West-Life Deliverable D2.3

Project Title:	World-wide E-infrastructure for structural biology	
Project Acronym:	West-Life	
Grant agreement no.:	**675858**	
Deliverable title:	Summary report of SB community engagement	
WP No.	2	
Lead Beneficiary:	7 - Instruct	
WP Title	Dissemination, Training, and Outreach	
Contractual delivery date:	30-April-2017	
Actual delivery date:	30-April-2017	
WP leader:	Instruct	7
Contributing partners:	STFC, NKI AVL, EMBL, MU, CSIC, CIRMMP, UU, INFN	

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Contents

1 Executive summary

West-Life VRE provides a platform offering variety of services and information on the services. Having an overview of experiments performed through an operational pipeline accessing different facilities in sequence would be extremely beneficial for the already well-informed community. This can be further publicised by West-Life presence at structural biology conferences, workshops and meetings. Flyers, presentations and posters at external meetings have already been made and will be continued. Through engagement channels like mailing lists identified by the workpackage, more than 5000 stakeholders from the structural biology community were contacted for information gathering exercised like surveys. The project website has news items that is updated with the latest structural biology happenings and is linked to the Structural Biology Research Infrastructure (Instruct). The project website also has an overview of the latest events in the community thus promoting collaboration and further engagement.

2 Project objectives

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

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

3 Detailed report on the deliverable

3.1 Background

A key part of delivering services to community at large is to promote the understanding and importance of structural biology by providing information on the value of the research being supported, the resources underpinning the service and to share knowledge and experiences arising from the project with a broader stakeholder community. Information on the services and their uses need to be disseminated to the well versed structural biology community through West-Life presence at various scientific conferences and meetings. The project website continues to be a major platform for providing updates on project delivery, training and scientific events and structural biology community news.

3.2 Engagement activities with Structural Biology community

3.2.1 Identification of structural biology user community and methods of engaging with them

As part of the work package 2 and 5, work was undertaken to identify and quantify users of structural biology community and users of tools and services provided through West-Life. Deliverable D5.2 Overview (baseline) of services and portals reported the total number of >16000 users for the portals providing access to services, who could be identified as the primary user community for West-Life. Some of the portals by West-Life partners, however, do not require authentication of users and thus are unable to accurately contribute to the above statistic, making the community of users a large number of scientists across the globe.

After identifying the user communities, it was important to find a way of communicating and engaging with these users. Milestone M2.2 Engagement Plan, recognised and reported different mailing lists within each partner of West-Life. These continue to provide an effective channel of engagement and was used to send survey for Workpackage 3. The survey was sent among communities for their use of structural biology data and tools/services, identifying gaps in data standards and software availability for broader usage of SB data. The survey is still open and is available at: https://goo.gl/forms/8Hkf7jtoendn3EWf2. The survey will close and results analysed before the West-Life Roundtable meeting (Deliverable D3.2 Organisation of a round table or joint meeting

involving ESFRIs), to be held at Brno on 24th May, 2017. The information gathered through the survey would feed into the strategic foresight of West-Life VRE and towards discussion with the biomedical ESFRIs at the roundtable mentioned above. Also, these will further be incorporated into deliverable D3.3 Report on requirements by other Research Infrastructures.

3.2.2 Presence at conferences and workshops

A recent CORBEL MIUF survey identified that the best means of dissemination and communication of Research Infrastructure information is via participation at scientific conferences and publication in the scientific literature[1]. As an eInfrastructure project, West-Life will also benefit from continued presence at conferences and workshops for better dissemination of information about the project and the VRE. Partners of West-Life presented 5 posters at different conferences and cited West-Life at 53 lectures at conferences worldwide (Appendix 3). West-Life was also acknowledged in more than 3 published journal articles. West-Life was also represented through presence at different events with a list of future events (Appendix 2) documented part of the engagement plan available in the internal wiki: http://internal-wiki.west-life.eu/w/index.php?title=Engagement_Plan. Project partners are continually encouraged to use West-Life branded templates for presentations and posters, use West-Life logos, namecheck other partners and distribute business cards when attending networking events.

3.2.3 Website and social media

Keeping the website current with up-to-date information and dynamic content is imperative for engaging with user communities. The West-Life website (https://west-life.eu/) pulls the news and events content from Instruct (https://www.structuralbiology.eu/), thus disseminating important structural biology information to West-Life users. The website also has Twitter widget engaging with different user communities, partners and collaborators. The @WestLifeSB twitter account has 102 followers and has 440 tweets engaging with policy makers, partners, collaborators and users, averaging excess of 100 profile views per month. Owing to the emergence of Twitter as a support platform, with specific instance of such support request in West-Life, the website also encourages users to contact West-Life using the twitter handle. Webinars and lecture, collected by WeNMR project, on the tools and services available to the users through West-Life are uploaded to the WeNMR YouTube Channel. More lectures from workshops will be added to this channel for further dissemination.

The West-Life website has also been improved with the facility of a forum facility for immediate support of user communities. While the tools and services provided through West-Life have their own established portals and support mechanisms, the forums and associated support pages in West-Life website will direct users to the correct help centre.

3.2.3 Flyer and promotional material

Workpackage 2 produced West-Life flyer after consultation with partners and it is made available for the everyone in the project to circulate among collaborators and at events. The flyer contents and the design were revisited through consultation with new user communities including public engagement expert, to make sure that the message and the text remain relevant to not just structural biology community but to a wider audience. The flyer is attached in Appendix 1.

References cited

1. CORBEL MIUF Survey: Conducted by Work Package 3 of CORBEL Project No. 654248

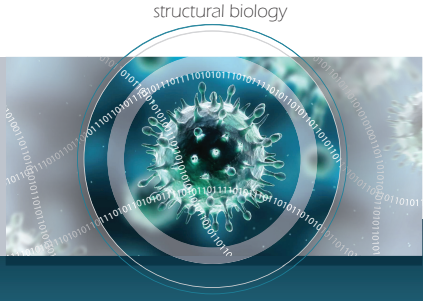
Appendix 1: West-Life Flyer

West-Life

West-Life: your virtual research environment for structural biology

Participants

West-Life is a Horizon 2020 Virtual Research Environment project (EINFRA No 675858) with 10 partners from 7 EU countries.



STFC, United Kindgom
NKI AVL, Netherlands
EMBL, Germany
Masarykova univerzita, Czech Republic
CSIC, Spain
CIRMMP, Italy
Instruct, United Kingdom
Universiteit Utrecht, Netherlands
LUNA, France
INFN, Italy

- Automated and integrated data management
- Provide access routes to cloud & grid resources
- Automated pipelines to process structural biology data
- Training on advanced computational solutions in structural biology

This project receives funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 675858.

- View all your data in a single, coherent place
- West-Life is your portal to processing data in the cloud
- Connect your processing together with a single portal

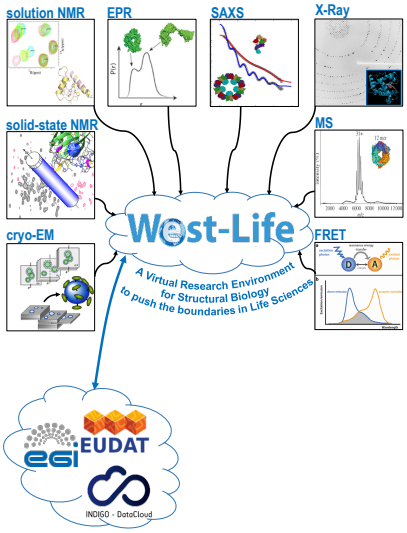
Visit: west-life.eu
Tweet: @WestLifeSB

West-Life
Life Sciences in the Cloud

West-Life pilots an e-infrastructure for providing data services and tools for structural biology

West-Life is a Virtual Research Environment (VRE) through which users from the life science research community can access services and tools that will advance their research in the area of structural biology.

- Support for experimental techniques and access generic data services developed by EUDAT and EGI
- Integrate existing data management services and develop new ones
- Building on strong foundations setup by WeNMR and European structural biology community under the umbrella of Instruct
- Integrated approaches to Bio Medical Sciences made more accessible



Integrate data management facilities

Integrate computational tools

West-Life

Appendix 2: Future events

Event	Location	Date	Target
FEBS Combined Practical and Lecture Course Chemistry of Metals in Biological Systems	Belgium	May 5 2017	New Communities
Instruct Biennial Structural Biology Meeting 2017	Brno, Czech Republic	May 21-24 2017	Structural Biology Community
iNEXT All Hands Meet	Brno, Czech Republic	May 21 2017	Structural Biology Community
GRC Computational Aspects of Biomolecular NMR	Sunday River ME, USA	June 11-16, 2017	Industry and new communities

CCP4/APS School in Macromolecular Crystallography	Argonne, USA	June 2017	Industry and Structural Biology Community
Biophysical Society Thematic Meeting	Berlin, Germany	August 25-29 2017	Structural Biology Community
PDBe API - search and entry API Workshop			Structural Biology Community
Drug Discovery 2017		2017	Industry and New communities
iNEXT training course Bridging solution methods: from NMR to X-ray scattering and biophysics	Patras, Greece	2017	Structural Biology Community and New Communities

Appendix 3: List of presentations by West-Life partners at various events

Lecture by Robbie Joosten. “How good is my model? And can it be improved?”, Computational Biotechnology at the Nanoscale, Faridabad, India, February 15-20, 2016.

Lecture by Alexandre Bonvin. “West-Life: A virtual research environment for structural biology”. International Symposium on Grid and Cloud Computing, Tapei, Taiwan, March 15-18th, 2016.

Lecture by Alexandre Bonvin. “High resolution modelling with 3D blurry images”. Institute of Biological Chemistry, Academia Sinica, Taipei, Taiwan, March 15th, 2016.

Lecture by Antonio Rosato. “The MoBrain Competence Center for Translational Research from Molecule to Brain”, EGI Conference 2016 - Opening science in Europe and in the World, Amsterdam, The Netherlands, April 4-6, 2016.

Lecture by Alexandre Bonvin. “Information-driven modelling of biomolecular complexes”. INSTRUCT practical course on “Advanced methods for the integration of diverse structural data with NMR data – 2nd Edition”, Utrecht, the Netherlands, April 11-15, 2016.

Lecture by Antonio Rosato. “Molecular dynamics for NMR-based protein structure refinement”, INSTRUCT practical course on “Advanced methods for the integration of diverse structural data with NMR data – 2nd Edition”, Utrecht, the Netherlands, April 11-15, 2016.

Lecture by Alexandre Bonvin. “Sense and simplicity in HADDOCK scoring: Lessons from CAPRI”. CAPRI meeting, Tel Aviv, April 17-20, 2016.

Lecture by Alexandre Bonvin. “Integrative modelling of biomolecular complexes using HADDOCK2.2”. BioExcel workshop, EBI, Hinxton UK, May 3-4, 2016.

Lecture by Alexandre Bonvin. “Integrative modelling of biomolecular complexes”, School on molecular modelling for life science, Pula, Italy, June 6-10, 2016.

Lecture by Alexandre Bonvin. “Structure, affinity and specificity riddles in biomolecular interactions”. 13th Annual Meeting of the Bioinformatics Italian Society - keynote lecture, Salerno, Italy, June 15-17, 2016.

Lecture by Alexandre Bonvin. EMBO Global Exchange Lecture Course on “Structural and Biophysical Methods for Biological Macromolecules in Solution”, Suwon, South Korea, June 19-26, 2016.

Lecture by Alexandre Bonvin. “Integrative modelling of biomolecular complexes: High-resolution modelling with blurry 3D images”, Summer Workshop by Biochemistry Division of Korean Chemical Society, KAIST, Daejon, South Korea, June 27, 2016.

Lecture by Robbie Joosten. “Validation & optimisation: From a solved structure to the final model”, CCP4/APS School in Macromolecular Crystallography, Argonne, IL, USA, June 21-29, 2016.

Lecture by Gregor Chojnowski. "Automated Protein Model Building with ARP/wARP 7.4", CCP4/APS School in Macromolecular Crystallography, Argonne, IL, USA, June 21-29, 2016.

Lecture by Gregor Chojnowski. "ARP/wARP Automatic Building", CCP4 SPring-8 school: From data processing to structure refinement and beyond January 23 – 27, 2017.

Lecture by Alexandre Bonvin. EMBO practical course on “Integrative modelling of biomolecular complexes”, Barcelona, Spain, July 4-9, 2016.

Lecture by Alexandre Bonvin. EMBO practical course on “Multidimensional NMR in Structural Biology”, Joachimsthal, Germany, July 11-15, 2016.

Lecture by Alexandre Bonvin. “Integrative modelling of biomolecular complexes”, Institute Pasteur course on integrative structural biology, Paris, France, July 20-21, 2016

Lecture by Marco Verlato at the DI4R conference, Krakow, Sept. 2016, Federated accelerated computing platforms for EGI

Lecture by Anastassis Perrakis, “From ARP/WARP to PDB_REDO: a short history and perspectives”. Joint International Conference of the HeCrA and the HSCCB, Athens, Greece, October 7-9, 2016.

Lecture by Wouter Touw (NKI), “Validation-driven model optimisation”. X-Ray Methods in Structural Biology, Cold Spring Harbour, NY, USA, October 10-15, 2016.

Lecture by Alexandre Bonvin, “West-Life: Structural biology in the clouds”. iNext user meeting, Alcala de Henares, Spain, October 19-21, 2016.

Lecture by Robbie Joosten, “PDB_REDO: What’s (i)NEXT? ”. iNext user meeting, Alcala de Henares, Spain, October 19-21, 2016.

Lecture by Alexandre Bonvin. “Structure, affinity and specificity riddles in biomolecular interactions”. Modelling of protein interaction conference, Lawrence KS, USA, October 27-29, 2016.

Lecture by Alexandre Bonvin. “High-resolution, integrative modelling of biomolecular complexes from fuzzy data”, Helmholtz Training Course on Integrative Structural Biology, Braunschweig, Germany, November 7-11, 2016

Lecture by Antonio Rosato. “INSTRUCT, a distributed infrastructure for integrated structural biology”, FAIR Data Management: best practices and open issues, Firenze, Italia, November 14-15, 2016.

Lecture by Alexandre Bonvin. “High-resolution, integrative modelling of biomolecular complexes from fuzzy data”, EMBO conference on Molecular Machines: Integrative Structural and Molecular, November 20-23, 2016

Lecture by Bart van Beusekom (NKI). “Homology-based restraints improve low-resolution protein structure models”, CHAINS 2016: Chemistry Matters for the Future, Veldhoven, The Netherlands, December 6-8, 2016.

Lecture by Robbie Joosten. “Model validation and optimisation”, DLS-CCP4 Data Collection and Structure Solution Workshop, Oxford, UK, December 13-20, 2016.

Lecture by Jose Miguel de la Rosa. INSTRUCT practical course: Advanced methods for the integration of diverse structural data with NMR data – 2nd Edition, Utrecht, Netherlands, April 11-15, 2016

Lecture by Jose Maria Carazo. INSTRUCT practical course: Advanced methods for the integration of diverse structural data with NMR data – 2nd Edition, Utrecht, Netherlands, April 11-15, 2016

Lecture by Jose Miguel de la Rosa. “Cryo EM solving the structure of macromolecular complexes: A hands on workshop One day practical workshop with Scipion”, International Symposium on Grids and Clouds", Taipei, Taiwan, March 14-17, 2016

Lecture by Jose Maria Carazo. “Soft validation in cryo EM”, Weizmann Center, Tel Aviv, Israel, March 2016

Lecture by Laura del Caño & Jesus Cuenca. “CryoEM: From Biomedical impact to Cloud deployment”, EGI Conference 2016, Amsterdam, Netherlands, April 8, 2016

Lecture by Jose Maria Carazo. “Cryo Electron Microscopy: The EM RESOLUTION REVOLUTION”, Leloir Foundation, Buenos Aires, Argentina, July 2016

Lecture by Jose Maria Carazo. “The EM RESOLUTION REVOLUTION”, Universidade de São Paulo, Sao Paulo, Brazil, July 2016

Lecture by Jose Maria Carazo. “The Electron Microscopy “Revolution” and the need of new data validation and data integration approaches”, National Institute of Medical Sciences and Nutrition Salvador Zubirán (INCMNSZ), Mexico DF, August 2016

Lecture by Jose Maria Carazo. “Pervasive data processing and information integration in Cryo Electron Microscopy”, EGI Conference 2016, New York, USA, August 2016

Lecture by Lucia Banci. “Cellular Structural Biology: from structures to functional processes”, 42nd Conference on "In the Vanguard of Structural Biology: Revolutionizing Life Sciences", 4-7 October 2016, Naito, Japan.

Lecture by Lucia Banci. “Cellular Processes Described at Atomic Resolution by NMR” , 27th International Conference on Magnetic Resonance in Biological Systems (ICMRBS), 21-26 August 2016, Kyoto, Japan

Lecture by Lucia Banci. “NMR in Cellular Structural Biology: combining atomic resolution with the cellular context” British Biophysical Society, Biennial Meeting, 6-8 July 2016, Liverpool, UK

Lecture by Lucia Banci. “NMR in Cellular Structural Biology: from structures to functional processes”, Euromar 2016, 3-7 July 2016, Aarthus, Denmark.

Lecture by Lucia Banci. “Spectral Assignment and Structure Calculation”, EMBO Global Exchange Lecture Course, 19-26 June 2016, Suwon, Korea.

Lecture by Lucia Banci. “What we learn from motions of the biomolecules?”, 14th International School of Biological Magnetic Resonance, 7-17 May 2016, Erice, Italy.

Lecture by Lucia Banci. “NMR in Cellular Structural Biology and few cool ways to do NMR” Scientific Symposium: 50 Cool Ways to Do NMR, 11 April 2016, Frankfurt, Germany.

Lecture by Martyn Winn. “What to do with all that Data” at “Advanced Data Collection for High Resolution cryoEM: How to make the most of your National Facility Visit”, Biochemical Society Training Day, Diamond National EM Facility (eBIC), 6 September 2016

Lecture by Martyn Winn. “Life Sciences work in STFC” at IBM-STFC workshop, IBM Yorktown, 13 April 2016

Lecture by Chris Morris. "DI4U" DI4R: The first cross e-infrastructure event for users, Krakow, 28-30 September 2016

Lecture by Alexandre Bonvin. High-resolution integrative modelling of biomolecular complexes from fuzzy data. ISGC 2017, Taiwan

Lecture by Alexandre Bonvin. The DisVis and PowerFit web servers: Explorative and Integrative Modeling of Biomolecular Complexes harvesting EGI GPGPU resources. ISGC 2017, Taiwan (https://indico4.twgrid.org/indico/event/2/session/30/contribution/4)

Lecture by Jose Maria Carazo. Image processing in cryo Electron Microscopy (cryo EM): Analyzing reliability and quality. ISCG 2017, Taiwan. (https://indico4.twgrid.org/indico/event/2/session/30/contribution/134)

Lecture by Jose Maria Carazo. Image Processing in cryoEM: Open problems and current perspectives. ISGC 2017, Taiwan

Lecture by Jose Maria Carazo. Image Processing in cryoEM: Quality checks. Netherland Center for Nanoscopi, Laiden, 27 January 2017

Lecture by Antonio Rosato. Molecular dynamics of proteins in the cloud. ISCG 2017, Taiwan.

(https://indico4.twgrid.org/indico/event/2/session/31/contribution/38)

Lecture by Marco Verlato. EGI federated platforms supporting accelerated computing. ISCG 2017, Taiwan. (https://indico4.twgrid.org/indico/event/2/session/47/contribution/6)

Lecture by Jose Maria Carazo. Image processing in cryoEM: Validation. Max F. Perutz Laboratories. Dept. of Structural and Computational Biology, University of Vienna, 16 March 2017