



# Discovering New Antimalarial Compounds Through Computational Modelling and Experimental Validation

Dr Fortunate Mokoena (North-West University)

Monday, 1 June 2026 | 16h00–17h00 SAST

## HOW TO ATTEND:

### In person (main venue):

- Road House Cinema (Neelsie) Stellenbosch University

### Watch at satellite venues:

- Room P215, 2nd Floor Physics Building University of the Witwatersrand
- Seminar Room K310 Physics Building G5 North-West University

### Online (live stream)

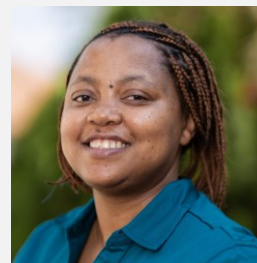
--- Please note, a recording of the lecture will be published on the NITheCS YouTube channel following the event ---

## ABSTRACT

The escalating challenge of antimalarial drug resistance underscores the pressing need for the discovery and development of novel pharmacological agents that engage unconventional mechanisms of action. Among potential therapeutic targets, the *Plasmodium falciparum* heat shock protein 90 (PfHsp90) stands out as a vital molecular chaperone that plays an essential role in the survival of the parasite and is linked to its drug resistance profile. This study employed an integrated computational drug discovery framework aimed at identifying selective inhibitors that target the N- and C-terminal domains of PfHsp90. The subsequent hit optimisation campaign was informed by structural insights derived from our findings. Molecular docking and molecular dynamics simulations indicated that the identified compounds interact selectively with PfHsp90, engaging specific residues that may disrupt ATPase activity and modulate the protein's allosteric properties. Biochemical analyses indicated that the diverse collection of hit compounds, uncovered through our integrated computational strategies, demonstrated moderate to high potency against both drug-sensitive and drug-resistant strains of *P. falciparum*. Furthermore, these compounds exhibited moderate biochemical and cellular selectivity, in addition to possessing overall favourable drug-like characteristics. The data generated from this investigation establishes a foundational basis for future optimisation efforts utilising deep learning methodologies, thereby heralding the potential for the accelerated development of effective lead compounds to combat malaria.

## BIOGRAPHY

Dr Fortunate Mokoena is a Senior Lecturer in the Department of Biochemistry at North-West University, where she leads research in infectious disease drug discovery. Her work focuses on the development of novel therapeutics for diseases that disproportionately affect children under the age of five, particularly malaria and pneumonia. She has published in internationally peer-reviewed journals and presented her research at major global conferences. Dr Mokoena has also secured competitive research funding from Grand Challenges Africa and South Africa's Technology Innovation Agency to support and advance her research programme. In addition, she is a full member of the Grand Challenges Drug Discovery Accelerator and serves as Deputy Programme Coordinator for the NITheCS Research Focus Area on health.



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