Abstract for SNS (end of April 2022)

Ersilia, a hub of open-source AI/ML models for drug discovery and global health

The Ersilia Open Source Initiative (EOSI; https://ersilia.io) is a non-profit organisation with the mission to strengthen the research capacity in low- and middle-income countries. In particular, EOSI is focused on disseminating and deploying artificial intelligence and machine learning (AI/ML) tools for drug discovery as a means to minimise the cost and number of laboratory experiments. The main asset of EOSI is the Ersilia Model Hub, a free, open-source platform where scientists can browse through a catalogue of AI/ML models, select the ones that are relevant to their research and run predictions online. We gather, in a single resource, two types of AI/ML models. On the one hand, we collect models developed by third parties and available in scientific publications. On the other hand, we develop models in-house and in collaboration with research groups that operate in the so-called Global South. In this presentation, I will explain how the Ersilia Model Hub can be deployed in the form of a fully functional, comprehensive virtual screening cascade that is coupled with medicinal chemistry, parasitology and ADME experimental pipelines.

Short Bio

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Miquel's research interests lay at the intersection between drug discovery and large-scale biological data analysis. During his PhD studies and early career, Miquel developed several in silico methods, producing scientific publications in a broad range of topics, from theoretical chemistry to cell-based data analysis. Along this process, he has worked at IRB Barcelona, the Massachusetts Institute of Technology (MIT), Tel Aviv University, ISGlobal-CISM (Mozambique), CIDRZ (Zambia) and H3D (South Africa). Currently, Miquel is Lead Scientist at the Ersilia Open Source Initiative. With Ersilia, he hopes to apply his data science skills in underfunded settings such as research institutes in low- and middle-income countries.