HADDOCK / WeNMR Suite for Structural Biology

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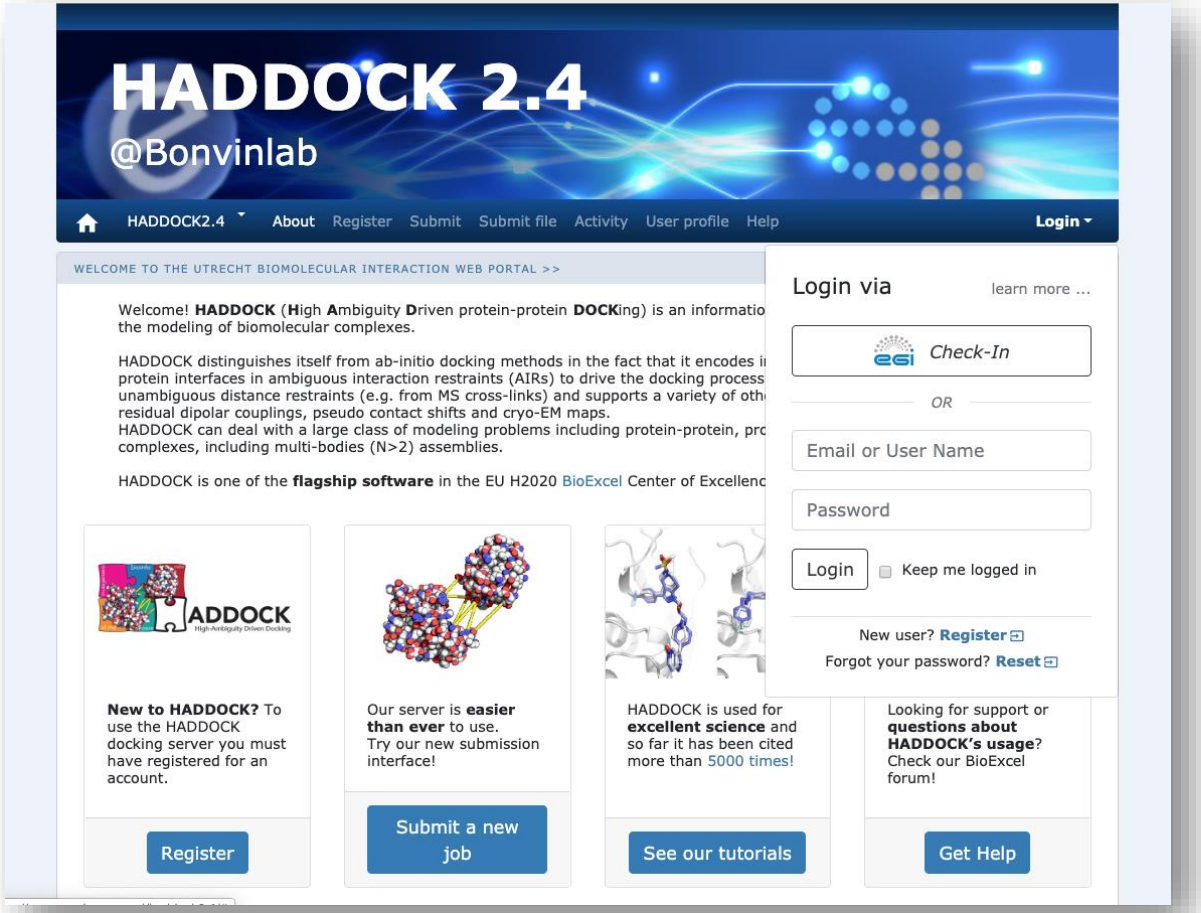
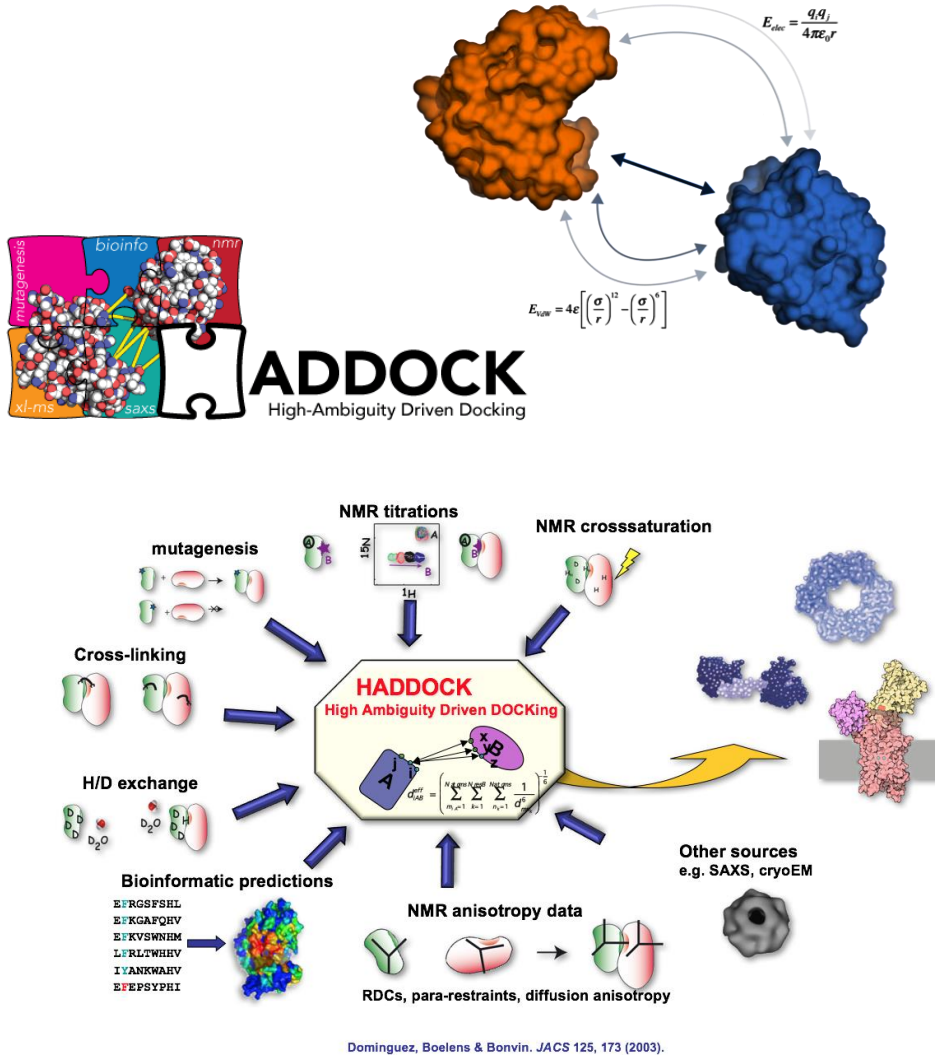
HADDOCK – integrative modelling platform

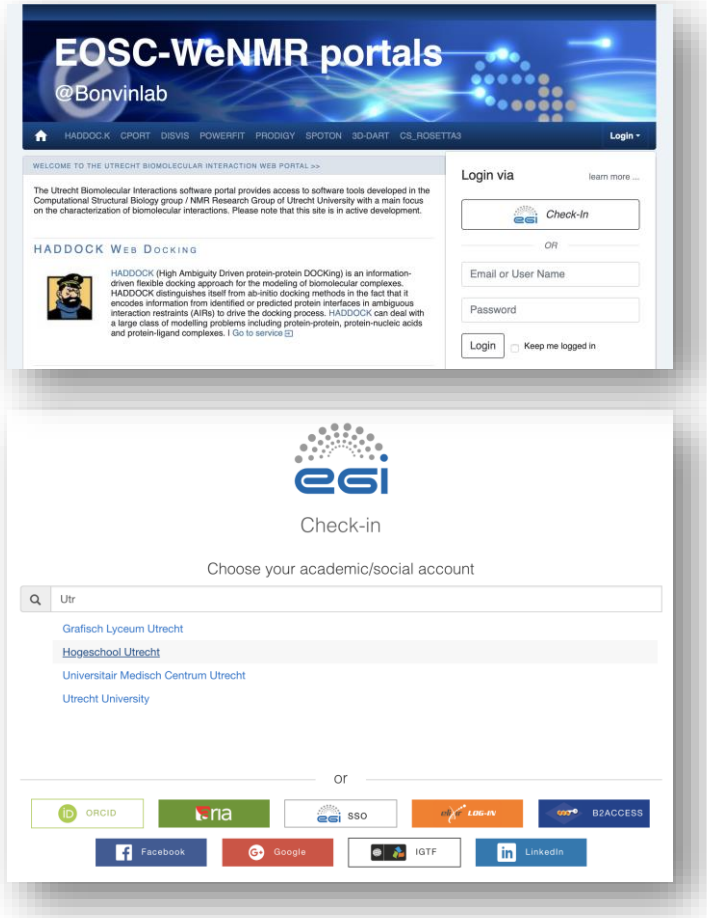




Dominguez, Boelens & Bonvin. *JACS* 125, 173 (2003).

WeNMR thematic services

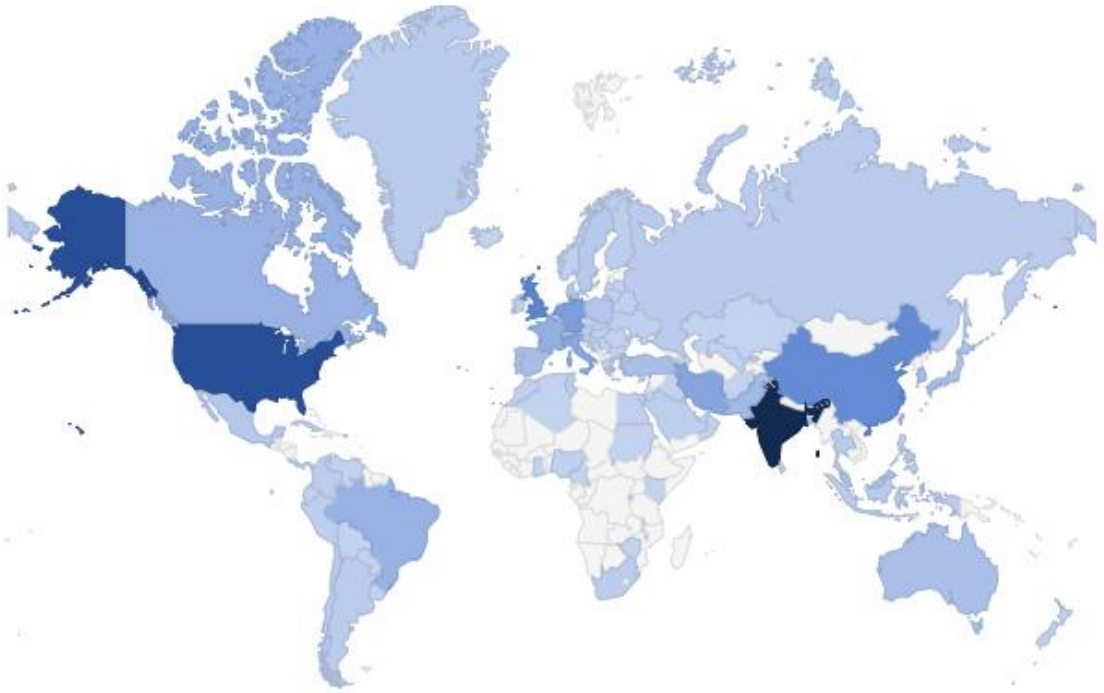
- The **WeNMR services** are based on:
  - A web page front end to the service exposed to the user
  - Back end consisting of a variety of software and scripts
  - Make use of the **DIRAC4EGI/EGI workload** service for distributing compute jobs and of some **gLite** components in some cases
  - Make use of the **HTC EGI resources (grid, cloud, GPGPUs)** of EOSC-Hub to distribute the computations
  - User registration and authentication mechanisms connected to **EGI Check-in**
  - Some portals make use of **OneData** for data management
  - Some portals use the **INDIGO-Datacloud udocker** solution



WeNMR/HADDOCK – Impact

- > 16’000 registered users
- > 110 countries reached
- > 25 millions jobs submitted to HTC resources per year
- Portals in grid operation mode since >10 years by now
- Supported by enmr.eu VO
- Make us of DIRAC for job submission/management

All_Users | HADDOCK | DISVIS | POWERFIT | SPOTON | CS_ROSETTA3

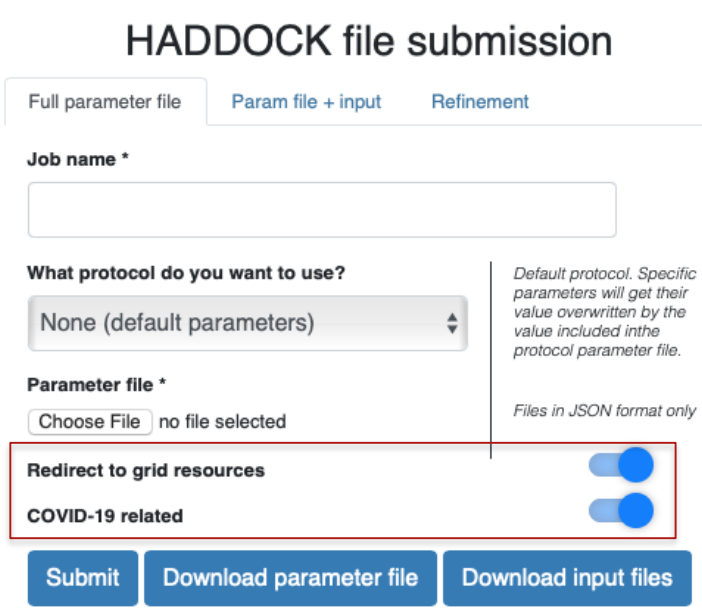


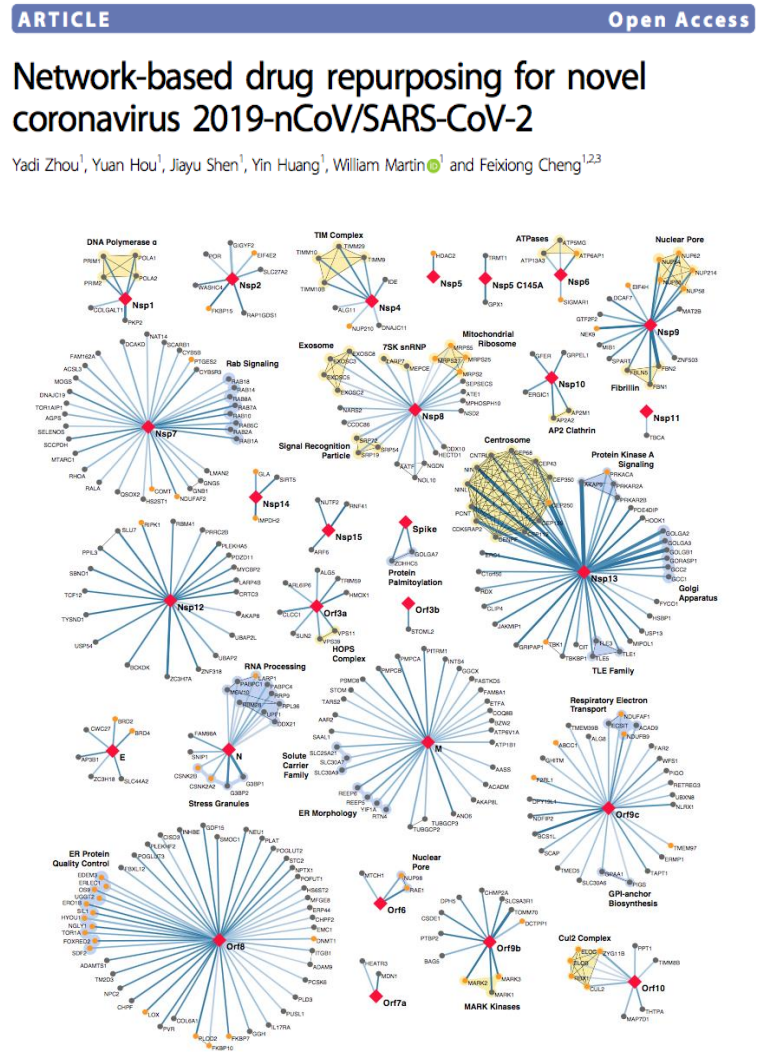
	Country	All_Users	HADDOCK	DISVIS	POWERFIT	SPOTON	CS_ROSETTA3
1	Total Users	16,824	16,147	1,784	1,363	1,493	1,152
2	India	3,625	3,553	331	289	334	239
3	EU Users	3,767	3,533	473	318	291	240
4	United States	2,550	2,448	253	166	210	156
5	United Kingdom	996	946	85	68	60	69
6	China	933	913	88	78	91	60

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

HADDOCK COVID-related activities

- **Modelling of Sarc-Cov-2 – human protein interactions**
- **Screening of approved drugs against the protease**
- **User activities…**
- **HADDOCK2.4 server ready to flag submission as COVID and DIRAC machinery can target those to specific sites** (thanks to Andrei Tsaregorotsev)





Thank you
for your attention!

Questions?

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