

H3D PARTNERS WITH ERSILIA OPEN SOURCE INITIATIVE TO BUILD CAPACITY IN ARTIFICIAL INTELLIGENCE AND MACHINE LEARNING FOR DRUG DISCOVERY IN AFRICA

The Holistic Drug Discovery and Development (H3D) Centre at the University of Cape Town (UCT), has entered into a partnership with Ersilia Open Source Initiative (EOSI), with a mission to incorporate artificial intelligence (AI) and machine learning (ML) tools into the H3D drug discovery pipeline.

AI holds great potential to accelerate the discovery and development of new medicines and increase the success rate in a time- and cost-efficient manner. H3D and EOSI are also both passionate about capacity building, and this partnership will be a unique opportunity to apply not only cutting-edge biological data and computational analysis to H3D's suite of experimental expertise, but also for the cross-pollination of ideas, techniques and skills.

The main objective of this collaboration is to develop AI/ML models tailored to key assays in H3D's malaria and Tuberculosis (TB) drug discovery pipelines, arranged in the form of a virtual screening cascade. Large chemical libraries can then be filtered through this cascade prioritizing compounds and thereby reducing the attrition rate of the real (experimental) pipeline.

Besides discovering new medicines for diseases that predominantly affect African populations, such as malaria, TB and antibiotic-resistant microbial diseases, H3D is focused on developing technology platforms that allow the customization of medicines specific to the needs of African patients. The Centre has been building one such platform over the last few years to investigate drug metabolism and disposition in the African population. As H3D begins to build much-needed skills in biological data analysis, the involvement of EOSI, amongst others, will lead to the introduction of predictive modeling of drug metabolism in livers and microbiomes specific to the African population. Ultimately, this will lead to a better understanding of the metabolism and disposition of drugs in the African populations in order to optimize dosing and minimize adverse effects.

According to H3D Director Professor Kelly Chibale, *'We are excited about this partnership with Ersilia as we look to develop a multi-disciplinary platform based on AI and ML for accelerating the delivery of clinical candidates at H3D. This technology will nicely augment our in-house abilities and skills.'*

H3D has a strong impetus for capacity building and supports drug discovery across Africa through fee-for-service offerings, research collaborations, expertise as well as scientific and technical guidance, and mentorship. Building AI/ML capacity at H3D through upskilling the Centre's staff will expand H3D's current offerings to its national and regional capacity development programs.

On the other hand, EOSI is working towards achieving a reference open-source online repository, named the Ersilia Model Hub, that serves pre-trained, ready-to-use AI/ML tools to the scientific community. The Hub contains curated AI/ML assets published in the literature in addition to in-house assets developed by EOSI in coordination with research institutions that are aligned with their mission.

"H3D is arguably the best possible partner when it comes to antimicrobial drug discovery. We are delighted about this opportunity. World-class laboratory data and access to experimental validation is rarely accessible to emerging initiatives like ours,"
said Dr Miquel-Duran Frigola, EOSI Co-founder and Chief Scientific Officer

About H3D

Founded and led by Professor Kelly Chibale, H3D is focused on developing technology platforms that allow customization of medicines to African patients' needs and discovering medicines for diseases that predominantly affect African populations. H3D is place where African scientists can utilize their scientific skills and education to improve the health of African patients and to educate the next generation of African pharmaceutical scientists. As the first and only centre of its kind on the African continent with world-class infrastructure, H3D undertakes drug discovery underpinned by the integration of chemistry, biology, and pharmacology, including drug metabolism and pharmacokinetics (DMPK).

About EOSI

EOSI is a UK-based non-profit organization specializing in AI/ML for drug discovery with a focus on urgent biomedical needs in Low- and Middle-Income Countries (LMICs). The goal of EOSI is to develop computational tools tailored to infectious and neglected diseases, including TB and malaria, by adapting existing data analysis techniques developed in the context of Westernised research.

