Contribution ID: **177** Type: **Invited Talk**

Molecular Modelling in Research: From Basic Research Methods to Advanced Research

Monday, 2 December 2024 11:55 (20 minutes)

Our research group utilizes High-Performance Computing (HPC) infrastructure to implement software programs facilitating calculations including, but not limited to, molecular docking, Quantum Mechanics/Molecular Mechanics (QM/MM), Molecular Dynamics Simulations (MDS), Molecular Mechanics Generalized Born Solvent Accessible Surface Area (MM-GB/SA), Quantitative Structure-Activity Relationships (QSAR), Pharmacophore modeling, Reaction-based Enumeration, Ligand Designer, and Free Energy Perturbation plus (FEP+) techniques. These molecular modeling methodologies are employed to engineer New Molecular Entities (NMEs), predict conformations, binding modes, pharmacophore features essential for binding, conduct library screening, and develop both training and testing models with an assessment of their relative and/or absolute binding affinities. This presentation will examine our application of these diverse molecular modeling techniques within research encompassing prostate and breast cancer, malaria, diabetes, SARS-CoV-2, tuberculosis, and Alzheimer's disease. Further investigation will address our utilization of Transition State Modeling to facilitate the study of functionalization of sp2-sp3 bonds of aryl halide coupling with α-ketones, exemplifying the significant utility of unliganded transition metal catalysts. This approach has enabled the synthesis of compounds conceived with molecular modeling techniques, achieving high yields. Consequently, this presentation will also demonstrate how contemporary medicinal chemistry methodologies assist synthetic organic chemists in designing synthesizable compounds. Additionally, the presentation will discuss the synthesis of various compounds, subsequently evaluated through cell-based and biophysical assays, providing insights into the synergistic effects of molecular modeling, synthesis, and bioassays within a university-affiliated drug discovery framework. Lastly, patents granted and publications by postgraduate students mentored within this research group will be presented.

Keywords: Molecular Modeling, High Performance Computing, NMEs, university-affiliated drug discovery

Student or Postdoc?

Email address

Co-Authors

CHPC User

CHPC Research Programme

Workshop Duration

Primary author: Dr GUMEDE*, Njabulo (Walter Sisulu Unibversity)

Presenter: Dr GUMEDE*, Njabulo (Walter Sisulu Unibversity)

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