Computational Biology and Drug Design

(CBDD)

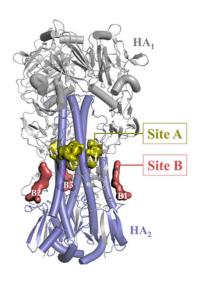


PhD Fellowship at the CBDD Lab

Institute of Theoretical and Computational Chemistry and Institute of Biomedicine - University of Barcelona

Project Summary

The emergence of resistant viral and bacterial strains challenges current therapeutic approaches in major global health threats, such as influenza and tuberculosis. Elucidating the molecular mechanisms of drug resistance and the design of novel strategies to evade these mechanisms is an urgent medical priority. The project aims to identify the resistance-based mechanisms in two key proteins: hemagglutinin in influenza A virus, and the reductase *ndh* protein in tuberculosis. Building on a consistent set of results that support the critical role played in the lifecycle of the infective organisms, and the encouraging results obtained by our team in a multidisciplinary collaboration with experimental groups, we aim to exploit this knowledge for the design of small compounds to inactivate these proteins.



Qualifications

Candidates must have obtained a MSc in Chemistry, Biochemistry, Biotechnology or related scientific disciplines. We are looking for a highly motivated researcher, interested in exploring the structure-dynamics-function properties of druggable targets and exploit this knowledge for the design of novel bioactive compounds. Creditable preliminary experience in molecular modeling, molecular simulations and/or computer-assisted drug design techniques will be assessed. Valued merits also include skills in English communication and preparation of scientific reports, as well as knowledge in scripting languages.

Contract conditions

A 4-year PhD position associated to the project entitled *New therapeutic strategies* against influenza and tuberculosis: Drug design based on multivalency, hydrophobic-guided screening and covalent modification (PID2023-147942OB-I00), financed by the *Spanish Ministerio de Ciencia, Innovación y Universidades*. The selected candidate is expected to start in January 2025.

Submission of online applications will be available from 9 - 27 September 2024.

Contact details

A motivation letter and an updated CV should be addressed to F. J. Luque (filuque@ub.edu). If available, include the name and email addresses of two senior scholars that have worked with the candidate.







