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# Inhibition of inosine monophosphate dehydrogenase in Lassa fever management by phenolics from (Telfairia Occidentalis ), an edible plant in Nigeria, using computational analysis

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## Introduction

Lassa fever is an acute viral hemorrhagic fever caused by a single-stranded RNA virus known as Lassa virus a member of the Arenaviridae family, and it poses a significant health threat with increasing mortality rate and paucity of concrete evidence on the efficacy of the only available drug, Ribavirin.

## Methods

This study employed a comprehensive computational approach, including molecular docking, MMGBSA (Molecular Mechanics Generalized Born Surface Area), induced fit docking, and pharmacokinetic analysis, to identify phenolic compounds of Telfairia occidentalis leaves to target Inosine Monophosphate dehydreognase (IMPDH) protein for the development of potential therapies for Lassa fever. The crystallographic structure of Inosine Monophosphate Dehydrogenase (PDB ID: 1JR1) for Homo sapiens was retrieved from the protein database repository (www.rcsb.org). The monomeric (chain A) protein was prepared using the protein preparation wizard of Schrodinger Suite (2021 v2). The receptor grid generation tool of the software was used to generate a grid coordinate (1JR1: x = 66.56, y = 81.89, and z = 84.83) at the binding domain of the co-crystallised ligand (phenolic acid).

## Results

Six (6) promising compounds were identified from phenolic compounds with better binding affinity with IMPDH, ranging from 10.375 to 6.902 (kcal/mol) compared to Ribavirin, a standard drug ( 6.838 kcal/mol). The six compounds formed a stable complex with IMPDH protein, and their predicted half-maximum inhibitory concentration (IC50) ranged from 5.035 to 4.597, when compared with the standard drug Ribavirin, with a 3.404 value indicating the lead compounds' bioactivity.

## Conclusion

The lead compounds passed Lipinski's rule of five and have good pharmacokinetic properties. This study revealed the inhibitory potential of the compounds (Rutin, Isoquercetin, Myricetin, Luteolin, Quercetin and Catechin identified from phenolic compounds that can be exploited for the development of therapies for Lassa fever and other viral infections.