SGR2021 EAPM: ELECTRONIC AND ATOMIC PROTEIN MODELLING

Description

We are devoted to the development of computational algorithms for LifeScience, using molecular modelling techniques, bioinformatics and machine learning methods.

Our molecular modeling software, PELE, is used worldwide through its public server, and commercialised through NBD since 2017, and clearly outperformed other tools in the CSAR blind competition. This status is the result of continuous algorithmic development, such as an adaptive procedure using reward functions. We also center on applications in drug targets, mostly in collaborations with Pharma companies such as Almirall or Jansen.

Other applications include enzyme engineering, where we have optimized several industrial enzymes and discovered a mechanism for adding new artificial sites into protein scaffolds: PluriZymes. Along these lines, we built a PluriZyme capable of one-pot two step cascade reactions (selected as cover in 2020 Nature Catalysis) and recently developed a nanopore capable of degrading plastic nanoparticles.

Barcelona Supercomputing Center - Centro Nacional de Supercomputación