

Deliverable D2.4

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Deliverable written by Narayanan Krishnan, Susan Daenke

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1 Executive summary

- From the inception of the project, West-Life has kept focus on engaging with Industrial partners. Through partner interactions with Industrial collaborators and establishing new interactions by representations at Industrial participant events, the project has been endeavouring to spread the achievements of West-Life enabled tools and services. West-Life has also been interacting with industrial scientists and solutions providers to understand their needs from the structural biology solutions and services and in training early career/established structural biologists. During the remainder of the project, West-Life will enable users from Industrial research to understand and utilise tools and services provided through the project through concerted efforts on engagement including website, social media, conferences and networking.

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		
2	Provide automated pipelines to handle multi-technique datasets in an integrative manner		
3	Provide integrated data management for single and multi-technique projects, based on existing e-infrastructure		
4	Foster best practices, collaboration and training of end users	Yes	

3 Detailed report on the deliverable

3.1 Background

One of the key factors defining the success of West-Life in structural biology research is to provide valuable tools and services to all stakeholders. While the different objectives and tasks within the project aim to deliver this, it is important that this includes a community beyond academic researchers. Work Package 2 focuses on dissemination, training and outreach of the project activities, outputs and achievements, focusing on developing engagements with industry. West-Life aims to leverage existing collaborations with Industry through the project partners and build new relationships to identify and establish users for VRE services and in doing so understand the needs of structural biology research in an industrial context.

3.2 Engagement Activities

3.2.1 Identification of Industrial Users

West-Life tools and services are predominantly developed and maintained by partners and funded independently through various funding sources and collaborations. Most publicly funded projects mandate the outcomes to be free for the public to use and this includes scientists/researchers from commercial entities, particularly where pre-clinical research is involved. This presents a hurdle in identifying and quantifying the user base of the different services enabled through West-Life.

Grid/Cloud resources provided through EGI are an essential resource, however, the funding/payment model for users from for-profit establishments needs to be clarified before jobs can be issued through West-Life for their services. This could take the form of a Memorandum of Understanding between the parties to provide a basis for use. West-Life is preparing Terms of Use suitable for both academic and industrial customers. In particular, these terms of use will make it clear that the service provider claims no ownership of the results of the computation.

For pharmaceutical companies of considerable size/revenues, this is relatively trivial – either a

payment model can be quickly established or they have sufficient compute power/storage within their own organisations to handle complex calculations and the requirements needed to run West-Life tools. The value of a ligand bound structure can be more than 100,000 Euros if the ligand is drug-like. Many companies will prefer to keep such data within their firewall. Certain software which is provided through West-Life is also available for use by industrial users. DevOps is a modern approach to server maintenance that makes it easier to clone a service and West-Life will look at facilitating industrial use in this way.

With the advent and increase in popularity of cryo-EM and integrative modelling techniques, small and medium sized pharmaceutical companies are increasingly looking for easy access to clusters of compute/storage infrastructure and West-Life could help them in this endeavour. However, industrial users are in the small minority of software users where this information is tracked. In most cases, the specific use by industry is not recorded (Table 1).

Table 1: Tracked users of West-Life software services

Portal	Method	Service	grid/ cloud- enabled	Total no. of Users	No. of Industrial Users
Scipion	Cryo-EM	3D electron microscopy online processing workflows	-/+	-	Free to use resource (when no FedCloud resources are used) – no industrial user tracking
GROMACS	Modelling	Molecular dynamics simulations	+/-	112	
ViCi	Modelling	In silico ligand-based drug design	-/-	292	
HADDOCK	NMR/modelling	Docking of biomolecular complexes	+/-	>9900	13 companies
DISVIS	NMR/modelling	Visualise distance restraints between macromolecular complexes			
AMPS-NMR	NMR	Molecular dynamics simulations with AMBER	+/-	300	None, but license allows them
CS-Rosetta3	NMR	Structure prediction with chemical shifts from NMR	+/-	51	

FANTEN	NMR	Determination of anisotropy tensors (NMR)	-/-	-	Free to use resource – no industrial user tracking
UNIO	NMR	Structure calculations including NOE assignment from NMR data	+/-	59	
XPLOR-NIH	NMR	Protein solution structure determination through structural restraints, simulated annealing calculations and energy minimization	+/-	100	License excludes for-profit users
ARP/wARP	X-ray	Crystallographic Macromolecular Model Building	-/-	4088	
Auto-Rickshaw	X-ray	Automated crystal structure determination platform	-/-	2319	
CCP4 - Ample*	X-ray	Automated search model generation and molecular replacement (MR)	-/-	20	
CCP4 - Balbes	X-ray	Automated MR pipeline	-/-	1155	
CCP4 - Crank2*	X-ray	Structure solution pipeline for experimental phasing	-/-	10	
CCP4 - MrBUMP	X-ray	Macromolecular structure solution by MR	-/-	580	
CCP4 - Shelx*	X-ray	SHELXC/D/E structure solution	-/-	19	
CCP4 - Zanuda	X-ray	Space group and crystallographic origin validation	-/-	264	
PDB-REDO	X-ray	Optimization of crystallographic structure models	-/-	1500	Free to use resource – no industrial user tracking
CCD	X-ray/Molecular Biology	Design of constructs for protein crystallography	-/-	-	Free to use resource – no industrial user tracking

West-Life tools and service portals rely heavily on EGI (<https://www.egi.eu>), negotiated mostly

by the project partners, for the use of Grid (<https://www.egi.eu/services/high-throughput-compute/>) and Cloud (FedCloud, <https://www.egi.eu/services/cloud-compute/>) computing resources. While West-Life have grid/cloud enabled tools and portals available for Industrial users, usage of EGI resources enabled through partners are restricted for for-profit use – unless there is an understanding between the EGI and the client (EGI terms of use: <https://www.egi.eu/terms-of-use/>). EGI has dedicated information for businesses on how they can access EGI services at <https://www.egi.eu/business/>. West-Life will present this information and guide industrial users to the above mentioned EGI business contact point.

3.2.2 Events

West-Life partners have developed existing and new connections with industrial collaborators using co-organised workshops and training workshops. One example is the Instruct (Partner 7) funded training course (Appendix 2) on *Image processing applied to the structural characterisation of biological macromolecules* co-hosted by CSIC (Partner 5) and FEI (<https://www.fei.com>). The trainers included eminent scientists from FEI along with scientists from the consortium partners. Participants were mostly doctoral students and post-doctoral scientists from academic institutions and also from pharmaceutical industry.

West-Life along with Instruct-Ultra (H2020 funded project led by Instruct, Partner 7), organised *Instruct Workshop on cryoEM best practices* (Appendix 3) where participants from both academic and industrial communities were selected to pilot a platform for sharing experiences and breakthroughs in the area of cryo-EM research and facility management.

West-Life will co-organise another industrial user meeting in partnership with iNEXT (H2020 funded project led by UU, Partner 8) on March 2018 in EMBL Grenoble. The meeting aims to provide a forum for students and researchers from both academic and industrial backgrounds, including pharmaceutical and biotech companies, to exchange and publicise information on the application of West-Life services to both user groups and to foster the transition of early career researchers from the academic community to industry.

West-Life partners have coordinated events specifically to bring communities together. As part of work towards project milestone M6, an engagement plan was created with specific actions for Industrial engagement: a list of events involving different communities were drawn up with

information exchange as the main objective (Appendix 1). Events included the Protein Structure Determination in Industry (PSDI, <http://www.psd2017.org/>) conference series and the Drug Discovery conference series (<http://elrig.org/portfolio/drug-discovery-2017-elrigdd17/>). At PSDI 2016, West-Life was represented by Instruct (Partner 7) and at PSDI 2017, there will be multiple partners (including CSIC - Partner 5, Instruct – Partner 7) presenting at workshops and training events.

3.2.3 Website and other outreach material

The CORBEL Medical Users Infrastructure Forum (MIUF) surveys identified the most effective ways of connecting Research Infrastructures to scientific communities as i) through collaborators (54.8%), ii) through a website (38.4%) and iii) through conferences (25%)¹. As an e-Infrastructure project, West-Life has built on this information to tailor its outreach approach where maximum impact can be achieved. West-Life partners have presented the project objectives and outcomes at many conferences and leveraged a close partnership with Industrial researchers. The MIUF also surveyed the satisfaction with Research Infrastructure websites and most respondents scored the description of services and the ease of finding information from project webpages very low. A more recent review by MIUF highlighted the importance of a web-services catalogue which can be used by all life sciences communities to find appropriate services and tools for their needs. Since the target life sciences communities include clinical practitioners through to basic science researchers, to ethicists and data managers, the challenge is to design a choice hierarchy that can guide users through a very comprehensive collection of services spanning all the biomedical sciences RIs to enable the appropriate choices to be made quickly. The process should provide a selection within 3 clicks of start and be searchable. This is a difficult challenge, but essential if the RI services are to be efficiently utilised by the large funded projects (e.g. ERAnets).

West-Life proposes to develop specific webpages with information relevant to business users. Services will be described with the applicable cost of access and any restrictions (licences, permissions). The pages can be designed in a simple tile layout to make choices easy and information clear and concise. In order to enhance collaborations with Industrial scientists, the Industry specific pages will also provide direct information of Principal Investigators of the different services and tools enabled through West-Life. The West-Life project website will have a menu tab 'Business', which will become the entry point for Industrial users. The Business

page could have the following:

1. Service catalogue of tools and portals provided through West-Life with information on the principal investigators for each of these resources;
2. Information and link to the EGI business portal – explaining the needs for industrial users to negotiate or establish an understanding with EGI to use Grid and/or Cloud resources;
3. Use cases of where industrial users have successfully used project tools and services and where the associated entities are happy to provide quotes and recommendations.

West-Life maintains contact with Industrial partners through social media platforms like Twitter with many followers from companies (643 tweets, 154 total followers, 25 industrial followers, averaging 200 profile visits a month). This is also enhanced through the regular interaction with the Instruct-ERIC twitter account – both managed by Instruct (Partner 7).

West-Life has also produced and distributed the flyer (Appendix 3), which was re-designed using feedback from researchers from varied scientific backgrounds, and from participants at conferences/workshops where the project was presented. The industry-specific flyer, providing tailored information will be designed to match the webpage structure and include successful use cases that demonstrate the West-Life services as value propositions to commercial science.

The project aims to deliver the Industry specific webpages and flyer in Month 30 of the project.

References cited

1. CORBEL 2nd Medical Infrastructure user forum reporting, Battaglia, Serena doi: 10.5281/zenodo.825054

Appendix 1: Events with Industrial user participants

Events where West-Life partners presented to Industrial community participants:

Event	Location	Date	Target
PSDI 2016	Malmö, Sweden	November 2016	Industry
CCP4 Study Weekend 2017	Nottingham, United Kingdom	January 9 2017	Industry and Structural Biology Community
CCP4 Crystallography School and Workshop at SPring-8	Japan	January 2017	Industry and Structural Biology Community
BCA spring meeting 2017	Lancaster, UK	March 10-13, 2017	Industry and Structural Biology Community
Experimental Nuclear Magnetic Resonance Conference	California, USA	March 26 - 31, 2017	Industry and New Communities
CryoEM Best Practices Workshop	Harwell, United Kingdom	May 9 2017	Industry and 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
Drug Discovery 2017	Liverpool, UK	October 2017	Industry and New communities
PSDI 2017	Cambridge, UK	November 2017	Industry

CCP4 Study Weekend 2018	Nottingham, UK	10- 12 January 2018	Industry and Structural Biology Community
PSDI 2018	Paris, France	13 November 2018	Industry

Appendix 2: Instruct Workshop on cryoEM best practices

Course Detail:

Venue: Research Complex at Harwell, Oxford, United Kingdom

Date: May 09, 2017

Website: <https://www.structuralbiology.eu/events/-instruct-workshop-on-cryoem-best-practices>

Course Programme:

Tuesday 9th May

13.00 Registration

13.45 Welcome & Introduction

Session 1: Operational methods

14.00 "New challenges in in situ cellular structural biology" Peijun Zhang (eBIC, Diamond light Source, Harwell).

14.30 "The Netherlands Centre for Electron Nanoscopy – How things have changed over the last year Ludo Renault (NeCEN, Leiden University, Leiden).

15.00 "Getting high-resolution structures from a cryo-EM facility" Bruno Klaholz (Integrated Structural Biology, IGBMC, Illkirch).

15.30 Coffee break

16.00 Breakout sessions

- sample quality assessment (rapporteur: Ludo Renault).

- microscope technology development (rapporteur: Alistair Siebert).

16.45 Report back

17.30 "Lessons learned in managing a large user facility" Bridget Carragher (Simons Electron Microscopy Centre, New York Structural Biology Center)

18.30 Drinks/buffet dinner

Wednesday 10th May

Session 2: Computational methods

9.00 "Taking your cryo-EM data and metadata through the structure solution pipeline" Martyn Winn (CCP-EM, STFC Daresbury).

9.30 "Image processing and its impact in cryoEM results: Assuring reproducibility" Jose-Maria Carazo (CNB-CSIC, Madrid).

10.00 "Streamlining cryo-EM data processing and method development with Scipion" Juha Huiskonen (OPIC, Division of Structural Biology, NDM, University of Oxford).

10.30- 11.00 Coffee Break

11.00 Breakout sessions

- software workflows (rapporteur: Jose-Maria Carazo)
- data management/storage (rapporteur: Martyn Winn)

11.45 Feedback
12.30 Lunch
13.30 eBIC tour
14.30 End of meeting