

Deliverable D2.5

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Deliverable written by Instruct Hub

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1 Executive summary

Disseminating information and training of existing user communities is at the heart of the work package. In this report we described the engagement activities carried out by West-Life in the form of presentations in conferences and workshops, organisation of meetings and dissemination events and organisation of training courses and workshops. The report also described our continuous effort on publications, social media and website. Previous reports included the preparation of dissemination material which are still available in our website.

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		

3 Detailed report on the deliverable

3.1 Background

A key part of delivering services to the 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 the structural biology community

3.2.1 Presence in conferences and workshops

Conference Title	Organiser	Country	No. of Participants	Date
Talk at Weizmann Center: Soft validation in cryo EM	Weizmann Center	Israel	16-50	14 March 2016
International Symposium on Grid and Cloud Computing. Talk: West-Life: A virtual research environment for structural biology	ISGC	Taiwan	> 150	15-18 Mar 2016
EGI Conference 2016. Talk: CryoEM: From Biomedical impact to Cloud deployment	EGI	Netherlands	> 100	08 April 2016
INSTRUCT practical course: Advanced methods for the integration of diverse structural data with NMR data – 2nd Edition	Instruct - Utrecht University	Netherlands	16-50	April 11 - 15, 2016
CAPRI meeting. Talk: Sense and simplicity in HADDOCK scoring: Lessons from CAPRI	CAPRI meeting	Tel Aviv	> 100	17-20 Apr 2016
BioExcel workshop. Talk: Integrative modelling of biomolecular complexes using HADDOCK2	EBI	Hinxton UK	24	3-4 May 2016

School on molecular modelling for life science. Talk: Integrative modelling of biomolecular complexes	BioExcel	Italy	30	6-10 Jun 2016
Gordon Research Conference on Computational Aspects of Biomolecular NMR. Talk: High-resolution, integrative modelling of biomolecular complexes from fuzzy data	Gordon Conferences	USA	> 100	11-16 Jun 2017
GRC 3D-EM conference. Poster "Overview of the CCP-EM project" including section on West-Life	GRC	Switzerland	200	11-16 June 2017
13th Annual Meeting of the Bioinformatics Italian Society. Talk: Structure, affinity and specificity riddles in biomolecular interactions	Bioinformatics Italian Society	Italy	> 200	15-17 Jun 2016
EMBO Global Exchange Lecture Course. Talk: Structural and Biophysical Methods for Biological Macromolecules in Solution	EMBO	South Korea	> 50	19-26 Jun 2016
Summer Workshop by Biochemistry Division of Korean Chemical Society. Talk: Integrative modelling of biomolecular complexes: High-resolution modelling with blurry 3D images	Korean Chemical Society	South Korea	> 200	June 27, 2016
EMBO practical course on "Integrative modelling of biomolecular complexes"	EMBO	Spain	30	4-9 Jul 2016
EMBO practical course on "Multidimensional NMR in Structural Biology"	EMBO	Germany	30	11-15 Jul 2016
Institute Pasteur course on integrative structural biology. Talk: Integrative modelling of biomolecular complexes	Institute Pasteur	France	24	20-21 Jul 2016
Talk at Universidade de São Paulo: Cryo Electron Microscopy: The EM RESOLUTION REVOLUTION	Universidade de São Paulo	Brazil	16-50	July 22 -29, 2016
Talk at the Leloir Foundation: Cryo Electron Microscopy:	Leloir Foundation	Argentina	16-50	01 August 2016

The EM RESOLUTION REVOLUTION				
Talk at INCMNSZ: 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	16-50	11 August 2016
Talk: Pervasive data processing and information integration in Cryo Electron Microscopy	Columbia University	USA	> 100	August 15 -29, 2016
Digital Infrastructures for Research 2016. Talk: Federated Accelerated Computing Platforms for EGI	EGI, EUDAT, GÉANT, OpenAIRE and RDA Europe, ACC Cyfronet AGH	Poland	>250	28-30 Sep 2016
Modelling of protein interaction conference. Talk: Structure, affinity and specificity riddles in biomolecular interactions	University of Kansas, Lawrence	USA	120	27-29 Oct 2016
Helmholtz Training Course on Integrative Structural Biology. Talk: High-resolution, integrative modelling of biomolecular complexes from fuzzy data	Helmholtz Training Course on Integrative Structural Biology	Germany	30	7-11 Nov 2016
EMBO conference on Molecular Machines: Integrative Structural and Molecular. Talk: High-resolution, integrative modelling of biomolecular complexes from fuzzy data	EMBL Heidelberg	Germany	> 200	21-23Nov 2016
12th Community Wide Experiment on the Critical Assessment of Techniques for Protein Structure Prediction. Talk: Evaluation of contact prediction in CASP12	CASP	Italy	> 100	10-13 Dec 2016
NECEN Cryo-EM School. Talk: Imagen Processing in cryoEM: Quality checks.	NECEN - FEI	Netherlands	16-50	Jan 22 - 27, 2017
Cryo-EM workshop at the International Symposium on Grid and Cloud Computing (ISGC) 2017	ISGC	Taiwan	>100	March 5 -10, 2017

International Symposium on Grid and Cloud Computing	ISGC	Taiwan	> 150	6-8 Mar 2017
BCA Spring Meeting 2017. Talk: Improving low-resolution protein structure models with knowledge-based and homology-based hydrogen bond restraints	British Crystallography Association	UK	>100	10-13 Mar 2017
Talk at University of Vienna: Validation and quality control all way through from maps to mode	Vienna University	Austria	16-50	16 March 2017
EMBL seminars. Talk: Optimising the crystallographic structure models of the past, present, and future	ESRF/EMBL-Grenoble	France	30-50	March 23, 2017
Experimental NMR Conference, Azilomar, Pacific Grove. Talk: High-resolution, integrative modelling of biomolecular complexes from fuzzy data	ENC	USA	> 600	26-31 Mar 2017
IG Structural Biology RDA 9th Plenary meeting	RDA	Spain	51-100	04 April 2017
Information-driven modelling of biomolecular interactions	Pasteur Institute	France	30	4-7 Apr 2017
3rd Icknield workshop on model building	CCP-EM @ STFC	UK	20	5-7 April 2017
Understanding Protein Interactions: From Molecules to Organisms	CNRS	France	> 100	24-26 Apr 2017
HEPIX Spring 2017 Workshop	Wigner Research Centre for Physics (Hungarian Academy of Sciences)	Hungary	125	24-28 Apr 2017
Instruct Best Practices workshop. Talk: "Taking your cryo-EM data and metadata through the structure solution pipeline"	Instruct	UK	29	9-10 May 2017
EGI Conference 2017 & INDIGO Summit 2017	INFN Catania	Italy	250	9-12 May 2017
2nd iNEXT AUM	iNEXT Consortium	Czech Republic	>100	May 22-24, 2017
3rd Instruct Biennial Structural Biology Conference 2017	Instruct EU	Czech Republic	250	May 24-26, 2017

HADDOCK workshop in information-driven modelling of biomolecular complexes	KAUST	Saudi Arabia	24	24-25 May 2017
3rd Instruct Biennial Structural Biology Conference 2017	Instruct	Czech Republic	250	24-26 May 2017
Dirac Workshop	Dirac Consortium	Poland	31	29-31 May 2017
3DEM Gordon Research Conference	GRC	Switzerland	200	June 11 - 16, 2017
Computation Drug Design course 2017. Talk: Macromolecular X-ray crystallography - Making and using structure models for CDD	BioSB	Netherlands	15	12-23 Jun 2017
BIOTEC 2017	BIOTEC	Spain	200	18-21 Jun 2017
CCP4/APS school in macromolecular crystallography. Talk: Model validation & optimization - From a solved structure to the final model	CCP4 + Advanced Photon Source	USA	30	19-26 Jun 2017
Platform for Advanced Scientific Computing conference. Talk: High-resolution, integrative modelling of biomolecular complexes from fuzzy data	PASC: sponsored by Association for Computing Machinery (ACM) and the Swiss National Supercomputing Centre (CSCS),	Switzerland	> 150	26-28 Jun 2017
Cryo-Electron Microscopy Symposium. Talk: Image processing in Cryo-EM: Quality checks	ESRF	France		July 6 - 7, 2017
Computation for Biomolecular Cryo-Electron Microscopy and Tomography. Talk: Validation and quality control all way through from maps to models	CCP-EM, CCPBioSim & University of Leeds	UK	50	July 13 -14, 2017
St Andrews PX Summer School. Talk: Model refinement	University of St Andrews + CCP4	UK	50	20-26 Aug 2017
Biophysical Society thematic meeting on conformational ensembles from simulation and experiment. Talk: High-resolution, integrative modelling of biomolecular complexes from fuzzy data	Biophysical Society	Germany	> 200	25-29 Aug 2017

Microscopy at the Frontiers of Science 2017 - 5th Joint Meeting of the Spanish and Portuguese Societies of Microscopy. Talk: Automatic calculation of Local Resolution with MonoRes: A new approach, its assessment and new applications	SME - SMP	Spain	200	September 5 - 8, 2017
Structure-Based Drug Design conference, ETH	EPFL	Switzerland	> 200	5-9 Sept 2017
iNext workshop on Bridging Solution Methods: From NMR to Xray Scattering And Biophysics	iNEXT H2020	Greece	30	18-22 Sept 2017
São Paulo School of Advanced Science on Biophysical Methods to Study Biomolecular Interactions, October 2017	São Paulo University	Brazil	40	01 October 2017
Drug Discovery 2017	ACC, Liverpool	UK	>500	3-4 Oct 2017
CryoEM Structure Challenges Workshop	NCMI	USA	73	October 6 - 8, 2017
São Paulo Advanced School of Science on Biophysical Methods to Study Biomolecular Interactions. Talk: Introduction to Cryo-Electron with key application examples / Computing cryo-EM maps: The image processing workflow to go from 2D to 3D	Brazilian Biophysical Society	Brazil	40	October 16 -27, 2017
HADDOCK workshop at Penn State University	Penn State University	USA	20	20 October 2017
CCP4 Crystallography School and Workshop: From data processing to structure refinement and beyond. Talk: Automated model completion and Model validation metrics	CCP4 + Chinese Academy of Sciences	China	100	23-27 Oct 2017
Structural Bioinformatics course at EMBL-EBI	EMBL-EBI	UK	24	25 October 2017
Protein Structures: production, prowess, power, promises, and problems. Talk: Using X-ray structures for bioinformatics	BioSB	Netherlands	10	30Oct-3Nov 2017

Netherlands Society for Biochemistry and Molecular Biology (NVBMB)meeting. Talk: High-resolution, integrative modelling of biomolecular complexes from fuzzy data	Netherlands Society for Biochemistry and Molecular Biology	Netherlands	80	01 November 2017
25th Protein Structure Determination in Industry Meeting. PSDI 2017. Talk Scipion - Data Processing Tutorial for Cryo-EM	PSDI	UK	50	Nov 12 - 14, 2017
BioExcel Community Forum. Talk: High-resolution, integrative modelling of biomolecular complexes from fuzzy data	BioExcel	Netherlands	30	21-23 Nov 2017
Digital Infrastructures for Research 2017	EGI, EUDAT, GÉANT, OpenAIRE, PRACE and RDA Europe	Belgium	500	30Nov-1Dec 2017
DLS-CCP4 Data Collection and Structure Solution Workshop. Talk: Model validation & optimisation	CCP4 + Diamond Light Source	UK	30	30Nov-7Dec 2017
ASCB/EMBO 2017	ASCB/EMBO	USA	>1000	1-6 Dec 2017
EMBO Global Exchange Lecture Course. Talk: Structural and Biophysical Methods for Biological Macromolecules in Solution	EMBO	Singapore	40	6-14 Dec 2017
Talk at Crick Institute London. Talk: Structural and Biophysical Methods for Biological Macromolecules in Solution	Crick Institute London	UK	50	14 December 2017
CCP4 Study Weekend 2018. Talk: PDB-REDO redone: Using homology for model building and refinement	CCP4	UK	400	8-10 Jan 2018
MeetU symposium. Talk: Structure, affinity and specificity riddles in biomolecular interactions	University Pierre et Marie Curie	France	50	10 January 2018
DNAREpairman workshop. Talk: The personal history of X-ray structure models	DNAREpairman ITN	Netherlands	15	15-19 Jan 2018

Instruct course on Image Processing for Electron Microscopy in the cloud.	Instruct- CNB	Spain	30	January 17 – 19, 2018
West-Life, Tools for Integrative Structural Biology	CERN, Meyrin	Switzerland	50	1-20 Feb 2018
ARIA 2 Workshop	Instruct-ERIC	Netherlands	25	02 February 2018
BPS18, 62nd Annual Meeting of the Biophysical Society	The Biophysical Society (BPS)	USA	500	17-21 Feb 2018
24th Conference of the National Magnetic Resonance Society of India	National Magnetic Resonance Society of India	India	300	16-19 Feb 2018
INSTRUCT course on "Advanced methods for the integration of diverse structural data"	Instruct - University of Florence	Italy	20	Feb 19 - 23, 2018
IT TRANSFORMATION AND CLOUD CONTENT MANAGEMENT FOR LIFE SCIENCES	Berlin	Germany	25	08-09 Mar 2018
International Symposium on Grids and Clouds (ISGC) 2018 in conjunction with Frontiers in Computational Drug Discovery (FCDD)	Academia Sinica in Taipei	Taiwan	180	16-23 Mar 2018
3rd AUM iNext	iNEXT consortium	France	80	19-21 Mar 2018
iNEXT Workshop: Translating Structural Biology into Biomedical Applications. Talk: PDB-REDO: high-throughput crystallographic model optimisation	iNEXT H2020	France	100	21-23 March 2018
EOSC-hub week	University of Malaga	Spain	>100	16-20 April 2018
CCP-EM Spring Symposium 2018. Talk: "Complex Image Processing Workflows and High-resolution reconstructions using Scipion" and others	CCP-EM @ STFC	UK	185	11-12 April 2018
1st CEITEC symposium on recent advances in cryo-electron microscopy	CEITEC	Czech Republic	>100	April 18 - 19, 2018

59th Experimental Nuclear Magnetic Resonance Conference	ENC	USA	500	29Apr-3May 2018
Instruct workshop on model building	Instruct	UK	20	1-4 May 2018
Remote X-ray Data Collection from European Synchrotrons	Open Sesame & Instruct-ERIC	Israel	20-40	14-18 May 2018
EMBO workshop Challenges for Magnetic Resonance in Life Sciences	CERM/Univ. of Florence and Fondazione L Sacconi	Italy	80	27May-1Jun 2018
DynaMoPPI: Dynamique et Modulation des Interactions Protéine-Protéine (PPI)	GGMM	France	20	28May-1Jun 2018
39th Steenbock Symposium "Iron-Sulfur Proteins- Biogenesis, Regulation and Function"	University of Wisconsin, Madison	USA	120	29May-2Jun 2018
Computation Drug Design course 2018	BioSB	Netherlands	10-20	11-22 Jun 2018
43rd FEBS Congress	Federation of European Biochemical Societies (FEBS)	Czech Republic	500	10-16 Jun 2018
BioExcel Summer School on Biomolecular Simulations 2018	BioExcel	Italy	30	17-22 Jun 2018
CCP4/APS school in macromolecular crystallography	CCP4 + Advanced Photon source	USA	30	18-25 Jun 2018
EUROMAR 2018	EUROMAR and AMPERE societies	France	200	1-5 Jul 2018
International Conference of Porphyrins and Phtalocyanine ICCP-10	Society of Porphyrins and Phtalocyanines	Germany	300	1-6 Jul 2018
Integrative modelling of biomolecular interactions	EMBO	Spain	30	2-6 Jul 2018
Integrative Structural Biology	Institut Pasteur	France	20-25	16-21 Jul 2018
XXVIII International Conference on Magnetic Resonance in Biological Systems, ICMRBS	International Council on Magnetic Resonance in Biological Systems (ICMRBS) / University College Dublin	Ireland	150	19-24 Aug 2018

14th Biennial Conference in Birmingham EuroBIC18	University of Birmingham	UK	200	26-30 Aug 2018
CCP4 Crystallography School and Workshop: From data processing to structure refinement and beyond	CCP4 + SPring-8	Japan	30	1-6 Oct 2018
Protein-peptide interactions: peptide identification, binding prediction and design	CECAM-FR-MOSER	Switzerland	30-40	16-19 Oct 2018
EGI User Forum. Talk: West-Life: A virtual research environment for structural biology	EGI	Italy	150	9-13 Nov 2015
Challenges and e-Solutions for Serving a Worldwide Structural Biology Community	SURFSara SuperD Event	Amsterdam	100	15 Dec 2016
EMBO Practical Course NMR 2017	EMBO	Basel, Switzerland	30	5-12 August 2017
EOSC Stakeholder Forum. Panelist.	EOSCpilot	Bruxelles, Belgium.	250	28-29 Nov 2017
Digital Infrastructures for Research	EGI/EUDAT/GEANT/OpenAIRE	Bruxelles, Belgium	400	30 Nov-Dec 1 2017
62nd Annual Meeting of the Biophysical Society	Biophysical Society	San Francisco, USA	150	17-21 February 2018
INSTRUCT practical course on Advanced methods for the integration of diverse structural data (3rd edition)	Instruct-ERIC, CERM-University of Florence	Florence, Italy	30	19-23 February 2018
COST FeSBioNet	CERM/CIRMMP	Zagreb, Croatia		12-13 June 2018
CCPN Conference 2018, University of Kent	CCPN	Canterbury, UK		6-8 September 2018
Open Science Fair	OSFAir	Athens	500	6-8 Sept 2017
OpenMinTeD: paving the way for text and data mining in science	OpenMinTeD	Brussels	200	24 May 2018
CernVM Users Workshop	CERN	CERN	100	20 Jan 2018
DI4R. Talk, posters and panel representation	EOSC-hub, GÉANT, OpenAIRE and PRACE	Lisbon, Portugal	>350	9-11 October

Events organised by West-Life

Title	Organiser	Type	No. of Participants	Date
West-Life: Structural biology in the clouds	West-Life	Meeting		19-21 Oct 2016
West-Life iNEXT round table. Satellite meeting to Instruct Biennial Structural Biology Conference 2017	West-Life/Instruct	Meeting	100	24 May 2017
West-Life all partners meeting	West-Life/CSIC	Meeting	27	3-5 May 2018
West-Life Hackathon	West-Life/Daresbury Laboratory	Workshop	4	13-14 Mar 2018
West-Life Hackathon	West-Life/Instruct	Meeting	7	26 Sep 2018
Webinar: "West-Life: Lessons learnt from developing a virtual research environment"	WestLife/Corbel/Instruct	Webinar	Online	23 Oct 2018

3.2.2 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 a Twitter widget engaging with different user communities, partners and collaborators. The @WestLifeSB twitter account has 231 followers and has 1039 tweets engaging with policy makers, partners, collaborators and users, averaging excess of 140 profile views per month and 1% engagement rate. Owing to the emergence of Twitter as a support platform, with specific instances of such support requests in West-Life, the website also encouraged users to contact West-Life using the twitter handle. Webinars and lectures, collected by the WeNMR project, on the tools and services available to the users through West-Life are uploaded to the WeNMR YouTube Channel (<https://www.youtube.com/c/WeNMRWestLifeVRC>) and are also available through the website. More lectures from workshops are added to this channel for further dissemination.



The West-Life website has also been improved with the provision 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 the West-Life website directs users to the correct help centre. Additional dynamic website content includes a publications page (<https://about.west-life.eu/network/west-life/outreach/publications>), with live data pulled from the OpenAire repository and the project page (<https://about.west-life.eu/network/west-life/about/project>), which displays a breakdown of KPI data from the EGI Accounting portal.

All publications arising from the project are deposited in the open to all resource [Zenodo](#). Zenodo assigns all publicly available uploads a Digital Object Identifier (DOI) to make the upload easily and uniquely citeable.

3.3 Training events

Title	Organiser	No. of Participants	Date
INSTRUCT practical course: Advanced methods for the integration of diverse structural data with NMR data – 2nd Edition	Instruct - Utrecht University	24	April 11 - 15, 2016
From 2D images to 3D structures: A practical course on Electron Microscopy Single Particle Analysis	West-Life/ Instruct/CSIC	20	May 17 – 20, 2016
Cryo EM Solving the Structure of Macromolecular Complexes: A Hands-on Workshop at International Symposium on Grids and Clouds 2016	West-Life	20	March 14-15, 2016
First I2PC-FEI “hands on” course on image processing applied to the structural characterization of biological macromolecules	West-Life/Instruct/FEI	20	October 17 – 20, 2016
Second Advanced methods for the integration of diverse structural data with NMR data	West-Life	20	April 11-15, 2016
Cryo-EM Workshop at International Symposium on Grids and Clouds 2017	West-Life	40	March 6-10, 2017
DIRAC Workshop for West-Life	West-Life	12	January 2017

Hands-On course on Cloud Orchestration	West-Life	9	April 2017
Hands-on in cryo Electron Microscopy image processing. São Paulo School of Advanced Science on Biophysical Methods to Study Biomolecular Interactions 2017	West-Life	80	15 – 19 Oct, 2017
Practical workshop on Cryo EM data analysis in Scipion	West-Life/MU/CSIC	20	25-26 Jan 2018
INSTRUCT course on "Advanced methods for the integration of diverse structural data"	West-Life/Instruct - University of Florence	20	Feb 19 - 23, 2018