

# WeNMR and applications portals

EOSC ask me anything webinar

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with

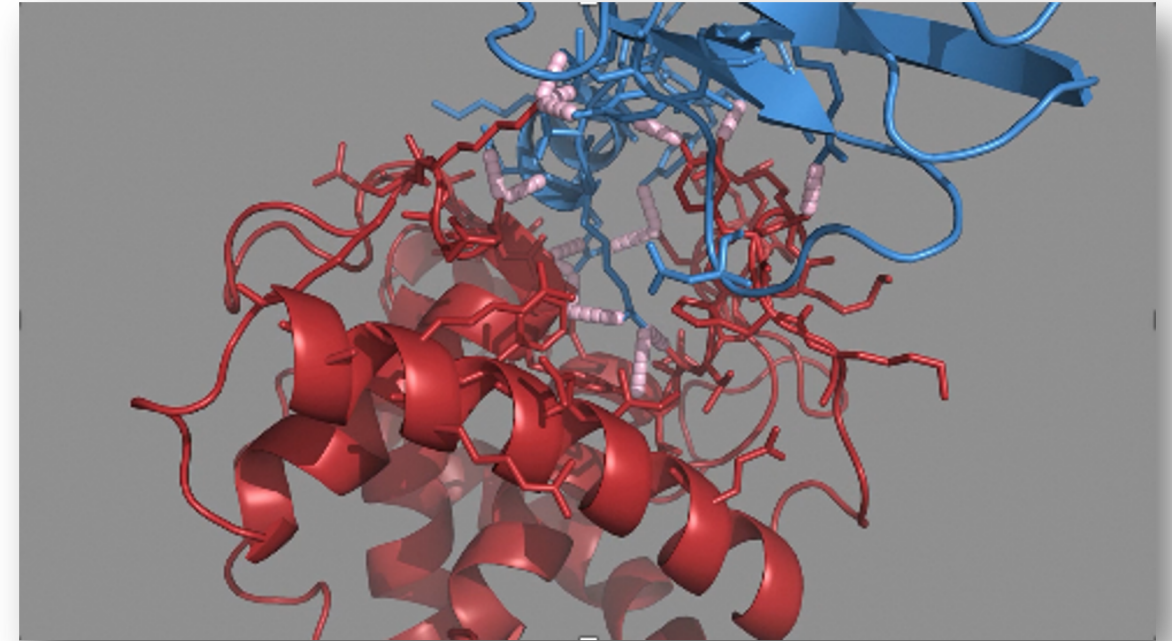
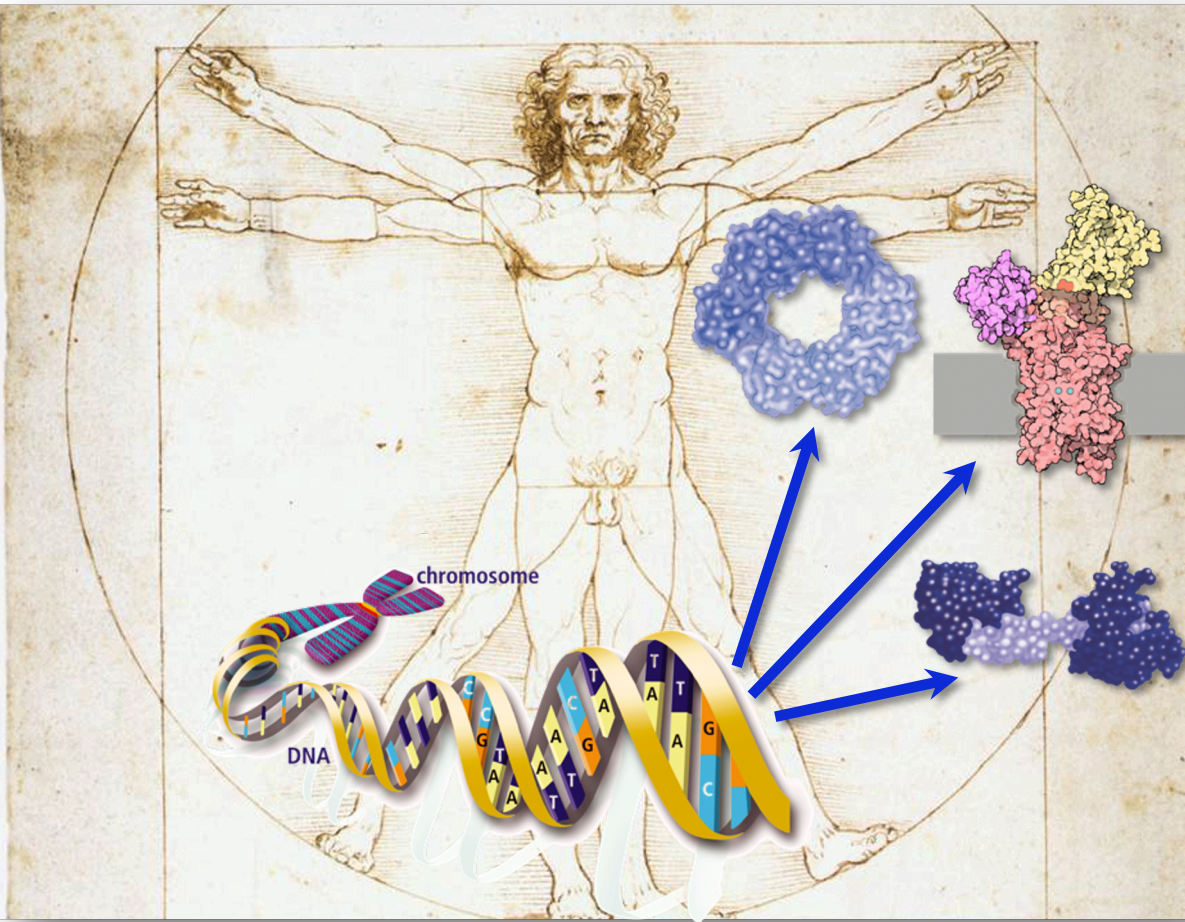


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# Domain: Life Sciences / Structural Biology

Understand life at a molecular level



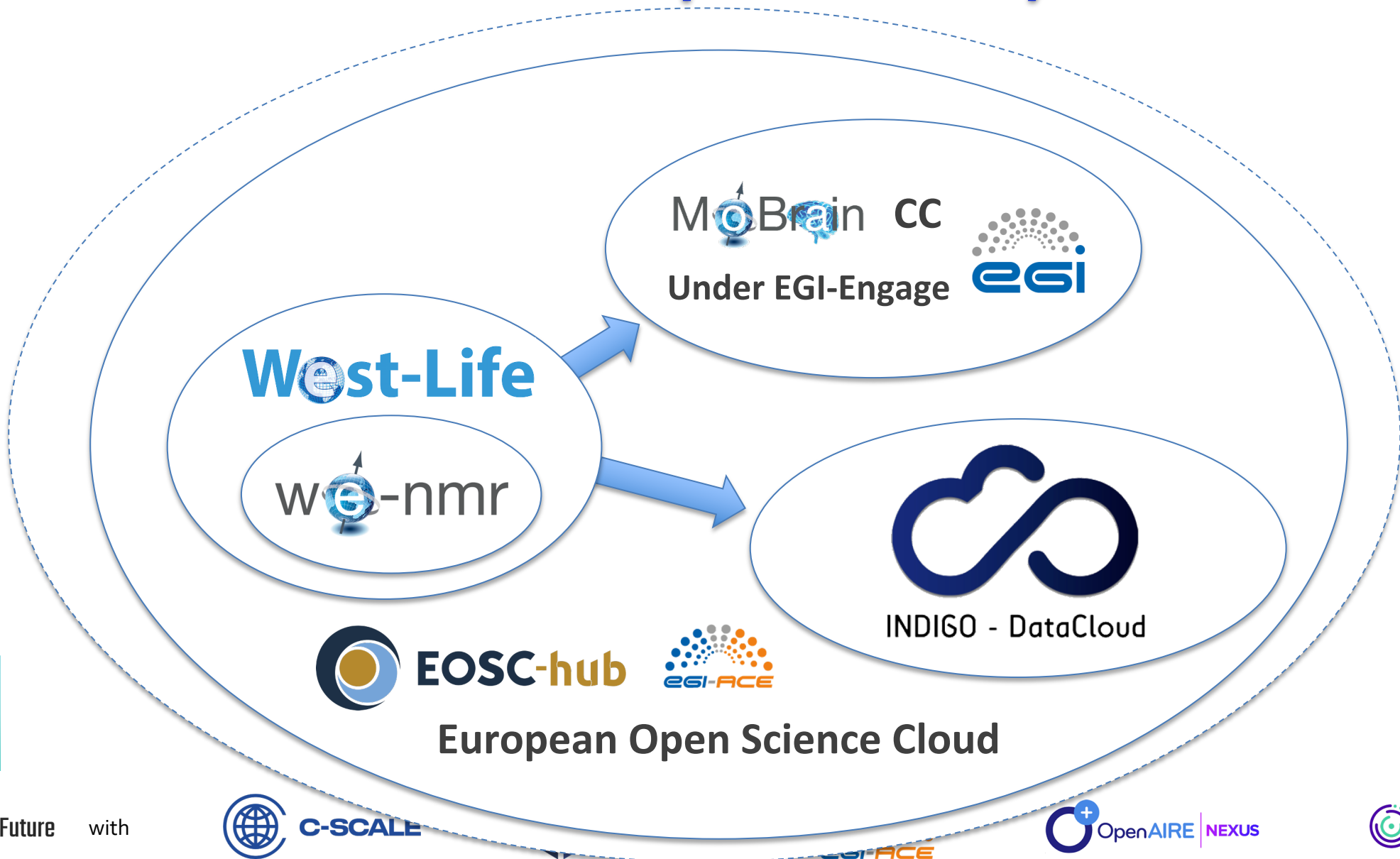
## Main use cases:

- Disease-causing mutations
- Engineer better molecules for material, health or food applications
- Obtain a starting point for drug design to combat disease





# The e-Infrastructure landscape over the years



[www.wenmr.eu](http://www.wenmr.eu)

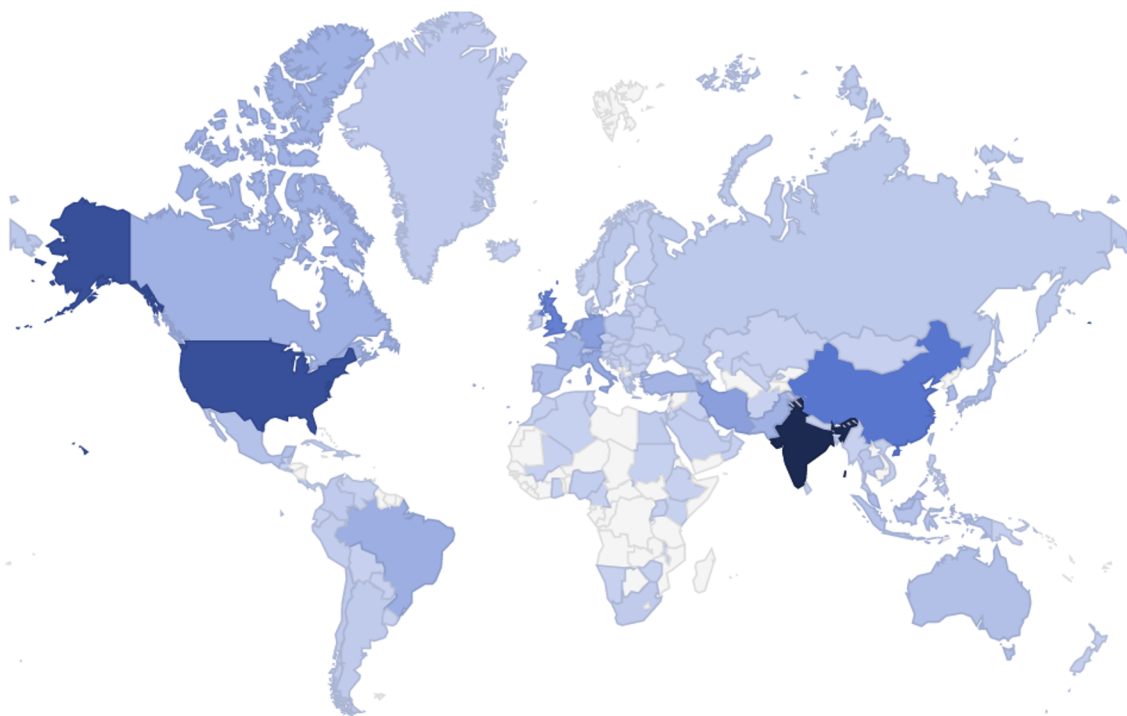


with



# Sustained growth of the WeNMR user base

All\_Users HADDOCK DISVIS POWERFIT SPOTON



	Country	All_Users ▼	HADDOCK	DISVIS	POWERFIT	SPOTON
1	Total Users	28,156	27,235	4,424	3,591	4,087
2	India	5,668	5,527	906	809	909
3	EU Users	5,622	5,362	851	591	678
4	United States	3,910	3,776	583	427	522
5	China	1,902	1,870	330	293	327

[https://wenmr.science.uu.nl/user\\_map](https://wenmr.science.uu.nl/user_map)

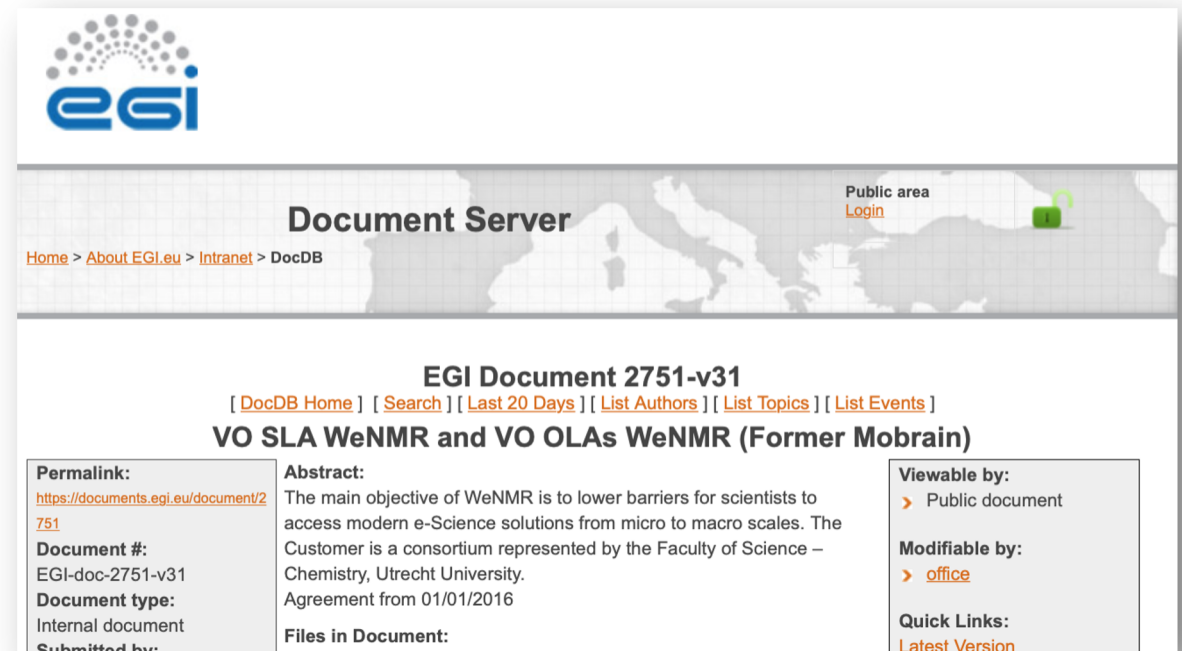


# Resources

The WeNMR services have been in production since >10 years under various projects (eNMR, WeNMR, West-Life, EOSC-Hub, EGI-ACE)

Access to resources formalized via EGI through a SLA agreement

- **50+** million CPU hours  
(opportunistic access)
- **500+** cloud CPU cores
- **~60** TB storage

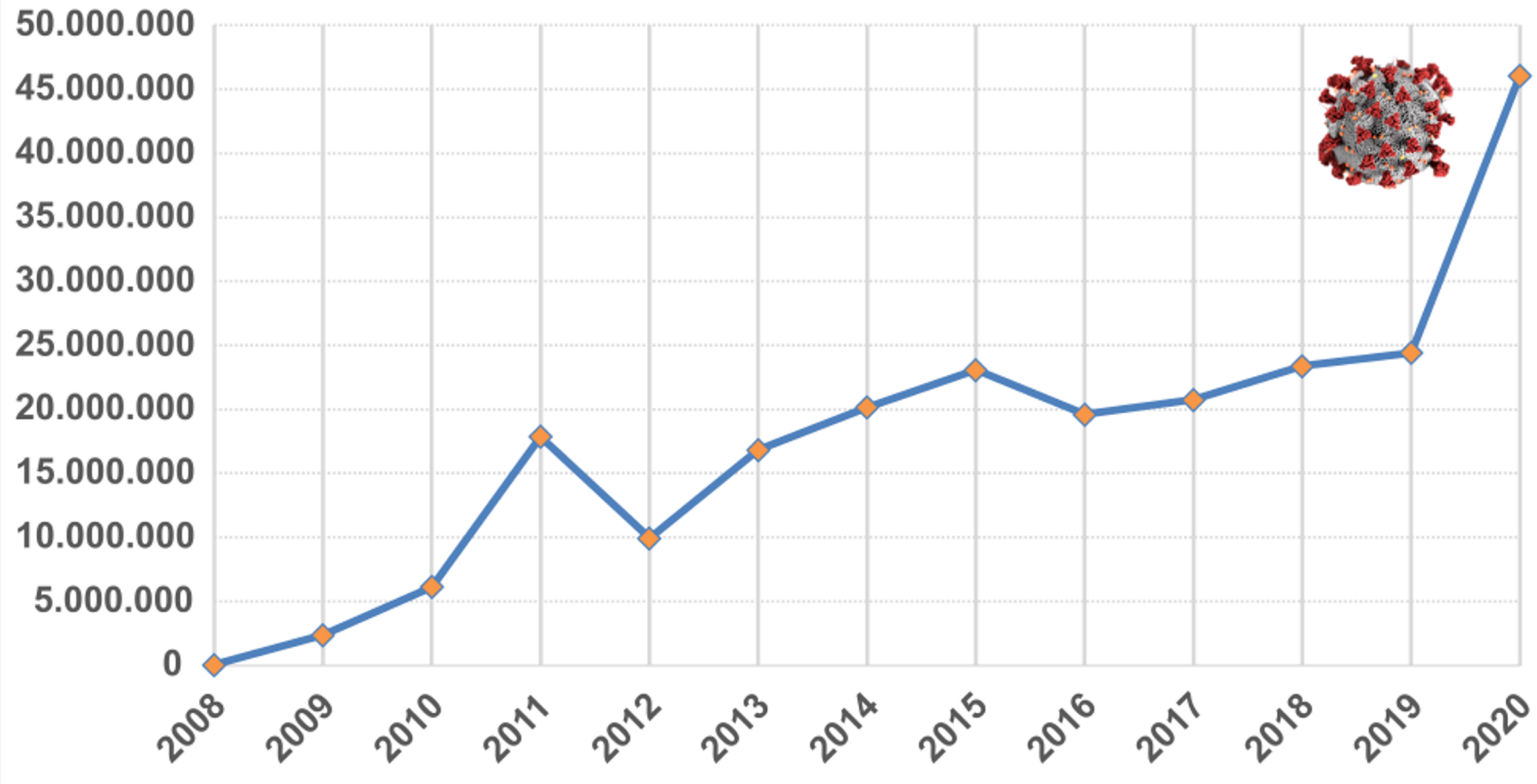


The screenshot displays the EGI Document Server interface. At the top, the EGI logo is visible. Below it, the page title "Document Server" is centered, with a "Public area Login" link on the right. A breadcrumb trail reads "Home > About EGI.eu > Intranet > DocDB". The main content area features the title "EGI Document 2751-v31" and a list of links: "[ DocDB Home ] [ Search ] [ Last 20 Days ] [ List Authors ] [ List Topics ] [ List Events ]". Below this, the document is identified as "VO SLA WeNMR and VO OLAs WeNMR (Former Mobrain)". A table-like layout provides details:

<b>Permalink:</b> <a href="https://documents.egi.eu/document/2751">https://documents.egi.eu/document/2751</a>	<b>Abstract:</b> The main objective of WeNMR is to lower barriers for scientists to access modern e-Science solutions from micro to macro scales. The Customer is a consortium represented by the Faculty of Science – Chemistry, Utrecht University. Agreement from 01/01/2016	<b>Viewable by:</b> ➤ Public document
<b>Document #:</b> EGI-doc-2751-v31	<b>Files in Document:</b>	<b>Modifiable by:</b> ➤ <a href="#">office</a>
<b>Document type:</b> Internal document		<b>Quick Links:</b> <a href="#">Latest Version</a>
<b>Submitted by:</b>		

# Resources usage

## enmr.eu VO normalized CPU hours/year







# The WeNMR services suite



with



# The WeNMR services portfolio over the years

The collage displays a variety of web portals and interfaces for NMR-related services. Key elements include:

- Xplor-NIH e-NMR GRID-enabled web portal:** A portal for Xplor-NIH simulations, featuring a login section and a "Parameters" table.
- AMBER e-NMR GRID-enabled web portal:** A portal for AMBER simulations, including an "INTRODUCTION TO AMBER WEB PORTAL" and a "Parameters" table.
- CYANA Web Portal:** A portal for CYANA simulations, featuring a "WELCOME TO CYANA WEB PORTAL" and a "RECOMMENDED BROWSER: MOZILLA FIREFOX" section.
- HADDOCK e-NMR GRID-enabled web portal:** A portal for HADDOCK simulations, including a "WELCOME TO THE e-NMR WEB PORTAL" and a "HADDOCK WEBSERVER" section.
- CS-ROSETTA e-NMR GRID-enabled web portal:** A portal for CS-ROSETTA simulations, featuring a "WELCOME TO THE e-NMR WEB PORTAL" and a "RECOMMENDED BROWSER: MOZILLA FIREFOX" section.
- MAXOCC WeNMR GRID-enabled web portal:** A portal for MAXOCC simulations, including a "WELCOME TO THE e-NMR WEB PORTAL" and a "RECOMMENDED BROWSER: MOZILLA FIREFOX" section.
- GROMACS e-NMR (GRID-enabled) web portal:** A portal for GROMACS simulations, featuring a "WELCOME TO THE e-NMR WEB PORTAL" and a "RECOMMENDED BROWSER: MOZILLA FIREFOX" section.
- 3DDART e-NMR (GRID-enabled) web portal:** A portal for 3DDART simulations, including a "WELCOME TO THE e-NMR WEB PORTAL" and a "RECOMMENDED BROWSER: MOZILLA FIREFOX" section.
- MARS Web Portal:** A portal for MARS simulations, featuring a "WELCOME TO THE e-NMR WEB PORTAL" and a "RECOMMENDED BROWSER: MOZILLA FIREFOX" section.
- AnisoFIT WeNMR GRID-enabled web portal:** A portal for AnisoFIT simulations, including a "WELCOME TO THE e-NMR WEB PORTAL" and a "RECOMMENDED BROWSER: MOZILLA FIREFOX" section.
- Antechamber GRID-enabled web portal:** A portal for Antechamber simulations, featuring a "WELCOME TO THE e-NMR WEB PORTAL" and a "RECOMMENDED BROWSER: MOZILLA FIREFOX" section.

The interfaces are predominantly blue and white, with a focus on providing user-friendly access to complex NMR data and simulation tools. Some portals include detailed instructions, while others offer more interactive features like parameter tables and search filters.



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C-SCALE

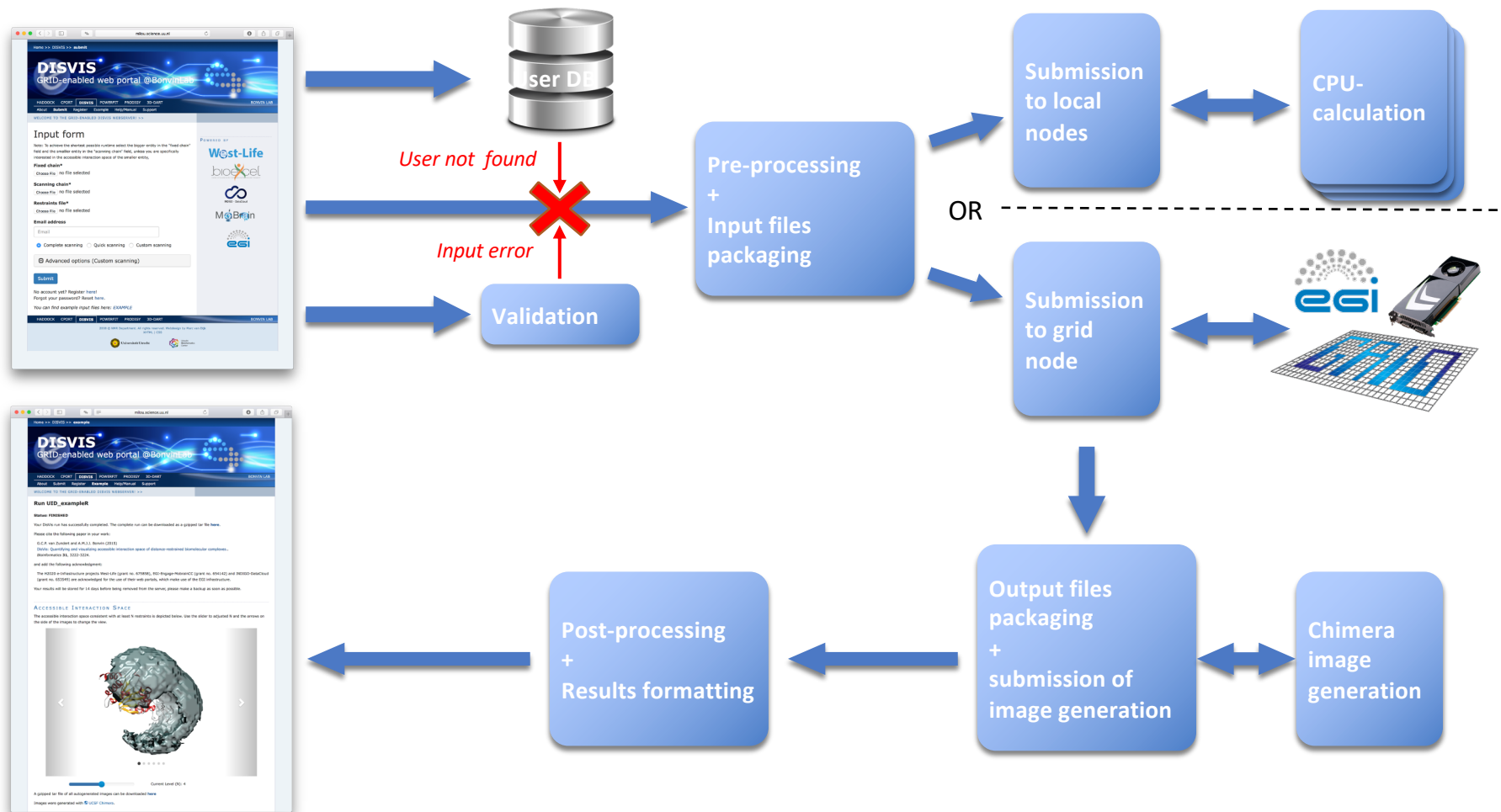



Data Infrastructure Capacity for EOSC





# Architecture behind the portals





# Supporting COVID-19 related research

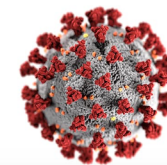


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# HADDOCK meeting the demand



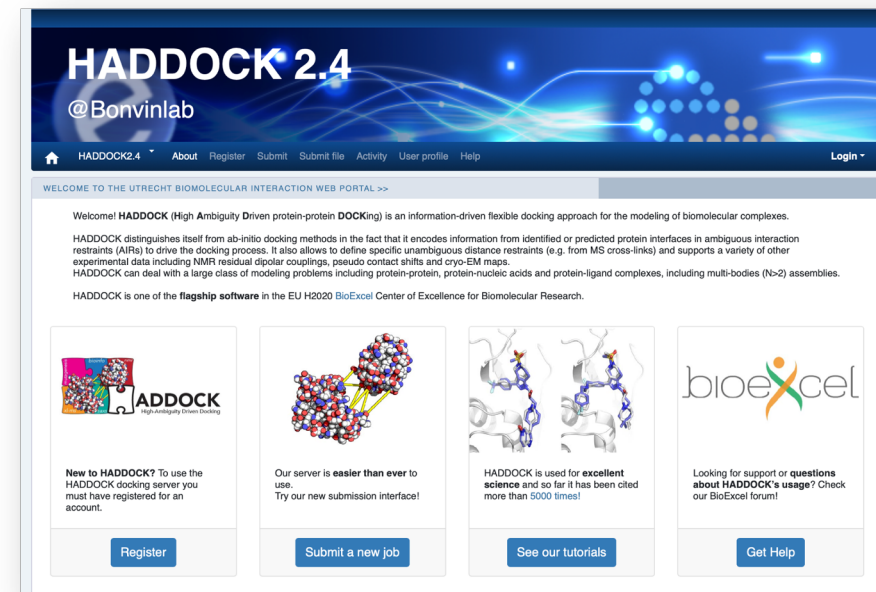
HADDOCK can be used to model interactions between virus and human proteins and for drug screening

Increased number of registrations since the lockdown measures in March 2020

We have tripled our processing capability by modifying the backend machinery managing the HADDOCK workflow

EGI additional HTC resources were allocated to WeNMR

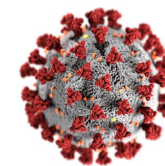
Users can now tag their submissions as COVID-related



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# Our own COVID efforts



<https://instruct-eric.eu/haddock-screen-of-2000-approved-drugs-for-covid19>

- **Modelling of various Sars-Cov2 – human protein interactions (also a CAPRI effort now)**
- **Screening of approved drugs against the protease with HADDOCK**
  - Could run on EGI/EOSC/OSG HTC resources in ~ 3 1/2 days docking of ~2000 approved drugs
- In a collaboration between MolSSI and BioExcl setup of a covid-related repository:

Initial results at:  
[bonvinlab.org/covid](https://bonvinlab.org/covid)

EUROPEAN OPEN SCIENCE CLOUD

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Home > trainings > HADDOCK to support COVID-19 research

**HADDOCK to support COVID-19 research**

06 Apr 2020

HADDOCK to support COVID-19 research

instruct ERIC

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Home > HADDOCK screen of 2000 approved drugs for COVID-19

**Resource Centre**  
Supporting research relating to SARS-CoV-2 and COVID-19

**HADDOCK screen of 2000 approved drugs for COVID-19**

Scientists at the Instruct Centre NL have led efforts to use a software tool called HADDOCK for a large drug screen in the search for new antivirals against COVID-19. HADDOCK (High Ambiguity Driven protein-protein DOCKing) was developed by Prof Alexander Bonvin at Utrecht University as a modelling tool to predict protein-protein interactions within biomolecular complexes.

One potential drug target for the COVID-19 virus is the SARS-CoV-2 protease, which has an essential role in processing the polyproteins that are translated from the viral RNA during replication. Therefore, a SARS-CoV-2 protease inhibitor could make for an effective anticonviral drug. Due to the urgent need for anti-COVID-19 therapies, researchers decided to screen for drugs that are already approved for other diseases. The strategy to repurpose existing drugs for new diseases is very appealing, as these drugs have already been fully tested in clinical trials to make sure that there is no toxicity or concerning side effects.

Using a platform such as HADDOCK, allows for rapid screening of thousands of chemical compounds against the protease structure, compared to reviewing compounds one-by-one after co-crystallisation or by Cryo-EM. In the first 24 hours, for example, an average of 731 jobs were completed per hour using HADDOCK.

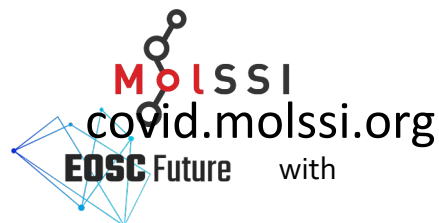
**Docking results: cluster-based**

score

target

Protease-inhibitors  
Antivirals  
Antiretrovirals  
Other  
NA


<https://www.eosc-portal.eu/news/haddock-support-covid-19-research>





# The WeNMR services portfolio in the EOSC

<https://marketplace.eosc-portal.eu/>



**EUROPEAN OPEN  
SCIENCE CLOUD**

Find resource...

Platform

My EOSC Marketplace

Resources > Sharing & Discovery > Software > Platform

All Resources 37

**CATEGORIES**

- Libraries 0
- Platform 7**
- Software Package 0
- Software Repository 0
- Other 0

**FILTERS**

**Scientific Domains**

Find or choose from the list below

- ☐ Natural Sciences 10
- ☒ **Biological Sciences 7**
- ☐ Earth & Related Environmental Sciences 2
- ☐ Computer & Information Sciences 1
- ☐ Other Natural Sciences 1
- ☐ Chemical Sciences 0
- ☐ Mathematics 0
- ☐ Physical Sciences 0

**FANTEN (Finding Anisotropy TENSOR)**

FANTEN for the analysis of magnetic anisotropy-induced NMR data

Organisation: A Worldwide e-Infrastructure for Structural Biology  
Provided by: Magnetic Resonance Center of the University of Florence - CERM, Interuniversity consortium CIRMMP  
Scientific domain: Biological Sciences

☐ Add to comparison ☐ Add to favourites

FULLY OPEN ACCESS

we-nmr

**HADDOCK2.4 web portal**

Integrative modelling of biomolecular complexes

Organisation: A Worldwide e-Infrastructure for Structural Biology  
Provided by: Bijvoet Centre - Utrecht University  
Scientific domain: Biological Sciences, Other Medical Sciences

☐ Add to comparison ☐ Add to favourites

OPEN ACCESS

HADDOCK

**PowerFit web portal**

Fit an atomic model with a electron density map.

Organisation: A Worldwide e-Infrastructure for Structural Biology  
Provided by: Bijvoet Centre - Utrecht University  
Scientific domain: Biological Sciences, Other Medical Sciences

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PowerFit

**SpotOn web portal**

Identify Hot-Spots at protein-protein interfaces.

Organisation: A Worldwide e-Infrastructure for Structural Biology  
Provided by: Bijvoet Centre - Utrecht University  
Scientific domain: Biological Sciences, Other Medical Sciences

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SpotOn

**AMBER-based Portal Server for NMR structures (AMPS-NMR)**

Web portal for the refinement of Nuclear Magnetic Resonance (NMR) structures of macromolecules

Organisation: A Worldwide e-Infrastructure for Structural Biology  
Provided by: Magnetic Resonance Center of the University of Florence - CERM, Interuniversity consortium CIRMMP  
Scientific domain: Biological Sciences, Other Medical Sciences

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AMPS-NMR

**DisVis web portal**

Visualisation of interaction space between two molecules

Organisation: A Worldwide e-Infrastructure for Structural Biology  
Provided by: Bijvoet Centre - Utrecht University  
Scientific domain: Biological Sciences, Other Medical Sciences

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OPEN ACCESS

DisVis

**PDB-Tools web**

Process and massage your PDB file using PDB-Tools

Organisation: A Worldwide e-Infrastructure for Structural Biology  
Provided by: Bijvoet Centre - Utrecht University  
Scientific domain: Biological Sciences, Other Medical Sciences

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PDB-Tools



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# Acknowledgements



**VICI  
TOP-PUNT**



**WeNMR  
West-Life  
EGI-Engage  
INDIGO-  
Datacloud  
BioExcel CoE  
EOSC-Hub  
EGI-ACE  
SURFSara**



**the CSB group@UU**

