



Early Stage Researcher Project

“Rational design of positive and negative allosteric modulators of pLGICs”

in

University of Strasbourg (Unistra), France

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 **Allostery in Drug Discovery (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: Unistra

Scientist-in-Charge: Prof. Marco Cecchini

Objectives:

- 1) The development of a state-based pharmacology approach for the rational design of PAMs and NAMs in allosteric proteins.
- 2) The development of an efficient methodology for massive rescoring of docking poses by simplified free energy approaches.
- 3) The discovery of novel PAMs and NAMs of the human glycine receptor $\alpha 1$.

Expected Results:

- 1) The identification of novel allosteric modulators of the human GlyR $\alpha 1$ to enter the lead optimization stage.
- 2) The development of a computational platform (ChemFlow) for the efficient evaluation of



protein-ligand binding affinities by docking with free energy rescoring on GPU computing.

Planned Secondement(s):

- **Host1:** FZJ, length: 2 months, purpose: in allosteric pathways for GPCRs,
- **Host2:** FMP, length: 2 months, purpose: Training in medicinal chemistry approaches to fragment design,
- **Host3:** Janssen, length: 3 months, purpose: Training in computer-aided drug design and AI methods for allosteric modulator development.

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.

Benefits

Enrollment in Doctoral degree(s): The ESR will be enrolled in the Ph.D. programme of Unistra.

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: mcecchini@unistra.fr

Apply until: 31 January 2022

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