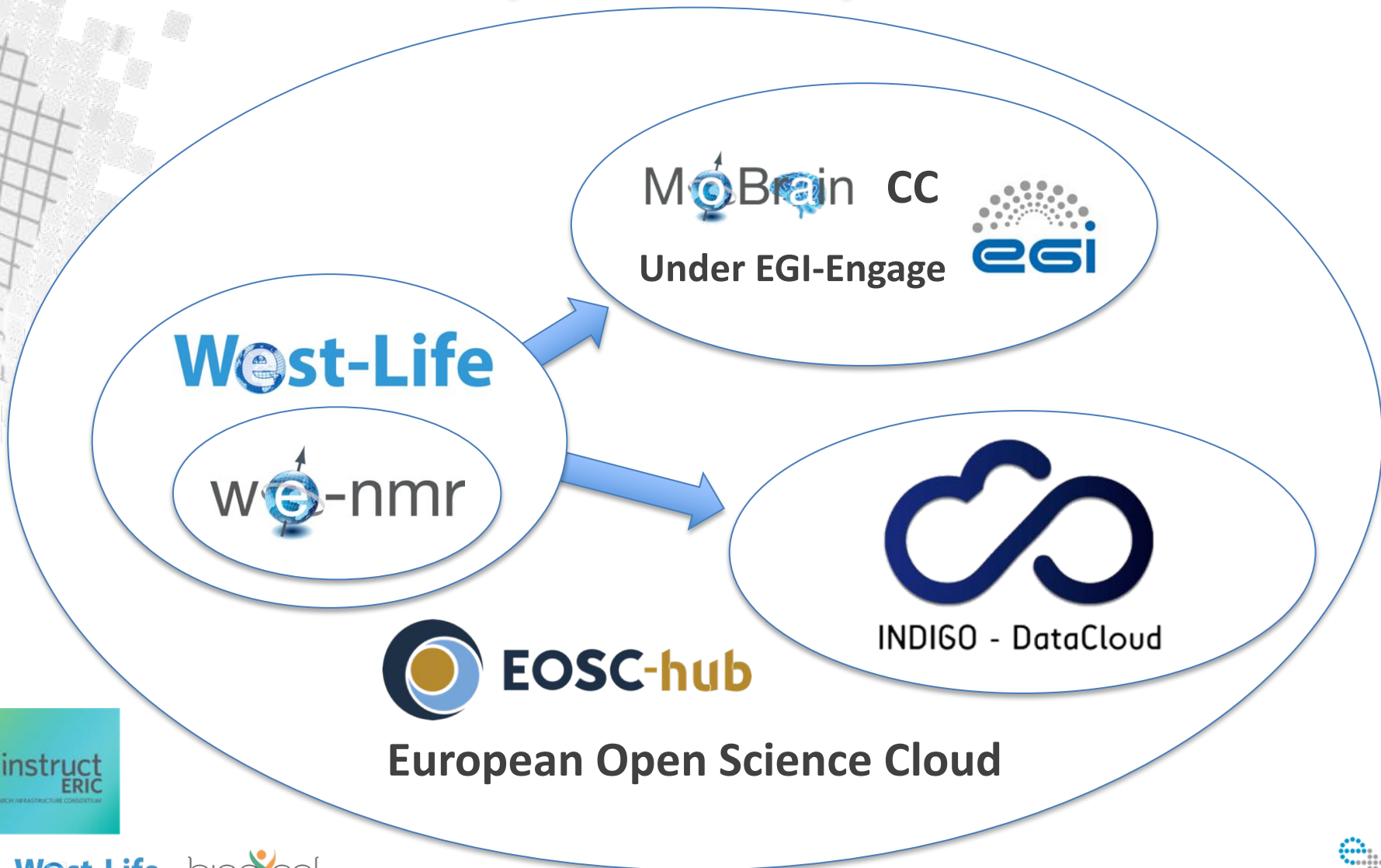


**Building bridges
between
services and e-Infrastructure
in structural biology**

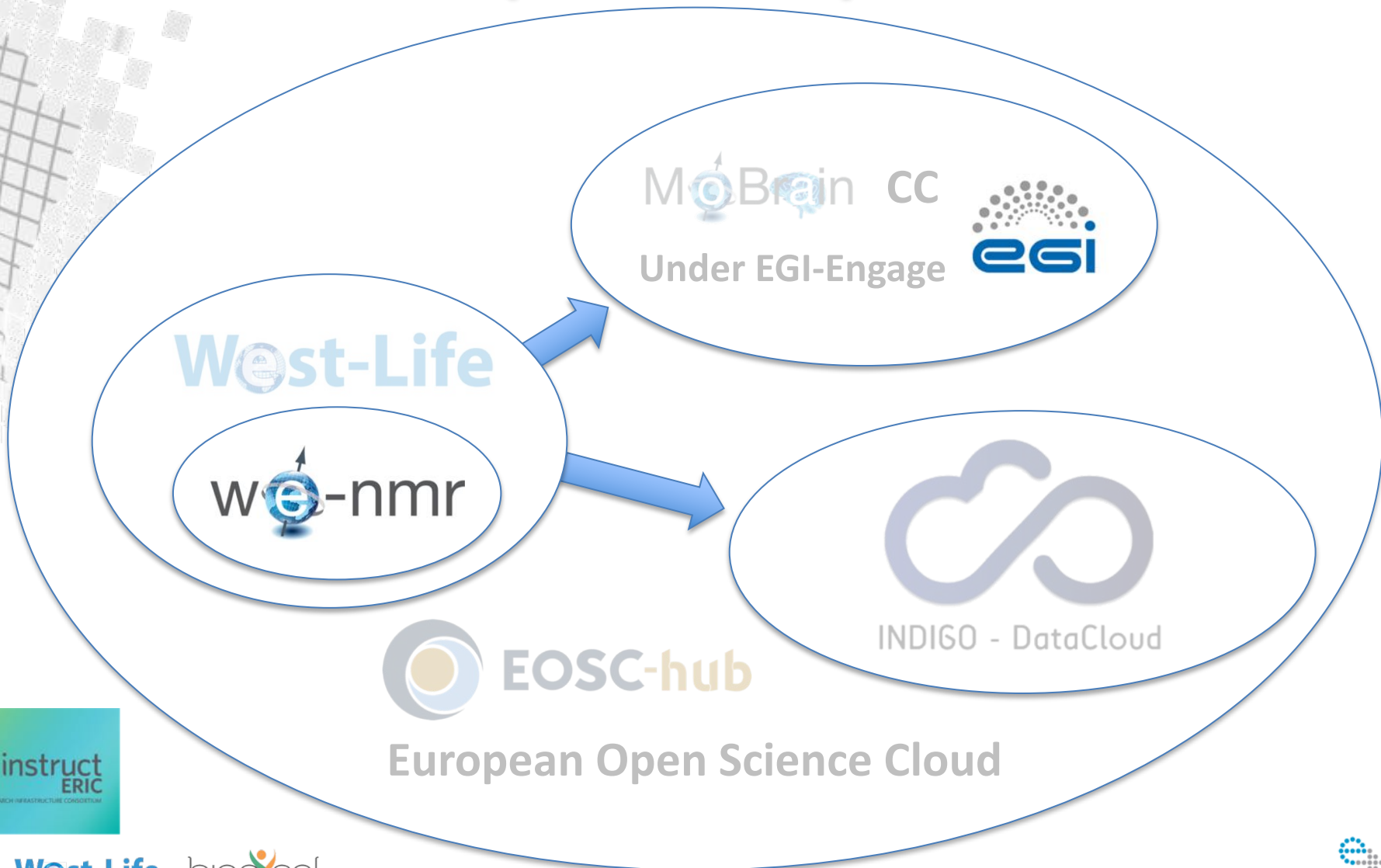
Alexandre Bonvin

Utrecht University
The Netherlands
a.m.j.j.bonvin@uu.nl

The structural biology e-Infrastructure landscape over the years



The structural biology e-Infrastructure landscape over the years





wE-nmr

Virtual Research Community

Exploiting GRID resources in structural biology...

NMR data collection and processing

SAXS data analysis

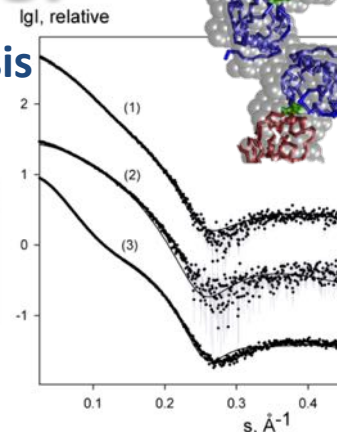


Table 2.2: Dihedral restraints

Dihedral	Angle limits (°)
ϕ Leu2	-160 to -30
ϕ Phe3	-160 to -80
ϕ Leu4	-160 to -80
ϕ Val8	-60 to -80
ϕ Val9	-15 to -80

Table 2.3: Hydrogen Bonding

Donor	Acceptor Pair	Distance
Leu7 HN	- Val9 O	3.00
Leu7 HN	- Val9 O	3.00
Val9 HN	- Leu2 O	3.00
Val9 HN	- Leu2 O	3.00
Val4 HN	- Leu7 O	3.00
Val4 HN	- Leu7 O	3.00
Leu7 HN	- Val4 O	3.00
Leu7 HN	- Val4 O	3.00

Table 1: NMR Param

Residue	HN ppm	HB ppm	others ppm	¹³ C _{alpha} Hz	Ala Type	K
Met1	5.66	1.75	H ₂ , 2.3, H ₃ , 1.84	8.43		6.92
Leu2	5.6	4.64	H ₁ , 4.6, H ₂ , 0.88	9.80		-6.10
Phe3	5.31	3.25	H ₁ , H ₂ , 7.05-7.22	9.30		-10.37
Val4	4.47	2.09	H ₂ , 0.92	9.60		-6.02
Phe5	4.43	2.21	H ₁ , 1.99, H ₂ , 3.45, 3.36			
Ala6	3.93	1.42		7.60		-9.85
Leu7	3.30	1.77	H ₁ , 6.0, H ₂ , 0.94	8.60		-2.70
Val8	3.21	4.47	H ₂ , 0.92	H ₁ , 0.63		9.13
Val9	3.01	4.32	3.92, 0.84	H ₁ , 0.92, 0.84		9.37
Val10	3.69	3.15, 2.97	H ₂ , H ₃ , 7.05-7.22	7.22		-9.12

```
# Number 1
# INAME 1
# INAME 2
12 2.137 387 1 T 0.00e+00 0.00e+00 - 0.2756 2760 0
14 2.36 40 1 T 0.00e+00 0.00e+00 - 0.2760 2752 0
32 1.849 40 1 T 0.00e+00 0.00e+00 - 0.2259 2257 0
36 1.849 3 143 1 T 0.00e+00 0.00e+00 - 0.2259 2587 0
assign ( resid 501 and name CO ) 0.00e+00 - 0.2260 2257 0
( resid 501 and name ) 0.00e+00 - 0.2260 2259 0
( resid 501 and name X ) 0.00e+00 - 0.2260 2587 0
( resid 501 and name Y ) 0.00e+00 - 0.2583 2257 0
( resid 501 and name Z ) 0.00e+00 - 0.2583 2259 0
(CA ) -0.1400 0.15000
```

Table 2.1: NOE restraints

Proton pairs	Intensity
Met 1 Ho - Leu 2 HN	Medium
Leu 2 Ho - Phe 3 HN	Weak
Phe 3 Ho - Val 4 HN	Weak
Pro 5 Ho - Ala 6 HN	Medium
Ala 6 Ho - Leu 7 HN	Medium
Leu 7 Ho - Val 8 HN	Medium
Val 8 Ho - Val 9 HN	Medium
Val 9 Ho - Phe 10 HN	Medium
Met 1 HN - Leu 2 HN	Medium
Leu 2 HN - Val 9 HN	Weak
Val 4 HN - Leu 7 HN	Weak
Ala 6 HN - Leu 7 HN	Medium
Met 1 Ho - Val 8 Ho	Medium
Phe 3 Ho - Val 4 Ho	Strong
Val 4 Ho - Pro 5 Ho	Strong
Val 4 Ho - Pro 5 Ho	Strong

Data interpretation

Computations



Structure, dynamics & interactions

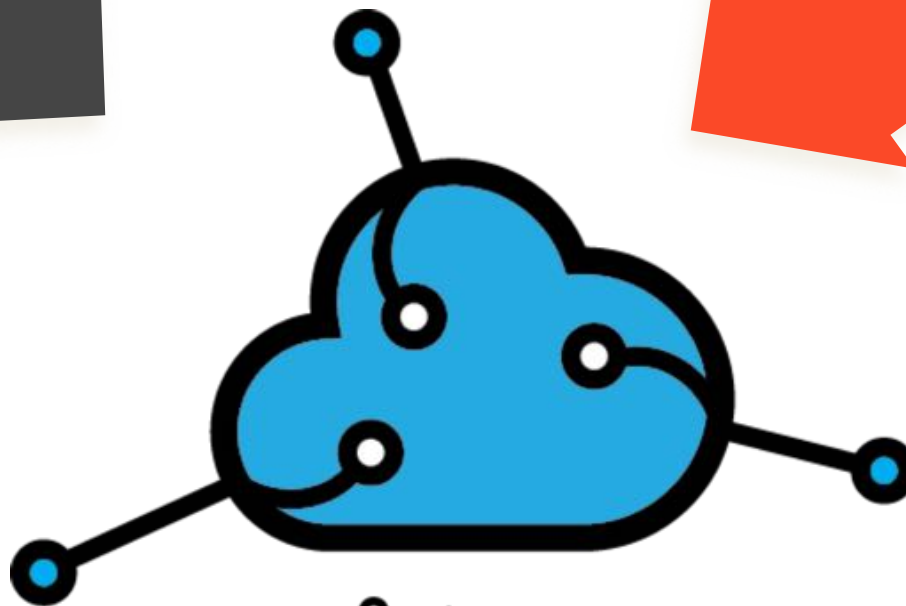
→ impact on research and health:

- origin of disease
- design of new experiments
- drug design...

The WeNMR VRC

Community

Infrastructure



eScience
hub in the Cloud

Science

Knowledge

eScience hub for NMR and structural biology

- Processing >
- Spectra&Assignment >
- Chemical Shifts >
- Structure Calculation >
- Analysis >
- Molecular Dynamics >
- Modeling >
- Tools >
- Structure Service >



WeNMR is both a three years project funded under the European Commission's 7th Framework Programme (e-Infrastructure RI-261571) and a Virtual Research Community supported by EGI, the largest one within the life science area. WeNMR aims at bringing together complementary research teams in the structural biology and life science area into a virtual research community at a worldwide level and provide them with a platform integrating and streamlining the computational approaches necessary for NMR and SAXS data analysis and structural modeling.

[Get Started >>](#)

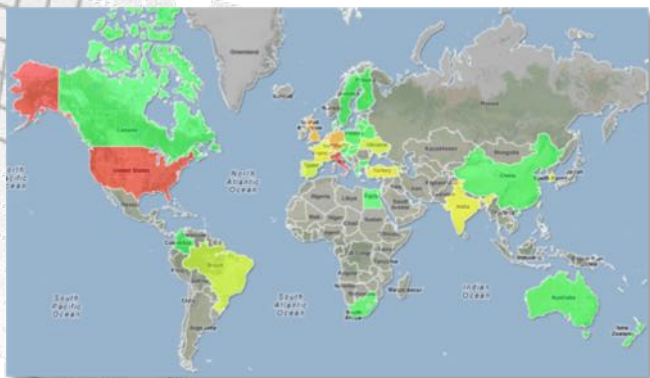
Harness the power of the GRID

[Highlights](#)
[News](#)
[Market](#)
[Resources](#)

- 2014-03-18 11:55 [Competition: Showcase your science at the EGI Community Forum](#)
- 2014-02-20 16:41 [Facing global challenges - Bio-NMR: Your partner in next generation sustainable health care.](#)
- 2014-02-03 10:50 [What is new in EGI? Inspired newsletter January 2014](#)
- 2014-02-03 09:41 [WeNMR within the top of European e-Infrastructure projects](#)
- 2013-12-17 22:54 [EGI Community Forum 2014](#)
- 2013-11-21 10:09 [WeNMR goes Chinese](#)

www.wenmr.eu

A worldwide e-Infrastructure for NMR and structural biology

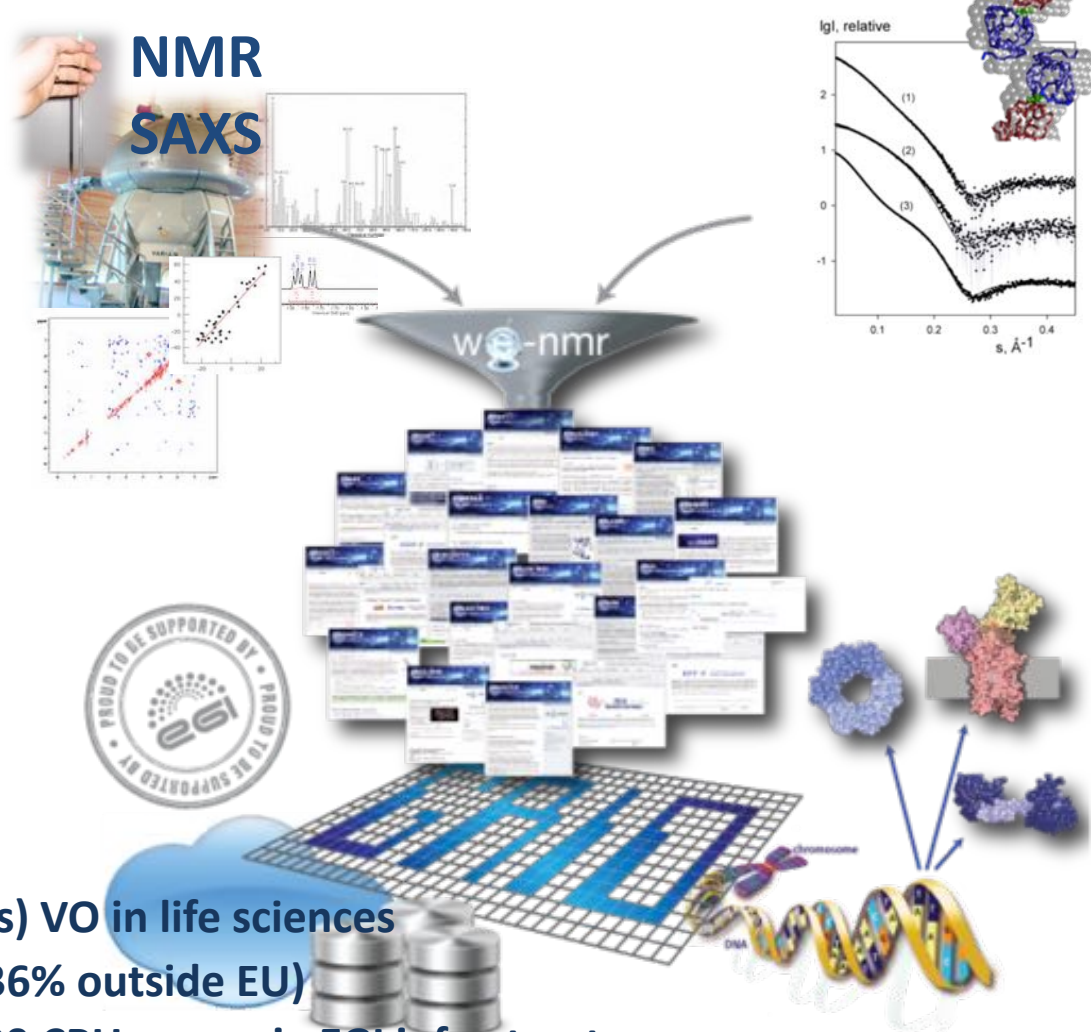


WeNMR VRC (February 2018)

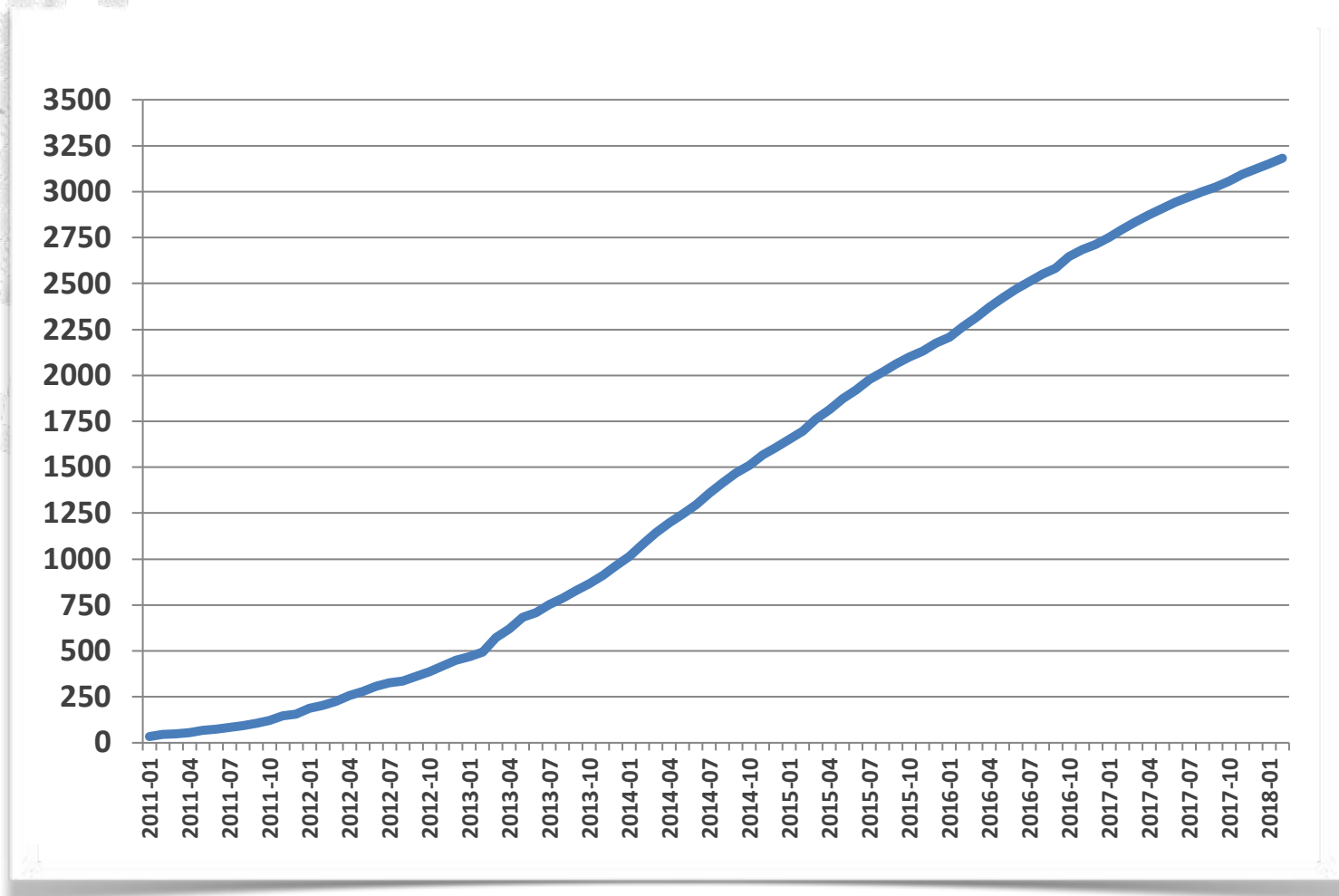
- enmr.eu: One of the largest (#users) VO in life sciences
- >830 users have registered so far(36% outside EU)
- Support from >40 sites for >200'000 CPU cores via EGI infrastructure
- User-friendly access to Grid via web portals
- Supported by an SLA (2016, updated in 2017) with EGI and NGIs

www.wenmr.eu

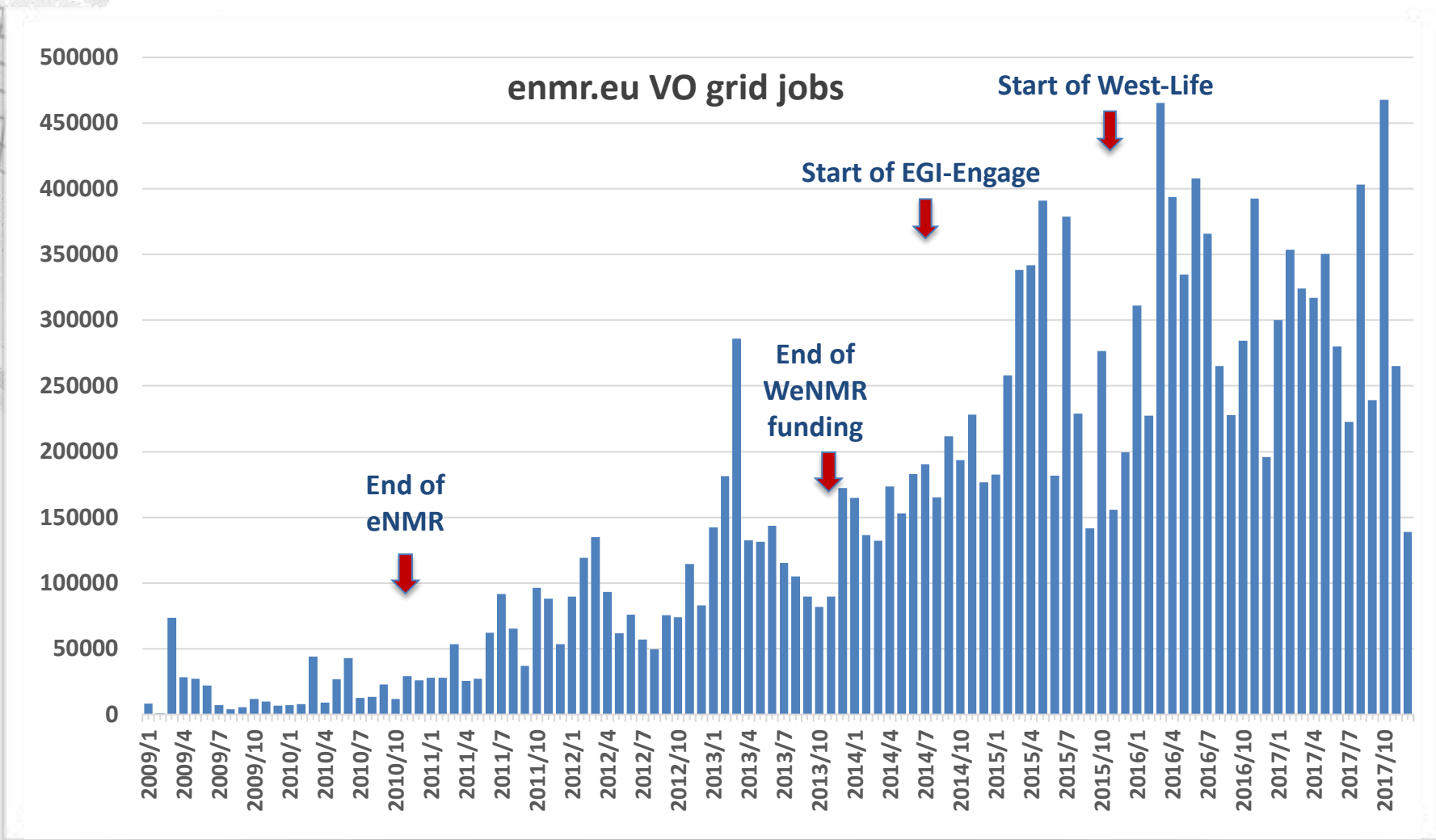
WeNMR



Sustained growth of the WeNMR VRC



Operational since 10 years



~2400 normalized CPU years over 2017

The West-Life VRE



Home Services ▾ Support ▾ News About ▾ Cloud Developers Contact Introduction

West-Life: Virtual Research Environment for Structural Biology



Computational and data management solutions for structural biology

Mission:

West-Life provides services for computation and data management to researchers in structural biology, integrating multiple approaches and experimental techniques. It builds on European e-infrastructure solutions from EGI and EUDAT and links together web services and repositories for structural biology. It is also engaged in the development and dissemination of best practices.

West-Life Twitter

Follow @WestLifeSB

West-Life @WestLifeSB
 This week @amjbonvin @WestLifeSB partner @UniUtrecht will be giving a keynote lecture at IT TRANSFORMATION AND CLOUD CONTENT MANAGEMENT FOR LIFE SCIENCES' @GlobalBSG conference bit.ly/2F6cDFk



IT TRANSFORMATION AND CLOUD CON...
 This event will serve as a business network...
 globallab.com

22h

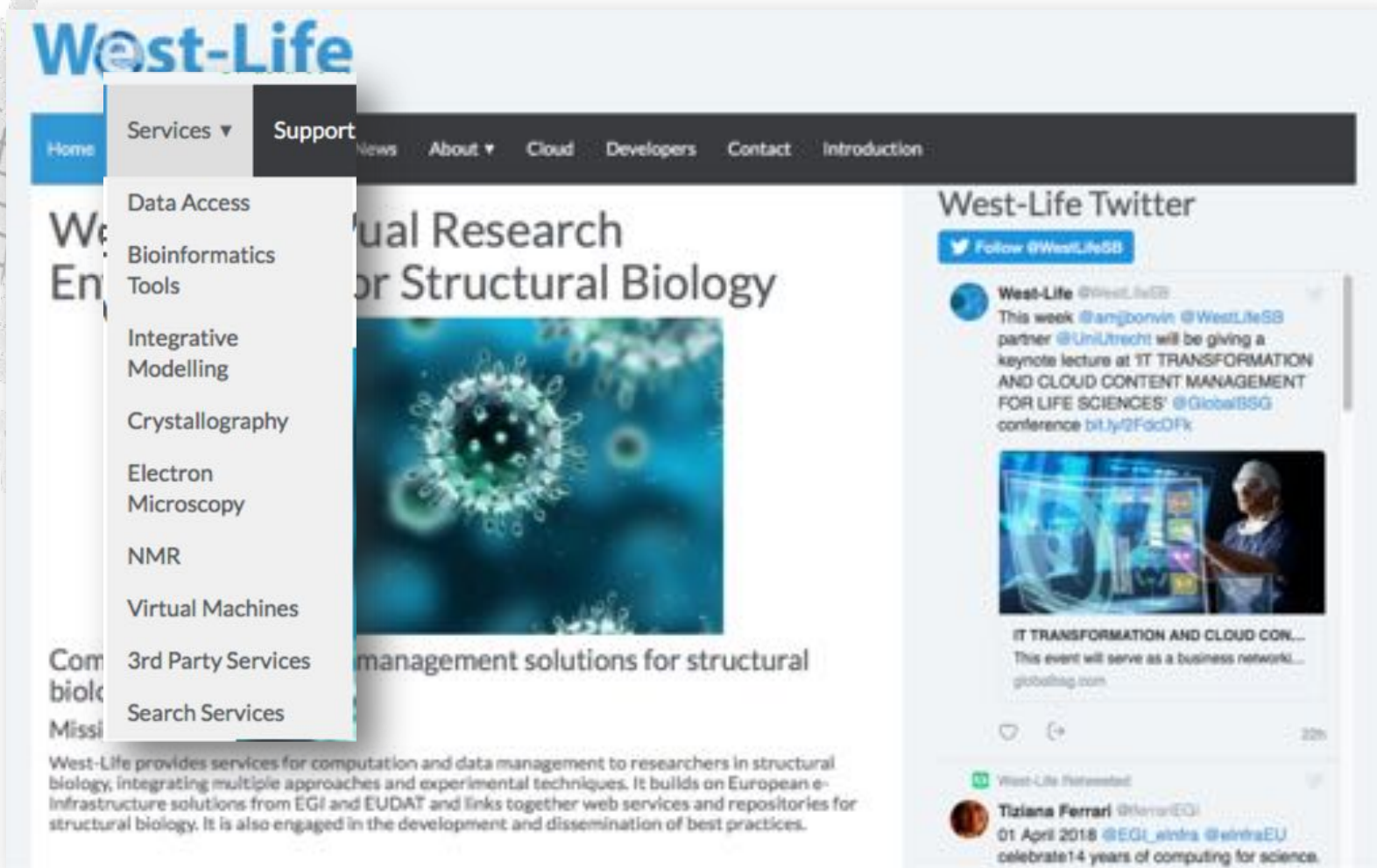
West-Life Retweeted
Tiziana Ferrari @FerrariEQI
 01 April 2018 @EGI_windra @windraEU celebrate 14 years of computing for science.

west-life.eu

Challenges & e-Solutions

- **Attract users!**
 - Offer them top of the line eScience solutions for their research ... which means top of the line software

The West-Life VRE



West-Life

Home Services **Support** News About **Cloud** Developers Contact Introduction

Virtual Research for Structural Biology

management solutions for structural

West-Life provides services for computation and data management to researchers in structural biology, integrating multiple approaches and experimental techniques. It builds on European e-infrastructure solutions from EGI and EUDAT and links together web services and repositories for structural biology. It is also engaged in the development and dissemination of best practices.

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IT TRANSFORMATION AND CLOUD CON...
This event will serve as a business network...
globallife.com

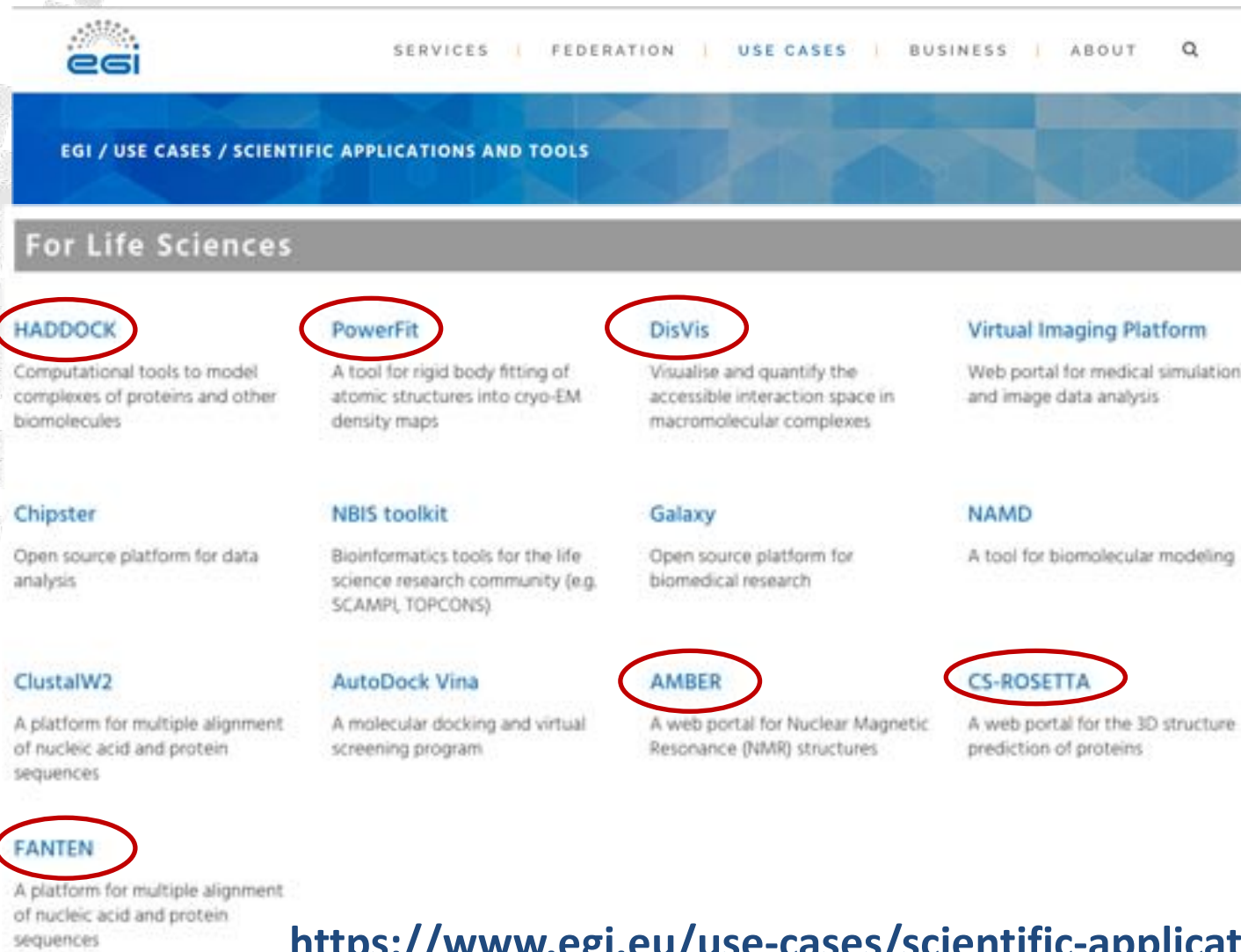
22h

West-Life Retweeted

Tiziana Ferrari @FerrariEQI
01 April 2018 @EGI_windra @windraEU celebrate 14 years of computing for science.

west-life.eu

Thematic services under EOSC-Hub



EGI / USE CASES / SCIENTIFIC APPLICATIONS AND TOOLS

For Life Sciences

<p>HADDOCK</p> <p>Computational tools to model complexes of proteins and other biomolecules</p>	<p>PowerFit</p> <p>A tool for rigid body fitting of atomic structures into cryo-EM density maps</p>	<p>DisVis</p> <p>Visualise and quantify the accessible interaction space in macromolecular complexes</p>	<p>Virtual Imaging Platform</p> <p>Web portal for medical simulation and image data analysis</p>
<p>Chipster</p> <p>Open source platform for data analysis</p>	<p>NBIS toolkit</p> <p>Bioinformatics tools for the life science research community (e.g. SCAMPL, TOPCONS)</p>	<p>Galaxy</p> <p>Open source platform for biomedical research</p>	<p>NAMD</p> <p>A tool for biomolecular modeling</p>
<p>ClustalW2</p> <p>A platform for multiple alignment of nucleic acid and protein sequences</p>	<p>AutoDock Vina</p> <p>A molecular docking and virtual screening program</p>	<p>AMBER</p> <p>A web portal for Nuclear Magnetic Resonance (NMR) structures</p>	<p>CS-ROSETTA</p> <p>A web portal for the 3D structure prediction of proteins</p>
<p>FANTEN</p> <p>A platform for multiple alignment of nucleic acid and protein sequences</p>			

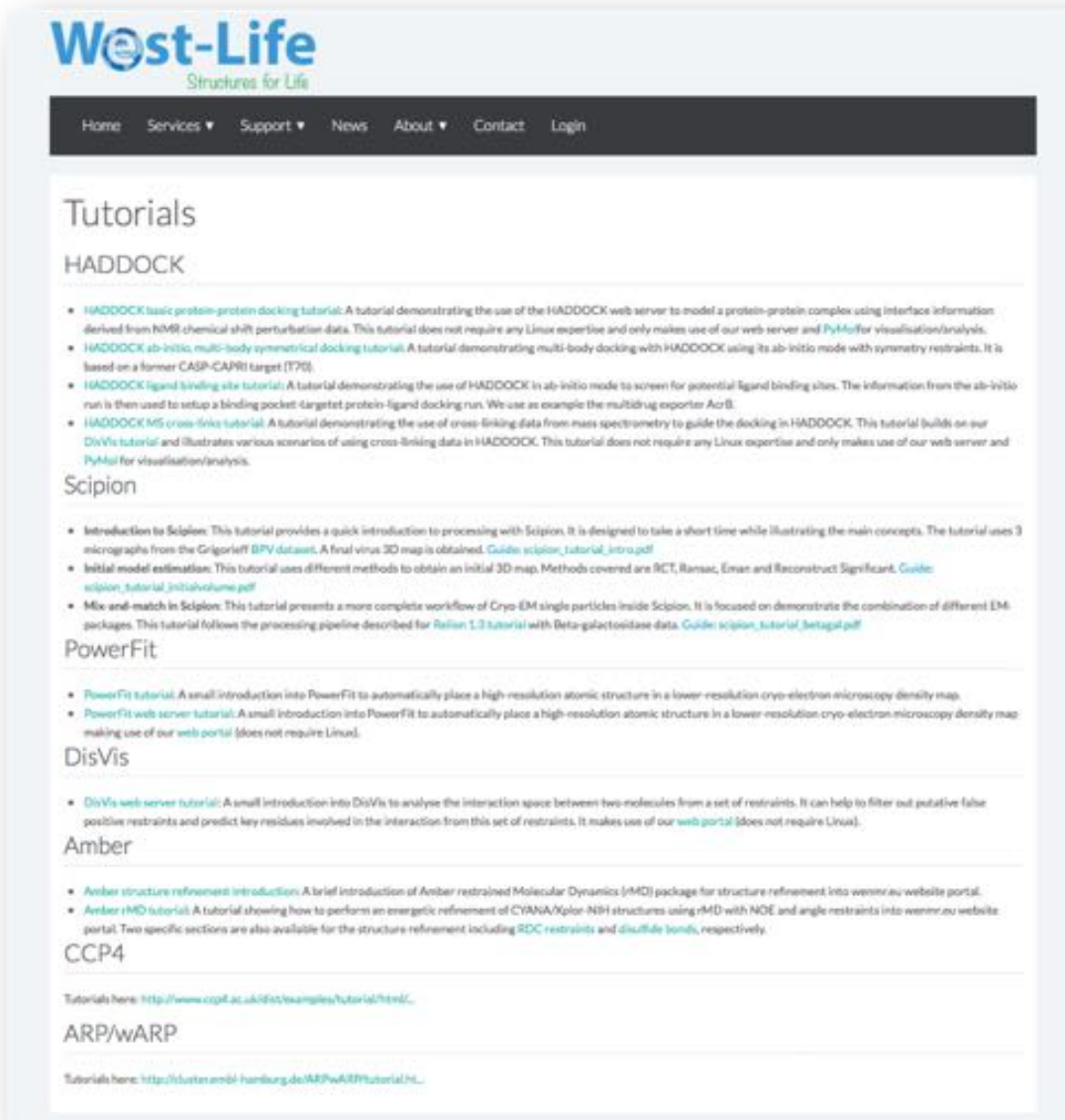
<https://www.egi.eu/use-cases/scientific-applications-tools/>

Challenges & e-Solutions

- **Attract users!**
 - Offer them top of the line eScience solutions for their research ... which means top of the line software
 - Provide them training, tutorials and support

West-Life knowledge and support center

- Various online tutorials aggregated in the support center



West-Life
Structures for Life

Home Services Support News About Contact Login

Tutorials

HADDOCK

- [HADDOCK basic protein-protein docking tutorial](#): A tutorial demonstrating the use of the HADDOCK web server to model a protein-protein complex using interface information derived from NMR-chemical shift perturbation data. This tutorial does not require any Linux expertise and only makes use of our web server and PyMol for visualisation/analysis.
- [HADDOCK ab-initio, multi-body symmetrical docking tutorial](#): A tutorial demonstrating multi-body docking with HADDOCK using its ab-initio mode with symmetry restraints. It is based on a former CASP-CAPRI target (T76).
- [HADDOCK ligand binding site tutorial](#): A tutorial demonstrating the use of HADDOCK in ab-initio mode to screen for potential ligand binding sites. The information from the ab-initio run is then used to setup a binding pocket-targeted protein-ligand docking run. We use as example the multidrug exporter AcrB.
- [HADDOCK MS cross-links tutorial](#): A tutorial demonstrating the use of cross-linking data from mass spectrometry to guide the docking in HADDOCK. This tutorial builds on our [DisVis tutorial](#) and illustrates various scenarios of using cross-linking data in HADDOCK. This tutorial does not require any Linux expertise and only makes use of our web server and PyMol for visualisation/analysis.

Scipion

- [Introduction to Scipion](#): This tutorial provides a quick introduction to processing with Scipion. It is designed to take a short time while illustrating the main concepts. The tutorial uses 3 micrographs from the Grigorieff BPV dataset. A final virus 3D map is obtained. [Guide: scipion_tutorial_intro.pdf](#)
- [Initial model estimation](#): This tutorial uses different methods to obtain an initial 3D map. Methods covered are RCT, Ransac, Eman and Reconstruct Significant. [Guide: scipion_tutorial_initvolume.pdf](#)
- [Mix and-match in Scipion](#): This tutorial presents a more complete workflow of Cryo-EM single particles inside Scipion. It is focused on demonstrate the combination of different EM packages. This tutorial follows the processing pipeline described for [Relion 1.3 tutorial](#) with Beta-galactosidase data. [Guide: scipion_tutorial_beta.pdf](#)

PowerFit

- [PowerFit tutorial](#): A small introduction into PowerFit to automatically place a high-resolution atomic structure in a lower-resolution cryo-electron microscopy density map.
- [PowerFit web server tutorial](#): A small introduction into PowerFit to automatically place a high-resolution atomic structure in a lower-resolution cryo-electron microscopy density map making use of our [web portal](#) (does not require Linux).

DisVis

- [DisVis web server tutorial](#): A small introduction into DisVis to analyse the interaction space between two molecules from a set of restraints. It can help to filter out putative false positive restraints and predict key residues involved in the interaction from this set of restraints. It makes use of our [web portal](#) (does not require Linux).

Amber

- [Amber structure refinement introduction](#): A brief introduction of Amber restrained Molecular Dynamics (rMD) package for structure refinement into [wemr.eu](#) website portal.
- [Amber rMD tutorial](#): A tutorial showing how to perform an energetic refinement of CVANA/npIor-NIH structures using rMD with NOE and angle restraints into [wemr.eu](#) website portal. Two specific sections are also available for the structure refinement including [SDC restraints](#) and [disulfide bonds](#), respectively.

CCP4

Tutorials here: <http://www.ccp4.ac.uk/Fts/examples/tutorial/html/>

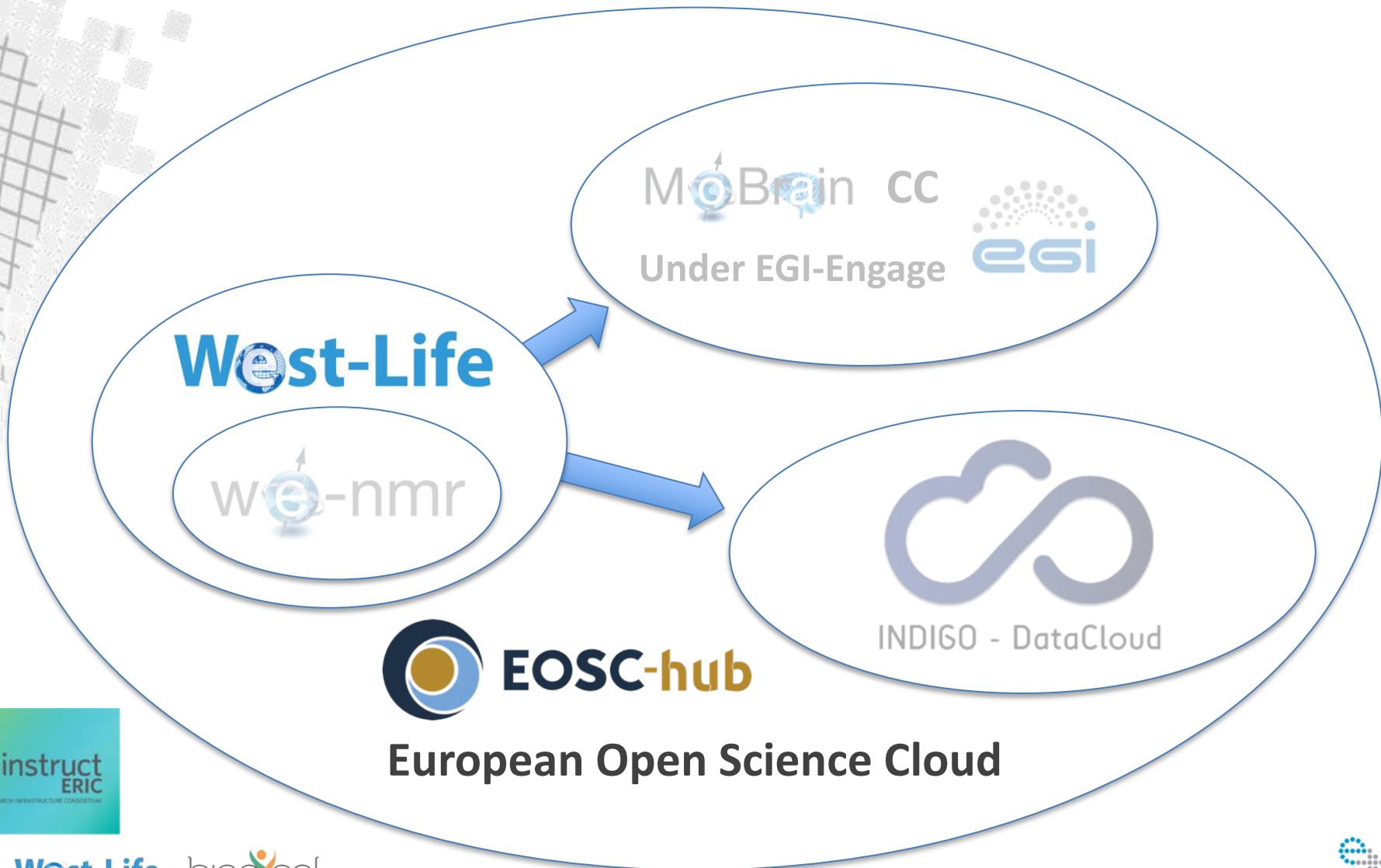
ARP/wARP

Tutorials here: <http://tutan.ambf-hamburg.de/ARPwARP/tutorial/HL/>

Challenges & e-Solutions

- **Attract users!**
 - Offer them top of the line eScience solutions for their research ... which means top of the line softwares)
 - Provide them training, tutorials and support
 - Make their life easier
 - ➔ SSO mechanisms
 - ➔ Build bridges between applications and with e-infrastructure solutions

Building bridges





Building bridges between services

West-Life: Cryo-EM in the clouds

SCIPION cloud server in production

scipionwebtools.westlife.fedcloud.eu/m/services/

SCIPION

Scipion web tools
Some of the Scipion framework methods available online to process your cryo electron microscopy data.

Align your movies
Try the Xmipp optical flow local alignment method to align your movies.
[My movie alignment](#)

Create your initial volume
You may want to try 3 different methods to generate an initial volume.
[My first map](#)

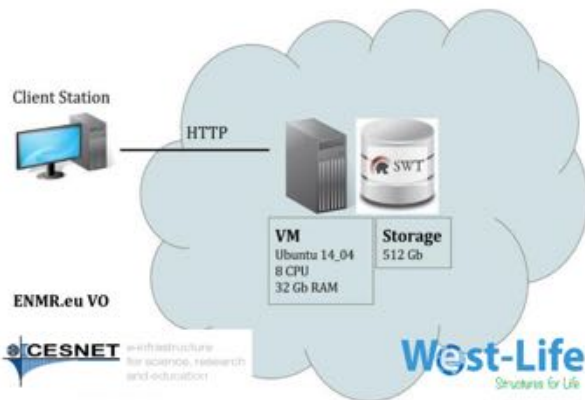
Get your map local resolution
Try 3 different methods to assess the local resolution of your map.
[My resolution map](#)

Explore protein interactions
Use 3D diana to explore possible domain-domain interactions.
[3D diana](#)

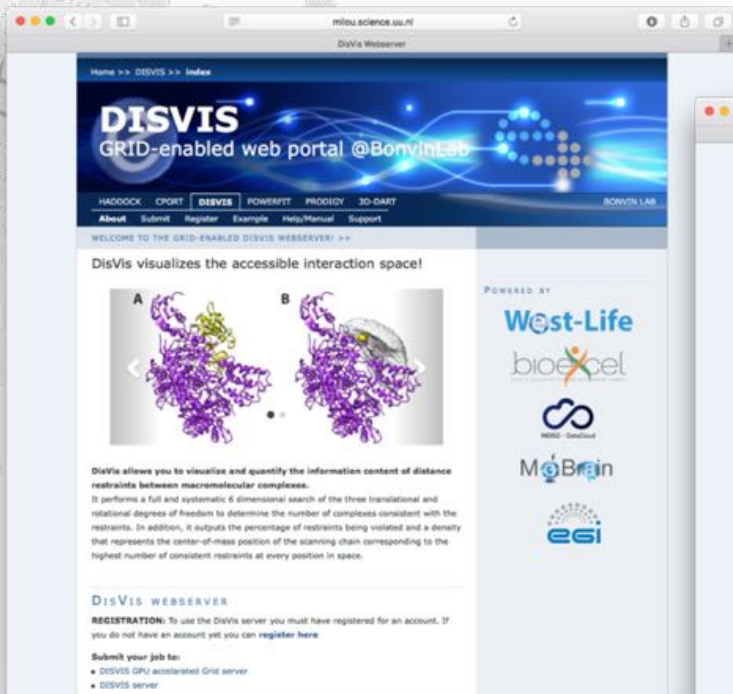
Can you trust your map?
Run 2 methods to assess the reliability of your map reconstruction.
[My reliability tool](#)

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Contact us

West-Life INEXT



New grid, GPGPU-enabled web portals: DISVIS & POWERFIT



indigodatacloudapps/disvis



indigodatacloudapps/powerfit



udocker

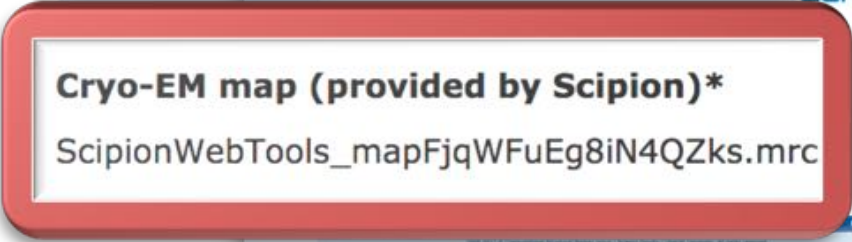
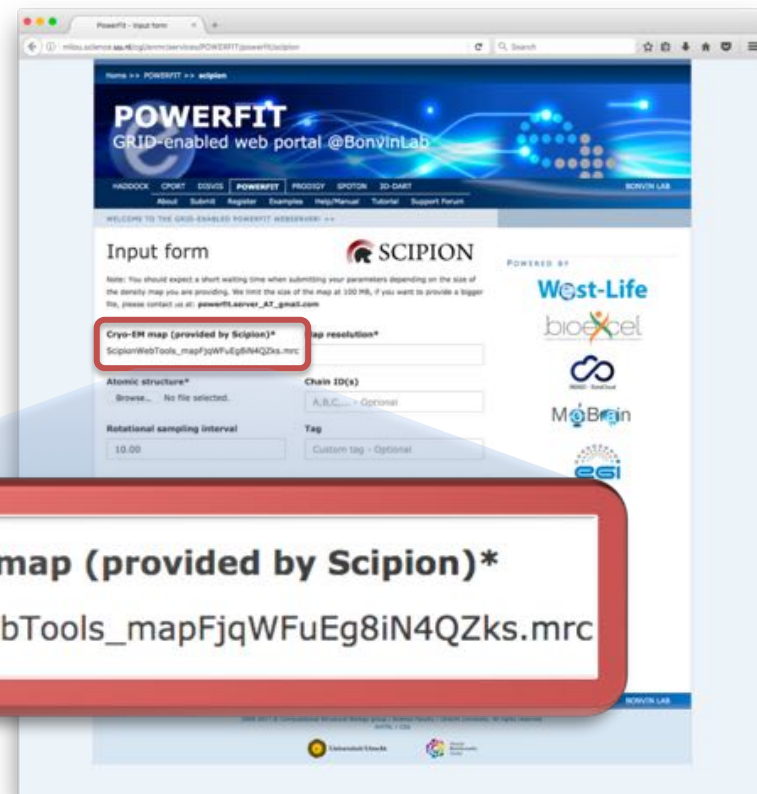
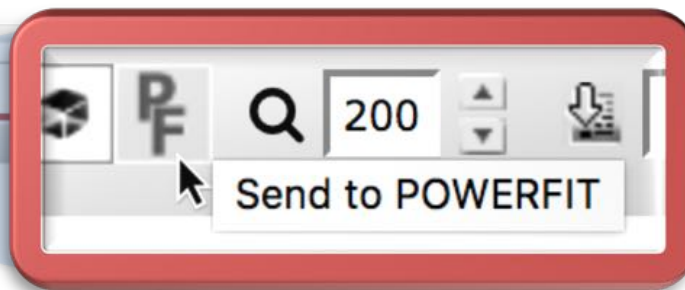
(Userspace Container Support)

<http://milou.science.uu.nl/enmr/services/DISVIS/>

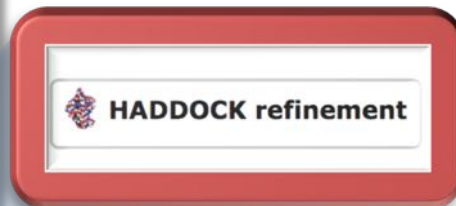
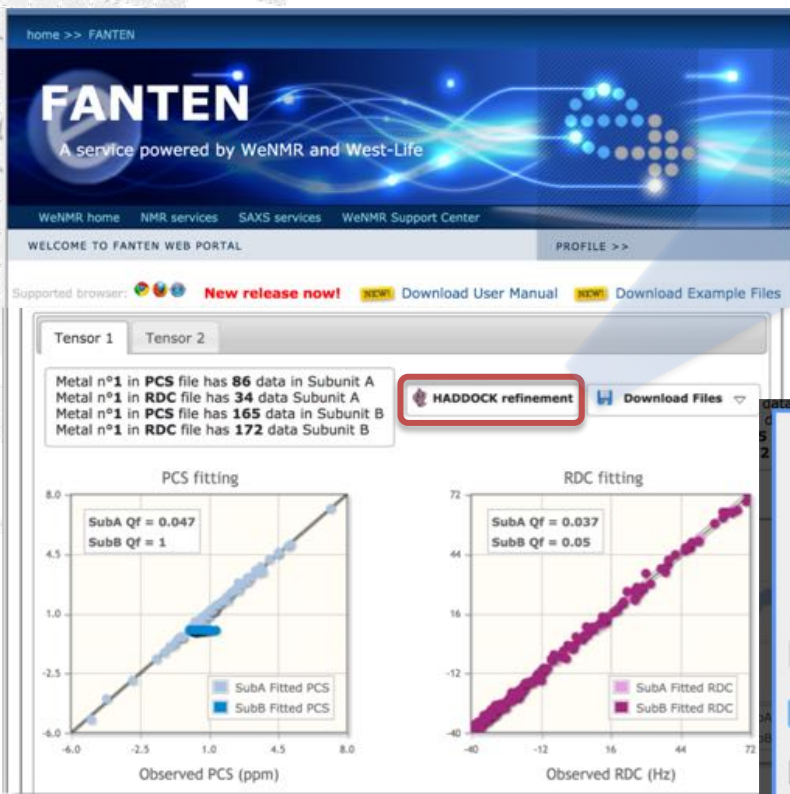
<http://milou.science.uu.nl/enmr/services/POWERFIT/>

- Hosted in Utrecht
- Implement INDIGO-Datacloud solutions
- Runs on GPGPU resources in Florence

Scipion – PowerFit workflow



FANTEN – HADDOCK workflow



HADDOCK

Username
mikaeltr

Password
.....

Register here

Login

Cancel

Powered by
West-Life
Structures for Life

HADDOCK2.2

WeNMR/West-Life (GRID-enabled) web portal

WeNMR home West-life home BioExcel home NMR services Support Center

WELCOME TO THE WENMR/WEST-LIFE WEB PORTAL >>

HADDOCK server status for docking run FANTEN-demo

Status: FINISHED

Your HADDOCK run has successfully completed. The complete run can be downloaded as a gzipped tar file [here](#). The file containing your docking parameters is [here](#).

Please cite the following paper in your work:
S.J. de Vries, M. van Dijk and A.M.J.J. Bonvin. **The HADDOCK web server for data-driven biomolecular docking**
Nature Protocols **5**, 883-897 (2010)
doi:10.1038/nprot.2010.32

Summary

HADDOCK clustered **190** structures in **5** cluster(s), which represents **95.0** % of the water-refined models HADDOCK generated. Note that currently the maximum number of models considered for clustering is 200.

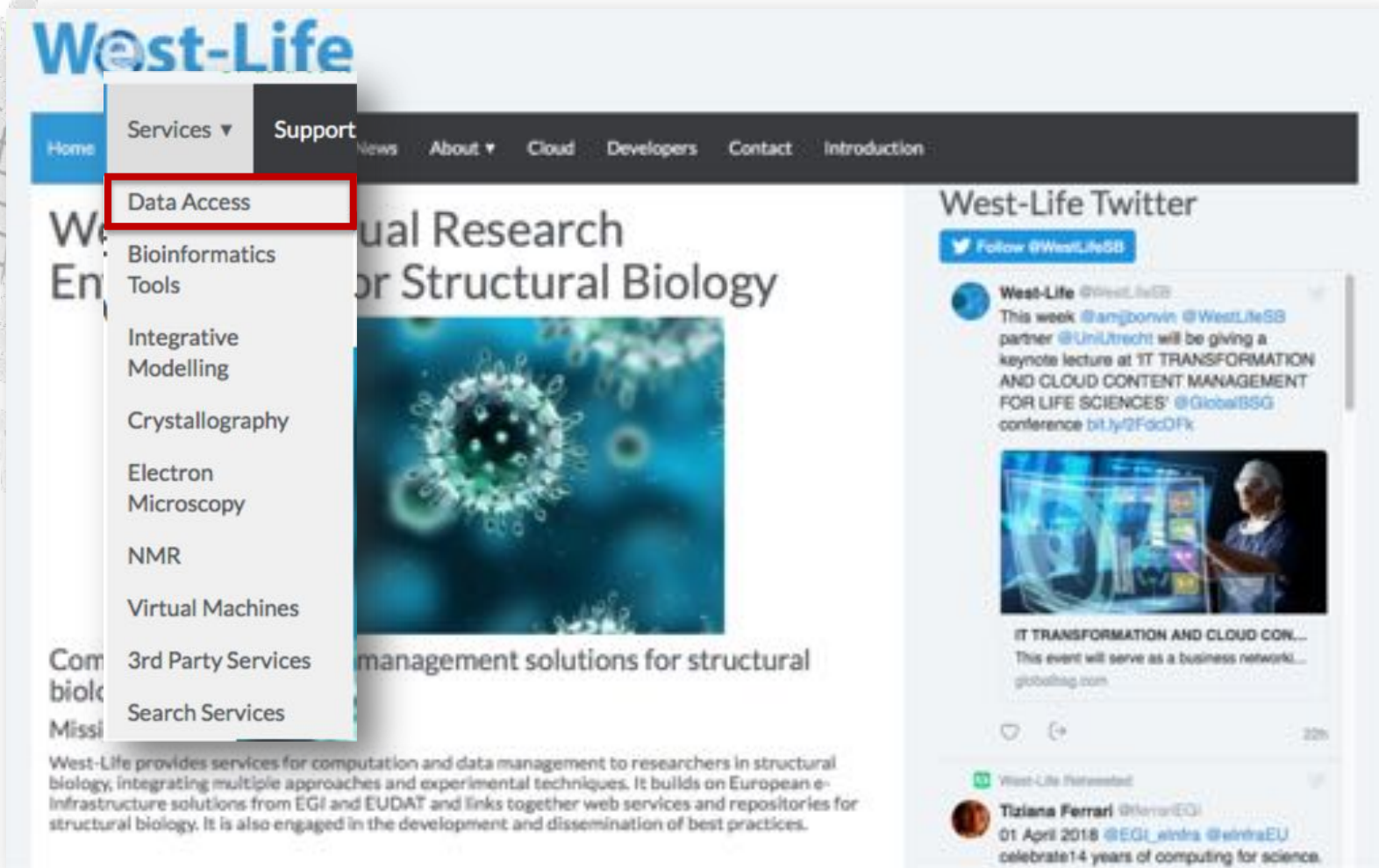
The statistics of the top 10 clusters are shown below. The top cluster is the most reliable according to HADDOCK. Its Z-score indicates how many standard deviations from the average this cluster is located in terms of score (the more negative the better).

A graphical representation of the results is also provided at the bottom of the page.



Building bridges with “cloud” storage

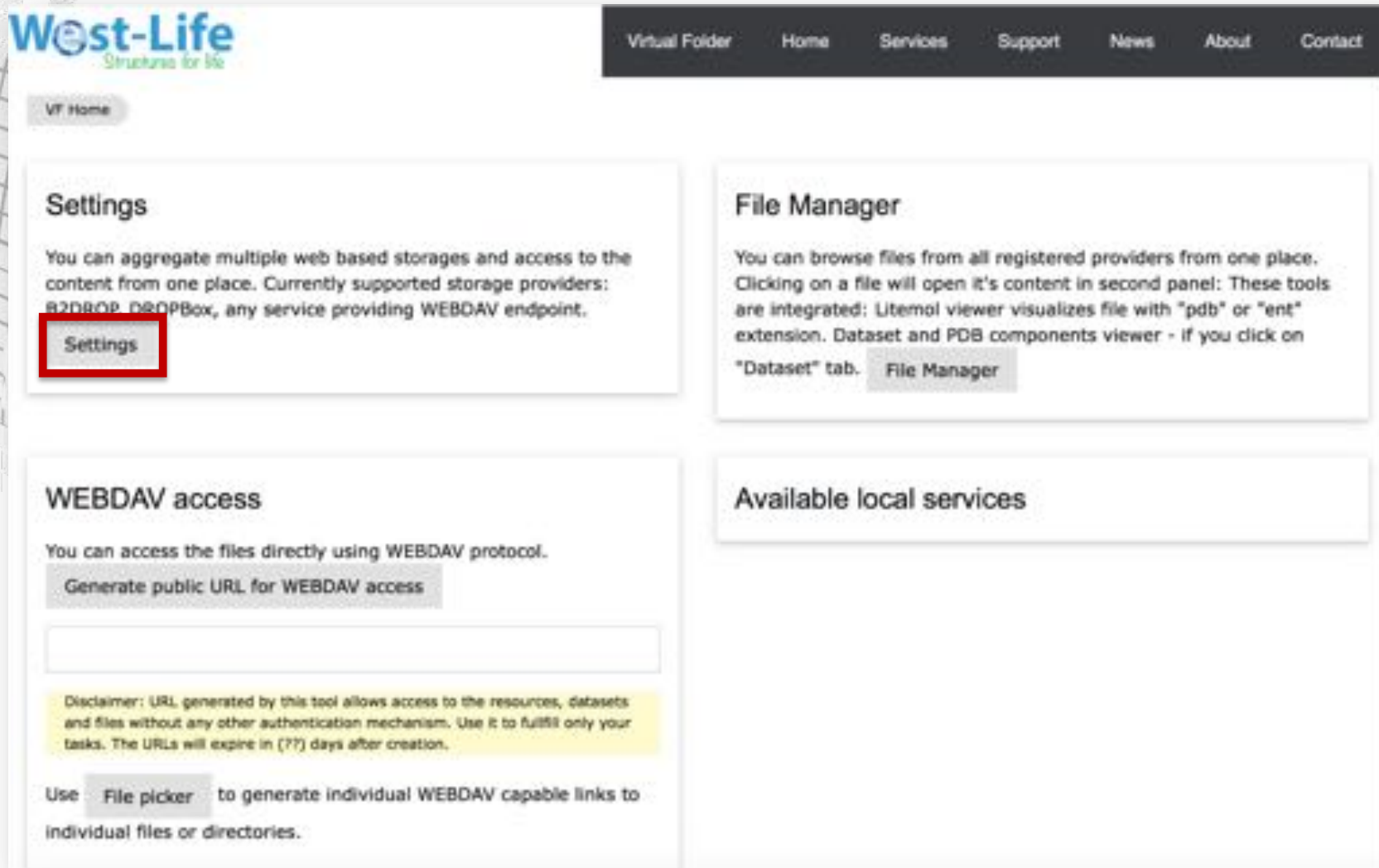
The West-Life VRE



The screenshot shows the West-Life website interface. At the top left, the 'West-Life' logo is displayed. Below it, a navigation bar includes 'Home', 'Services', and 'Support'. A dropdown menu is open under 'Services', with 'Data Access' highlighted by a red border. Other items in the menu include 'Bioinformatics Tools', 'Integrative Modelling', 'Crystallography', 'Electron Microscopy', 'NMR', 'Virtual Machines', '3rd Party Services', and 'Search Services'. The main content area features a large image of a protein structure and the text 'Virtual Research for Structural Biology'. On the right side, there is a 'West-Life Twitter' section with a 'Follow @WestLifeSB' button and a tweet from West-Life (@WestLifeSB) dated 01 April 2018.

west-life.eu

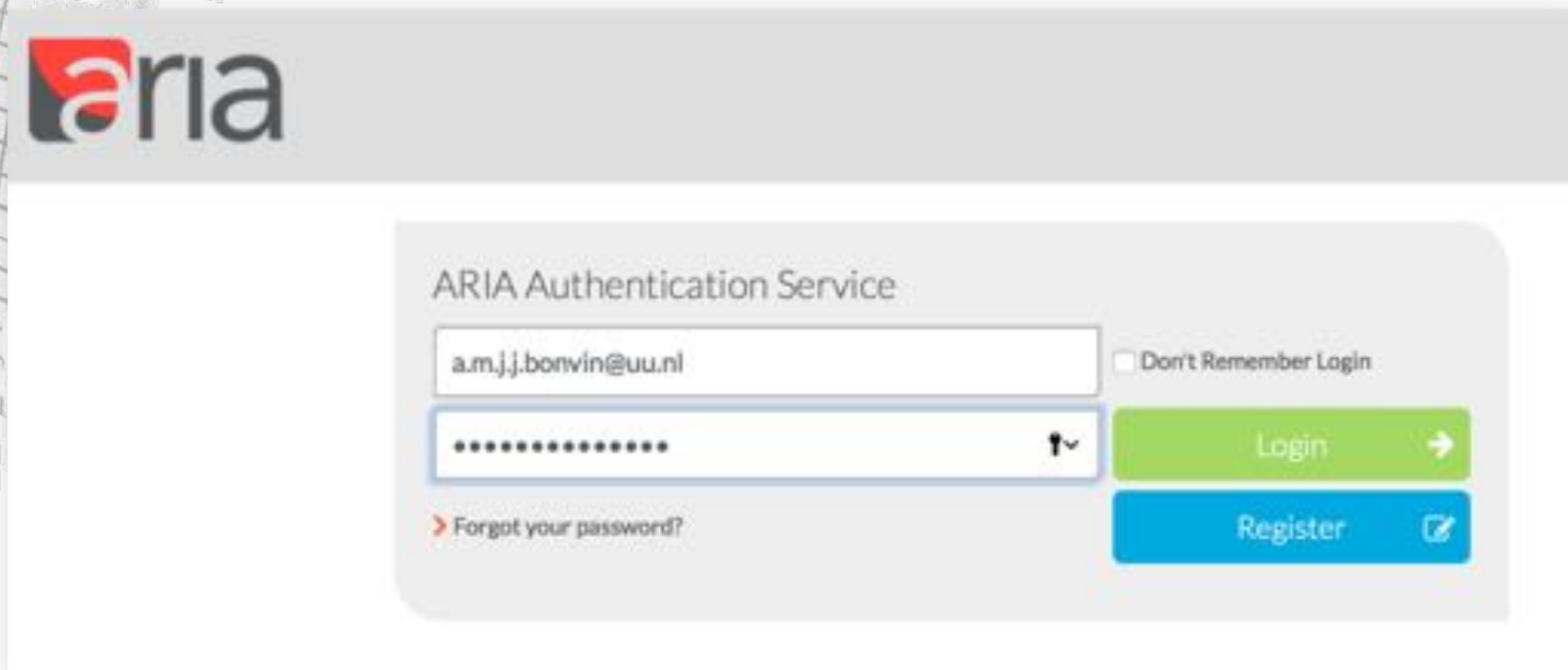
The West-Life Virtual Folder



The screenshot shows the West-Life Virtual Folder web interface. At the top left is the West-Life logo with the tagline "Structures for life". A dark navigation bar contains links for "Virtual Folder", "Home", "Services", "Support", "News", "About", and "Contact". Below the navigation bar is a "VF Home" button. The main content area is divided into four panels:

- Settings:** Contains the text "You can aggregate multiple web based storages and access to the content from one place. Currently supported storage providers: B2DROP, DROPBox, any service providing WEBDAV endpoint." Below this text is a button labeled "Settings", which is highlighted with a red rectangular box.
- File Manager:** Contains the text "You can browse files from all registered providers from one place. Clicking on a file will open it's content in second panel: These tools are integrated: Litemol viewer visualizes file with ".pdb" or ".ent" extension. Dataset and PDB components viewer - if you click on "Dataset" tab." Below this text is a button labeled "File Manager".
- WEBDAV access:** Contains the text "You can access the files directly using WEBDAV protocol." Below this text is a button labeled "Generate public URL for WEBDAV access". Underneath is an empty text input field. A yellow disclaimer box states: "Disclaimer: URL generated by this tool allows access to the resources, datasets and files without any other authentication mechanism. Use it to fulfill only your tasks. The URLs will expire in (??) days after creation." At the bottom of the panel, it says "Use File picker to generate individual WEBDAV capable links to individual files or directories."
- Available local services:** This panel is currently empty.

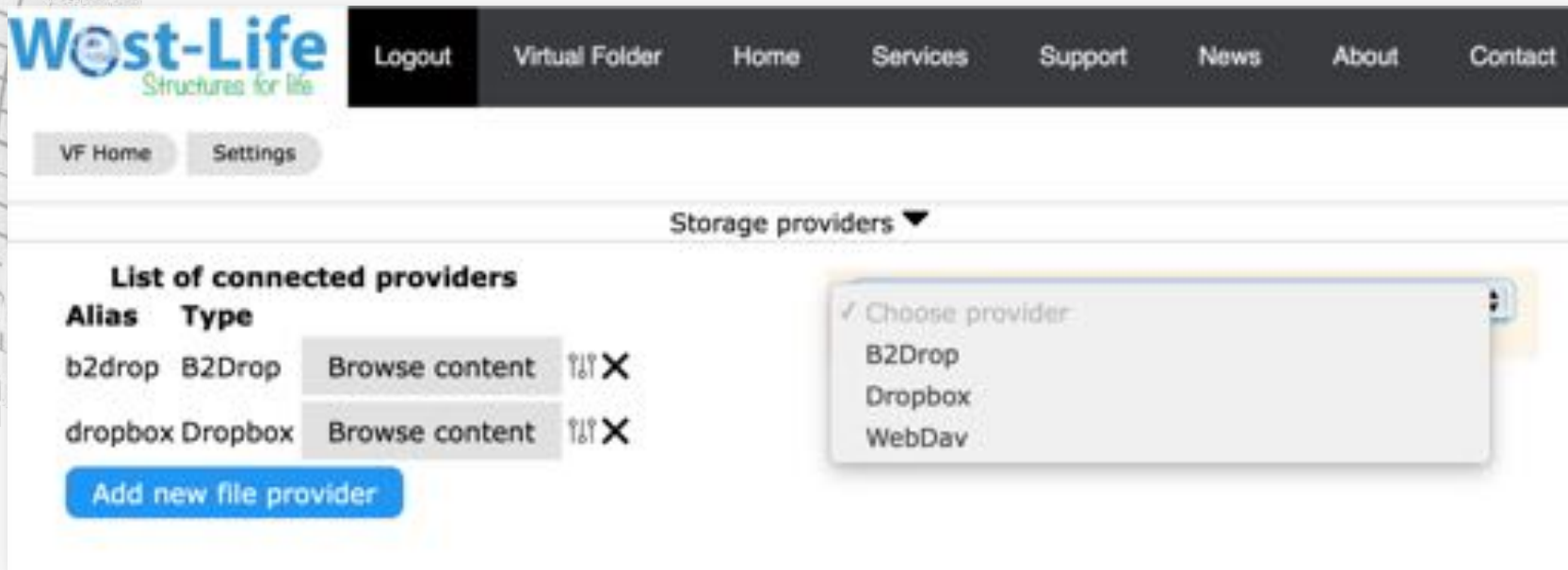
The West-Life Virtual Folder



The screenshot shows the ARIA Authentication Service login interface. At the top left is the 'aria' logo. The main heading is 'ARIA Authentication Service'. Below this, there is a text input field containing the email address 'a.m.j.j.borvin@uu.nl'. To the right of this field is a checkbox labeled 'Don't Remember Login'. Below the email field is a password input field with a masked password of ten dots and a small eye icon to toggle visibility. To the right of the password field are two buttons: a green 'Login' button with a right-pointing arrow, and a blue 'Register' button with a checkmark icon. Below the password field, there is a link '> Forgot your password?'. The entire form is set against a light gray background.

SSO authentication via INSTRUCT-ERIC

The West-Life Virtual Folder



The screenshot shows the West-Life Virtual Folder interface. At the top, there is a navigation bar with the West-Life logo and the tagline "Structures for life". The navigation menu includes "Logout", "Virtual Folder", "Home", "Services", "Support", "News", "About", and "Contact". Below the navigation bar, there are two buttons: "VF Home" and "Settings".

The main content area is titled "Storage providers" with a dropdown arrow. Underneath, there is a section titled "List of connected providers" which contains a table:

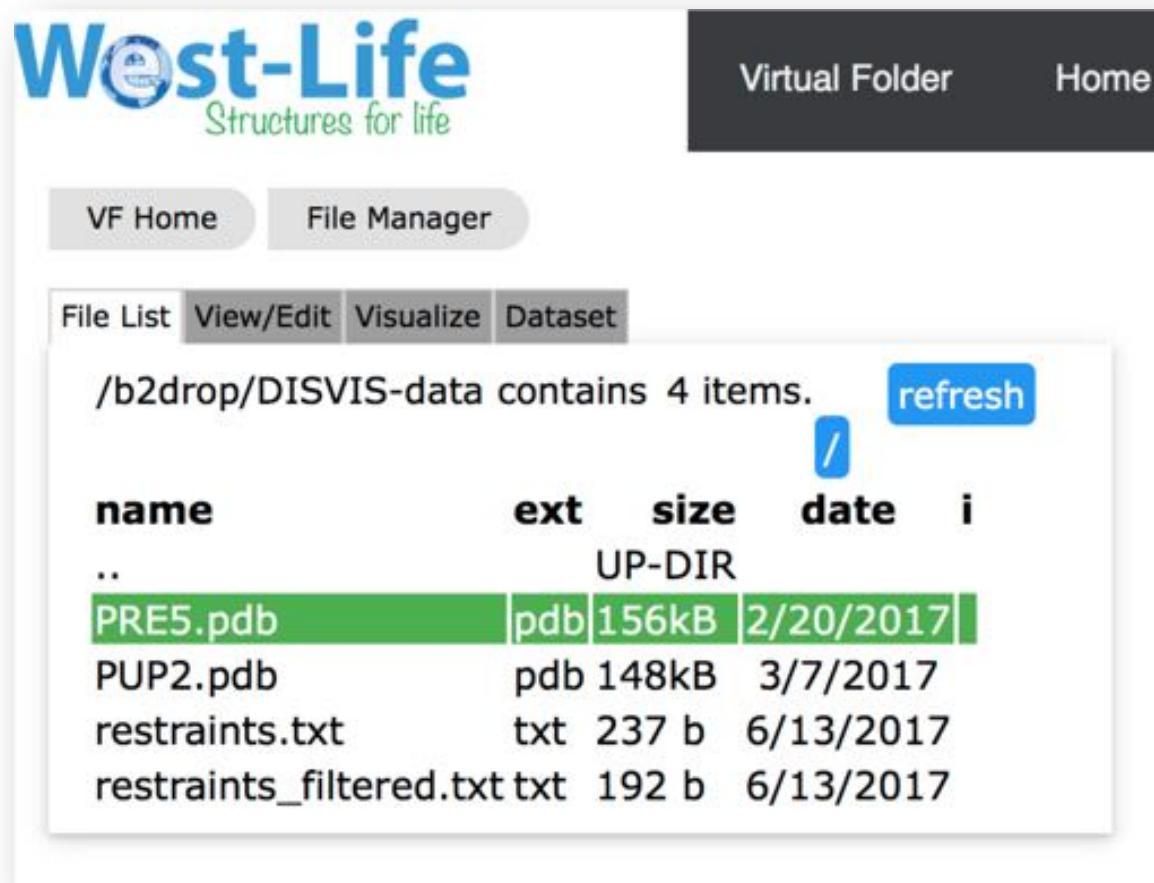
Alias	Type	Actions
b2drop	B2Drop	Browse content [lock icon] [X icon]
dropbox	Dropbox	Browse content [lock icon] [X icon]

Below the table is a blue button labeled "Add new file provider". To the right of the table, there is a dropdown menu with the following options:

- ✓ Choose provider
- B2Drop
- Dropbox
- WebDav

Allows to aggregate storage providers

The West-Life Virtual Folder



The screenshot displays the West-Life Virtual Folder interface. At the top left is the West-Life logo with the tagline "Structures for life". To the right, there are navigation tabs for "Virtual Folder" and "Home". Below the logo, there are buttons for "VF Home" and "File Manager". A menu bar contains "File List", "View/Edit", "Visualize", and "Dataset". The main content area shows the path "/b2drop/DISVIS-data contains 4 items." with a "refresh" button and a folder icon. Below this is a table listing files and directories.

name	ext	size	date	i
..		UP-DIR		
PRE5.pdb	pdb	156kB	2/20/2017	
PUP2.pdb	pdb	148kB	3/7/2017	
restraints.txt	txt	237 b	6/13/2017	
restraints_filtered.txt	txt	192 b	6/13/2017	

Allows to browse storage

West-Life VMs



West-Life
Structures for Life

Home Services Support News About Cloud Developers Contact Introduction

Virtual Machine Services

- **ScipionCloud_v1.0** 
app01.epi.eu
- **West-life VM with Virtual Folder for OpenNebula or Virtualbox** 
Continuously updated Scientific Linux 7.2 delivered by CernVM 4.0 configured with West-life feature - D6.1-VirtualFolder and West-life related software (CCPA, Scipion, ...). This virtual machine takes operating system (Scientific Linux 7.2) from cernvm.ch and software from west-life.epi.eu sites
- **West-life VM with Virtual Folder for OpenStack** 
Clone of West-life VM compatible with OpenStack.

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West-Life is part of the e-Infrastructure Virtual Research Environment (VRE) project No. 675858

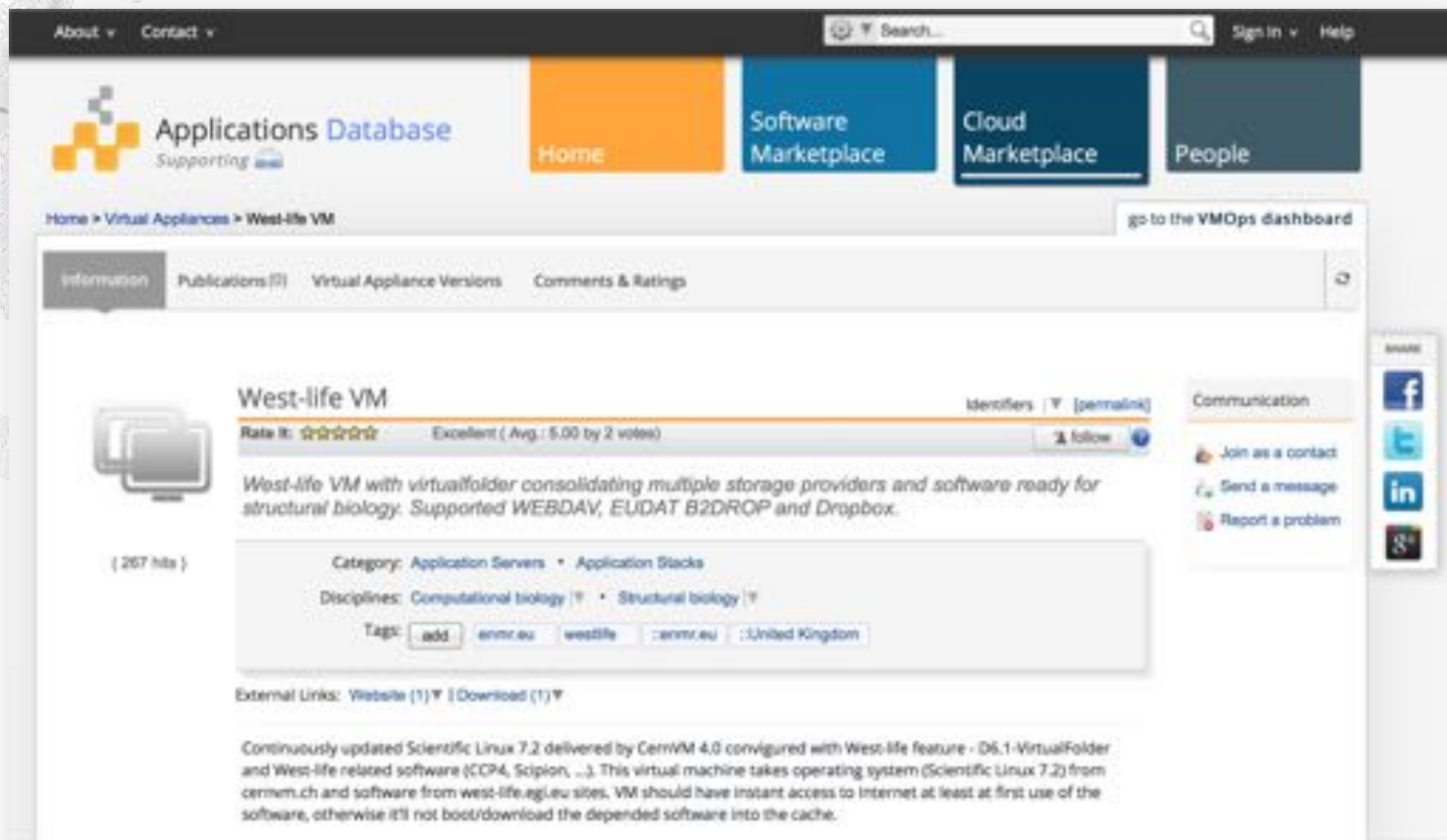
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OFI



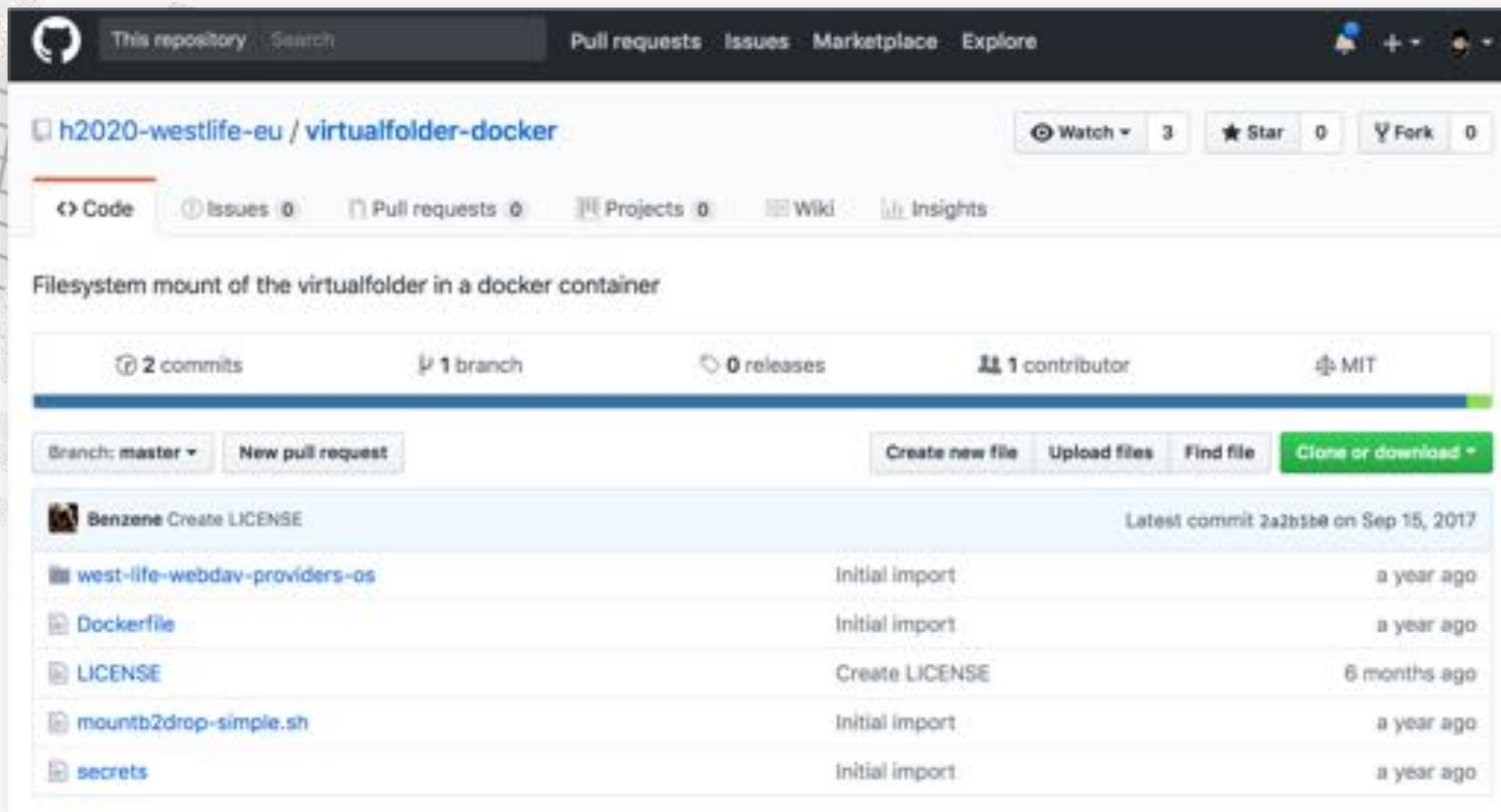
West-Life VMs



The screenshot shows the 'Applications Database' website. The main navigation bar includes 'Home', 'Software Marketplace', 'Cloud Marketplace', and 'People'. The current page is 'Home > Virtual Appliances > West-life VM'. The entry for 'West-life VM' is displayed with a rating of 5.00 (Excellent) based on 2 votes. The description states: 'West-life VM with virtualfolder consolidating multiple storage providers and software ready for structural biology. Supported WEBDAV, EUDAT B2DROP and Dropbox.' The category is 'Application Servers' and 'Application Stacks'. Disciplines include 'Computational biology' and 'Structural biology'. Tags include 'enmr.eu', 'westlife', and 'United Kingdom'. External links for 'Website' and 'Download' are provided. A detailed description at the bottom explains that it is a continuously updated Scientific Linux 7.2 delivered by CernVM 4.0, configured with West-life feature - D6.1-VirtualFolder and West-life related software (CCPA, Scipion, ...).

Available from EGI AppDB

West-Life Virtual Folder



This repository: Search Pull requests Issues Marketplace Explore

h2020-westlife-eu / virtualfolder-docker Watch 3 Star 0 Fork 0

Code Issues 0 Pull requests 0 Projects 0 Wiki Insights

Filesystem mount of the virtualfolder in a docker container

2 commits 1 branch 0 releases 1 contributor MIT

Branch: master New pull request Create new file Upload files Find file Clone or download

File Name	Commit Message	Time Ago
Benzene Create LICENSE	Latest commit 2a2b5b8 on Sep 15, 2017	
west-life-webdav-providers-os	Initial import	a year ago
Dockerfile	Initial import	a year ago
LICENSE	Create LICENSE	6 months ago
mountb2drop-simple.sh	Initial import	a year ago
secrets	Initial import	a year ago

More on the West-Life GitHub repo

Implementation in a web portal

Home >> DISVIS >> submit

DISVIS
@BonvinLab
DEVELOPMENT
VERSION

HADDOCK CPDRT **DISVIS** POWERFIT PRODIGY SPOTON 3D-DART
BONVIN LAB

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WELCOME TO THE DISVIS WEBSERVER! >>>

Input form

Note: To achieve the shortest possible runtime select the bigger entity in the "fixed chain" field and the smaller entity in the "scanning chain" field, unless you are specifically interested in the accessible interaction space of the smaller entity.

Tag

Fixed chain*

Choose File no file selected

OR select fixed chain from your VRE
Choose VRE file.

Scanning chain*

Choose File no file selected

OR select scanning chain from your VRE
Choose VRE file.

Restrains file*

Choose File no file selected

OR select restraints file from your VRE
Choose VRE file.

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Implementation in a web portal



Input form

Note: To achieve the shortest possible "scanning chain" field, unless you s

Tag

Custom tag - Optional

Fixed chain*

Choose File no file selected

Scanning chain*

Choose File no file selected

Restrains file*

Choose File no file selected

portal.west-life.eu/virtualfolder/filepickercomponent.html

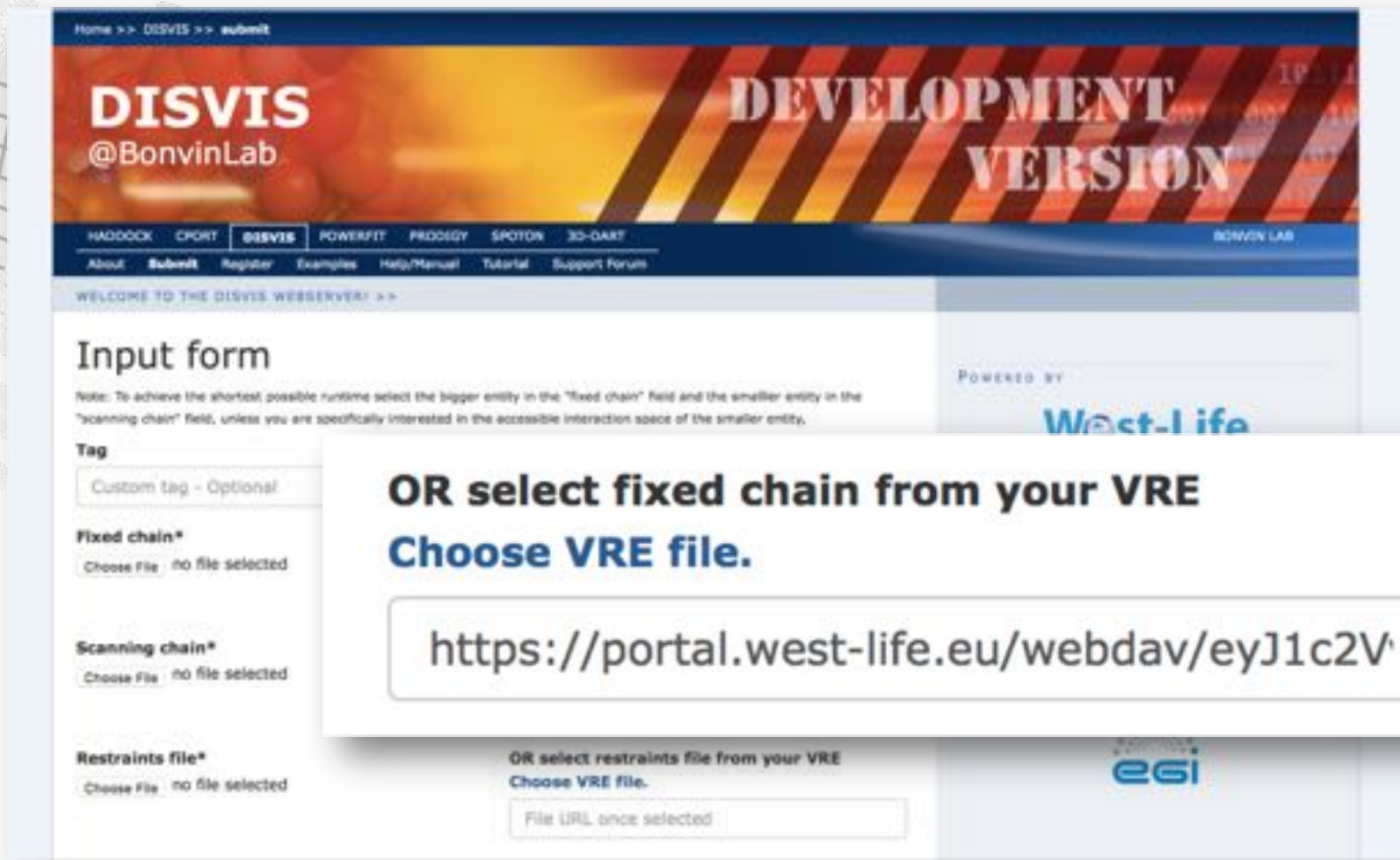
Virtual Folder - File Picker

/b2drop/DISVIS-data contains 4 items.

/ refresh

name	ext	size	date	i
..		UP-DIR		
PRE5.pdb	pdb	156kB	2/20/2017	
PUP2.pdb	pdb	148kB	3/7/2017	
restraints.txt	txt	237 b	6/13/2017	
restraints_filtered.txt	txt	192 b	6/13/2017	

Implementation in a web portal



Home >> DISVIS >> submit

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DEVELOPMENT VERSION

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WELCOME TO THE DISVIS WEBSERVER! >>>

Input form

Note: To achieve the shortest possible runtime select the bigger entity in the "fixed chain" field and the smaller entity in the "scanning chain" field, unless you are specifically interested in the accessible interaction space of the smaller entity.

Tag
Custom tag - Optional

Fixed chain*
Choose File no file selected

Scanning chain*
Choose File no file selected

Restraints file*
Choose File no file selected

**OR select fixed chain from your VRE
Choose VRE file.**

`https://portal.west-life.eu/webdav/eyJ1c2V'`

**OR select restraints file from your VRE
Choose VRE file.**

File URL once selected

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Conclusions

- **Life of users made easier by offering direct connections between portals (no need to download and upload data)**
- **West-Life Virtual Folder solution**
 - **Aggregated view of data**
 - **Direct transfer to portal via webdav**
- **Future: Direct upload of results to Virtual Folder**

Conclusions

- Life of users made easier by offering direct connections between portals (no need to download and upload data)
- West-Life Virtual Folder solution
 - Aggregated view of data
 - Direct transfer to portal via webdav
- **Present Future:** Direct upload of results to Virtual Folder

Implementation in a web portal



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Virtual Folder - Upload-dir Picker

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WELCOME TO THE LOCAL DISVIS WEBSERVER! >>

Run aaa_3qUIF3Kp

Status: **FINISHED**

Your DisVis run has successfully completed.

Archive of the complete run: [aaa_3qUIF3Kp.tgz](#)

Upload results to West-Life Virtual Folder: [Upload archive to VF](#) Status: SUCCESS - Open VF

Archive of all autogenerated images: [aaa_3qUIF3Kp_images.tgz](#)

Please cite the following papers in your work:

G.C.P. van Zundert, M. Trellet, J. Schaarschmidt, Z. Kurkcuoglu, M. David, M. Verlets, A. Rosato and A.M.J.J. Bonvin.
The DisVis and PowerFit web servers: Explorative and Integrative Modeling of Biomolecular Complexes. *J. Mol. Biol.*, Advanced Online Publication (2016).

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Thank you for your attention!

<http://bonvinlab.org>