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RESEARCH PAPER

# MOLECULAR DOCKING STUDIES OF PHYTOCONSTITUENTS IDENTIFIED FROM TRADITIONAL MEDICINAL PLANTS FOR PROTEASE AND REVERSE TRANSCRIPTASE TARGETED ANTI-HIV ACTIVITY

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**The aim of the present study was to identify specific phytoconstituents by *in silico* molecular docking studies on selected medicinal plants for AIDS which is an autoimmune disorder caused by immunodeficiency virus (HIV). The replication of HIV virus inhibition was studied by the ligand docking result of phytoconstituents such as Calanolide C, Calanolide B, Calanolide A, Buchenavianine, Agastenol, O-Demethyl buchenavianine and Artemisinin on the medicinal plants *Callophyllum lanigerum*, *Buchenavia capitata* and *Artemisia annua* respectively with that of HIV Integrase and HIV Reverse transcriptase. The molecular docking study was carried by using Molegro Virtual Docker and the results were expressed based on the ability of the chemical constituents to bind with the targets given in terms of MolDock score, Rerank score and Hydrogen bond binding energy. Calanolide C and Calanolide $E_2$ have least MolDock score than Buchenavianine, as compared with that of standard anti-HIV drugs such as Indinavir and Saquinavir. According to the docking studies, least MolDock score have high anti-HIV activity and phytoconstituents from *Callophyllum lanigerum* predicted for better anti-HIV activity through molecular docking studies.**

**Key words:** Phytoconstituents, Anti-HIV activity, MolDock score, *Callophyllum lanigerum*.

## INTRODUCTION

AIDS is caused by infectious virus which is known as human immunodeficiency virus (HIV). It is an immunosuppressant disease which results into life threatening action. According to United Nation, 36 million people were infected by AIDS globally every year. AIDS has worldwide approach and most commonly in South Africa and Swaziland [1]. The replication of HIV virus in a host cell is majorly done by three important enzymes namely HIV-protease, HIV-reverse transcriptase and HIV-protease with two glycoproteins [2].

The pathogenesis of human immunodeficiency virus is to attack on immune system and central nervous system and hence suppress the immunity. The first step is entry of HIV into the cell required certain receptor and the cell surface CD4 receptor and co-receptor such as