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The use of Cheminformatics in understanding the molecular mechanisms of South African Phytochemicals in the treatment of metabolic diseases

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Cheminformatics has gained traction over recent years. Under the large umbrella term, there are a plethora of in silico techniques that can be used to gather information at the molecular level, with high importance in numerous research niches including biology, biochemistry and drug discovery. Our research group utilizes these techniques within the drug discovery domain. Our current research focuses on the molecular understanding of phytochemicals identified in South African traditional plant extracts. This includes the pharmacokinetic and toxicological profiling of compounds, biological target identification and network pharmacology analysis, as well as mechanistic analysis through molecular dynamic simulations. The CHPC has been vital in this pipeline. Hosting the AMBER suite, CHPC has created the environment to set up, equilibrate, run and analyze these biomolecular simulations. The GPU version offered through AMBER has also optimized and shortened the time required for trajectory generation. Our research group currently has 11 active members on the cluster that have used 587973 CPUh over the last 3 months. This has allowed our students to train and run their research without the need of expensive equipment. The above-mentioned biomolecular cheminformatics techniques, through CHPC, have and will continue to revolutionize drug lead optimization, personalized therapy, and infectious disease therapeutics within Africa.

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