

SCIENTIFIC SEMINAR



Miquel Durán

Ersilia Open Source Initiative

The Ersilia Model Hub: Open Source AI for Antimicrobial Drug Discovery

The Ersilia Open Source Initiative is a research-oriented charity aimed at equipping laboratories in low-income countries with artificial intelligence (AI) tools for infectious disease research. Over the last three years, Ersilia has been focused on automating and simplifying access to predictive tools for medicinal chemistry and beyond. Ersilia's tools encompass quantitative structure-activity/property relationship (QSAR/QSPR) modelling pipelines and generative chemistry methods applied to a broad set of tasks and datasets, with a focus on pathogens that predominantly affect the Global South. In this talk, we will describe an end-to-end implementation of Ersilia at the H3D Centre, the leading integrated drug discovery unit in Africa, at which no prior AI capabilities were available. By leveraging in-house data collected over a decade, we have developed a virtual screening cascade for malaria and tuberculosis drug discovery comprising 15 models for key decision-making assays. In addition, we will illustrate how Ersilia's unique expertise in embedding techniques unlocks the potential of AI in low-data scenarios, including pharmacogenomics studies in Africa and chemoproteomics studies for fragment-based drug discovery.

CIC bioGUNE

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SEVERO
OCHOA

Friday
September 26
Atrio 800
12.00H



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