PhD Position in Computational Chemistry. Marie Sklodowska Curie ITN

An Early Stage Researcher (ESR) position is available within the EU-funded Marie Skłodowska Curie Innovative Training Network on Allostery in Drug Discovery (ALLODD) under Grant Agreement No. 956314, in the Curutchet Lab (https://www.ub.edu/cplab), at the Faculty of Pharmacy & the Institute of Theoretical and Computational Chemistry, University of Barcelona.

Network Description: The ALLODD project is a collaboration between 13 academic and industrial organizations with 14 PhD students in total. The aim of ALLODD is to train a new generation of scientists to exploit the concept of allostery in drug design, putting together a whole array of technologies to identify and characterize allosteric modulators of protein function that will be applied to therapeutically relevant systems.

PhD Project: The Förster resonance energy transfer (FRET) technique is an important tool in structural biology, due to its ability to monitor and measure distances in biological systems. The Curutchet lab investigates the spectroscopy and FRET properties of biosystems using multiscale QM/MM computational models. In the project, a novel multiscale strategy combining Molecular Dynamics simulations and efficient models to estimate FRET couplings will be used to help in the structural characterization of allosteric binding sites and ligand binding modes.

Offer Description:
• We are seeking an Early Stage Researcher willing to pursue a PhD in allosteric and structure-based drug discovery with interest in photophysics.
• The work involves the use of computational methods to: 1) Develop a Python-based tool to generate FRET observables from MD trajectories; 2) Select a library of promiscuous fragments with tailored FRET properties; 3) Assess the ability of FRET simulations to characterize allosteric binding sites and ligand binding modes for drug discovery targets.
• The main computational methods in use will be Molecular Dynamics simulations and excited state polarizable multiscale QM/MM calculations.
• Computational work will be complemented with experiments on adjacent scientific areas.
• The ESR will carry out the following secondments:
o Gain Therapeutics SA (Spain) – 2 months. Purpose: Application of the developed computational tools to assess the binding site of allosteric pharmacological chaperones developed at GTx.
o Heptares Therapeutics Ltd (United Kingdom) – 3 months. Purpose: application to undisclosed allosteric target + training in computer-aided drug design.
o University of Vienna (Austria) – 3 months. Purpose: training in NMR for allostery.

Specific Requirements: Bachelor's or Master's degree in Chemistry, Physics, Pharmacy, Biochemistry, or related field. Excellent English oral and writing skills. Experience in computational chemistry and knowledge in programming with Python or other languages is desirable.

We Offer:
• Structured 3-year cutting-edge Research/PhD training program in the field of structure-based drug discovery and theoretical photophysics/spectroscopy of biomolecules.
• Stimulating, interdisciplinary research in a high-quality international scientific environment.
• Participation in ALLODD's workshops, summer schools and internships, providing excellent training on research and transferable skills.
• Excellent working environment.
Eligibility: Applicants must be in the first 4 years after obtaining their Master´s degree and/or Bachelor's degree and must not have resided or carried out their main activity (work, studies, etc.) in Spain for more than 12 months in the 3 years immediately before the recruitment date. Applicants must be eligible to work in Spain.
Expected starting date: 1 January 2022
To apply: Interested candidates should send a letter of motivation and CV (including two potential referees) to carles.curutchet@ub.edu, indicating as reference "ALLOD_ESR4" as soon as possible and no later than 24/10/2021