



LEIBNIZ
FORSCHUNGSINSTITUT
FÜR MOLEKULARE
PHARMAKOLOGIE

Early Stage Researcher Project

**“Design and synthesis of allosteric
phosphatase inhibitors”**

In

Forschungsverbund Berlin EV (FMP), Germany

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: FMP

Scientist-in-Charge: Dr. Marc Nazaré

Objectives:

- 1) Identification and chemical optimization of novel allosteric inhibitors of SHP2 and PTP1B from biochemical screening and by fragment hybridization.
- 2) Identification of minimal binding fragments by deconstruction of known allosteric ligands for addressing the binding site of SHP2 and PTP1B.
- 3) Characterization of synergistic effects of dual inhibition of the active site and allosteric site in SHP2 and PTP1B.

Expected Results:

- 1) Toolbox of allosteric ligands for phosphatase inhibition based on novel chemotypes.
- 2) Characterization of the energetic contribution
- 3) Understanding of the interrelationship of synergistic combinations of active site and allosteric inhibitors of SHP2 or PTP1B.



Planned Secondement(s):

- **Host1:** RCNS, length: 3 months, purpose: training in covalent ligand synthesis ,
- **Host2:** UNIGE, length: 3 months, purpose: training in metadynamics protein simulations.
- **Host3:** GTx, length 2 months, purpose: training in non-competitive pharmacological chaperones.

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) MSc degree, excellent knowledge in Synthetic Organic Chemistry and Biochemistry.
- 2) Very good communication and writing skills in English.

Desirable Skills: Knowledge of in-silico docking and molecular dynamics simulation and NMR spectroscopy.

Benefits

Enrollment in Doctoral degree(s):

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 Nazare@fmp-berlin.de indicating Reference: ALLODD_ESR8.

Apply until: 31 January 2022

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