

RESEARCH POSITION IN COMPUTATIONAL CHEMICAL BIOLOGY

A research position is offered at the Computational Chemical Biology Laboratory at the CIB Margarita Salas of the Spanish Research Council (CSIC) in Madrid (Spain).



Group Leader: Dr. Sonsoles Martín-Santamaría.

Project: Computational studies of eco-efficient carbon capture and mineralization by dynamic enzyme-boosted approach.

Ref.: TED2021-132094B-I00

<https://cib.csic.es/research/structural-and-chemical-biology/computational-chemical-biology>

We are involved in an innovative approach to Integrated Absorption and Mineralization wherein CO₂ is captured and mineralized in efficient and environmentally benign conditions. Effective and fast capture by carbonation will be ensured by using aminoacid-based sorbents in the presence of carbonic anhydrase (CA). By tuning the inner active pocket of CA and/or by designing a novel polymeric outer shell for the CA, fast kinetics and low retention in the final inorganic product will be attained.

In the project, we combine computational methodologies such as QM, QM/MM and MD simulations, in close collaboration with the experimental chemists.

Key References: *J. Med. Chem.* **2023**, 3010; *Sci. Rep.* **2022**, 12, 19474; *Chem. Eur. J.* **2021**, 27, 15406; *ACS Omega*, **2021**, 6, 6041; *Front. Immunol.* **2022**, 12, 748303; *J. Med. Chem.* **2021**, 64, 12261.

Duration: 12-18 months.

Required qualifications and experience:

- Training in the Computational Chemistry field with proven experience in multiscale simulations of biomolecules. PhD will be valued.
- Solid background in Chemistry, Biophysics, Biochemistry, and/or Pharmaceutical Chemistry.
- Knowledge and experience in modern coding languages are beneficial.
- Very good communication skills in English and ability to produce acceptable drafts and scientific reports are a must.
- Motivated and committed to research excellence, and ability to work in a team.

Application: We are looking forward to receiving your email application including a letter of motivation (one page), a short CV (two pages), and contact details of two referees. The email must be addressed to smsantamaria@cib.csic.es.