

<u>About Service</u>
1. Service name: ARIA (Access to Research Infrastructure Administration)
2. What does the service provide? Please give technical details (approx. 100 words). NB: Information can be copied/adapted from deliverable 5.7
   https://zenodo.org/record/1039054#.WseHd9PwY3g
   ARIA provides, an integrated cloud-based solution for:
   - Peer review of research proposals
   - Research visit management or remote sample processing workflow
   - Instrument booking calendar with user training levels
   - User forums
   - Web-page management with WYSIWYG custom pages and templated branding options for different companies and projects.
   - Event/News/Job posting
   - Document hosting
   - Surveys
   - Reports (on visits, proposals, bookings, surveys)
3. What benefit does this service give to its user base?
   Although the features offered by ARIA are individually available elsewhere (e.g. booking calendar) ARIA offers all of this together in a modular yet integrated manner so that peer review can be linked to visit management and internal instrument booking. Customers can choose to use the complete ARIA offering, or a subset with ease.
4. What are the competing or alternative services (if any)?
   a. BBMRI Negotiator https://negotiator.bbmri-eric.eu/
      Provides access to biobank samples through an online communication tool with communication between multiple biobanks
   b. Agendo http://www.cirklo.org/
      Facility booking including charged access to instruments. Customizable access forms for each instrument.
   c. Elixir Galaxy (see https://www.elixir-europe.org/about/groups/galaxy-wg)

5. What demonstrable benefit does this service provide over these competing services?
   a. Negotiator is well tailored to provide communication between service providers (a similar development is planned as a plug-in tool for ARIA) but ARIA provides more general access which is appropriate for a wider range of services. ARIA enables planning of physical or remote visits/access whereas biobank samples and services are provided remotely.
   b. Agendo is a commercial competitor which provides the ability to request access to instruments, and booking calendar for instruments, but without the higher level organization of 'access routes' provided by ARIA which makes it less appropriate as a tool for distributed research infrastructures especially those providing access funding from different sources. Agendo does not provide the 'Community' functions offered in ARIA
6. How is the service currently provided? (e.g. Online software provided through webserver) Please give a short description and links to all modalities of access.
   Online software either managed on servers operated by Instruct-ERIC hub or offered as a development instance.
7. Is the service available through direct routes other than West-Life; if so which?

ARIA is the software through which Instruct access is managed. It also supports additional access routes iNEXT, CORBEL, EMBRIC; Websites West-Life, Instruct-ULTRA.

Registered Users
8. Is service-specific registration required to use the service? (Yes/No) Yes
   If "Yes"
   9. How many registered users in total? 6323
   10. How many new registered users in the last year (2017)? 1509
   11. How many new registered users in the previous year (2016)? 1267

Active Service Usage
12. If submissions are connected to registered users
    How many users placed submissions in the last year (2017)?

    i. 130 (NB a submission can be placed by a team of multiple users)

    ii. 513
13. If submissions are connected to registered users
    How many users placed submissions in the previous year (2016)?

    i. 150

    ii. 212
14. What is the submission unit recorded (task, job, hour, data (bytes)…)?

    iii. Access Visit approved (i.e. after peer review) (physical or remote) to an instruct Service/Technology

    iv. Instrument bookings placed
15. How many submissions were made in the last year (2017)?

    v. 104

    vi. 10685
16. How many submissions were made in the previous year (2016)?

    vii. 110

    viii. 2683

Service support
17. Is there support for service users in place (e.g. Manuals, Help guides, telephone help desk, tutorials, use cases, software updates, user forums)? If so give details on:
    18. The type of support available.

       i. Help Guides (Available at structuralbiology.eu/help)

       ii. Support tickets (emails to admin@structuralbiology.eu / aria@structuralbiology.eu)

       iii. Telephone helpline (Instruct Hub office)
    19. The frequency of maintenance of support material.

       iv. Guides first published 13/12/2017, no scheduled maintenance but some edits to help guide content are made each month

       v. Tickets are responded to on a daily basis

       vi. Phone calls accepted daily Monday-Thursday 10:00am - 3:30pm

20. Metrics on usage of help material (e.g. number of web page views in the past year, number of downloads in the past year, number of emails requesting support in the past year)

     vii. 56 guides currently available

     viii. 738 unique (1444 total) page views of help pages since launch (13/12/2017);
- 459 support tickets resolved 06/04/2016-05/04/2017
- 625 support tickets resolved 06/04/2017-05/04/2018

21. Is training provided for the service? (Yes/No) If yes give details of:

22. Type of training

     ix. Workshops

     x. Webinars

23. Frequency of training

     xi. Once or twice a year

     xii. Only started webinars this year: Once so far this year but another planned for May 2018 (now completed)

24. Outcome of training
- Familiarity with the features available in ARIA
- Able to use the ARIA GUI in the administration pages to perform management actions
- Participant issues/questions addressed
- Suggestions received from participants for new features and developments

25. Number of participants in training (per training event)

     xiii. Workshop (02/02/2018) 20 participants

     xiv. Webinar (16/01/2018) 26 participants and 60 views of webinar recording

26. Resources required to provide this training
- Staff (2-4) staff per workshop (1-2) staff per webinar
- Funds for transport, accommodation and refreshments for each workshop
- Webinar platform for webinars (currently supported by CORBEL project funded GoToWebinar platform)
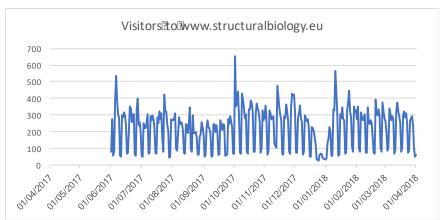
Commitment to service

27. How long has the service been operational? (via ARIA)
Version Drupal: 2011
Version 1: 2013
Version 2: 15/08/2017

28. Do you log service outages? Yes (indirectly through web analytics collected using piwik since 01/06/2017)

29. Please provide details of service outages in the last year. (e.g. graphical representation of service provision showing downtime).

Visitors to www.structuralbiology.eu

30. Explain any significant (> 1 day) service outages in this period.
    - No outages >1 day since records began.
    - 5hr scheduled outage on 15/08/2017 to migrate to from ARIA V1 to ARIA V2.
    - There was intermittent service disruption on 22/12/2017 due to a planned internal switch upgrade.

31. What is the penetrance of the service in the structural biology community?
    The Instruct member countries have a total of 4.116.920 HRST researchers. Researchers either interested or using structural techniques are estimated at less than 3% of the biology community (<1% in 1991, 1% in 2010 (doi:10.3390/su4123234); 3% 2017 WOS. If we use this as a baseline, Instruct reaches 5% of its potential user community.
32. Is the service scalable to increase penetrance? Yes

Impact of service
33. What is the total number of publications acknowledging the use of the service? 373 acknowledging Instruct (NB: We do not ask users to acknowledge ARIA however users of Instruct must use ARIA system to apply for access, and acknowledge Instruct in publications)
34. How many of these publications were published within the last year (2017)? 63

Sustainability of service
35. Give details of past developments (with dates) to the service which have been made to ensure the service provision remains up-to-date with the needs of users and/or scientifically at the cutting-edge.

    xv. Version 2.0 release (15/08/2017) - Complete rewrite of the code. Simplified interfaces and menus in the administration pages.

    xvi. Instruct-ERIC website – Rewrite and reorganization of the user-facing pages of the Instruct website. Pages have been updated with a fresh look and to be more mobile friendly. (05/2018)

36. Do you have a plan for future developments of the service over the next 2 years to keep the service relevant and at the cutting-edge (Yes/No). Yes
    a. If "yes" please give details.
       - Continued expansion of ARIA to more organisations (RIs, academic institutions)

- API development to allow flow of data back into ARIA (currently data can only be pulled from ARIA).
- Help-desk feature to allow the creation of user generated help content, help content tagging with keywords for navigation.
- Notes feature to add text comments to a particular visit/proposal.
- Integration with Life Science AAI (pending successful H2020 INFRAEOSC-04 application)

37. What resources (infrastructure and support) are required to continue operation of the service? Please select all that apply and add any resources not included in the list under "other":
   - ☐ Grid/Cloud - currently no provision, but EOSC should become available as it develops. Instruct is a partner in this development for biomedical sciences RIs. GRID services are currently utilized independently through each facility (e.g. CNB Madrid)
   - ☐ Local servers - 4 servers
   - ☐ Staff [Maintenance/Support/] (please give the number of person months required per year) 2.5 FTE = 30pm
   - ☐ Other (please specify) none declared

38. For each of the resources listed above, please give an estimated financial cost (per year), and explain how these resources are supported (e.g. funded by X, Staff employed by X).
   2.5FTE Staff employed by Instruct-ERIC = €150K per year full costs

West-Life Sustainability Questionnaire: Services

The following services were surveyed:

Service	Link to portal
3DBionotes	https://3dbionotes.cnb.csic.es/ws
AMPS-NMR	http://py-enmr.cerm.unifi.it/access/index
ARP/wARP	https://arpwarp.embl-hamburg.de/
Auto-Rickshaw	http://webapps.embl-hamburg.de/cgi-bin/Auto-Rick/arinitAR1.cgi
CCD	https://ccd.rhpc.nki.nl/
CCP4	https://portal.west-life.eu/static/ccp4.html
CS - ROSETTA	http://milou.science.uu.nl/enmr/services/CS-ROSETTA3
DisVis	http://milou.science.uu.nl/cgi/services/DISVIS/disvis/
FANTEN	http://fanten-enmr.cerm.unifi.it:8080/
GROMACS	http://haddock.science.uu.nl/enmr/services/GROMACS/main.php
HADDOCK2.2	http://haddock.science.uu.nl/enmr/services/HADDOCK2.2
MetalPDB	http://metalweb.cerm.unifi.it/
PDB-REDO	https://pdb-redo.eu/
PowerFit	http://milou.science.uu.nl/enmr/services/POWERFIT
Scipion Web Tools	https://structuralbiology.eu/network/west-life/documentation/scipion-web-tools
ScipionCloud_v1.0	https://appdb.egi.eu/store/vappliance/scipion.v1.0
SpotON	http://milou.science.uu.nl/cgi/services/SPOTON/spoton/
ViCi	https://www.embl-hamburg.de/vici/index
Virtual Folder	https://portal.west-life.eu/virtualfolder/

Questions posed per service:

1. **Name of service**
2. **What does the service provide?**
3. **What benefit does this service give to its user base?**
4. **Are there any competing services?**
5. **What demonstrable benefit does this service provide over these competing services?**
6. **How is the service currently provided?**
7. **Is the service available through direct routes other than West-Life; if so which?**
8. **Is service-specific registration required to use the service?**
9. **If registration is required, how many registered users are there in total for the service?**
10. **If registration is required, how many new registered users were there in 2017?**
11. **If registration is required, how many new registered users were there in 2016?**
12. **If submissions are connected to registered users, how many users placed submissions in 2017?**
13. **If submissions are connected to registered users, how many users placed submissions in 2016?**

14. What is the submission unit recorded?
15. How many submissions were made in 2017?
16. How many submissions were made in 2016?
17. Is there support for service users in place?
18. If support is provided, please give details of the type of support available.
19. If support is provided, please give details of the frequency of maintenance of the help material.
20. If support is provided, please give metrics on usage of help material.
21. Is training provided for the service?
22. If training is provided, give details of the type(s) of training.
23. If training is provided, give details of the frequency of training.
24. If training is provided, please state the outcome(s) of training.
25. If training is provided, please give the number of participants (per training event).
26. If training is provided, please list the resources required to provide this training
27. How long has the service been operational?
28. Do you log service outages? If [Yes], please explain how outages are logged.
29. If outages are logged, provide (upload) details of service outages in the last year. (e.g. graphical representation of service provision showing downtime).
30. If outages are logged, explain any significant (> 1 day) service outages in the last year (planned or unplanned).
31. What is the penetrance of the service in the structural biology community?
32. Is the service scalable to increase penetrance?
33. What is the total number of publications acknowledging the use of the service?
34. How many of these publications were published in 2017?
35. Give details of past developments (with dates) to the service which have been made to ensure the service provision remains up-to-date with the needs of users and/or scientifically at the cutting-edge.
36. Do you have a plan for future developments of the service over the next 2 years to keep the service relevant and at the cutting-edge? If [Yes] give details.
37. What resources (infrastructure and staff) are required to continue operation of the service? Please list all that apply and include the number of person months per year for staff required.
38. For each of the resources listed above, please give an estimated financial cost (euros per year), and explain how these resources are supported (e.g. funded by X, Staff employed by X).

Responses to the survey of services was comprehensive. The full dataset is available in Appendix 1.

West-Life Questionnaire: End-Users

Questions posed per user:

1. **Which West-Life tool were you using?**
2. **Which route(s) do you use to access this tool?**
3. **On a scale of 1-5 how easy to use was the tool (where 1= extremely difficult to use and 5= extremely easy to use)**
4. **How satisfied were you with the outcome after using the tool (where 1= extremely dissatisfied and 5= extremely satisfied)**
5. **Free comments about the tool [text box].**

255 responses were received to the user survey. A summary of responses is shown in Appendix 2.

Analysis of the responses to the questionnaires indicated that ARIA could provide a sustainable platform for some of the West-Life services and provide access to the structural biology community without a break to service. Further, mechanisms were already demonstrable to support the service into the future (Instruct-ERIC has core funding until 2022).

3.2.3   Execution of the sustainability plan

Recommendations were made by the SAB and the working group nominated by the ERP and these formed the bases of a plan for sustainability.

Most services existed before the West-Life project, and will continue to be operated by their host organisations after West-Life. For example, the CCP4 services for crystallography have been under continuous development by STFC since 2013, and will continue to be supported by the CCP4 project. The WeNMR services are now operating as thematic services under the EOSC-Hub (https://www.eosc-hub.eu/catalogue/WeNMR%20suite%20for%20Structural%20Biology). West-Life support has enabled specific enhancements in the interoperability of these services.

The West-Life website provides a convenient entry point for new users, and much of its content will be migrated onto equivalent pages on the Instruct-ERIC website, to be maintained and updated by Instruct-ERIC. A new cloud instance of the Virtual Folder will be operated by Instruct-ERIC, eventually replacing the version at portal.west-life.eu/virtualfolder.

Migration of services from West-Life to the Instruct-ERIC platform were mapped onto the page structure of the Instruct website. Some services pre-dated Instruct and West-Life and will continue to be operated by their host institutions after West-Life. Other compute/grid-related portals could not be supported by ARIA and their support will remain with the present provider (see Table 1). Migration of the services tagged for transfer to ARIA was planned for execution at a Hackathon undertaken on Wednesday 26th September at the Instruct Hub offices. Attendees were: Chris Morris (STFC), Tomas Kulhanek (STFC), Fiona Sanderson (Instruct), Claudia Alen Amaro (Instruct), Twba Al Shaghdari (Instruct), Martyn Winn (STFC), François Ruty (Luna).

West-Life Hackathon: 26th September 2018
Agenda

Transfer Virtual Folder and related services:

   11:00 - 11:15 - (15 mins) Introduction
   11:15 - 11:45 - (30 mins) Virtual Machines templates, containers - preparation, reuse, CernVM 4.0, Scientific Linux 7.5
   11:45 - 12:15 - (30 mins) Bootstrapping - VM, container preparation, configuration with SSO, VRE, ...

(lunch time)

   13:00 - 13:30 - (30 mins) Backend services - WEBDAV API, strategy for mounting/unmounting, REST API, message driven services, common storage location (/srv/virtual folder) source code organization, build and test
   13:30 - 14:00 - (30 mins) Frontend UI - components (Setting, Settings Export/Import, File Manager, File picker, Viewer, Metadata), source code organization, build

(break 15 mins)

   14:00 - 16:00 - (2 hours) Integration into partner/third party services. files - WEBDAV, metadata - REST API, auth - SSO; Deep dive into picked features; Additional use case discussion/prototyping

Table 1: Migration plan for West-Life services to the Instruct website.

Menu	Page	Page section			
			West-Life = current site which will last at least 2 years, but not be updated		
			Instruct = computational area of structuralbiology.eu to be actively maintained		
Menu	**Page**	**Page section**			
Home		Project progress	West-Life	keep up-to-date until project signed-off	
		Twitter	West-Life	freeze	
		Events	West-Life	freeze	
Services	Data Access		Instruct	Virtual Folder, main one for migration	
	Bioinformatics		Instruct	catalogue of services (services are external, but we want Instruct to host the catalogue)	
	Integrative		Instruct	catalogue of services	
	Crystallography		Instruct	catalogue of services	
	EM		Instruct	catalogue of services	
	NMR		Instruct	catalogue of services	
	VM		Instruct	catalogue of services	
	3rd party		West-Life	Instruct will support links to W-L services but not 3rd party ones	
	Search		Instruct	searches Elixir Tools registry	
Support	Data Access		Instruct	link to gitbooks site	
	Bioinformatics		Instruct	catalogue of docs (these could be in separate Support section, or merged with services catalogue)	
	Integrative		Instruct	catalogue of docs	
	Crystallography		Instruct	catalogue of docs	
	EM		Instruct	catalogue of docs	
	NMR		Instruct	catalogue of docs	
	VM		Instruct	link to gitbooks site, keep and merge with Cloud below	
	Login ARIA		West-Life	this should be unnecessary when users on Instruct site	
	EGI		Instruct	documentation on available hardware platforms	
	Tutorials		Instruct	catalogue of tutorials	
	Webinars		Instruct	catalogue of webinars (videos of old ones?)	
	Forums	top list	Instruct	catalogue of forums	
		W-L forums	West-Life	not active	
		individual forums	West-Life	these already listed in main catalogue	
	Search		Instruct	Google search targeted at support sites	
News			West-Life	freeze	
About	Project		Instruct	could we place a shorter edited version on Instruct, as a historical record of West-Life?	
	Partners		West-Life	freeze	
	Advisory Board		West-Life	freeze	
	WP		West-Life	freeze	
	Deliverables		West-Life	keep up-to-date until project signed-off	
	Milestones		West-Life	keep up-to-date until project signed-off	
	Internal wiki		Is this a separate site?		
	Publicity		West-Life	keep up-to-date until project signed-off	
	Flyer		West-Life	freeze	
Cloud			Instruct	merge with Support page for VM	
Developers			Instruct	links to internal-wiki, gitbooks, readythedocs	
Contact			West-Life	freeze	
Introduction			West-Life	freeze	
Login			West-Life	this is replaced by Instruct login	

A summary of the work achieved during the Hackathon was drafted and circulated to the Evaluation Review Panel and other stakeholders (appended below).

Summary report of the outcome of the Hackathon migration and future plans for sustainability of collateral West-Life services (Chris Morris, October 2018)

The meeting at Instruct-ERIC at Oxford on 26/9/18 considered the transfer of online resources and services from West-Life to Instruct-ERIC. Specifically, these include catalogues of computational services, catalogues of support sites, search facilities (Elixir tools registry and targeted Google), guides for developers and advanced users, the Virtual Folder distribution and the hosted service. Note that the catalogues contain links to services and support from West-Life partners, but not the services themselves which will be maintained by partners.

Instruct-ERIC staff will transfer the content to https://www.structuralbiology.eu/ in an area called "Computational Services". This will be linked from the Service/Technology Catalogue. There is no contractual obligation to maintain the West-Life branding, though these pages should acknowledge their origins in the West-Life project. Instruct-ERIC staff will provide technical assistance in maintaining the Computational Services pages, but are not expected to provide expert support for all services. Chris Morris will provide additional technical support on a best effort basis.

The Instruct-ERIC Computational Services pages will need oversight, to ensure that all links and services remain working, up-to-date and relevant. A new Instruct-ERIC working group will be formed to provide this oversight, with suggested members Martyn Winn, Tassos Perrakis, Laura Del Cano and Antonio Rosato. In addition, this working group will draft a paper for the Instruct Executive outlining the future of computational services within Instruct-ERIC. While starting from the West-Life contribution, the proposal should consider the wider issue of how computational services and software should be organised alongside physical infrastructure.

Claudia Alen (Instruct Hub) will continue to operate the West-Life twitter account.

West-Life SSO accepts "Sign in with Google". However, this does not grant access to the services for someone with only a Google ID. It is an authentication method, which can be used to access services only after someone has merged identities.

Currently, the only area requiring authentication is the hosted Virtual Folder service (http://portal.west-life.eu/). It is hosted now by Francois Ruty at Luna, and allows login via West-Life SSO or ARIA. This will be migrated to Instruct at https://vf.structuralbiology.eu but this is not an urgent task, as Francois has promised to maintain the existing service past the end of the West-Life grant. Chris Morris will be responsible for the maintenance of this code.

Other Instruct services require ARIA authentication. Navigation will be possible between the VF and Instruct services without logging in again. This will be discussed further at a later date.

4. Conclusion

This report describes the process and the execution of a sustainability plan for West-Life services beyond the term of the project. Instruct-ERIC will periodically evaluate the access to these services (via the Instruct website) by the user community, using their internal Data Management Group. This group will identify changes to the management of the services that may be required to keep them current and relevant including updates, changes to the platform or removal.

Service Name	What does the service provide?	What benefit does this service give to its user base?	Are there any competing services?	What demonstrable benefit does this service provide over these competing services?	How is the service currently provided?	Is the service available through direct routes other than West-Life; if so which?	Is service-specific registration required to use the service?	If registration is required, how many registered users in total?	If registration is required, how many new registered users in 2017?	If registration is required, how many new registered users in 2016?	If submissions are connected to registered users, how many users placed submissions in 2017?
3DBIONOTES-WS	3DBIONOTES is a web platform designed to integrate structural information with proteomic, genomic, and interactomic annotations. The framework aligns protein sequences of PDB entries with sequences of the UniProt and ENSMBL databases in such a way that any biological annotation can be mapped at structural and protein and gene sequence level. Current sources of information include post-translational modifications, genomic variations associated to diseases, short linear motifs, immune epitopes sites, disordered regions and domain families. The application can be accessed submitting a protein structural model or using a particular EMDB, PDB or UniProt identifier.	Mapping of biomedical and biochemical annotations at structural and sequence level including protein and gene sequences.		N/A	Web application accessible through a webserver.	Web server accessible at http://3dbionotes.cnb.csic.es, from the different web pages of the EMDB entries, from PDB_REDO entries and from the HADDOCK web server.	0	N/A	N/A	N/A	N/A
AMPS-NMR	AMPS-NMR is a web interface to set up and run calculations with the AMBER package. In particular, the interface allows the refinement of NMR structures through restrained Molecular Dynamics. Some predefined protocols are provided for this purpose. The portal uses both grid CPU and local GPU resources.	Easy access to computational resources and a convenient user-friendly interface to set up restrained Molecular Dynamics simulations. It takes care automatically of all format conversions needed for NMR restraints			Online software provided through webserver. The local users can access using login and password provided internally, all other users can access using Single Sign On authentication provided by West-Life https://auth.west-life.eu/ or IAM https://iam-test.indigo-datacloud.eu provided by the INDIGO Datacloud project.	direct link at http://py-enmr.cerm.unifi.it/access/index	0	468	78	90	34
ARIA	ARIA provides, an integrated cloud-based solution for: Peer review of research proposals; Research visit management or remote sample processing workflow; Instrument booking calendar with user training levels; User forums; Web-page management with WYSIWYG custom pages and templated branding options for different companies and projects. Event/News/Job posting; Document hosting; Surveys; Reports (on visits, proposals, bookings, surveys)	Although the features offered by ARIA are individually available elsewhere (e.g. booking calendar) ARIA offers all of this together in a modular yet integrated manner so that peer review can be linked to visit management and internal instrument booking. Customers can choose to use the complete ARIA offering, or a subset with ease.	BBMRI Negotiator https://negotiator.bbmri-eric.eu/ Provides access to biobank samples through an online communication tool with communication between multiple biobanks; Agendo http://www.cirklo.org/ Facility booking including charged access to instruments. Customizable access forms for each instrument. Galaxy (see https://www.elixir-europe.org/about/groups/galaxy-wg) Many online tools for data analysis with customizable data analysis workflows.	Negotiator is well tailored to provide communication between service providers (a similar development is planned as a plug-in tool for ARIA) but ARIA provides more general access which is appropriate for a wider range of services. ARIA enables planning of physical or remote visits/access whereas biobank samples and services are provided remotely. Agendo is a commercial competitor which provides the ability to request access to instruments, and booking calendar for instruments, but without the higher level organization of 'access routes' provided by ARIA which makes it less appropriate as a tool for distributed research infrastructures especially those providing access funding from different sources. Agendo does not provide the 'Community' functions offered in ARIA or the field functionality that generates custom forms with automatic field detection. Galaxy is focused on data analysis pipelines and therefore it does not provide peer reviewed access management for the tools/services. Galaxy is for remote (cloud based) computational tools and resources only, and not physical visit management.	Online software either managed on servers operated by Instruct-ERIC hub or offered as a development instance.	ARIA is the software through which Instruct access is managed. It also supports additional access routes iNEXT, CORBEL, EMBRIC; Websites West-Life, Instruct-ULTRA.	1	6323	1509	1267	130 (NB a submission can be placed by a team of multiple users) 513
ARP/wARP	ARP/wARP webservice provides computational services for crystallographic macromolecular model building of proteins, RNA/DNA, secondary structure, side chains, loops, solvent and ligands. It also provides de-novo model building in cryo-electron microscopy density maps at resolution better than 4 A.	Automatic and objective interpretation of the experiment and provision of a highly complete built and refined model	There are computational services for macromolecular crystallography and cryo-electron microscopy but to our knowledge there is none comparable to the broad services provided by ARP.wARP	see above	Online computation is provided via the webserver which contains sufficient explanations therein	https://arpwarp.embl-hamburg.de/ or google for ARP/wARP remote service	1	We have 4000 unique users (defined by their email addresses)	Approximately 400-500 every year	Approximately 400-500 every year	931
Auto-Ricksha	Auto-Rickshaw web service provides computational service for crystal structure determination for macromolecule by various phasing methods including molecular replacement, starting from intensity data to partially refined structure.	Validation of the X-ray diffraction experiment at the Beamline and provision of highly complete and partially refined crystal structure.	There are computational services for macromolecular crystallography but to our knowledge there is none comparable to the service provided by Auto-Rickshaw.	see above	Online computation is provided via webserver which contains adequate explanation therein.	http://www.embl-hamburg.de/Auto-Rickshaw or google for Auto-Rickshaw and EMBL.	1	We have 3000 unique users (defined by their email address).	Approximately 400 – 500 every year	Approximately 400 – 500 every year	824
CCD	It is a meta-server providing visualisation of multiple sequence alignments and secondary structure predictions for the designing clones for protein expression experiments.	Easy analysis, design, and logistics for PCR-based cloning for structural biology		n/a	Webserver / metaserver integrating data and displaying in concise format	No.	0	n/a	n/a	n/a	n/a
CCP4 (all portals)	Provides services for macromolecular crystallography. 4 are for structure solution via molecular replacement, 2 are for structure solution via experimental phasing, and 1 is for space group and crystallographic origin validation.	Allows automated structure solution from experimental diffraction data. Most services will output an atomic model. This will need further rounds of checking and improvement, but the major step of obtaining good phase estimates will have been completed.	These are not competing services, but ones in a similar area. All services differ slightly in requirements and approach used. Hamburg services: ARP/wARP, auto-Rickshaw	Different approaches (CCP4 vs other software, and between different CCP4 pipelines). Sometimes one works, sometimes the other. For hard problems, good to have the choice. For easy problems, anything will work.	Online software provided through a webserver. http://www.ccp4.ac.uk/ccp4online Initial login gives access to all 7 services.	Normally available directly from CCP4 www.ccp4.ac.uk/ccp4online	Until recently, a CCP4-specific login was required. We now allow login via ARIA authentication.				Ample: 194 Balbes: 684 Crank2: 105 MorDa: 446 MrBUMP: 512 SHELX: 128 Zanuda: 224 SIMBAD: 70
CS-ROSETTA	CS-Rosetta is a protocol which generates 3D models of proteins, using only the 13CA, 13CB, 13C', 15N, 1HA and 1HN NMR chemical shifts as input. Based on these parameters, CS ROSETTA uses a SPARTA-based selection procedure to select a set of fragments from a fragment-library (where the chemical shifts and the 3D structure of the fragments are known). The fragments are assembled using the Rosetta protocol. The generated models are rescored based on the difference between the back-calculated chemical shifts of the generated models and the input chemical shifts, and when available, with a post-scoring procedure based on unassigned NOE lists. The CS-Rosetta3 grid-enabled web server, originally developed under the WeNMR e-Infrastructure project (www.wenmr.eu) uses resources provided by the EGI (www.egi.eu) and the associated National Grid Initiatives (NGIs).	CS-Rosetta is computationally highly demanding. Users can run calculations using the EGI HTC infrastructure. Further they are provided with a graphical representation and reliability estimate of the results.	BMRB in Wisconsin USA is operating another CS-Rosetta server. See https://csrosetta.bmrb.wisc.edu/csroset ta/submit	Never used the BMRB server - can't answer. Our portal was in production prior to the NMRFAM one and provides a graphical overview of the results.	Online web portal at: http://haddock.science.uu.nl/enmr/services/CS-ROSETTA3/	Available directly from haddock.science.uu.nl (the location of the portal at Utrecht University). But also links from West-Life, WeNMR (www.wenmr.eu), the EOSC-Hub marketplace (marketplace.eosc-hub.eu/thematic-services/94-wenmr.html)	1	239	0 (the portal was down since April and only put back in production in November)	9	
DisVis	DisVis allows to visualize and quantify the information content of distance restraints between macromolecular complexes. It performs a full and systematic 6- dimensional search of the three translational and rotational degrees of freedom to determine the number of complexes consistent with the restraints. In addition, it outputs the percentage of restraints being violated and a density that represents the center-of-mass position of the scanning chain corresponding to the highest number of consistent restraints at every position in space.	Easy access to DISVIS and use of the computational resources of the EGI grid, including GPGPU resources. Guided interpretation of results. No need for complex local installation.		Easy access to DISVIS and use of the computational resources of the EGI grid, including GPGPU resources. Guided interpretation of results. No need for complex local installation.	Web portal at: http://haddock.science.uu.nl/enmr/services/DISVIS	Available directly from haddock.science.uu.nl (the location of the portal at Utrecht University). But also links from West-Life, WeNMR (www.wenmr.eu), the EOSC-Hub marketplace (marketplace.eosc-hub.eu/thematic-services/94-wenmr.html), and EGI (www.egi.eu/use-cases/scientific-applications-tools).	0	296 See: https://nestor.science.uu.nl/user_map	121	38	
FANTEN	The program performs the calculation of the magnetic susceptibility anisotropy tensor for paramagnetic metalloproteins. Pseudocontact shifts and/or residual dipolar couplings and protein atom coordinates are needed as input data.	An extensive approach to the analysis of paramagnetic NMR data, from fitting to rigid docking, in a unified interface	NUMBAT	Interactive graphical interface. More extensive analysis	Online software provided through webserver. No registration needed. Has been linked to the VirtualFolder for data upload	direct link (in publication) http://abs.cerm.unifi.it:8080/	0				

Service Name	What does the service provide?	What benefit does this service give to its user base?	Are there any competing services?	What demonstrable benefit does this service provide over these competing services?	How is the service currently provided?	Is the service available through direct routes other than West-Life; if so which?	Is service-specific registration required to use the service?	If registration is required, how many registered users in total?	If registration is required, how many new registered users in 2017?	If registration is required, how many new registered users in 2016?	If submissions are connected to registered users, how many users placed submissions in 2017?
GROMACS	GROMACS (www.gromacs.org) is a versatile package to perform molecular dynamics, i.e. simulate the Newtonian equations of motion for systems with hundreds to millions of particles. GROMACS is able to work with many biochemical molecules like proteins, lipids and nucleic acids. The WeNMR GROMACS grid-enabled webportal combines the versatility of this molecular dynamics package with the calculation power of the WeNMR grid. This will enable the user to perform many simulations from the comfort of his/her internet browser anywhere in the world. The server is furthermore aimed to provide a user friendly and efficient MD experience by performing many preparation and optimization steps automatically. The GROMACS web server, originally developed under the WeNMR e-Infrastructure project (www.wenmr.eu) uses resources provided by the EGI (www.egi.eu) and the associated National Grid Initiatives.	Easy setup of molecular dynamics simulations for standard protein systems. Provides an equilibrated system that can be moved for production to other computational resources. Allows non-experts to run simple MD simulations.	Most likely, but not aware of any similar user-friendly setup		Via its web portal at: http://haddock.science.uu.nl/enmr/services/GROMACS/main.php	Available directly from haddock.science.uu.nl (the location of the portal at Utrecht University). But also links from West-Life, WeNMR (www.wenmr.eu), the EOSC-Hub marketplace (https://marketplace.eosc-hub.eu/thematic-services/94-wenmr.html)	1	121	0 (service was down)	9
HADDOCK	HADDOCK2.2 (High Ambiguity Driven protein-protein DOCKing) is an integrative, information-driven flexible docking approach for the modeling of biomolecular complexes. HADDOCK distinguishes itself from ab-initio docking methods in the fact that it encodes information from identified or predicted protein interfaces in ambiguous interaction restraints (AIRs) to drive the docking process. HADDOCK can deal with a large class of modeling problems including protein-protein, protein-nucleic acids and protein-ligand complexes.	Unique ability to incorporate a large variety of experimental data (biochemical, bioinformatics, NMR, cryo-EM, MS, …). Access to computational resources (local clusters and EOSC HTC resources)	There are other docking servers available online, but most are rather ab-initio docking server with limited if any capability to use experimental restraints.	Unique ability to incorporate a large variety of experimental data (biochemical, bioinformatics, NMR, cryo-EM, MS, …).	Web portal requiring registration (free for non-profit users). Different levels of access are provided that define the features/options that a user has access to.	Available directly from haddock.science.uu.nl (the location of the portal at Utrecht University). But also links from West-Life, WeNMR (www.wenmr.eu), the EOSC-Hub marketplace (marketplace.eosc-hub.eu/thematic-services/94-wenmr.html), and the EGI scientific applications and tools (www.egi.eu/use-cases/scientific-applications-tools/). And next to that the portal is referenced in a variety of web sites.	1	To date >11'000 from >90 countries See: https://nestor.science.uu.nl/user_map	1870	1621	1371
MetalPDB	MetalPDB is a public database that collects and allows easy access to the knowledge on metal sites in biological macromolecules, starting from the structural information contained in the Protein Data Bank (PDB)	Direct information on metal-binding sites in biological macromolecules of known 3D structure, including both functional and structural features. Ancillary services allow sites to be compared at the structural level			Online database. Flat copy downloadable.	direct link at http://metalweb.cerm.unifi.it/	0			
PDB-REDO	PDB-REDO is an expert system to optimise crystallographic structure models of macromolecules based on their experimental data. The input models are refined, rebuilt, and validated resulting in new models that better reflect the experimental data and our prior knowledge of (macro)molecular structure. The PDB-REDO system is available in three modalities: a web server for practicing crystallographers (accessible through the website pdb-redo.eu and web-service APIs), a databank of 'redone' PDB entries for the wider structural biology community (accessible through the website and multiple (third-party) services and programs), and as a downloadable software package for expert and high-throughput (industrial) users.	Server/service users get access to a comprehensive, yet minimal-effort, way to obtain high quality models of their own experimental data. Databank users have access to a huge dataset of high quality, consistently treated, structure models that are an excellent starting point for downstream research.			Webserver, databank, software package are available through https://pdb-redo.eu directly. Webservice interfaces exist from ARP/wARP (arpwarp.embl-hamburg.de) and CCP4 online (ccp4serv7.rc-harwell.ac.uk/ccp4online) PDBe(www.ebi.ac.uk/pdbe) and 3D-Bionotes (3dbionotes.cnb.csic.es/ws) display PDB-REDO data. The programs COOT (www2.mrc-lmb.cam.ac.uk/personal/pemsley/coot), YASARA (yasara.org), CCP4mg (www.ccp4.ac.uk/MG), and VHELIBS (urvnutrigenomica-ctns.github.io/VHELIBS) have native databank interfaces. Access to databank entries is described in detail at https://pdb-redo.eu/download-info.html	Directly through pdb-redo.eu	1	1800 registered users	450	500	790
PowerFit	PowerFit automatically fits high-resolution atomic structures into cryo-EM densities. To this end it performs a full-exhaustive 6-dimensional cross-correlation search between the atomic structure and the density. It takes as input an atomic structure in PDB- or mmCIF-format and a cryo-EM density with its resolution and outputs positions and rotations of the atomic structure corresponding to high correlation values. PowerFit uses the local cross-correlation function as its base score. The score is by default enhanced with an optional Laplace pre-filter and a core-weighted version to minimize overlapping densities from neighbouring subunits.	Easy access to Powerfit and use of the computational resources of the EGI grid, including GPGPU resources. No need for complex local installation.		Easy access to Powerfit and use of the computational resources of the EGI grid, including GPGPU resources.	Web portal at: http://haddock.science.uu.nl/enmr/services/POWERFIT	Available directly from haddock.science.uu.nl (the location of the portal at Utrecht University). But also links from West-Life, WeNMR (www.wenmr.eu), the EOSC-Hub marketplace (marketplace.eosc-hub.eu/thematic-services/94-wenmr.html), and the EGI scientific applications and tools (www.egi.eu/use-cases/scientific-applications-tools/).	1	To data 161. See: https://nestor.science.uu.nl/user_map	78	21	
Scipion Web Tools	Scipion Web Tools (SWT) is a web application built over Scipion framework software, offering access to predefined image processing workflows over the web. Current tools are divided in two sections: "Single particle analysis tools" which includes initial volume estimation, movie alignment and local resolution and "Validation tools" that focuses on ways to analyze some quality parameters of maps ('My reliability tool') and a protein interaction explorer tool accessing 3DIANA. SWT are technically a "web wrapper" for Scipion software, therefore it offers most of its features over the web. One of the Scipion features is the ability to easily switch from one Cryo-EM software package to another, allowing users to make the output data from one package, the input data for different package smoothly, thus trying out different software methods without installing and configuring anything.	Possibility to try some of the typical CryoEM processing workflows using Scipion framework software without any installation (online access).		N/A	Online software provided through a webserver.	Web server hosted at other location (http://scipion.cnb.csic.es/m/service s/) and linked from Scipion website (http://scipion.i2pc.es/).	0	N/A	N/A	N/A	N/A
Scipion Cloud	ScipionCloud and ScipionCloud-GPU are virtual appliances available at the EGI AppDB that can be used to deploy a Virtual Machine in the EGI Federated Cloud containing ready-to-use Scipion software with the most common EM-packages, plus remote desktop installed and configured to access the Virtual Machine through a Web Browser. GPU appliance is ready to be used on a GPU enabled virtual machine.	It can be used to deploy its own Scipion service on a machine in the Federated Cloud sites that support enmr.eu VO.	Scipion Web Tools	Scipion Web Tools only offer a set of predefined workflows to test Scipion on the web while ScipionCloud offers the whole Scipion functionality accessible also through a web browser.	Virtual Appliance on EGI AppDB catalog and also as images available at the FedCloud sites who endorse the image and enmr.eu VO.	Amazon Web Services AMI.	0	N/A	N/A	N/A	N/A
SpotON	SpotOn is a robust algorithm developed to identify and classify the interfacial residues as Hot-Spots (HS) and Null-Spots (NS) with a final accuracy of 0.95 and a sensitivity of 0.95 on an independent test set. The predictor was developed using an ensemble learning algorithm with up-sampling of the minor class and was trained on a large number of complexes and on a high number of different structural- and evolutionary sequence-based features.	Online tool for hot-spot identification. No need for complex local software installation.	There are other published hot-spot prediction methods. We compared our performance with those in our 2017 paper showing that SpotOn currently has the best performance. See SpotOn: High Accuracy Identification of Protein-Protein Interface Hot-Spots IS Moreira, PI Koukos, R Melo, JG Almeida, AJ Preto, J Schaarschmidt, ... Scientific Reports 7 (1), 8007	Better prediction performance	Via its web portal at: milou.science.uu.nl/enmr/services/SPOTON	Available directly from haddock.science.uu.nl (the location of the portal at Utrecht University). But also links from West-Life, WeNMR (www.wenmr.eu), the EOSC-Hub marketplace (marketplace.eosc-hub.eu/thematic-services/94-wenmr.html)	0	193 See: https://nestor.science.uu.nl/user_map	105	N.A.	
Virtual Folder	Virtual folder delivers a uniform way to integrate scattered data from different storage providers. Provided as public web application - with interface to connect scattered data storage. User can browse all the data from connected providers using VF interface or generate link to download/upload content hosted by the data storage providers via WEBDAV protocol using unique link which doesn't need any further authentication. This allows e.g. grid jobs as well as other services to access user's data and upload results to user's preferred data storage.	Uniform interface and way to perform data management of scattered data.	EUDAT B2DROP and B2... services	EUDAT B2DROP can be integrated into Virtual Folder as a provider. Other data can be made accessible from services based on WEBDAV or DROPBOX.	Online server as webserver. Scripts to deploy this service as private service e.g. for facility or lab use-cases		0				

Service Name	If submissions are connected to registered users, how many users placed submissions in 2016?	What is the submission unit recorded?	How many submissions were made in 2017?	How many submissions were made in 2016?	Is there support for service users in place?	If support is provided, please give details of the type of support available.	If support is provided, please give details of the frequency of maintenance of the help material.	If support is provided, please give metrics on usage of help material.	Is training provided for the service?	If training is provided, give details of the type(s) of training.	If training is provided, give details of the frequency of training.	If training is provided, please state the outcome(s) of training.	If training is provided, please give the number of participants (per training event).	If training is provided, please list the resources required to provide this training
3DBIONOTES-WS	N/A	Task (step)	9011	N/A	1	Online help and howto examples.	When new functionality are available.		0	N/A	N/A	N/A	N/A	N/A
AMPS-NMR	69	job	1383	3655	1	Email contact.			1	Training on the portal at training events (e.g. INSTRUCT training courses https://www.structuralbiology.eu/events/advanced-methods-for-the-integration-of-diverse-structural-data-/)	Yearly	Users learn how to submit calculations with different combinations of restraints and/or macromolecule types via the portal	20	staff
ARIA	i. 150 ii. 212	Access Visit approved (i.e. after peer review) (physical or remote) to an instruct Service/Technology Instrument bookings placed	i. 104 ii. 10685	i. 110 ii. 2683	1	Help Guides (Available at structuralbiology.eu/help) Support tickets (emails to admin@structuralbiology.eu / aria@structuralbiology.eu) Telephone helpline (Instruct Hub office)	Guides first published 13/12/2017, no scheduled maintenance but some edits to help guide content has been made each month so far Tickets responded to on a daily basis Phone calls accepted daily Monday-Thursday 10:00am - 3:30pm	56 guides currently available 738 unique (1444 total) page views of help pages since launch (13/12/2017). 459 support tickets resolved 06/04/2016-05/04/2017 625 support tickets resolved 06/04/2017-05/04/2018	1	Workshops Webinars	Once or twice a year Only started webinars this year: Once so far this year but another planned for May 2018	Familiarity with the features available in ARIA Able to use the ARIA GUI in the administration pages to perform management actions Participant issues/questions addressed Suggestions received from participants for new features and developments	i. Workshop (02/02/2018) 20 participants ii. Webinar (16/01/2018) 26 participants and 60 views of webinar recording	Staff (2-4) staff per workshop (1-2) staff per webinar Funds for transport, accommodation and refreshments for each workshop Webinar platform for webinars (currently supported by CORBEL project funded gotowebinar platform)
ARP/wARP	635	This is a set of files required for specific computational task	6100	3480	1	Every premature software termination (most typically due to file format and data content) is investigated and the users receive advice. There is a helpdesk and email notification of job submission, start and completion	The help material is updated at every new software release. Troubleshooting for data formats and contents is, wherever possible, incorporated into the software for future updates.	We provide support by communicating directly with the users . We do not count these but my guess would be about 100 ommunications per annum	1	As we advise the users on the best usage, this can be regarded as training. The webservice provides means of automatic re- submission of computational tasks with modified parameters.	As we advise the users on the best usage, this can be regarded as training. The webservice provides means of automatic re- submission of computational tasks with modified parameters.	I guess the users submit more jobs and obtain better results. We do not count this.	As written above, there are about 100 users per annum receiving advice on their specific computational task	Troubleshoot in one user's case takes anything between 10 minutes and several person-days.
Auto-Rickshaw	729	This is a set of intensity data files required for specific computational task.	4514	4353	1	Every premature software termination (most typically due to file format and data content) is investigated and the users receive advice. There is a email notification of job submission and successful completion.	Troubleshooting for data formats and contents is, wherever possible, incorporated into the software as soon it is realised and the help material is updated accordingly.	We provide support by communicating directly with the users, which is about 150 communications per annum.	1	We advise the users on the best usage and this can be regarded as training.	We advise the users on the best usage and this can be regarded as training.	I guess, the users submit more jobs and obtain better result. We do not count this.	As mentioned above, there are about 150 users per annum receiving advice on their specific computational task.	Toubleshooting one user's case takes anything between 10 minutes and several person days.
CCD	n/a	Hits and Unique visitors	6787 and 1271	3800 and 720 (953 and 240 from Sep/oct/Nov/Dec that logs started, a year [over]estimate is provided)	1	Help Page / FAQ / Dedicated email	Support is provided on demand, the help function is updated if specific questions arise to warrant such an update	300 hits on Help/FAQ	0	n/a	n/a	n/a	n/a	n/a
CCP4 (all portals)	Ample: 187 Balbes: 700 Crank2: 94 MorDa: 202 MrBUMP: 453 SHELX: 151 Zanuda: 196 SIMBAD: 15	Job	Ample: 667 Balbes: 3508 Crank2: 543 MorDa: 1777 MrBUMP: 1682 SHELX: 612 Zanuda: 489 SIMBAD: 341	Ample: 535 Balbes: 3148 Crank2: 587 MorDa: 790 MrBUMP: 1721 SHELX: 656 Zanuda: 598 SIMBAD: 148	1	Email to ccp4@ccp4.ac.uk	n/a	Queries received around once a week. Usually around submission problems, rather than how to use the service.	1	No specific training for CCP4Online, but often included in broader CCP4 training courses.				
CS-ROSETTA		User submissions (jobs) to the portal	20	33	1	There was a support mechanism in the old WeNMR site (now migrated). And otherwise via email			0	Only tutorial at haddock.science.uu.nl/wenmr/services/CS-ROSETTA3/csr-tutorial.html	No training events in the last years			
DisVis		User submissions (jobs) to the portal	553		0	DISVIS forum: ask.bioexcel.eu/c/disvis Online tutorials from www.wenmr.eu/tutorials	Tutorials are added on irregular basis.	So far little use of the forum (6 posts viewed ~3000 times in total)	0	Online tutorials from www.wenmr.eu/tutorials Used in various workshops around the world				
FANTEN		We are tracking contacts and fittings	6149 contacts; 1808 calculations	Not available	1	Email of IT staff at CERM/CIRMMP				Demonstration of the interface within training courses on biological (paramagnetic) NMR	occasional	Capability to use the interface	Average 20	none
GROMACS		User submissions (jobs) to the portal	0 (service was down)	107	1	There was a support mechanism in the old WeNMR site (now migrated). And otherwise via email. Or making use of the BioExcel forum.			0	Simple online manual: http://haddock.science.uu.nl/enmr/services/GROMACS/usage.php p				

Service Name	If submissions are connected to registered users, how many users placed submissions in 2016?	What is the submission unit recorded?	How many submissions were made in 2017?	How many submissions were made in 2016?	Is there support for service users in place?	If support is provided, please give details of the type of support available.	If support is provided, please give details of the frequency of maintenance of the help material.	If support is provided, please give metrics on usage of help material.	Is training provided for the service?	If training is provided, give details of the type(s) of training.	If training is provided, give details of the frequency of training.	If training is provided, please state the outcome(s) of training.	If training is provided, please give the number of participants (per training event).	If training is provided, please list the resources required to provide this training
HADDOCK	1319	User submissions (jobs) to the portal	33300	27291	1	HADDOCK forum: http://ask.bioexcel.eu/c/haddock Email support: haddock.support@gmail.com Online tutorials from http://www.wenmr.eu/tutorials HADDOCK software online manual at http://www.bonvinlab.org/softwa re/haddock2.2/manual/	Tutorials are added on irregular basis. The online manual is updated with new software versions (unfrequent)	The forum gets about 9k views per month	1	Online tutorials from http://www.wenmr.eu/tutorials Various workshops (from 1 to 3 days duration) around the world.	Usually in the order of 5 workshops per year, depending on demand.		Since training involved computer practical parts, the number of participants is limited (typically between 10 and 30)	1 to 2 persons depending on the size of the audience.
MetalPDB		Unique IP contacts	18442	14866	1	Email contact	The database is automatically updated on a monthly basis		0					
PDB-REDO	725	Jobs	5500	4500	1	Support by e-mail to pdbredo@gmail.com, directly to PDB-REDO developers, or to the CCP4 bulletin board, proactive support (developers contact users before support request are made), and a FAQ.	FAQ is updated when new question arise (rarely) other modes of support do not use ready-made material.	>175 support e-mails were received in 2017	1	Training for PDB-REDO is given in the context of international crystallography workshops and national structural biology workshops.	~6 times per year	The users have a better understanding of the algorithms in the PDB-REDO system and know how to interpret the results (crystallography workshops). Users understand the purpose and benefits of using the PDB-REDO databank as data source for downstream research (all workshops).	10-100 (typically 20)	Staff: 1 person month Travel/accommodation: EUR 7k / year
PowerFit		User submissions (jobs) to the portal	150	34	0	POWERFIT forum: http://ask.bioexcel.eu/c/powerfit Online tutorials from http://www.wenmr.eu/tutorials	Tutorials are added on irregular basis.	So far little use of the forum (5 posts viewed ~2750 times in total)	1	Online tutorials from http://www.wenmr.eu/tutorials				
Scipion Web Tools	N/A	Task (step)	30045	1970	1	Video tutorials, embedded help, Github issues. Users mailing list.	When new functionality or bugs appear.	Video tutorial number of visualizations on Youtube: 48, 28 and 48. Number of user mails (71 for Scipion questions).	1	Not for SWT. Yes for Scipion software. Workshop, practical courses.	Around 20 training events per year.	Train new users on the usage of Scipion software.	Around 20 students per event.	Scipion development team (and research staff) do it. Virtual machines are set up for the practical part, usually in AWS cloud.
Scipion Cloud	N/A	N/A	N/A	N/A	1	Documentation wiki and email support account.	When new version of appliance appears.	Number of support email received.	1	Practical course.	So far just one course (January 2018)	Train users to use Scipion in the cloud.	Around 20 students.	Scipion team and virtual machines on AWS cloud.
SpotON		User submissions (jobs) to the portal	165	N.A.	0	http://milou.science.uu.nl/cgi/services/SPOTON/spoton/help And via http://ask.bioexcel.eu	Rather simply submission process - no need for complex help material. The portal itself provides the required example and help manual	No support/help requests received so far.	0	N.A.	N.A.	N.A.	N.A.	N.A.
Virtual Folder					1	Only online documentation at https://h2020-westlife-eu.gitbook.io/virtual-folder-docs/virtual-folder	No maintenance. Documentation provided/updated at the end of release cycle. (once a year?)		0					

Service Name	How long has the service been operational?	Do you log service outages? If [Yes], please explain how outages are logged.	If outages are logged, provide (upload) details of service outages in the last year. (e.g. graphical representation of service provision showing downtime).	If outages are logged, explain any significant (> 1 day) service outages in the last year (planned or unplanned).	What is the penetration of the service in the structural biology community?	Is the service scalable to increase penetration?	What is the total number of publications acknowledging the use of the service?	How many of these publications were published in 2017?	Give details of past developments (with dates) to the service which have been made to ensure the service provision remains up-to-date with the needs of users and/or scientifically at the cutting-edge.	Do you have a plan for future developments of the service over the next 2 years to keep the service relevant and at the cutting-edge? If [Yes] give details.	What resources (infrastructure and staff) are required to continue operation of the service? Please list all that apply and include the number of person months per year for staff required.	For each of the resources listed above, please give an estimated financial cost (euros per year), and explain how these resources are supported (e.g. funded by X, Staff employed by X).
AMPS-NMR 3DBIONOTES-WS	from 2017	Downtime due to server maintenance (99,9% up time)	null	Server crash.			0	2	1	Update of the integrated databases (March 2018).	Expanding the integrated sources of informations and including new genomic and interactomic tools and functionalities. Different workshops and seminars will be done to have users feedback during 2018.	1 full time software developer for 1 year. 32-core Intel Xeon with 128GB ram server.	The server is allocated at CNB-CSIC.
AMPS-NMR	Since 2011		null		Medium	1	49 in Goggle Scholar 46 in Scopus	7 in Scopus	in 2018: implemented West-Life SSO and DIRAC submission	link to cloud storage	0.75 FTE	30000, funded by European Commission via H2020 projects
ARIA	Version Drupal: 2011 Version 1: 2013 Version 2: 15/08/2017	Indirectly through web analytics collected using piwik/matomo since 01/06/2017.		No outages >1 day since records began. 5hr scheduled outage on 15/08/2017 to migrate to from ARIA V1 to ARIA V2. There was intermittent service disruption on 22/12/2017 due to a planned internal switch upgrade.	The Instruct member countries have a total of 4.116.920 HRST researchers. Researchers either interested or using structural techniques are estimated at less than 3% of the biology community (<1% in 1991, 1% in 2010 (doi:10.3390/su4123234); 3% 2017 WOS . If we use this as a baseline, Instruct reaches 5% of its potential user community.	1	373 acknowledging Instruct (NB: We do not ask users to acknowledge ARIA however users of Instruct must use ARIA system to apply for access, and acknowledge Instruct in publications)	63	Version 2.0 release (15/08/2017) - Complete rewrite of the code. Simplified interfaces and menus in the administration pages. Instruct-ERIC website – Rewrite and reorganization of the user-facing pages of the Instruct website. Pages have been updated with a fresh look and to be more mobile friendly. (05/2018)	Continued expansion of ARIA to more organisations (RIs, academic institutions) API development to allow flow of data back into ARIA (currently data can only be pulled from ARIA). Help-desk feature to allow the creation of user generated help content, help content tagging with keywords for navigation. Notes feature to add text comments to a particular visit/proposal. Integration with Life Science AAI (pending successful H2020 INFRAEOSC-04 application)	Grid/Cloud: Currently no provision, but EOSC should become available as it develops. Instruct is a partner in this development for biomedical sciences RIs. GRID services are currently utilized independently through each facility (e.g. CNB Madrid) Local servers: 3 servers (plus 1 backup) Staff: 2.5 FTE = 30pm Small number of paid-for libraries	Server warranty/maintenance/replacement costs estimated at ??? per year funded by Instruct ERIC 2.5 FTE Staff employed by Instruct-ERIC = €150K per year full costs funded by Instruct ERIC Library licenses c. £30 per year, funded by Instruct-ERIC
ARP/wARP	Its first generation since January 2004 and the second, current generation since June 2017.	All computational jobs and their results are stored to the extent which is subject to the user- defined dissemination level (world, developers, confidential) described on the web service.	NULL	The service normally runs 24x7 unless there are accidental hardware or power-supply problems. Out IT group has statistics on the downtimes.	The service provided more than 30,000 computational jobs and its usage increases exponentially with about 6000 jobs provided in 2017. For the first half of 2018 we already have 5000 jobs, thus this number may double	1	A dedicated publication for the webservice does not exist and is currently being submitted. The use of ARP/wARP has been cited in about 7000 publications.	We have not yet done this analysis for 2017	The web service always uses the latest ARP/wARP software. 2004 version 6.1 2005 version 6.2 2006 version 7.0 2009 version 7.1 2010 version 7.2 2012 version 7.3 2013 version 7.4 2015 version 7.5 2016 version 7.6 2018 version 8.0		Infrastructure support - compute cluster, storage and server computers, network, web access Staff support - in addition to the involvement of our IT, one engineer and 5 researchers are currently involved in service and software support and development	Out of engineer and 5 researchers 3 are supported form external funds
Auto-Rickshaw	Its first generation since Junary 2005 and the second , current generation mid 2018.	All computational jobs and their results are stored to the extent which is subject to the user- defined dissemination level (world, developers, confidential) described on the web service.	null	The service normally runs 24 x 7 unless there are accidental hardware or power-supply problems. EMBL- Hamburg IT group has statistics on the downtimes.	The service provided more than 60000 computational jobs and its usage in 2017 increased to 4500.	1	The use of Auto-Rickshaw web service has been cited in about 500 publications.	The use if Auto-Rickshaw web service has been cited in about 30 publications in 2017.	The web service always used the latest Auto-Rickshaw software. The latest software has been updated on 16th June 2018.		Infrastructure support at the EMBL – compute cluster, storage and server computer, network, web access staff support in addition to the involvement of EMBL IT group. One engineer from EMBL (Victor Lamzin's group) and 1 researcher (myself) are involved in service and software support and development.	Myself employed by the Australian Synchrotron
CCD	About one year		null	n/a	Its the only tool of its kind publicly available - awareness needs to be improved though!	0	29	2	Completely re-implemneted in the context of West-Life.	Implementing better integration with PDB structures analysis	0.2 person months a year for regular maintenance	1,000 Euro salary costs, funded from various sources 1,000 Euro sever cost write-off value, funded from various sources
CCP4 (all portals)	First service was Balbes in 2013 (inherited from York). MrBUMP and Zanuda added in 2014. Others added in 2016.		null		Hard to separate from usage of downloadable CCP4 suite. CCP4 is ubiquitous in MX community. Pipelines in CCP4Online are also available in downloadable version.	0						
CS-ROSETTA	Jun-13		null		The service is rather specific to NMR and is not used heavily.	1	Total number of citations for the original WeNMR paper describing this (and other) service (J. Grid. Comp. 2010) and server related publications (J. Biomol. NMR 2013, 2015): 129	21	The most recent development is the porting of the service to make use of DIRAC4EGI for submitting to EGI HTC resources. Further an improved protocol and reliability metric was published in 2015 (J. Biomol. NMR)	The service is part of the EOSC-Hub WeNMR thematic services and we are planning to connect it to the EGI CheckIN SSO and possibly also to EUDAT for direct data download.	Operation of such portals is a team effort and difficult to measure in terms of PMs. An minimum estimate just to keep all the Utrecht portals operating and providing registration and support would be 1 FTE per year. This does not include any new development.	Funding comes from national and EU grants. There is no permanent staff (except for the PI) supported by the university.
DisVis	Since August 1st 2016		null		This is a rather new service so difficult to say. But since it allows analysis of MS cross-links we do expect a lot of interest. Even ThermoFischer a major producer of MS equipment is interested.	0	Two publications describe DisVis, one for the original software in 2015 (10 citations) one for the web server in 2017 (8 citations)		Most recent development has been a new registration system to comply with GDPR rules.		Operation of such portals is a team effort and difficult to measure in terms of PMs. An minimum estimate just to keep all the Utrecht portals operating and providing registration and support would be 1 FTE per year. This does not include any new development.	Funding comes from national and EU grants. There is no permanent staff (except for the PI) supported by the university.
FANTEN	Since 2015		null		Good	0	10	6			1 technical staff to maintain the web server operational: 0.5 PM/y	45,000 euro/year funded by CIRMMP

Service Name	How long has the service been operational?	Do you log service outages? If [Yes], please explain how outages are logged.	If outages are logged, provide (upload) details of service outages in the last year. (e.g. graphical representation of service provision showing downtime).	If outages are logged, explain any significant (> 1 day) service outages in the last year (planned or unplanned).	What is the penetration of the service in the structural biology community?	Is the service scalable to increase penetration?	What is the total number of publications acknowledging the use of the service?	How many of these publications were published in 2017?	Give details of past developments (with dates) to the service which have been made to ensure the service provision remains up-to-date with the needs of users and/or scientifically at the cutting-edge.	Do you have a plan for future developments of the service over the next 2 years to keep the service relevant and at the cutting-edge? If [Yes] give details.	What resources (infrastructure and staff) are required to continue operation of the service? Please list all that apply and include the number of person months per year for staff required.	For each of the resources listed above, please give an estimated financial cost (euros per year), and explain how these resources are supported (e.g. funded by X, Staff employed by X).
GROMACS	Since April 2011		null			0	Total number of citations for the original WeNMR paper describing this (and other) service (J. Grid. Comp. 2010) and server related publications (Journal of Chemical Theory and Computation 2012): 120	20	See plans.	The server is currently not in production. Its interface is being completely rebuilt in Flask and the Gromacs version will be updated to the latest 2018 version. The service is part of the EOSC-Hub WeNMR thematic services and we are planning to connect it to the EGI CheckIN SSO and possibly also to EUDAT for direct data download.	Operation of such portals is a team effort and difficult to measure in terms of PMs. An minimum estimate just to keep all the Utrecht portals operating and providing registration and support would be 1 FTE per year. This does not include any new development.	Funding comes from national and EU grants. There is no permanent staff (except for the PI) supported by the university.
HADDOCK	Since June 2008.		null	We have redundancy in our servers, so usually we can redirect from one portal to another in case of major outages. There has not been any outage longer than max 24 hours over the last years.	>11'000 registered users from >90 countries. Heavily used and cited.	1	Counting only citations to the HADDOCK web server publications (Nature Protocol 2010, JMB 2016 and J Grid Comp 2012): - 2017 citations: 201 (source Google Scholar)	Counting only citations to the HADDOCK web server publications (Nature Protocol 2010, JMB 2016 and J Grid Comp 2012): - 2017 citations: 201 (source Google Scholar)	See the HADDOCK-related publications at bonvinlab.org/publications Some highlights: Complete rewrite of the web Implementation of cryo-EM restraints (will be put in production in the course of 2017) Most recent development has been a new registration system to comply with GDPR rules	New developments are part of our continues research efforts funded by national and EU grants. We are going to put into production this year a completely new implementation of the HADDOCK portal supporing cryo-EM data. The new machinery will allow smoother updates and additions in the future.	Operation of such portals is a team effort and difficult to measure in terms of PMs. An minimum estimate just to keep all the Utrecht portals operating and providing registration and support would be 1 FTE per year. This does not include any new development.	Funding comes from national and EU grants. There is no permanent staff (except for the PI) supported by the university.
MetalPDB	Since 2012		null		High	0	62 in Google Scholar 44 in Scopus	18 in Scopus	In 2017 several improvements and extensions to the initial MetalPDB database have been finalized and reported in https://doi.org/10.1093/nar/gkx989		1 FTE	48000, funded by the Italian Ministry of University, CIRMMP and grants from regional charities
PDB-REDO	Databank since 2007, webserver since 2014	Manual records	null	There were none	PDB-REDO is a unique tool and visibility in the crystallographic community is high. Visibility in the overall structural biology community is good, but can be increased.	1	~800	~125	Over the past 3 years: 2018 incorporation of automated loop building, support for mmCIF input, various new algorithms 2017 integration of databank with web server on pdb-redo.eu, redesign of databank, addition of SSO login system, incorporation of homology-based restraints, full databank update, databank interface with 3d-bionotes, mmCIF output, various new algorithms 2016 parallelisation of computing for speed, databank interface with PDBe, new algorithms	Gridification of calculations to allow large scale-out required for fragment-based drug design campaigns. Major rewrite of the PDB-REDO system to ensure longterm maintainability. Expansion of scope to electron microscopy. New algorithms to deal with non-protein parts of structure models.	Minimal operation requirement: 5 person months/year + EUR 4k in hardware Operation plus further development: 24 person months year + EUR 12k in hardware + grid resources	Minimal operation: EUR 40k / year, staff employed by NKI, funded by institute and national grants Full operation: Eur 160k /year, staff employed by NKI, funded by institute and grants
PowerFit	Since August 2016		null		This is a rather new service so difficult to say.	0	Two publications describe PowerFit, one for the original software in 2015 (8 citations) one for the web server in 2017 (8 citations)		Most recent development has been a new registration system to comply with GDPR rules		Operation of such portals is a team effort and difficult to measure in terms of PMs. An minimum estimate just to keep all the Utrecht portals operating and providing registration and support would be 1 FTE per year. This does not include any new development.	Funding comes from national and EU grants. There is no permanent staff (except for the PI) supported by the university.
Scipion Web Tools	Since 2016	Local instance had minimal downtime due to server maintenance (99,9% up time). Federated Cloud instance had larger outages due to cloud maintenance tasks at CESNET.	null	Cloud maintenance tasks at CESNET	The instance running at our local server is being widely used, more after last publication. CESNET instance is not that used. Duplication of instances is not good for this but we cannot leave only CESNET instance without knowing the future of that SLA when Westlife finishes.	0	2	2	SWT last service update was on February 2018 to improve one of the tools (monores).	Expanding the number of tools. Increasing the hardware resources of the server hosting the service (number of CPU's, GPU's, memory and disk). Implement a user model to keep track of users and improve privacy. SWT is build on top of Scipion framework software and it will be kept up-to-date when future releases of Scipion software appear. Besides, new tools will be added to SWT when users request them or new protocols of interest are implemented.	Software developer with apache-django experience (half person month). System admin to maintain infrastructure (half person month or less). Hardware resources (local or cloud) to guarantee new users a reasonable performance in the use of the tools: disk, GPUs, CPUs and RAM.	65.559 euros per full year (staff employed by CNB) per person
Scipion Cloud	Since May 2017 (first version)		null		Advertised but not used due to the difficulty to request access to FedCloud for biologists (belong to VO, grid certificates...). A solution is to deploy the service for them and give them access.	1			Last appliance version released on May 2018.	New version releases to keep up to date with Scipion releases and other bug fixes and improvements. Extension of this service with the development of automatic deployment tool by MU partner.	Extend SLA between enmr.eu VO and FedCloud sites to provide cloud resources that endorse these appliances. Maintenance is hard to estimate but minimum 2PM to keep versions updated and give support / training.	65.559 euros per full year (staff employed by CNB)
SpotON	Since March 2017		null	N.A.	This is a rather new service so difficult to say. But the number of users has been growing quite fast so far.	0	4 citations of our August 2017 publication so far.	0 - all citations are from 2018	This is a very recent service	The service is part of the EOSC-Hub WeNMR thematic services and we are planning to connect it to the EGI CheckIN SSO	Operation of such portals is a team effort and difficult to measure in terms of PMs. An minimum estimate just to keep all the Utrecht portals operating and providing registration and support would be 1 FTE per year. This does not include any new development.	Funding comes from national and EU grants. There is no permanent staff (except for the PI) supported by the university.
Virtual Folder	2 years		null		New service. About 10-20 users.	1	0				staff 1-2 PM in order to keep updated security mechanisms as the service holds credentials/access token to user's data, staff 1-2 PM if new feature is requested (e.g. to integrated, support new data storage provider)	Staff employed by any organization or university who will maintain the service.

Appendix 2 – Responses to West-Life Questionnaire: End-Users

Tool	Responses	Link from west-life.eu website	Link from tool's own website	Link from your institution's website	Other	Ease of use (1-5)	Satisfaction with outcome (1-5)
3DBionotes	8	50.0%	12.5%	25.0%	12.5%	4.63	4.71
AMPS-NMR	10	0.0%	60.0%	30.0%	10.0%	4.40	4.20
ARP/wARP	3	0.0%	100.0%	0.0%	0.0%	5.00	4.67
Auto-Rickshaw	1	0.0%	100.0%	0.0%	0.0%	5.00	5.00
CCD	8	12.5%	37.5%	25.0%	25.0%	4.88	5.00
CCP4	11	9.1%	90.9%	0.0%	0.0%	4.45	4.09
Rosetta	4	50.0%	0.0%	25.0%	50.0%	4.25	4.25
DipCheck	0						
DisVis	3	0.0%	66.7%	33.3%	0.0%	4.67	4.67
FANTEN	1	100.0%	0.0%	0.0%	0.0%	5.00	5.00
GROMACS	4	0.0%	75.0%	0.0%	25.0%	4.00	4.33
HADDOCK2.2	159	10.7%	74.2%	11.9%	11.3%	4.18	4.26
MetalPDB	4	0.0%	75.0%	25.0%	0.0%	5.00	4.50
PDB-REDO	32	9.4%	71.9%	3.1%	28.1%	4.75	4.66
PowerFit	1	0.0%	100.0%	0.0%	0.0%	5.00	3.00
Scipion	2	50.0%	50.0%	50.0%	0.0%	3.50	4.50
SpotON	5	0.0%	80.0%	20.0%	0.0%	4.80	4.00
UNIO	0						
ViCi	0						
XPLOR-NIH	0						
Virtual Folder	1	100.0%	0.0%	0.0%	0.0%	3.00	5.00
Overall	255	11.4%	70.2%	11.8%	13.3%	4.36	4.35

Tool	Free comments
3DBionotes	The tool is good. However, sometimes it appears that its results show more interaction amongst proteins than they really do so..
AMPS-NMR	unable to successfully run NMR structure calculations using various tools (ARIA, XPLOR, etc.). Very frustrating.
AMPS-NMR	AMPS-NMR's water refinement tool worked very well for me, but it was difficult to extract stats for the calculation.
Auto-Rickshaw	Best thing that has ever been programmed.
CCD	Alignment, structure predictions and creation of plasmid maps have made the CCD the perfect tool for designing DNA/protein constructs for recombinant expression.
CCP4 - Crank2	Verg good experience with CRANK2
CCP4 - MRBUMP	Molecular replacement using CCP4 online programs is very useful. Thanks, Tomas

Tool	Free comments
HADDOCK2.2	A little more difficult to navigate/use but found the results very useful.
HADDOCK2.2	I would like Haddock to perform blind docking as well. The current tools is great though.
HADDOCK2.2	Very useful tool
HADDOCK2.2	it is a very much good tool ,i like it but i does not support multiple job simultaneously form single user id.
HADDOCK2.2	good work. please keep it up
HADDOCK2.2	Nice program. good for all structural biologist around the world. Please do continue the service.
HADDOCK2.2	used it for a course
HADDOCK2.2	The HADDOCK tool, especially the website, is very useful in studying protein ligand interaction.
HADDOCK2.2	Its hard to understand what is what in the results from the docking simulation
HADDOCK2.2	Please also mention in results the most appropriate binding residues between interacting partners like proteins.
HADDOCK2.2	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!
HADDOCK2.2	1. Response times are a little slow. 2. The energy scale provided is an arbitrary measure and not very applicable.
HADDOCK2.2	If docking parameters for membrane protein and their ligands are included in the portal, then it will be highly beneficial for users working on membrane protein docking.
HADDOCK2.2	In fairness, this was for a protein engineering project so I wasn't exactly expecting anything fantastic. I had a pretty good idea of interacting residues but I certainly wasn't 100% certain.
HADDOCK2.2	In my opinion HADDOCK is an extremely powerful tool, and the web-based version of the program is very easy to use and allows users to get rapid results.
HADDOCK2.2	Ignition way too long to get the results from the tool and in the end I had to use a different one.
HADDOCK2.2	It would be good to integrate FireDock and XSCORE scoring of the complexes automatically like the HADDOCK Score, BSA, and other energies are include in the analysis directory.
HADDOCK2.2	Extremely valuable resource. Has already yielded important observations for my research which could not have been obtained without access to this platform.
HADDOCK2.2	Excellent. It is an easy to follow web interface. Well designed. Leaves enough flexibility for the user to optimally design calculations.
HADDOCK2.2	Thanks bonvin good job
HADDOCK2.2	Great opportunity tool! Thank you very much and looking for accepting carbohydrates.pdb for docking too!
HADDOCK2.2	Very easy to use
HADDOCK2.2	Extremely good explanations and tutorials. The team responds to any questions quickly.
HADDOCK2.2	Easy to handle and interpret the result
HADDOCK2.2	Carbohydrates(.pdb) are highly desirable type of structures to dock to proteins
MetalPDB	The tool is well devised, easy to use and extremely useful!
PDB-REDO	Good experience with PDB-redo, but still prefer to re-refine manually myself using different programs (BUSTER, Phenix) for comparison.
PDB-REDO	great tool!
SpotON	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?).