

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

By

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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<sup>1</sup>
- Lassa Fever, an acute viral hemorrhagic fever was first described in 1969, in the town of Lassa in Borno State, Nigeria<sup>2</sup>
- It is a zoonotic infectious disease<sup>3</sup>

1. Ogbu et al. "Lassa fever in West African sub-region: an overview". *Journal of vector borne diseases* 2007; 44(1): 1-11
2. Frame et al. "Lassa fever, a new virus of man from West Africa". I. Clinical description and Pathological findings. *Am J. Trop. Med. Hyg.* 19(4): 670-676
3. Healing et al. Report on an assessment visit to Sierra Leone, April 12<sup>th</sup> – 30<sup>th</sup> 2001. London: Merlin, 2001.

# 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<sup>1,2</sup>
- 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<sup>3</sup>

1. McCornick et al. A prospective study of the epidemiology and ecology of Lassa Fever. *J. Infect. Dis.* 1987; 155: 437.
2. Fisher-Hoch et al. Review of cases of nosocomial Lassa Fever in Nigeria: The high price of poor medical practice. *Br. Med. J.* 311: 857.
3. McCornick et al. Lassa Fever; Effective therapy with Ribavirin. *The New England Journal of Medicine.* 1986: 344; 20-26.

# INTRODUCTION

- Ribavirin, a guanosine analogue displays broad antiviral activity against several RNA and DNA viruses<sup>1,2</sup>
- 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<sup>3,4</sup>

1. Sidwell et al. Broad-Spectrum antiviral activity of Virazole: 1-f8-D-Ribofuranosyl-1,2,4-triazole-3-Carboximide. Science:1972;177, 705-706.
2. Streeter et al. Mechanism of action of 1-D-ribofuranosyl-1,2,4-triazole-3-carboxamide (Virazole), a new broad spectrum antiviral agent. Proceedings of the National Academy of Sciences of the United States of America 1973: 70; 1174-1178.
3. Jassim et al. Novel antiviral agents; a medicinal plant perspective. J. Appl. Microbiol. 2003; 95: 412-427.
4. Naithani et al. Antiviral activity of phytochemicals: a comprehensive review. Mini Rev. Med. Chem. 2008; 8: 1106-1133.

# METHOD

- Nucleoprotein structure of Lassa Fever Virus (LASV) with ID number **3MX2** was downloaded from Protein Data Bank<sup>1</sup>. 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<sup>2</sup>.

1. <https://www.rcsb.org/>

2. Ashfaq et al. Medicinal plants against Hepatitis C Virus. World J. Gastroenterol 2014; 20 (11): 2941-2947.

# METHOD

- These compound structures were downloaded from PubChem with compound ID numbers; **11168203, 1548994, 31553, 53208441, 3218, 932, 9972913<sup>1</sup>**
- The Nucleoprotein structure was docked with the chemical structures of the compounds using PyRx, a docking software.

1. <https://pubchem.ncbi.nlm.nih.gov>.

# 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.

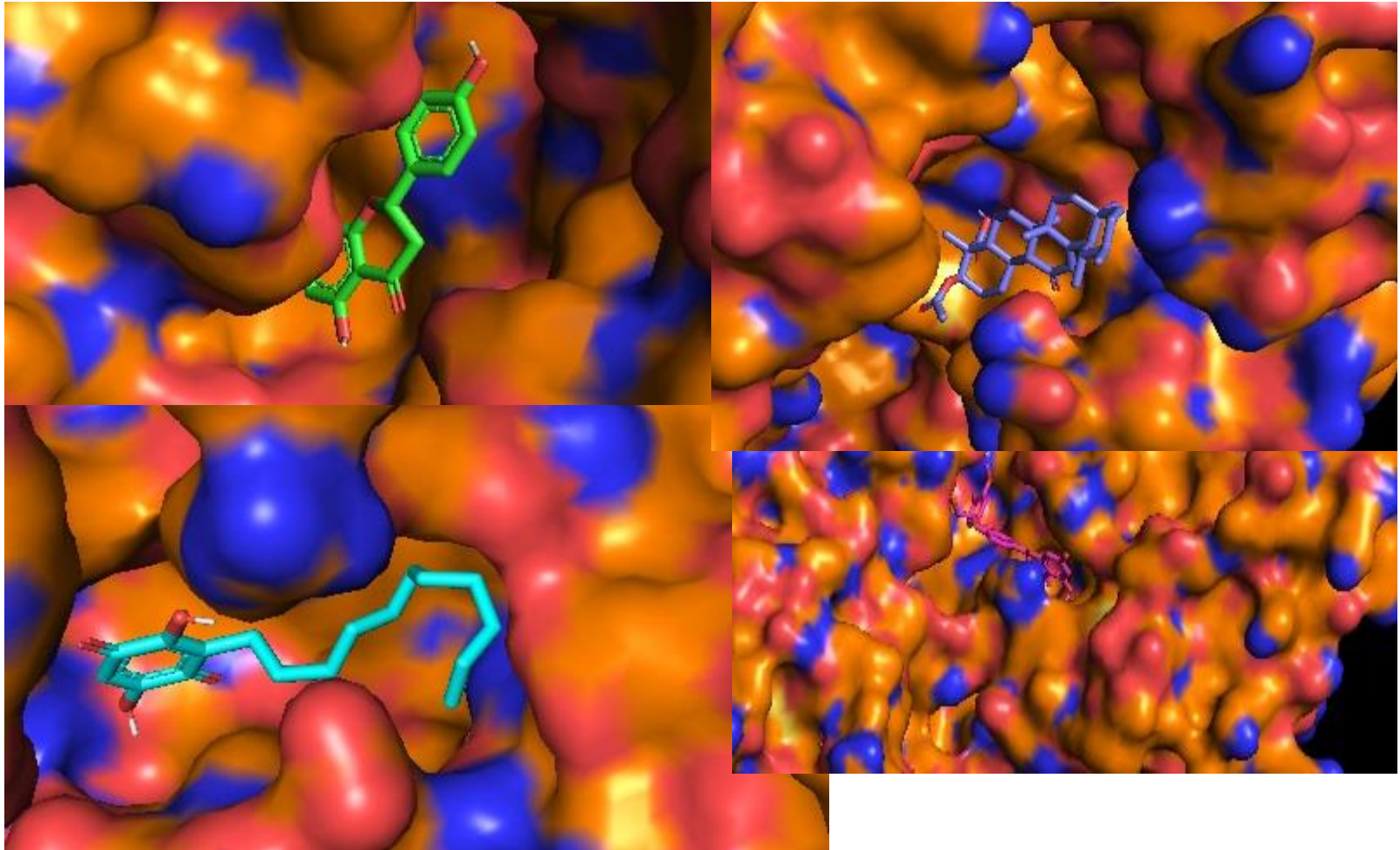
# RESULTS

LIGAND	BINDING AFFINITY	RMSD/UB	RMSD/LB
3mx2_31553_uff_E=443.51	-10.1	0	0
3mx2_1548994_uff_E=464.56	-9.8	0	0
3mx2_5320844_uff_E=613.59	-9.6	0	0
3mx2_11168203_uff_E=675.55	-8.3	0	0
3mx2_932_uff_E=195.80	-8.1	0	0
3mx2_9972913_uff_E=515.77	-7.5	0	0
3mx2_3218_uff_E=108.24	-6.5	0	0

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.