A L L O X

Computational Chemist

Barcelona, Spain
Full-Time / On-Site, Hybrid or Remote
Starting date: April 2025

Who We Are

ALLOX is a spin-off of the Centre for Genomic Regulation (CRG) and draws on the expertise and technology developed in the lab of Ben Lehner. The company was born out of the realisation that combining systematic mutagenesis, high-throughput phenotyping and biophysical modelling has the potential to revolutionise drug development but also transform biotechnology in general. In February 2025 we will be relocating to a new incubation space in the Barcelona Science Park (surrounded by 3 research institutes and over 70 different companies), and our immediate goal is to identify allosteric switches in all proteins and then leverage this unprecedented resource to rapidly develop novel medicines to treat human diseases. Our long-term vision is to become a leader in programmable biology, building the next generation of tools to predict, design and engineer new protein functions. We believe in a future where humanity will be able to harness the power of biology to solve our most pressing issues. We are expanding our interdisciplinary team with highly motivated individuals who are excited by this bold vision, share our sense of urgency, but are not willing to compromise on integrity. At ALLOX the success of our revolutionary scientific approach is as important to us as our mission to create a healthy, honest and respectful culture, both internally and with our partners.

For additional information, please visit: https://www.allox.bio/

Who You Are

ALLOX is seeking a highly motivated and ambitious **Computational Chemist** to join our growing startup and spearhead our in-house drug discovery efforts. As a key member of our multidisciplinary team you will play a pivotal role in translating the allosteric maps generated by our platform into actionable chemical strategies for modulating protein function and addressing unmet medical needs. Your primary responsibility will be to leverage ALLOX's unique data on protein function to design and optimise novel small-molecule allosteric modulators. This will involve: (1) applying virtual screening techniques to identify promising drug candidates that bind to allosteric sites, (2) performing molecular dynamics simulations and free energy calculations to assess the stability and activity of these molecules, (3) making use of structure-based drug design and cheminformatics approaches to optimise their pharmacological properties, and (4) collaborating closely with experimental scientists to validate and refine your computational predictions. The ideal candidate possesses a strong background in computational chemistry and drug discovery, with demonstrated experience in techniques such as virtual screening, molecular docking, pharmacophore modeling, and QSAR. A deep understanding of protein structure and function, as well as familiarity with allosteric regulation, is essential. Excellent communication and collaboration skills are crucial, as you will be working closely with both computational and experimental scientists to drive our drug discovery efforts forward. If you are a passionate and results-oriented scientist eager to contribute to the development of novel therapeutics and thrive in a dynamic and collaborative environment, we encourage you to apply. Join ALLOX and help us revolutionize drug discovery by unlocking the potential of allosteric modulation!

What You'll Do

<u>Drug Development</u>

- Apply structure-based, ligand-based and machine learning/generative design approaches to advance **drug discovery projects** (small molecules and short peptides).
- Analyse potential drug targets to assess their **druggability**, help identify best modality and contribute to developing the screening strategy.
- Perform **virtual screening** campaigns to identify novel starting points for drug development.
- Drive the design of **medicinal chemistry** efforts by applying in-depth knowledge of structure-activity relationships (SAR), a profound understanding of target biology, and predictive methods for assessing drug-like properties.
- Develop algorithms to prioritise target protein pockets, cryptic sites or surface patches for downstream drug discovery efforts.
- Participate in the **decision-making** process of target selection and pocket prioritisation for drug development.

<u>Research and Platform Development</u>

- Develop and implement computational methods to integrate ALLOX's proprietary allosteric maps with structural data and other relevant information (e.g., predicted binding affinities) to enhance the drug discovery process.
- Design and implement algorithms to predict the impact of small molecule binding on protein function, leveraging allosteric information and machine learning techniques.
- Contribute to the development of new computational tools and workflows that leverage ALLOX's unique datasets to improve the efficiency and success rate of drug discovery.
- Explore and evaluate emerging computational methods and technologies in drug discovery and assess their potential for integration into ALLOX's computational platform.

Communication, Teamwork and Culture

- Establish clear communication channels with the different working teams.
- Keep stakeholders informed about workload, progress, results, and innovations.
- Exemplify best practices and positive behaviours.
- Foster a productive and inclusive working environment.
- Participate in general company duties and contribute to overall success.

Job & Technical Competencies Requirements

Essential:

- **Master's/PhD** degree in Computational Chemistry, Chemical Physics, Physical Chemistry, Chemical Engineering, Computational Biology, or a related field. We also welcome applications from candidates with a wet laboratory background in chemistry, supplemented with strong computational experience.
- **5+ years** experience in computational chemistry and/or medicinal chemistry (in industry or academia).
- Strong knowledge or research experience in the fields of **Computational** and **Medicinal Chemistry**.
- Familiarity with a range of **computational chemistry software for drug design** (e.g., molecular docking, molecular dynamics, quantum chemistry).
- Strong programming skills in **Python**, including experience with relevant scientific libraries (e.g., RDKit, PyMOL, Biopython).
- Experience with **UNIX** OS and Bash/Shell scripting.
- Knowledge of **version control systems** (e.g., Git and GitHub) and high-performance computing infrastructure.
- Strong **teamwork** and collaborative attitude.
- **Adaptable**, capable of managing **multiple projects** concurrently and adept at shifting focus between them in line with the company's evolving priorities.
- Strong **organisational** and record-keeping skills.
- Organised **thinker** with excellent **communication** skills, thriving in a multidisciplinary, fast-paced team environment.
- Fluent **English**.

Desirable:

- Thorough **understanding of the drug discovery process** from lead screening to late-stage optimization and knowledge of how to maximise the impact of computational modeling.
- Familiarity with **cloud-based computing** (preferably GCP) environments.
- Strong publication history in peer-reviewed journals.
- Expert in the field of computational chemistry in an industry setting and good knowledge of related and adjacent disciplinary areas.
- Fluent Spanish and/or Catalan.

Compensation & Benefits

To determine starting pay, we consider multiple job-related factors including a candidate's skills, education and experience, the level at which they are actually hired, market demand, business needs, and internal parity. We may also adjust this range in the future based on market data.

This role is eligible for participation in our Annual Performance Bonus Plan (based on company goals by role level and annual company performance) and all employees are offered Equity, subject to the terms of those plans and associated policies.

In addition, ALLOX also provides our employees:

- 25 days annual leave (excluding public holidays)
- Paid parental leave
- Free drinks, snacks and regular team meals

This position is available for full-time on-site work at Barcelona Science Park, a hybrid model combining on-site and remote work, or fully remote work depending on the role and your individual circumstances. We are open to discussing the best option for you during the interview process.

Let's make programmable biology a reality

The startup nature of ALLOX provides multiple growth opportunities into other areas of the company. As one of the early employees at ALLOX, your work will have a direct impact on the foundation of a groundbreaking new approach to biotechnology.

Application Process

Apply for this job here. The interview process includes a take-home assignment to assess your practical skills.

The closing date for applications is **February 28th, 2025**. We encourage applicants to submit their application at the earliest opportunity as the closing date may be brought forward if a high volume of applications are received.

**Please note jobs may be taken down from our website, this does not mean they have been filled. This is to maintain our candidate experience for current applicants. If you are in the interview process and would like to request a copy of the job description, reach out to your recruiting contact.*