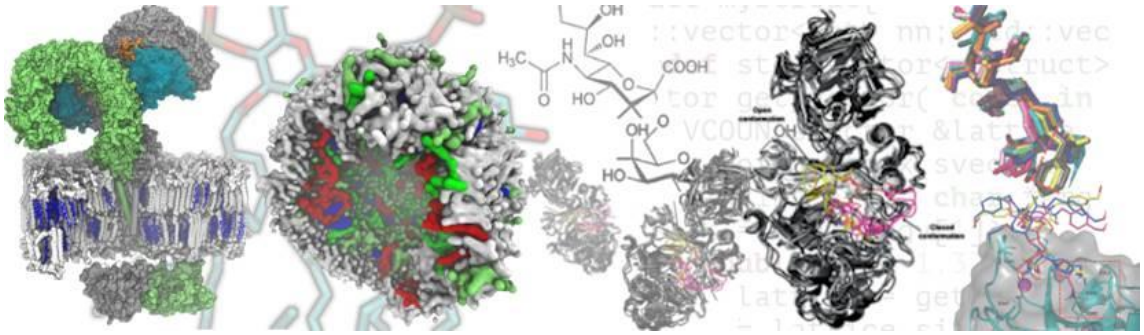

Computational Chemical Biology (CCB) Group,

Centro de Investigaciones Biológicas Margarita Salas, CSIC.

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

The research interests of the CCB group lie at the interface between Chemistry and Biology, by means of molecular modeling and computational chemistry applied to the understanding of ligand-receptor interactions and molecular recognition processes relevant for drug design. We combine these investigations with structural studies, synthesis of compounds, and biological studies in close collaboration with international groups, within a multidisciplinary and integrative approach.

We are focused on the study of the molecular recognition processes involving Pattern Recognition Receptors (PRRs), such as Toll-like receptors (main actors in innate immunity), and lectins (carbohydrate-binding proteins with important roles in infection, inflammation, and tumor progression). Our global goal is to understand the molecular details of ligand recognition as a source of new compounds able to modulate the target behaviour with possible therapeutic applications.

Group Leader: Sonsoles Martín-Santamaría

♦Scientific works: over 100 articles published, Editor of 2 books, and co-author of 3 book chapters.

♦Supervision experience: 9 PhD supervised and defended; 1 PhD Thesis in progress; 15 TFMs and 12 TFGs supervised and defended.

♦Postgraduate teaching in 3 Master programs: “Integrative Synthetic Biology” (UIMP/CSIC); “Drug Discovery” (Interuniversity UCM/UAH/USP-CEU); “Organic Chemistry” (Univ. Valencia). SMS is also Invited Professor at the Dep. of Chemistry of the Univ. of Osaka (since 2021).

♦Membership and collaboration with **Scientific Societies:** EuChemS (Chair, Division of “Chemistry for Life Sciences”, two mandates 2017-23); RSEQ [Secretary General, since 2018; Associate Editor “Anales de Química” 2009-12 & 2015-17; Web Coordinator, 2012-17; Division of “Chemical Biology”: Co-founder, Secretary (2011-16), President (2016-19)]; SEBBM (WP “Chemical Biology” Coordinator, 2016-18, and 2021-24). Member of the SEQT since 2004.

♦Corresponding Academician of the Royal National Academy of Pharmacy (2023).

Requirements for the PIF2024 contract:

Degree in Pharmacy, or degree in Chemistry, Biochemistry, Biotechnology plus Master in areas related to computational chemistry, biophysics and/or drug design.

Level of Englidh: high.

Basic knowledgements of linux and python are required.

We seek outstanding individuals with initiative, creativity and team-working ability. Previous experience in research activities in computational chemical biology and/or computational drug design will be highly considered.

The name and email of two contacting professors or researchers that know the candidate should be provided (e.g., TFG and/or TFM supervisors).

Training program planned:

The research group provides an excellent international training environment within a comprehensive and multidisciplinary approach:

1-Doctorate Program, the PhD student will join the Doctorate Program in Medicinal Chemistry of the UCM within the Paul Ehrlich MedChem Euro-PhD Network. The Doctorate Committee keeps track of the student training on a yearly basis by following the up-load information at the UCM platform (RAPI): (i) the activities carried out within the PhD program; (ii) the activities outside the PhD Program; and (iii) their research plan indicating the yearly progress of the specific activities and up-dating the tasks for upcoming year. Workshops and PhDay are organized every year with keynote lectures by prestigious researchers, in order to instruct PhD students in advanced topics, and to build a network of contacts with senior researchers, and with other PhD students.

2-Personalized training at the host laboratory, while developing the challenging research project here proposed, in the fields of Computational Chemical Biology and Pharmaceutical Chemistry with a multi/inter-disciplinary exposure and integrative perspective. The PhD student will learn various essential techniques, and will develop research skills, in molecular modeling and computer-aided drug design with extensive impact in the area of modern Science in both, pharmaceutical industry and Academia environments, as drug design, multiscale MD simulations, docking, VS, quantum mechanics, and ML-based techniques. To complete a multidisciplinary training, PhD students work in close involvement with the collaborators from various disciplines, national and international, by means of regular on-line/in-person research meetings and seminars. Also, they present the work progress in our regular group meetings and in conferences, participate in specific workshops (*e.g.*, Gaussian users, CECAM courses, etc.) and are offered to perform 3-month stays allowing to get the "International Mention".

3-Complementary training involves a wide range of courses (scientific integrity, scientific/grant writing, communication, critical thinking, and career development). These courses are offered by the CIB (CIB4future), by the Master MISB Module 3-Extension opened to CIB PhD students, and by the CSIC. CSIC also offers the participation in the mentorship program CAMINO.