Molecular Docking Studies of Compounds from Medicinal Plants on Lassa Fever Virus.

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INTRODUCTION

• Lassa virus which causes Lassa fever is of the family of the Arena Viridae; is an enveloped single stranded bi-segmented RNA virus

• Lassa Fever, an acute viral hemorrhagic fever was first described in 1969, in the town of Lassa in Borno State, Nigeria

• It is a zoonotic infectious disease


INTRODUCTION

• Humans become infected through contact with infected specimen of these multi-mammate rats, and also human to human transmission of the virus is possible\(^1,2\)
• Currently, no vaccine is available against Lassa Fever Virus in humans, but treatment of the virus is the administration of Ribavirin,
• It is only effective if administered early on the onset of the infection\(^3\)

INTRODUCTION

• Ribavirin, a guanosine analogue displays broad antiviral activity against several RNA and DNA viruses\textsuperscript{1,2}

• Its also used in the treatment of Hepatitis C.

• Many medicinal plants have been tested against Hepatitis C virus and has showed some antiviral activities.

• The phytochemicals of medicinal plants are considered important because of their efficiency in hampering viral entry, blocking, limiting RNA/DNA genome replication\textsuperscript{3,4}


METHOD

• Nucleoprotein structure of Lassa Fever Virus (LASV) with ID number 3MX2 was downloaded from Protein Data Bank\(^1\). The water molecules, ligand in complex with the 3MX2 structure was removed using Discovery Studio Visualizer.

• The Chemical structure of some compounds were randomly selected from a list of medicinal plants known to have antiviral activity on Hepatitis C\(^2\).

1. https://www.rcsb.org/
METHOD

• These compound structures were downloaded from PubChem with compound ID numbers; 11168203, 1548994, 31553, 53208441, 3218, 932, 9972913

• The Nucleoprotein structure was docked with the chemical structures of the compounds using PyRx, a docking software.

RESULTS

From the docking result it was observed that the seven compounds from medicinal plants that was docked on the nucleoprotein structure of Lassa Fever Virus (LASV) have low docking energy with good binding affinity and thus have potential to inhibit the activity of nucleoprotein of Lassa virus.
## RESULTS

<table>
<thead>
<tr>
<th>LIGAND</th>
<th>BINDING AFFINITY</th>
<th>RMSD/UB</th>
<th>RMSD/LB</th>
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</table>

RMSD/UB: Root Mean Square Deviation/Upper Bound
RMSD/LB: Root Mean Square Deviation/Lower Bound
CONCLUSIONS

• Docking studies of the nucleoprotein structure of Lassa Fever Virus (LASV) with seven compounds from medicinal plants showed that the docked medicinal plants have effective antiviral activities against Lassa virus.

• ADME properties and QSAR of the molecules can be considered for further studies.

• Thus the compounds from the medicinal plants can be considered for developing into a potent antiviral drug.