

Assessment of the Mechanism of Anticancer Interaction of the Bioactive Compounds of *Xylopia Aethiopica* Against Bcl-2 Protein Associated with Cancer

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Introduction

BCl-2 protein is among the family of key regulator protein with pro and anti-apoptotic activity. It has been implicated in the expression of various cancer cells. This study is aimed at investigating the mechanism of anticancer interaction of the bioactive compounds of *Xylopia aerthiopica* against BCl-2 protein associated with cancer.

Materials and methods

The quantitative screening of the phytochemicals of the methanol extract of *Xylopia aerthiopica* was carried out using standard method. Characterization of the bioactive compounds was carried out using GC-MS method. The ligand and protein selection, preparation, and docking were carried out using PyRx and Auto Dock vina, while the ADMET predict was carried out using ADMET LAB and SWISSADMET.

Results and discussion

The result of the phytochemical screening revealed the presence of ten (10) compounds ranging from 0.00065 mg/l to 25.70mg/l. Glycoside was observed to be higher with 25.70mg/l followed by phytate 21.39mg/l. The compound with the least value is tanine with 0.00065mg/l. The characterized extract using GC-MS, revealed forty-eight compounds which cut across the groups of secondary metabolites from plants. the molecular interaction of the ligands with the BCl-2 protein revealed the presence of three compounds namely 2(4(4(diphenylmethylmethylene piperion-1-yl)-hydroxyl butyl phenyl), with the highest binding affinity of -7.6 followed by levopinaric acid with -7.3 and pimaric acid with -7.2. these compounds had more bonding affinity than obatoclax (the standard) with -6.7. the three ligands also proved to follow the Lipinski “rule of five” and are drugable compounds than obatoclax as revealed by ADMETLAB and SWISSADMET. The interaction of the ligands and the binding site of the BCl-2 protein involved up to five binding forces which are categorized with Hydrophobic and hydrophilic interaction as demonstrated by their interaction with the amino acids between the ligands and the binding site of the protein.

Conclusions

This study has demonstrated the potential of the three compounds with the higher binding affinity as good alternative compounds than the standard drug for the treatment of cancer condition

Keywords: Binding, cancer, BCl-2 protein, molecular docking, *Xylopia aerthiopica*