

## **Adam Hospital – talk information and short bio**

**Talk title** Biomolecular simulations and macromolecular flexibility databases in the EBRAINS research infrastructure: exploring the dynamics of central nervous system molecules.

**Subject:** Atomistic and molecular dynamics in the brain: We will present new advances to bridge the gaps between different levels of brain organisation through computational modeling. For the event we will focus on the areas spanning from atomistic simulation, to molecular dynamics, to the cellular level. We will present tools for simulation offered on our research infrastructure EBRAINS. An application example will be the investigation of Covid-19 and the brain and Alzheimer's disease.

### **Short biography**

Adam Hospital is a Postdoctoral fellow at the Molecular Modeling and Bioinformatics Unit (MMB) – Institute for Research in Biomedicine in Barcelona (IRB-Barcelona) and research software engineer for the Spanish National Institute of Bioinformatics (INB, ELIXIR-ES). From a computer science background, he jumped to the bioinformatics world and got trapped by the fascinating field of structural bioinformatics. He has been involved in scientific projects at IRB and at the Barcelona Supercomputing Center (BSC), and he is currently leading the workflows team in the BioExcel CoE. While working as a bioinformatician, he obtained his PhD in Biotechnology from the University of Barcelona with his thesis *“High Throughput Computational Studies of Macromolecular Structure Flexibility”*. He has developed and coordinated a set of public web servers and databases related to macromolecular structure flexibility, included in the INB integrated platform for macromolecular flexibility.