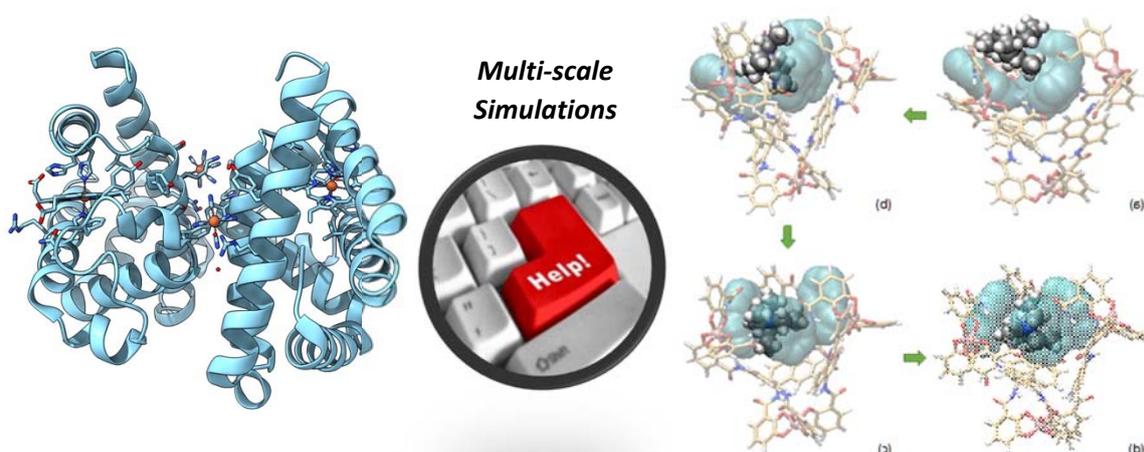


Predocctoral Position in SupraMolecular and Biological Chemistry

A 4-year predoctoral fellowship in computational chemistry from the Spanish Ministry of Science and Innovation (FPI contract) is offered at the Chemistry Department of the Universitat Autònoma de Barcelona (Spain). The grant is associated to the project **PID2020-116861GB-I00** entitled “**Frontiers in Molecular Modeling of Metal-Mediated Catalytic and Recognition Processes**”.

The successful candidate will be part of a group with a long and internationally recognized track record in molecular modelling of supramolecular systems, metal-mediated catalysis, and biological processes (<https://insilichem.com/>). Depending on her/his background and interests, he/she would participate in lines related to enzyme design, supracatalytic systems, software development (e.g., GaudiMM) and/or identification of antiviral and antibacterial molecules.



The candidates are expected to own a B.Sc. in Chemistry and/or closely related areas like Physics, Biochemistry or Biotechnology and a scientific M.Sc in relation to the line of research (Theoretical and/or Computational Chemistry, Biophysics, Nanosciences, Catalysis, Bioinformatics).

The student will be trained in a series of computational techniques and multi-scale procedures in a competitive and interdisciplinary group that includes chemists, biochemists, biotechnologists, informaticians, and physicists. Interest in programming and scripting is not mandatory but positively valued. Open mind, motivation in working at frontline and challenging research and good idiomatic skills will be appreciated.

Official deadline for application is November **11th, 2021**. Interested candidates should contact one or both principal investigators of the project, Dr. Jean-Didier Maréchal (jeandidier.marechal@uab.cat or jeandidier.marechal@gmail.com) and Dr. Gregori Ujaque (gregori.ujaque@uab.cat) NO LATTER than **8/11/2021**.

Candidates could refer to these publications: *Nat. Catal.* 2021, 4, 643–653 / *J. Am. Chem. Soc.* 2019, 141, 33, 13114–13123, *Evidence-Based Alternative Med.* 2020, 4932572