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Drug Design, Resistance and Metabolisms through CHPC

Monday, 1 December 2025 11:35 (20 minutes)

One major health challenge in the Continent is the underrepresentation of African populations in the various aspects of drug development. Firstly, drug development is a long and expensive process. Hence, the focus of drug companies is often towards more profitable markets, leaving the specific needs of Africa populations out of their scope. This results in limited development of treatments for diseases that disproportionately affect African populations. Even when there are drugs against pathogenic diseases, pathogens ultimately gain resistance against any drugs, leaving drugs, which take years of work and millions of dollars to develop, ineffective. Thus, scientific priority should be not only on the design of new efficacious drugs, but also on drugs capable of bypassing pathogen's resistance. Secondly, the African Continent hosts the most genetic diversity in the world. This diversity is not well studied, and the incorporation of the unique genetic make-up of African populations into clinical trials is limited. As a result, medications are not optimized for African populations, which may lead to variability in drug metabolism, i.e. lack of efficacy due to insufficient drug exposure or adverse reactions due to increased exposure. Furthermore, there is also a growing hypothesis on the connection between drug resistance and drug metabolism (human pharmacogenomics). This becomes particularly important in the African context, as the Continent has the highest incident rates in many diseases, and equally very high unique population specific variation profiles in the human genomes.

The integration of different aspects of bioinformatics, computational chemistry, population genomics, and intelligent systems for drug development and pharmacogenomics holds enormous potential to address these gaps. Our research aims to revolutionize drug development for diseases related to Africa, preempt drug resistance issues while developing drugs, and advance pharmacogenomics by bringing together cutting-edge computational technologies that would not be feasible without CHPC. This talk will present some case studies from our recent research and demonstrate the need for HPC resources.

Presenting Author

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Student or Postdoc?

CHPC User

CHPC Research Programme

Workshop Duration

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