Early Stage Researcher Project

"Development of a computational methodology to detect allosteric pathways in proteins and application in drug discovery"

in

Biomedical Research Foundation, Academy of Athens, Athens

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: BRFAA

Scientist-in-Charge: Dr. Zoe Cournia

Characterize protein conformational ensembles (from NMR or clustering MD trajectories) based on their aminoacid physico-chemical properties, produce features from these properties and select the most discriminant using Linear Discriminant Analysis or Principal Component Analysis, train, test, and validate multiple Machine Learning, Deep Learning, and Ensemble Learning algorithms on proteins with known allosteric pathways in order to classify aminoacids that contribute to protein allosteric pathways. Assess the viability of binding sites as allosteric pockets using normal mode analysis or elastic network models. Perform computer-aided drug design in the identified pockets.

Expected Results: Creation of a predictive platform for identifying allosteric networks in proteins; assessment and improvement of current methods to assess the implication of binding pockets in large scale protein motions. Delivery of putative allosteric modulators by computer-aided drug design.

Planned Secondement(s):

Host1: Charité, length: 3 months, purpose: training in X-ray crystallography

Host2: KI, length: 3 months, purpose: training in HDX experiments

Host3: Janssen, length: 2 months, purpose: training in computer-aided drug design.

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/Quaifications:

- Experience with biomolecular simulations, computational chemistry and/or programming skills are **desirable**.
- Bachelor's or Master's degree in Chemistry, Physics, Pharmacy, Biochemistry, Engineering, Computer Science, or related field is **required**.
- Excellent oral and writing skills are **required**.

Benefits

Enrolment in Doctoral degree(s): The ESR will have the possibility to be enrolled in any European University upon mutual agreement.

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: zcournia@bioacademy.gr

Apply until: 31 January 2022

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