

POSTDOCTORAL POSITION IN COMPUTATIONAL CHEMICAL BIOLOGY

A postdoctoral 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 chemistry approaches to molecular mechanisms of innate immunity and bacterial resistance.

Ref.: PID2020-113588RB-I00

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

We are devoted to the study of the molecular mechanisms involved in the Toll-like receptors functionality, and in the recognition by PAMPs, such as natural lipopolysaccharides and lipopeptides, with special focus in the design and identification of new compounds able to modulate the TLRs behaviour with possible therapeutic applications. We also pursue to deepen in antimicrobial resistance-related molecular mechanisms, in particular: bacterial envelope and bacterial conjugation proteins. We combine computational methodologies at different resolution scales, docking, and all-atom and coarse-grained MD simulations, and works in close collaboration with international specialists in medicinal chemistry, biochemistry and cell biology.

Key References: *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:

- PhD in the Computational Chemistry field with proven experience in multiscale simulations of biomolecules.
- Solid background in Chemistry, Biophysics, Biochemistry, and/or Pharmaceutical Chemistry.
- Knowledge and experience in chemical glycobiology is beneficial.
- 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.