Bioinformatics Approaches for

Biocontrol of Foot-and-Mouth Disease

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Abstract

Foot-and-Mouth Disease (FMD), is an acute highly contagious viral disease that can infect cloven-hooved animals such as cattle, buffaloes, pigs, and sheep. The disease can cause a drop in meat and milk production and high mortality rates among young animals, causing severe economic losses according to the World Organization

for Animal Health. Foot-and-Mouth Disease Virus (FMDV), which is the causative agent of this disease is highly mutable and includes seven serotypes (A, O, C, Asia1, SAT1, SAT2, and SAT3) and several subtypes. No specific treatment against FMDV is available, and only symptomatic treatment can be performed. Moreover,

available vaccination programs against FMDV cannot prevent infection or virus replication. Therefore, this study aims to use computational and bioinformatics approaches to develop a specific antiviral drug against FMDV. The FMDV genome and polyprotein were scanned, and three viral proteins that are indispensable to the

FMDV life cycle were chosen to be targeted by competitive inhibition strategy. The three viral targeted proteins are RNA Dependent RNA Polymerase (RdRP_1), Peptidase_C3, and L-pro. In

this study, sequence and evolutionary analysis were carried out on the three viral enzymes. Accurate 3D models of the three viral proteins were predicted and validated. The predicted models were docked against 623 compounds stored at the South African natural compound database. The docking identified three compounds with IDs: SANC00257, SANC00380, and SANC00585, that can act as ii potential inhibitors against the three FMDV proteins and consequently used as specific antiviral drugs against FMDV.

Keywords: Foot-and-Mouth Disease Virus (FMDV); Antiviral drug;

Competitive inhibition; Protein structure prediction; Molecular docking