Contribution ID: **18** Type: **Poster**

Molecular dynamic study of multitargeting ligands – A new strategy for the treatment of Mycobacterium tuberculosis (TB)

ABSTRACT
Tuberculosis (TB) remains one of the leading causes of mortality worldwide, it kills approximately 1.5 million people annually, while the spread of multidrug-resistant strains is of great global concern. Thus, continuous efforts to identify new anti-tubercular drugs as well as novel targets are crucial. Recently, Compounds 11426026, CDD-823953 and GSK735826A had shown to act as dual targeting ligands individually against Mycobacterium tuberculosis PanK and PyrG protein simultaneously. These enzymes are crucial to the survival of the tuberculosis bacterial. The results reported in this study shows apo conformation to be less stable, as compared to bound conformation. Principal component analysis further justifies the same findings, whereby the apo enzyme exhibits a higher fluctuation compared to the bound complex. Findings reported in this study further enhance the understanding of Mycobacterium tuberculosis Pank and PyrG as a lead to the development of multitargeting potent tuberculosis drugs.

Presenter Biography

Primary authors: Mr EJALONIBU, Murtala Adegbola (College of Health science University of KwaZulu-Natal); Mr ELRASHEDY, Ahmad (College of Health Sciences University of KwaZulu-Natal); Dr KUMALO, Hezekiel (Medical college University of KwaZulu-Natal); Dr NDUMISO, Mhlongo (Medical college University of KwaZulu--Natal); Prof. SOLIMAN, Mahmoud (College of Health sciences University of KwaZulu-Natal)

Presenter: Mr EJALONIBU, Murtala Adegbola (College of Health science University of KwaZulu-Natal)

Session Classification: Poster session

Track Classification: Computational Chemistry