



## Computational Chemical Biology (CCB) Group

Centro de Investigaciones Biológicas Margarita Salas, CSIC.

<https://www.cib.csic.es/research/cellular-and-molecular-biology/computational-chemical-biology>

### PhD CONTRACT OFFER IN COMPUTATIONAL CHEMICAL BIOLOGY

**We seek** motivated scientists with integrity, initiative, creativity and team-work ability.

**We offer** a 4-year-long contract for a PhD Thesis project at the CIB Margarita Salas of the CSIC in Madrid (Spain).

**Group Leader:** Dr. Sonsoles Martín-Santamaría.

**Project:** Understanding molecular mechanisms of immunomodulation and bacterial resistance using computational chemistry approaches (PID2023-152271NB-I00).

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 work in close collaboration with international specialists in medicinal chemistry, biochemistry and cell biology.

**Key References:** *Angew. Chem.* **2024**, *63*, e202401541; *J. Med. Chem.* **2023**, *66*, 3010; *Sci. Rep.* **2022**, *12*, 19474; *Front. Immunol.* **2022**, *12*, 748303; *Chem. Eur. J.* **2021**, *27*, 15406; *ACS Omega*, **2021**, *6*, 6041; *J. Med. Chem.* **2021**, *64*, 12261.

**Starting date (tentative):** January 2025

#### Required qualifications and experience:

- Master of Science: Pharmacy, Chemistry, Biochemistry, Biotechnology, plus Master in areas related to computational chemistry, biophysics and/or drug design.
- Previous experience in multiscale simulation, biophysics techniques and/or drug design will be considered.
- Knowledge and experience in modern coding languages are beneficial.

**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](mailto:smsantamaria@cib.csic.es).