SLJID 2026 Vol 15 (Supplement 7):S16
DOI : https://doi.org/10.4038/sljid.v15i5.8932

In silico screening of *Cyperus rotundus* phytochemicals targeting African swine fever virus MGF 505-7R

Manathunga MJB[1], Ranathunga LN[2], Karunarathne KKP[2], Adhikari AAHR[1], Wijekoon WMHNTK[1], Aberathna WAKL[2], Nanayakkara PRS[1], Somarathna MSSP[2], Ariyasinghe AHTDK[2], Samadhi KGA[3]

Introduction and Objectives: African swine fever (ASF) is a highly lethal and contagious viral disease that affects both domestic and wild pigs. Its causative agent, African swine fever virus (ASFV) is a double-stranded, large, complex DNA virus that belongs to the *Asfarviridae* family. The viral genome encodes 150 to 200 proteins, including MGF 505-7R, which plays a crucial role in the virus's life cycle, making it a viable target for antiviral drug development. *Cyperus rotundus* is a traditional medicinal plant with a rich history in Ayurveda. In the present study, we employed an *in silico* remodeling approach to assess the antiviral properties of bioactive compounds from the *C. rotundus* plant, specifically targeting the function of MGF 505-7R. To our knowledge, no previous computational studies have been conducted on this plant against ASFV, making this work the first attempt in this direction.

Methods: In order to determine the bioactive components from *C. rotundus*, a thorough literature study was carried out. Drug-likeness and safety of the plant compounds were tested using DataWarrior with the help of Lipinski's Rule of Five, and 4 toxicity parameters. The target protein, MGF 505-7R, 3D structure was modelled using Alphafold3, and its structural accuracy was confirmed. PyRx 0.8 was used for virtual screening in order to assess the filtered compounds' binding affinities against MGF 505-7R. Compounds exhibiting binding affinities over a threshold were further investigated using CB-Dock2. The types of interactions between the chosen ligand and the protein active site were examined using molecular visualisation methods of the Discovery Studio.

Results: A total of 40 bioactive compounds of *C. rotundus* were identified through literature review, of which 11 compounds met the criteria of Lipinski's Rule of Five and passed toxicity screening. The 3D structure of the MGF 505-7R was generated with high confidence scores (ipTM=-pTM=0.77). Among the compounds screened via PyRx, 6H-[1]Benzothiopyrano[4,3-b]quinoline, 6,6,7-trimethyl showed a binding affinity exceeding the threshold -6 kcal/mol. Specifically, this compound demonstrated a superior binding affinity of -7.4kcal/mol, forming strong interactions at the MGF505-7R active site, with hydrophobic contacts contributing significantly to the stability and strength of the docking pose.

Conclusion: Taken together, our data revealed that the compound 6H-[1]Benzothiopyrano[4,3-b]quinoline, 6,6,7-trimethyl found in *C. rotundu*s showed promising stable binding to ASFV MGF 505-7R, warranting further research as a potential ASFV therapeutic.

***Keywords**: African Swine Fever Virus (ASFV), MGF 505-7R, Cyperus rotundus, Molecular Docking, Phytochemicals*

Acknowledgement: University Research Council (URC) Multidisciplinary Grant (No.516)

[1]*Department of Agricultural Biology, Faculty of Agriculture, University of Peradeniya, Sri Lanka*
[2]*Department of Animal Science, Faculty of Agriculture, University of Peradeniya, Sri Lanka*
[3]*Standard Seed Corporation, Wilmington, Delaware, USA, 19977*

Address for correspondence: Dr. L.N Ranathunga: Department of Animal Science, Faculty of Agriculture, University of Peradeniya, Sri Lanka ; Telephone:+94775207815; Email: lakmalr@agri.pdn.ac.lk

https://orcid.org/0000-0003-2904-4018