Predoctoral Position in Theoretical Molecular Biology

A 4-year predoctoral fellowship in Biomolecular Simulations from the Spanish Ministerio de Ciencia e Innovación (FPI contract) is offered at the Dynamics and Mechanisms of Chemical and Biochemical Reactions (Chemistry Department) of the Universitat Autònoma de Barcelona (Spain). The grant is associated to the project **PID2020-113764GB-I00** entitled **"Using theoretical biomolecular engineering and photopharmacology to design and get new therapeutic drugs for human diseases, including COVID-19"**.

Currently our goal in the field of Theoretical Molecular Biology is to use QM/MM and Molecular Dynamics methods to carry out Biomolecular Simulations to predict how the activity and functions of biomolecules (especially lipoxygenase and cyclooxygenase enzymes) can be controlled and modified, so that they perform the functions that we have previously defined. This line of research should lead to significant and experimentally tangible progress, for example in the field of inflammatory processes (which are at the source of many diseases), photopharmacology, the design of active biomarkers in the optical window of mammalian tissues near infrared, and the rational design of new methods and medicines to act on human diseases with as few undesirable side effects as possible for human health. In the field of Biotechnology, we intend to design new enzymes as engineered biomolecular catalysts for the preparation of relevant organic molecules with better, faster, cheaper and with more selective synthetic processes than the ones currently available. Specifically, we focus on the design of two different kinds of drugs that can play an especially important role in the control and treatment of several life-threatening human diseases: Drugs related to lipoxygenases and cyclooxygenases for inflammatory-based diseases, and photoswitchable drugs, and their transfer to the production sector (Biotechnology and Pharmaceutical industry).

See orcid.org/0000-0002-7536-1869 for a list of the research publications of our group.

This grant is specifically focused on the "**Theoretical design of drugs related to lipoxygenases and cyclooxygenases for inflammatory-based diseases: Combining Molecular Dynamics Simulations and QM/MM calculations**". This interdisciplinary PhD Thesis in the field of Theoretical Molecular Biology, with a very long journey from Theoretical Chemistry (on the border with Molecular Physics) to Biology (on the border with Biotechnology and Pharmacology), is very suitable to provide adequate training in multidisciplinary scientific research, since our PhD students have to acquire a solid knowledge of Mathematics, Physics, Chemistry, Biochemistry, Biology and Computer Science. It is not simply about training researchers who know how to use certain techniques, more or less routinely, but also to teach them to think and develop new solutions and methods to face and solve the problems that appear throughout their research work. All this is very enriching, and, after their PhD, our students are excellently prepared to choose from many different professional careers.
Official deadline for telematic application is **14:00 h**., **November 11th, 2021**. Interested candidates can contact one of the IPs of the project, Dr. Àngels González-Lafont (angels.gonzalez@uab.cat) or Dr. José M. Lluch (JoseMaria.Lluch@uab.cat). Anyway, the complete information and the instructions to directly apply can be found in
http://www.aei.gob.es/portal/site/MICINN/menuitem.dbc68b34d11ccbd5d52ffeb801432ea0/?vgnextoid=4c6c68d98570c710VgnVCM1000001d04140aRCRD&vgnextchannel=305938bc8423c710VgnVCM1000001d04140aRCRD