



UNIVERSITAT DE
BARCELONA

Early Stage Researcher Project

“Allosteric modulators of Fbw7 E3 ligase”

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, www.ub.edu/bl

Scientist-in-Charge: Prof. Xavier Barril

Objectives:

- 1) Detect cryptic pockets in Fbw7.
- 2) Determine binding site and binding mode of existing Fbw7 ligands.
- 3) Improve potency and modulate allosteric response of ligands.

Expected Results:

Structural, dynamic and druggability characterization of Fbw7 allosteric pockets. Structural characterization of existing Fbw7 ligands and fragments. Optimization of allosteric ligands as chemical probes for this tumour suppressor. Understand wider implications for other WD40 repeat domain proteins, as this is one of the most common protein-protein interaction domains.



Planned Secondement(s):

- **Host1:** KI, length: 3 months, purpose: application of HDX experiments on Fbw7,
- **Host2:** RCNS, length: 3 months, purpose: synthesize reactive analogues for confirmation of binding mode.
- **Host3:** Novo Nordisk, length 2 months, purpose: training in modelling of peptides as allosteric modulators

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:

- MSc Computational Chemistry, Bioinformatics or similar
- Background (BSc) in chemistry, physics, pharmaceutical sciences or molecular life sciences.
- Excellent oral and writing skills.

**Desirable but not Required Skills:**

- Experience/interest in biophysics, structural biology and/or synthetic chemistry. Programming and scripting skills.
- Experience in the simulation of biomolecular systems.
- Good interpersonal skills will facilitate fruitful collaborations within the consortium.

Benefits

Enrolment 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:

- 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 xbarril@ub.edu indicating Reference: ALLODD_ESR3.

Apply until: 31 January 2022

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