



Early Stage Researcher Project

“Design and synthesis of covalent allosteric probes”

In

Research Center for Natural Sciences (RCNS), Hungary

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: RCNS

Scientist-in-Charge: Dr. György Keserű

Objectives:

Develop computational tools to analyse and predict druggable allosteric sites suitable for covalent targeting. Develop workflows for optimizing covalent allosteric probes. Deliver high affinity and specific covalent probes for the identification of allosteric pockets on selected protein targets.

Expected Results:

Established methodology to predict druggable allosteric sites and to design covalent allosteric probes. Validated protocol for optimizing high affinity and specific covalent allosteric probes. Covalent allosteric probes for the targets investigated by the network.



Planned Secondement(s):

- **Host1:** Heptares, length: 2 months, purpose: modelling water networks using WaterFLAP and WaterMAP,
- **Host2:** UB, length: 2 months, purpose: training in dynamic undocking and MDmix methodologies.
- **Host3:** FMP, length 3 months, purpose: training in fragment synthesis.

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 and/or Medicinal Chemistry.
- 2) Good communication and writing skills in English.

Benefits

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

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 keseru.gyorgy@ttk.hu indicating Reference: ALLODD_ESR7.

Apply until: 31 January 2022

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