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The effect of South African Natural Compounds on Type II NADH: quinone oxidoreductase (NDH2): a relative bioinformatics study

Malaria is caused by Plasmodium parasites, spread to people through the bites of infected female Anopheles mosquitoes. The study focused on all 5 (Plasmodium falciparum, P. knowlesi, P. malariae, P. ovale and P. vivax) parasites that causes malaria in humans. Africa is a developing continent, and it is the most affected with an estimation of 90% of more than 400 000 deaths reported by the World Health Organization (WHO) report in 2020, in which 61% of that number are children under the ages of five. Malaria resistance originally was observed in early 1986 and with the progression of time anti-malarial drug resistance has only increased. As a result, there is a need to study the malarial proteins mechanism of action and identify alternative treatment strategies for this disease. Type II NADH: quinone oxidoreductase (NDH2) is a monotopic protein that catalyses the electron transfer from NADH to quinone via FAD without a proton-pumping activity, and functions as an initial enzyme, either in addition to or as an alternative to proton-pumping NADH dehydrogenase (complex I) in the respiratory chain of bacteria, archaea, and fungal and plant mitochondrial. The structures for the other plasmodium species were modelled from the crystal structure of Plasmodium falciparum (5JWA). South African natural compounds database (SANCDB) were docked against the NDH2 crystal structure and modelled structures. By performing in silico screening the study aims to interrupt the electron transfer to quinone therefore disturbing the enzyme's function and possibly elimination of the plasmodium parasite. CHARMM-GUI was used to create the membrane and orient the protein on the membrane using OPM server guidelines, the interface produced Gromacs topology files that were used in molecular dynamic simulations. Molecular dynamic simulations were performed in the Centre for high performance computing (CHPC) cluster under the CHEM0802 project and the trajectories produced were further analysed.

Student?

Yes

Supervisor name

Prof Kevin Lobb

Supervisor email

k.lobb@ru.ac.za

Primary author: Ms BAYE, Bertha (Rhodes University)

Presenter: Ms BAYE, Bertha (Rhodes University)

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