WeNMR and applications portals

EOSC ask me anything webinar

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EOSC Future with C-SCALE DICE Data Infrastructure Capacity for EOSC EGI-ACE OpenAIRE NEXUS Reliance

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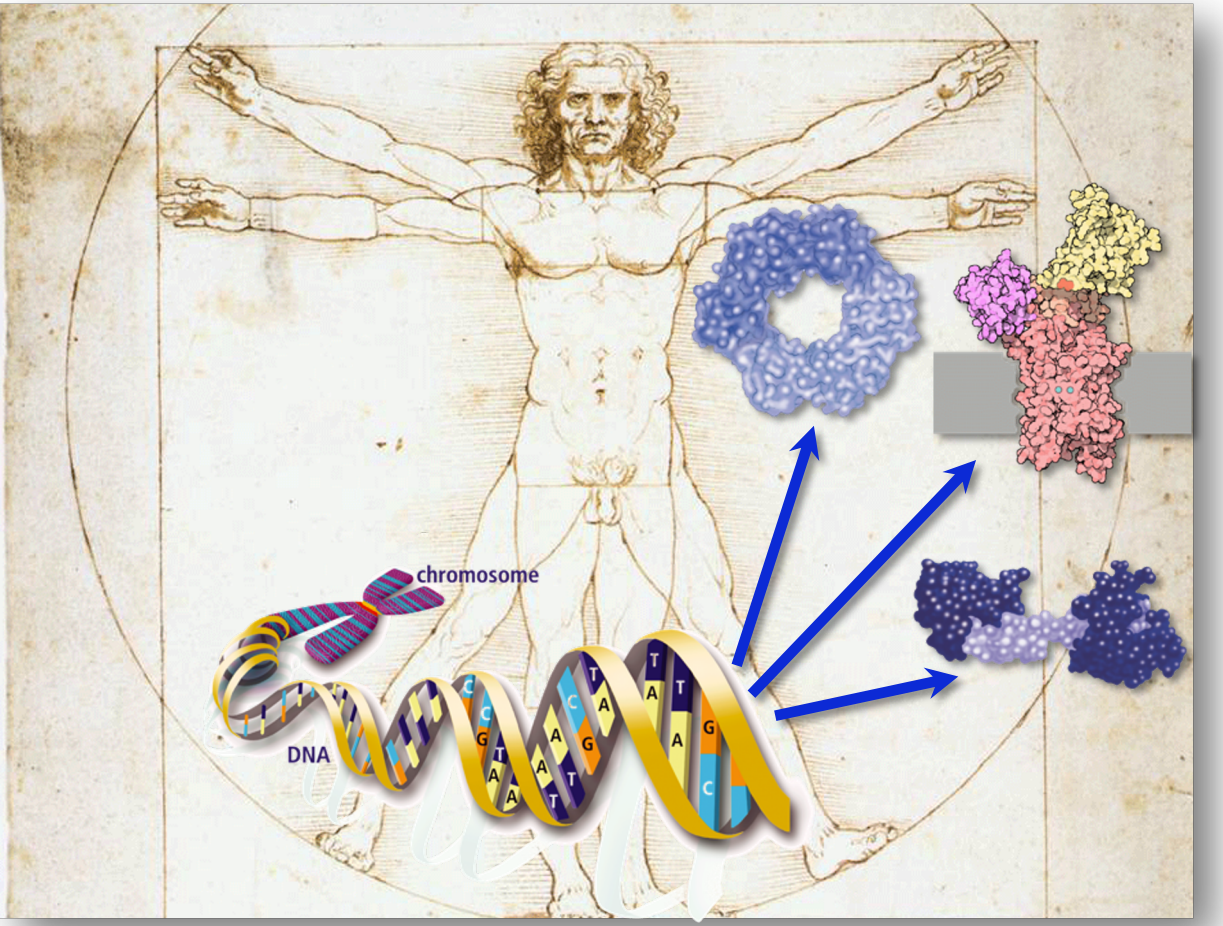
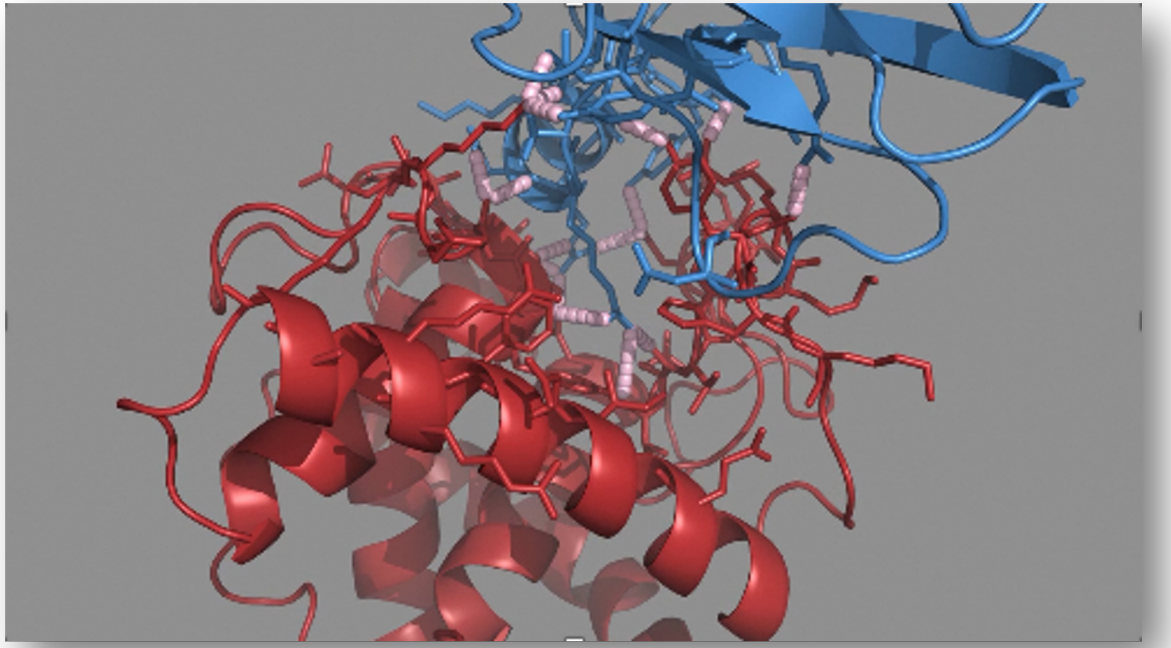
Domain: Life Sciences / Structural Biology

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

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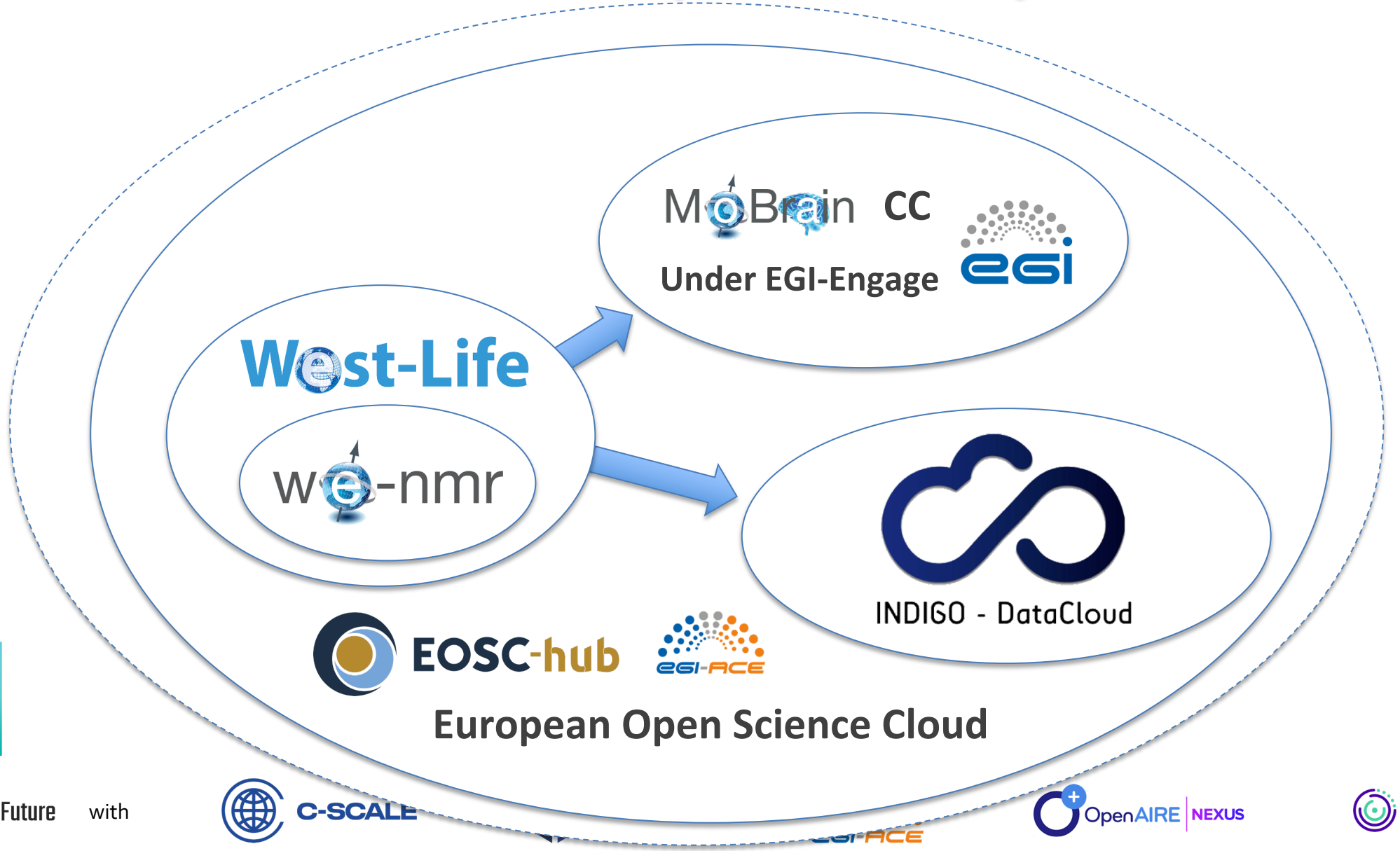
The e-Infrastructure landscape over the years



www.wenmr.eu

instruct ERIC
EUROPEAN RESEARCH INFRASTRUCTURE CONSORTIUM

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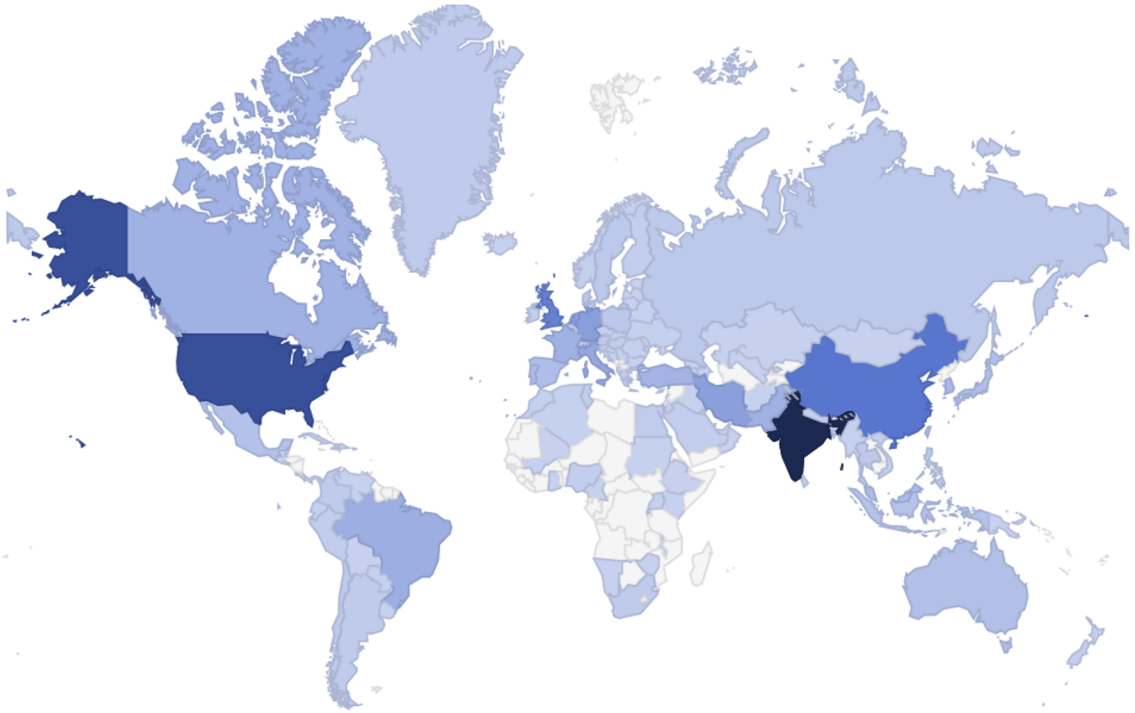
Sustained growth of the WeNMR user base

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

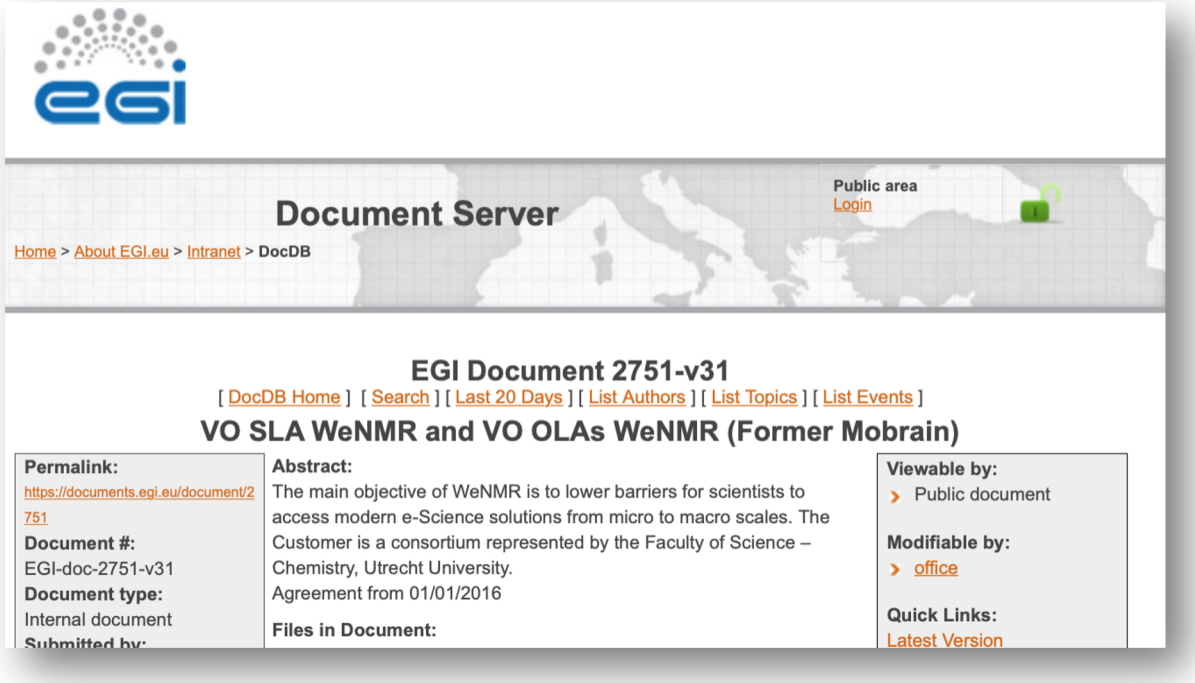
https://wenmr.science.uu.nl/user_map

Resources

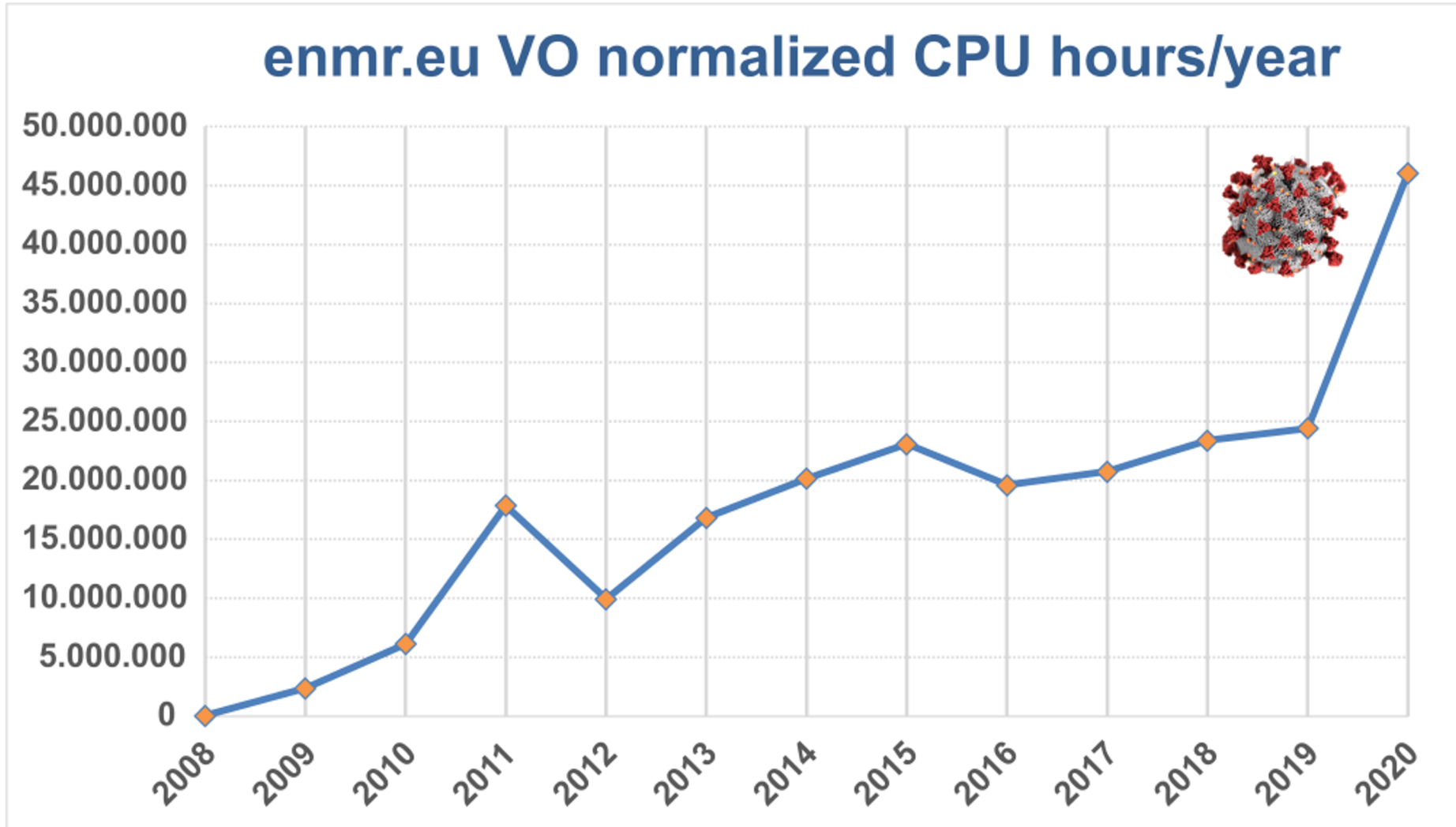
The WeNMR services have been in production since >10 years under various projects (eNMR, WeNMR, West-Life, EOSC-Hub, EGI-ACE)

Access to resources formalized via EGI through a SLA agreement

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



Resources usage



The WeNMR services suite

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The WeNMR services portfolio over the years

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Architecture behind the portals

User DB

User not found

Input error

Validation

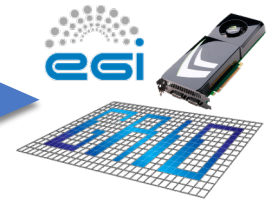
Pre-processing
+
Input files packaging

Submission to local nodes

CPU-calculation

OR

Submission to grid node



Output files packaging
+
submission of image generation

Chimera image generation

Post-processing
+
Results formatting

WEB CLIENT

WEB SERVER

MASTER NODE

WORKING NODE

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Supporting COVID-19 related research

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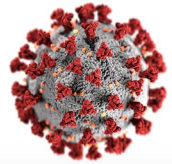
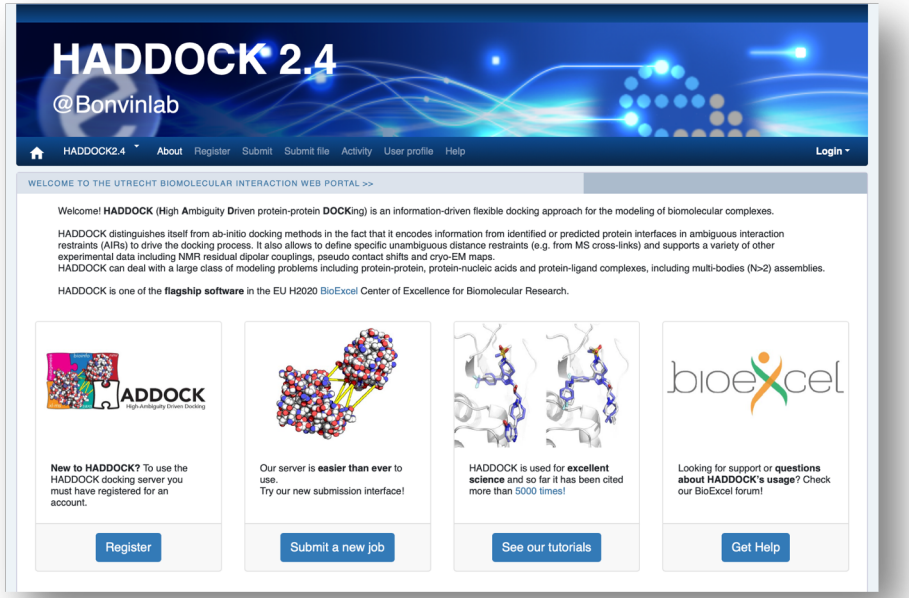
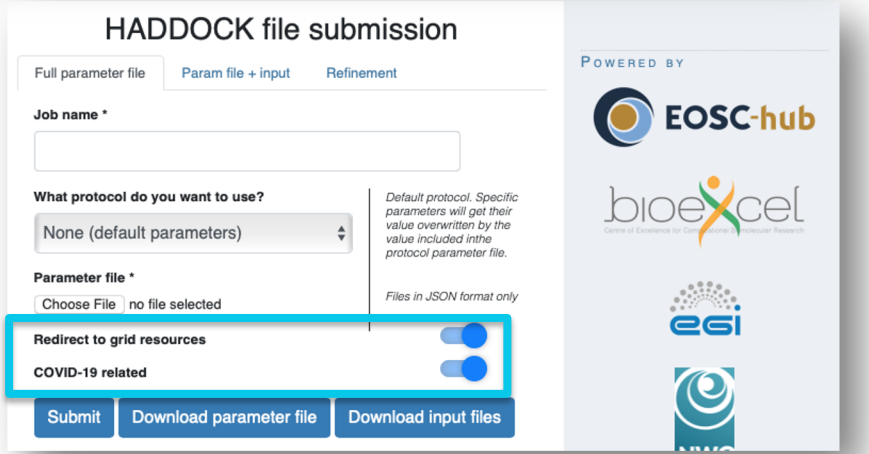
HADDOCK meeting the demand



- 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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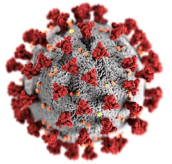
Our own COVID efforts



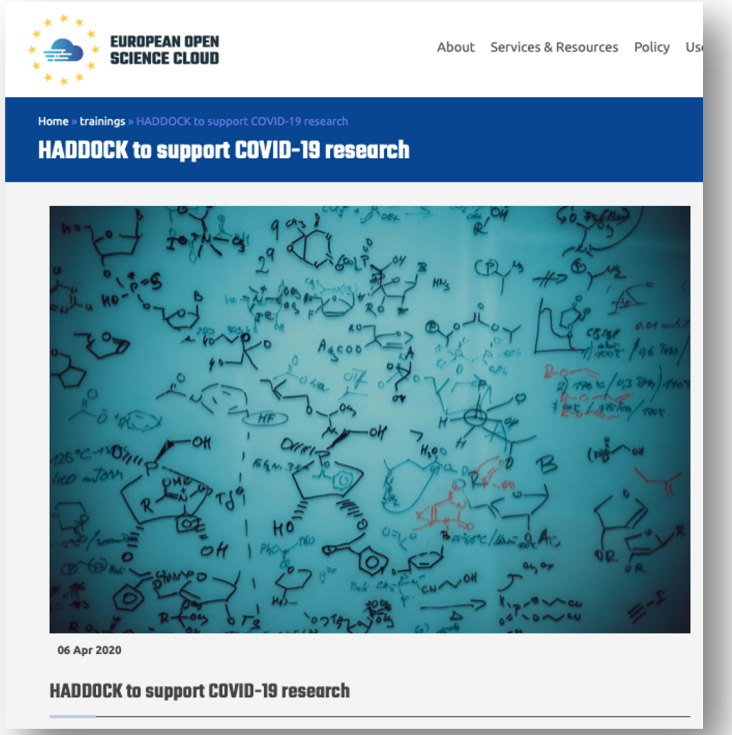
https://instruct-eric.eu/haddock-screen-of-2000-approved-drugs-for-covid19

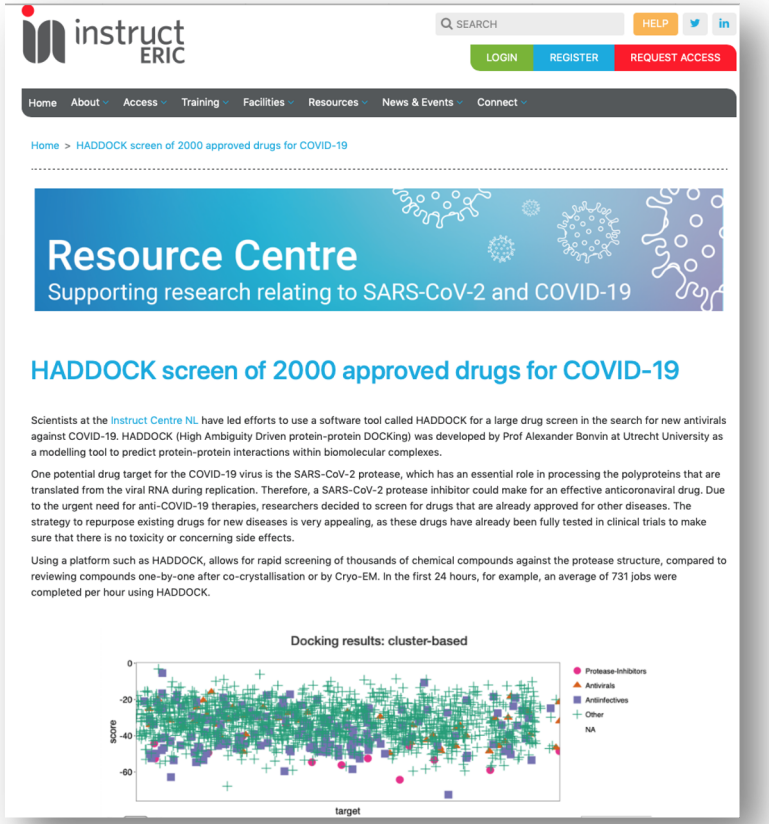
- **Modelling of various Sars-Cov2 – human protein interactions (also a CAPRI effort now)**

- **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://www.eosc-portal.eu/news/haddock-support-covid-19-research

MolSSI
covid.molssi.org
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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

FULLY OPEN ACCESS

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

OPEN ACCESS

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

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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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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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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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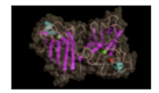

OPEN ACCESS

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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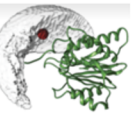

FULLY OPEN ACCESS

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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