



## Early Stage Researcher Project

**“Computer-aided drug discovery of GPCR allosteric modulators”**

In

Heptares Therapeutics Limited (Heptares), United Kingdom

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:** Sosei Heptares

### Company Description

Sosei Heptares (the corporate brand of Sosei Group Corporation) is a research-focused biotechnology group, publicly listed in Japan (TSE: 4565) and with sites in Tokyo, London and Cambridge (UK).

Our mission is to make a significant contribution to improving the quality of life and health of people around the world. To achieve this, we will discover, design and develop the most innovative and effective medicines for patients worldwide, through our world-leading patent-protected technology and platform.

Our primary focus is the discovery and early development of new medicines originating from our proprietary G Protein-Coupled Receptor (GPCR)-targeted StaR® technology and Structure-Based Drug Design (SBDD) platform capabilities. We are advancing a broad and deep pipeline of



## ALLOstery in Drug Discovery

novel medicines across multiple therapeutic areas, including CNS, immuno-oncology, gastroenterology, inflammation and other rare/specialty indications.

We have established partnerships with some of the world's leading pharmaceutical companies, including AbbVie, AstraZeneca, Biohaven, Genentech (Roche), GSK, Novartis, Pfizer and Takeda and additionally with multiple emerging technology companies. Sosei Heptares is headquartered in Tokyo, Japan with corporate and R&D facilities in Cambridge, UK.

Sosei Heptares has approximately 161 employees based at its new R&D research facility at Granta Park. The size of the company ensures a transparent linkage between all activities from early discovery through to clinical development.

**Scientist-in-Charge:** Dr. Chris de Graaf

### Objectives:

- 1) Develop a structural cheminformatics platform that integrates chemical, biological and structural data on allosteric interactions with GPCRs.
- 2) Identify structural determinants of allosteric modulation of GPCRs for structure-based ligand design.
- 3) Develop computer-aided drug discovery methods for virtual screening and structure-based design of allosteric modulators of GPCRs.

### Expected Results:

The cheminformatics platform integrating chemical, bioactivity, and structural data on allosteric GPCR binding sites will increase our understanding of the structural determinants of GPCR allosteric modulation. Insights in the role of water networks and lipophilic hot spots in allosteric modulation of GPCRs will enable the development of virtual screening and computer-aided drug design approaches to identify and design allosteric modulators of GPCRs.

### Planned Secondement(s):

- **Host1:** RCNS, length: 2 months, purpose: Training FTMap methodologies for the identification of receptor-ligand interaction hotspots in allosteric GPCR binding sites,
- **Host2:** UB, length: 2 months, purpose: Training dynamic undocking and MDmix methodologies to investigate transient allosteric GPCR binding sites,
- **Host3:** UNIURB, length: 2 months, purpose: Training MD methods to investigate binding kinetics of allosteric GPCR modulators



## 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) A Master's degree in Chemistry or a related discipline
- 2) Keen interest in applying computational tools to address complex chemical and biological questions
- 3) Excellent inter-personal, oral and written communication skills in a collaborative working environment
- 4) Experience in computational chemistry, cheminformatics, and/or computer-aided drug discovery is desirable.

## Benefits

**Enrollment in Doctoral degree(s):** The ESR will have the possibility to join a three-year PhD program at UNIURB starting Autumn 2022, under the supervision of Dr. de Graaf (Heptares) and Prof. Bottegoni (UNIURB).

**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.

### Other information

Heptares is an equal opportunities employer.



## To be a part of ALLODD:

Applications should include a covering letter, providing a short description of the background to their interest in the role, with curriculum vitae including the names and contact details for two referees.

**Application information:** Please apply through Sosei Heptares [on-line jobs' portal](#) with your application in pdf format, quoting reference number 2021-ALLODD-ESR10.

Sosei Heptares does not accept speculative or unsolicited CVs from agencies. All speculative or unsolicited CVs submitted without an agreement in place will be considered Sosei Heptares' property and will not obligate us to pay a referral fee.

**Apply until:** 15 November 2021