



UNIVERSITAT DE
BARCELONA

Early Stage Researcher Project

“Excitation energy transfer applied to drug design”

in

University of Barcelona, Spain

You want to participate in a training programme in and beyond the fields of physical chemistry of biological systems, theoretical and computational chemistry, biological chemistry, biochemistry, targeted drug delivery/discovery and medicinal chemistry?

14 Early Stage Researcher (ESR) positions are available within the EU-funded Marie Skłodowska Curie Innovative Training Network on **Allo**stery in **D**rug **D**iscovery (**ALLODD**) under Grant Agreement No. 956314.

The ALLODD project is a collaboration between 13 academic and industrial organizations with 14 ESR/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.

Project Description

Host Organisation: UB

Scientist-in-Charge: Prof. Carles Curutchet

Objectives: 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 computational models. In this context, multiscale strategies combining Molecular Dynamics simulations and efficient models to estimate FRET couplings will be used to help in the structural characterization of allosteric binding sites/modes and allosteric conformational transitions, including the following objectives:

- 1) Develop a tool to generate FRET observables from MDs;
- 2) Determine the impact of flexible/rigid linkers on FRET;
- 3) Assess the ability of FRET simulations to characterize binding sites and binding modes.

Expected Results:

- 1) Release a computational toolbox to generate FRET data from MDs;



- 2) Quantify the gain in resolution provided by FRET studies based on rigid linkers;
- 3) Determine the binding sites of different ligands for drug discovery targets.

Planned Secondement(s):

- **Host1:** GTx, length: 2 months, purpose: Application of the developed computational tools to assess the binding site of allosteric pharmacological chaperones developed at GTx;
- **Host2:** Heptares, length: 3 months, purpose: application to undisclosed allosteric target + training in computer-aided drug design.
- **Host3:** UNIVIE, length: 3 months, purpose: training in NMR for allostery.

Eligibility Criteria

There are **strict eligibility requirements** to apply for participation in a Marie Skłodowska Curie Innovative Training Network:

- Applicants for the ESR/PhD positions should be in the first 4 years (full-time equivalent) of their research careers and not yet have been awarded a doctorate.
- Applicants must not have resided or carried out their main activity (work, studies, etc.) in the host country for more than 12 months in the 3 years immediately before the recruitment date. In addition, local regulations of the host countries may apply.

Specific Requirements/Qualifications:

- 1) Bachelor's or Master's degree in Chemistry, Physics, Pharmacy, Biochemistry, or related field.
- 2) Excellent English oral and writing skills.
- 3) Experience in computational chemistry is **desirable**.
- 4) Knowledge in programming with Python or other languages is **desirable**.

Benefits

Enrollment in Doctoral degree(s): The ESR will be enrolled in the Ph.D. school at the University of Barcelona (UB).

We are offering a competitive, interdisciplinary environment with a track record of intense mutual collaboration. In addition to the individual training-through-research, our program includes further elements such as workshops, summer schools, internships and secondments to the partners' laboratories.

The successful candidate:



ALLODD in Drug Discovery

- will be funded for 36 months with a competitive salary in accordance with the MSCA regulation for Early Stage Researchers, including living allowance, mobility allowance and a family allowance (if married).
- will have to perform the secondments defined in his/her personalized career development programme.

To be a part of ALLODD:

Apply to and contact for further information: Applicants should apply by email to carles.curutchet@ub.edu indicating Reference: ALLODD_ESR4.

Apply until: 31 January 2022

Starting date: The earliest starting date will be **1 November 2021** The latest will be **1 September 2022**.