



Early Stage Researcher Project

“Validation and prospective application of allosteric binding site detection and ligand identification”

in

Janssen Pharmaceutica NV (Janssen), Belgium

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: Janssen

Scientist-in-Charge: Dr. Herman van Vlijmen

At the Janssen Pharmaceutical Companies of Johnson & Johnson, what matters most is helping people live full and healthy lives. We focus on treating, curing and preventing some of the most devastating and complex diseases of our time. And we pursue the most promising science, wherever it might be found. Janssen Research & Development, LLC discovers and develops innovative medical solutions to address important unmet medical needs in oncology, immunology, neuroscience, infectious diseases and vaccines, and cardiovascular and metabolic diseases. Please visit <http://www.janssenrnd.com/> for more information.

Objectives: We are looking for a skilled and motivated computational chemist for the position of PhD Student, at our Antwerp, Belgium site. The position is part of the EU Horizon2020 project ALLODD, an Innovative Trainings Network (ITN) in the Marie Skłodowska-Curie Actions program.

You will assess how well structure-based methods can identify ligandable allosteric sites and



how well ligands for these sites can be identified. For this you will use several conformational sampling methods to identify allosteric sites in disease relevant protein targets. You will apply virtual screening using docking, pharmacophore-based, and AI methods to see if known allosteric ligands can be identified. In addition, you will apply the developed approach prospectively to targets of interest and select compounds for purchase or for synthesis. These compounds will then be tested for activity.

Expected Results:

- 1) Develop and execute in silico structure-based methods to identify allosteric binding sites on protein targets. Validate performance on a set of known allosteric modulation sites.
- 2) Develop and execute in silico methods to identify small molecule allosteric modulators via structure-based and ligand-based methods, both physics-based and AI-based.
- 3) Collaborate with other PhD students and partners in the ALLODD project.

Planned Secondment(s): Your primary location will be at Janssen in Belgium, and the program foresees two 2-month secondments at other academic partner locations.

- **Host1:** BRFAA, length 2 months, purpose: training in allosteric modulation at the protein-membrane interface,
- **Host2:** UNIGE, length 2 months, purpose: training in SWISH methodology for discovering cryptic pockets,
- **Host3:** UB (Barril), length: 2 months, purpose: Training dynamic undocking and MDmix methodologies to investigate transient allosteric binding sites.

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) Bachelor's or Master's degree in Chemistry, Biochemistry, or related field. Knowledge and



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strong interest in computational methods.

- 2) Comfortable with the Python programming language
- 3) Good multidisciplinary teamwork and communication skills

Bonus qualifications (nice to have, but not required!):

- 1) Knowledge of organic chemistry
- 2) Experience with machine learning programming (e.g. PyTorch, TensorFlow)
- 3) Experience with cheminformatics or computer-aided drug discovery
- 4) Appointment: The position will be for 4 years.

We will ensure that individuals with disabilities are provided reasonable accommodation to participate in the job application or interview process, to perform essential job functions, and to receive other benefits and privileges of employment. Please contact us to request accommodation.

Johnson & Johnson is an Affirmative Action and Equal Opportunity Employer. All qualified applicants will receive consideration for employment without regard to race, color, religion, sex, sexual orientation, gender identity, age, national origin, or protected veteran status and will not be discriminated against on the basis of disability.

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: hvvljme@its.jnj.com

Apply until: 31 January 2022

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