



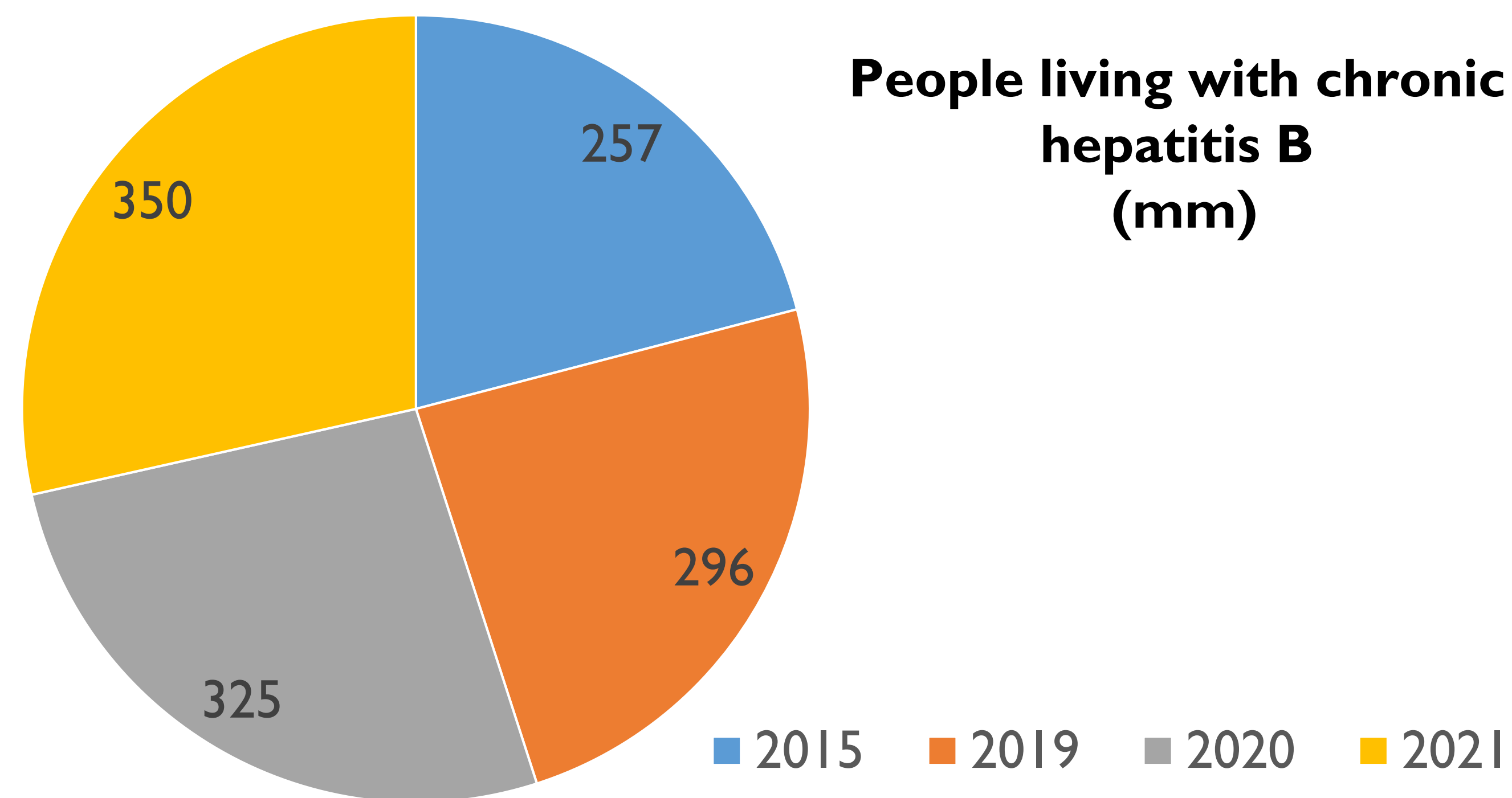
Phyllanthus amarus as a potential drug candidate for the management of hepatitis B

P.O Usman, M.U Okoro, I.A Duru and C.O Akalezi

Department of Chemistry, Federal University of Technology Owerri, P.M.B 1526, Owerri, Nigeria

3rd Commonwealth Poster Presentation 2022

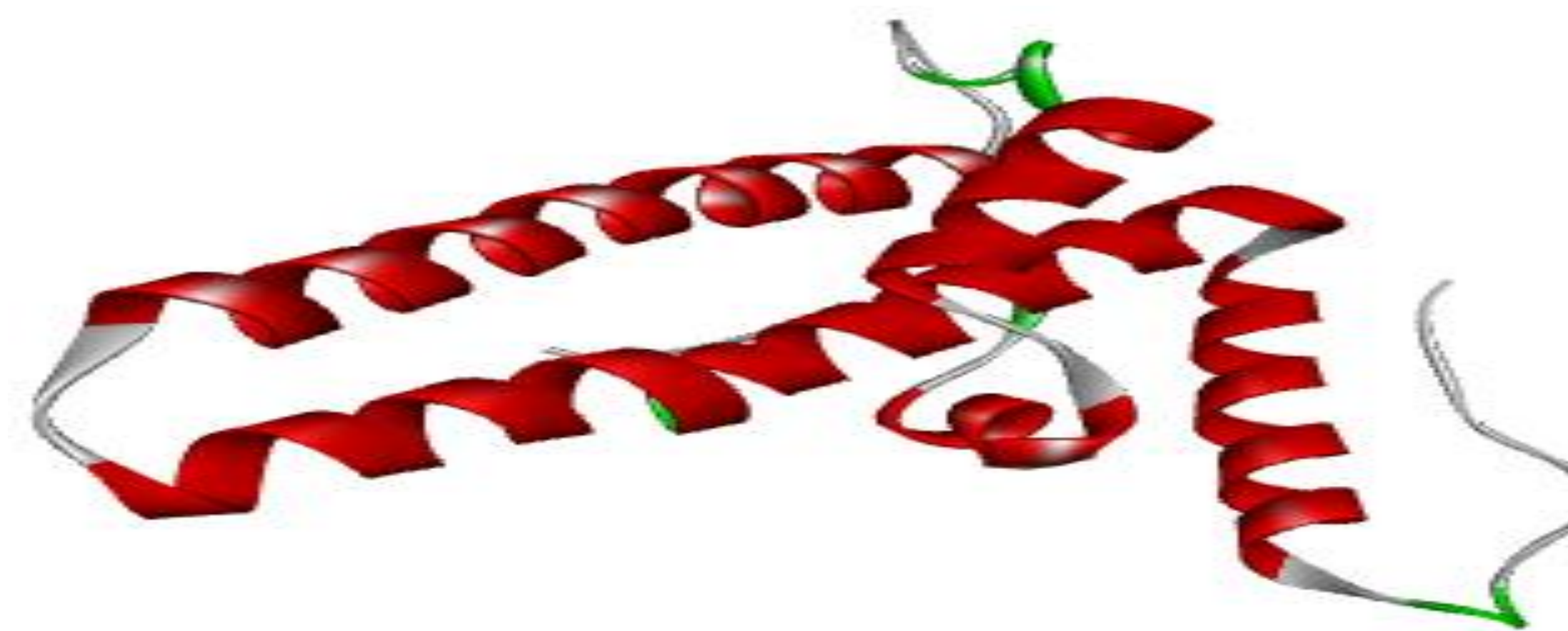
Globally



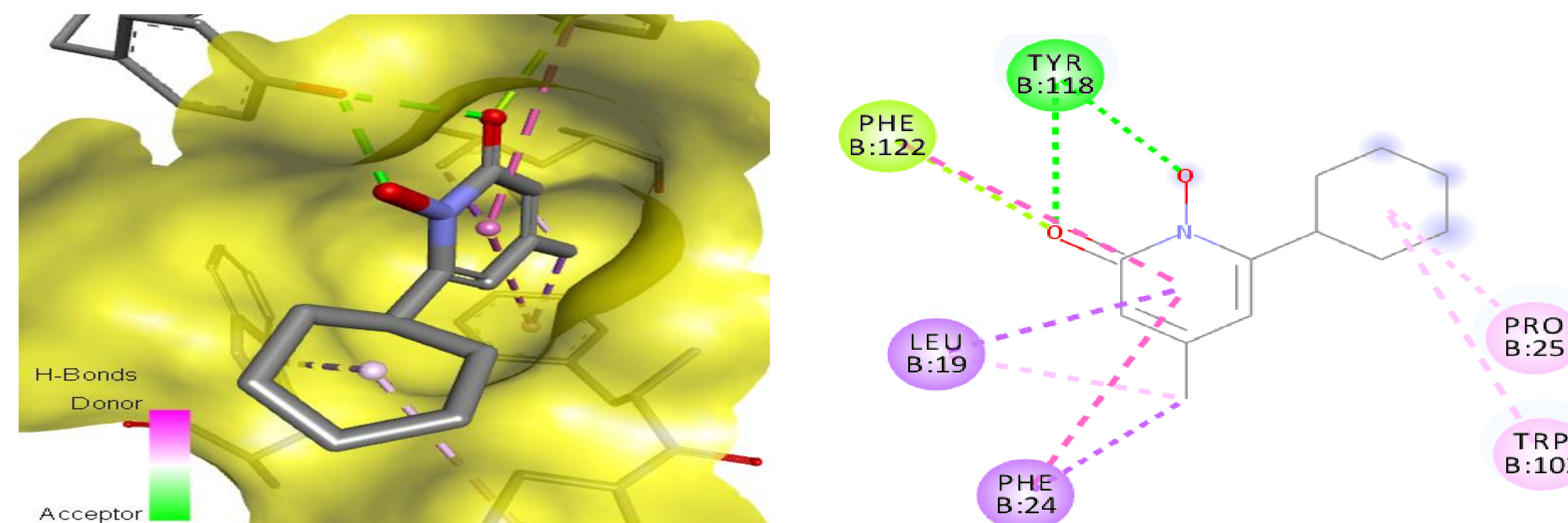
Method

- Extraction of plant root and characterization of extract
- Docking studies of phytochemicals in plant root extract against hepatitis B core protein Y132A mutant using Autodock Vina in PyRx software, version 0.8.

Protein chain B: Y132A



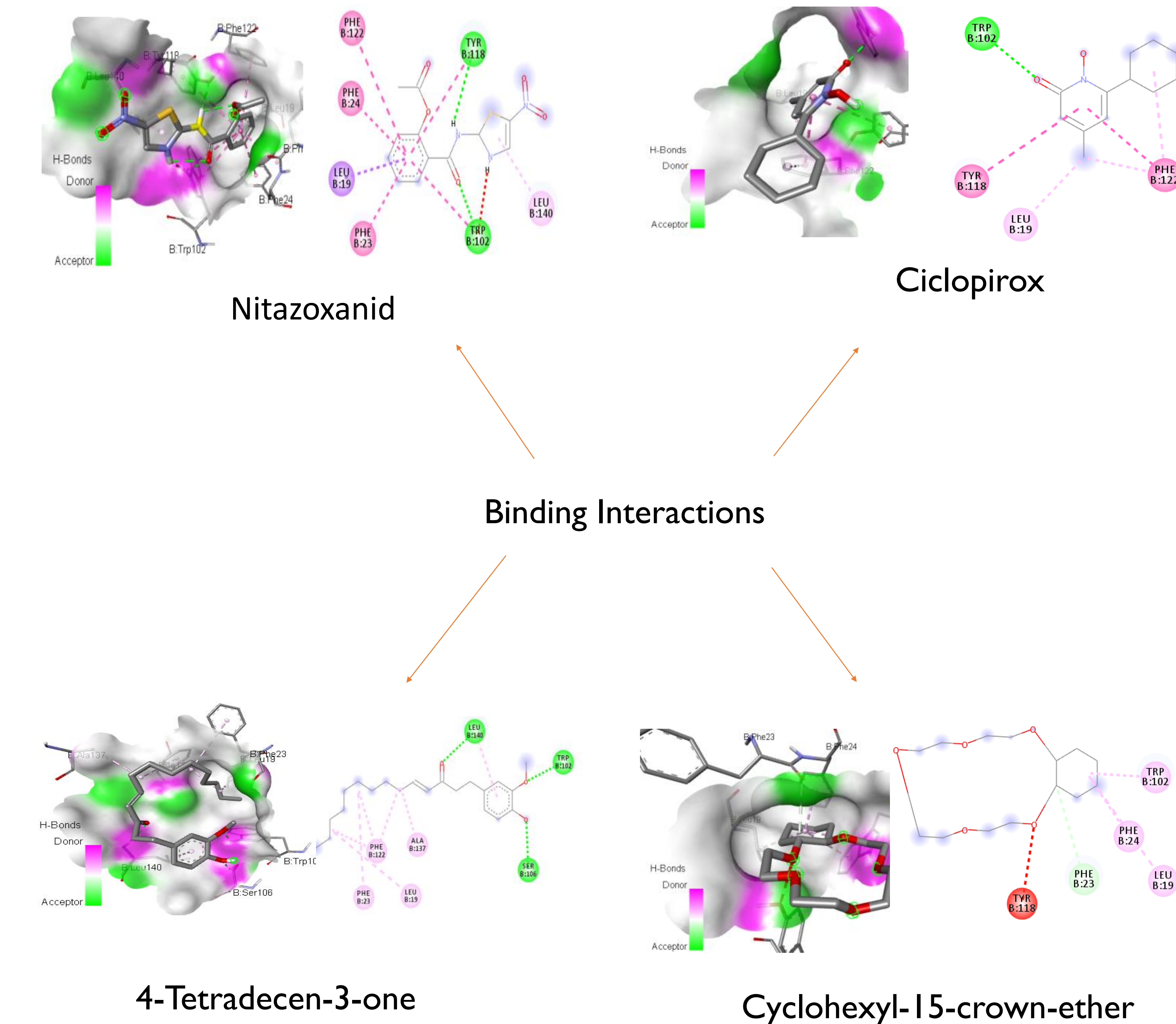
Amino acid residues at binding sites



Literature

- Sankar, N.K., Esack, E.R., Radhapriya, P., Gopal, V.B, Muthu S, and Perumal P. (2018). Impact of geography on adaptation of P. amarus. J. Abbr. Biotech
- Tesfa T, Hawuite B, Tolera D, Abaje D. (2021). Hepatitis B virus infection and associated risk factor among medical students in eastern Ethiopia. Plos one.
- World Health Organization (WHO) HBV Report 2017.06

Docking Result



What we observed

From the table and binding energy data, 4-tetradecen-3-one and cyclohexyl-15-crown-5 show the possibility to inhibit the cellular gene required for HBV replication. Thereby serving as drug lead for the management/treatment of HBV infection and providing a novel route to combat chronic HBV infection by blocking HBV capsid assembly.

Our Conclusion

Inhibition of Hepatitis B Virus secretion by blocking capsid assembly or Targeting Hepatitis B virus (HBV) capsid assembly modulators (CpAMs) can open a wide range of opportunities for drug design

The Plant



Phytochemicals

Compound	Percentage composition	Binding affinity
I-Nonadecene	0.57	-4.3
4-Tetradecen-3-one	3.16	-5.8
Dibutyl Phthalate	3.20	-5.4
Butanoic Acid	0.46	-3.7
n-Hexadecanoic Acid	32.08	-4.3
Octadecanoic Acid	4.63	-4.2
Oleic Acid	49.06	-4.7
Cyclohexyl-15-crown-5-ether	1.55	-5.8
(Z)-9-Octadecenamide	3.21	-4.4
(Z)-6-Octadecenoic Acid	2.10	-4.4
Nitazoxanid (Control)	-	-6.1
Ciclopirox (Control)	-	-5.5