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A panoptic uncovering of the dynamical evolution of the Zika Virus NS5 methyltransferase binding site loops—zeroing in on the molecular landscape

The global threat of the Zika virus to humanity is real. Innovative and potent anti-Zika virus drugs are still at large, due to the lack of anti-Zika virus drugs that have passed phase 1 trials. Experimental research has revealed novel inhibitors of Zika virus NS5 methyltransferase enzyme. This study has taken a step further to provide insight into the molecular dynamics of Zika virus and inhibitor binding, which have not been established experimentally. Movements of the methyltransferase binding site loops have a large role to play in the methylation of the viral mRNA cap, which is essential for Zika virus replication. Here, we pinpoint the binding interactions between each potential inhibitor and the methyltransferase, residues that are responsible for binding, as well as which inhibitor-bound complex renders the methyltransferase more stable. We also highlight the conformational changes that occur within the methyltransferase to accommodate binding of inhibitors and consequences of those changes upon the RNA-and cap-binding sites in the methyltransferase. This research will improve the understanding of the Zika virus NS5 methyltransferase enzyme, and will be beneficial in driving the development of anti-Zika virus drugs.

Presenter Biography

My name is Nikita Devnarain, I'm a second year PhD student in Pharmaceutical Chemistry at UKZN supervised by Professor Mahmoud E.S. Soliman, Dean and Head of School of Health Science. I have a BSc Biomedical Science degree, and honours and masters in Medical Science (Medical Biochemistry). I am currently undergoing in silico studies on the Zika virus enzymes and its potential inhibitors.

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