



## Early Stage Researcher Project

**“Development of a computational methodology to detect allosteric pathways in proteins and application in drug discovery”**

Biomedical Research Foundation, Academy of Athens, Greece

Do 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:** BRFAA, Greece

**Scientist-in-Charge:** Dr. Zoe Cournia

A PhD or young researcher (ESR) position is available to work in the laboratory of Dr. Zoe Cournia at the Biomedical Research Foundation, Academy of Athens, Greece.

The researcher will work on the development of a computational methodology to detect allosteric pathways in proteins and application in drug discovery within the EU-funded Marie Skłodowska Curie Innovative Training Network on Allostery in Drug Discovery (ALLODD):

<http://www.allodd-itn.eu>.

The young researcher will work on allosteric regulation of proteins, identification of cryptic binding pockets and performing computer-aided drug design. More specifically, the study focus is on the characterization of protein conformational ensembles (from NMR or clustering MD trajectories) based on their amino acid physicochemical properties, produce features from these properties and select the most discriminant ones, train, test, and validate multiple Machine



Learning, Deep Learning, and Ensemble Learning algorithms on proteins with known allosteric pathways in order to classify amino acids 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:** UNIGE, length: 3 months
- **Host2:** Merck, length: 2 months
- **Host3:** Janssen, length: 2 months

### Eligibility Criteria & Qualifications:

- Diploma in Computer Science Chemistry, Physics, Pharmacy, Biology or related discipline
- Applicants should be in the first 4 years (full-time equivalent) of their research career and not yet have been awarded a doctorate. This 4-year period is measured from the date of obtaining the undergraduate or Master's degree, which would formally entitle to embark on a doctorate.
- Applicants should not have resided or performed their main activity (work, studies, etc.) in Greece for more than 12 months in the 3-year period immediately prior to the start date of the position.
- Be eligible to work in Greece
- Experience in computational chemistry and molecular simulation techniques
- Programming experience is not required, but will be viewed favorably
- Excellent knowledge (written and spoken) in English

### Benefits

**Enrolment in Doctoral degree(s):** The ESR will enrol at the University of Vienna.

**Salary:** 3500 EUR per month (brutto)

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](mailto:zcournia@bioacademy.gr)

**Apply until:** 31 August 2022

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

For more information on the Cournia lab research interests and ALLODD, please refer to the webpages:

<http://www.drugdesign.gr>

<http://www.allodd-itn.eu>