Insights of Antiplasmodial Potentials of Secondary Metabolites from *Cylicodiscus gabunensis*: Virtual Screening, Drug-likeness and Molecular Docking

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Introduction

Malaria chemotherapy has recently come under increasing challenge because *Plasmodium falciparum*, has developed diverse forms of resistance to available antimalarial drugs.

Despite all effort to eliminate malaria, it remains a life threatening disease. There is an urgent need to develop new antimalarial potentials with novel modes of action. Secondary metabolite from *Cylicodiscus gabunensis* a medicinal plant, have shown broad spectrum of activities. This study therefore, investigated the antimalarial potentials of the secondary metabolites from *Cylicodiscus gabunensis* using virtual screening, drug-likeness and molecular docking analyses.

Results

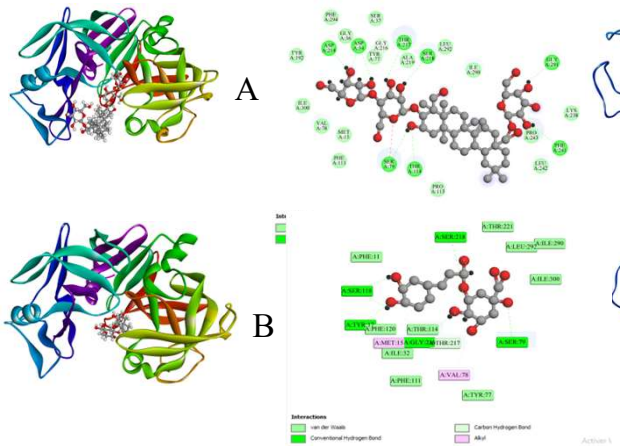

Figure 1: 3D poses and 2D interaction of maslinique acid – 1me6 (A), Araliasaponine I -1me6 (B)

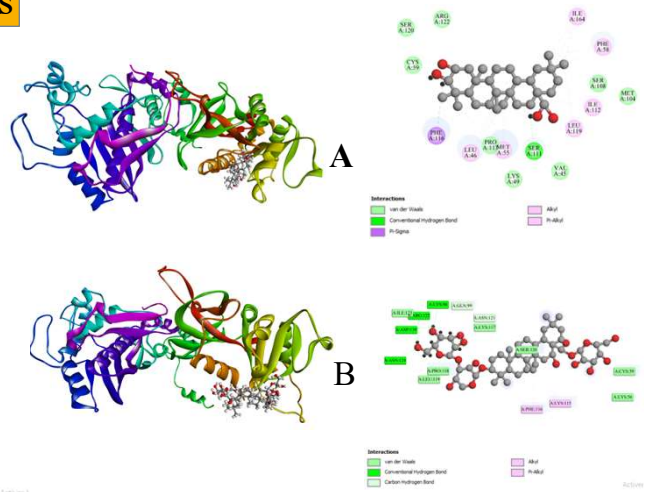

Figure 2: 3D poses and 2D interaction of maslinique acid - 4DPD (A), Araliasaponine I -4DPD (B)

Discussion

The results of molecular docking revealed significant binding affinities for several compounds, with favorable binding energies for chlorogenic acid (−12.317 kcal/mol) and ellagic acid (−10.874 kcal/mol) against 1me6, as well as maslinic acid (−11.077 kcal/mol) and araliasaponin I (−10.983 kcal/mol) against 4DPD. These values, lower than −10 kcal/mol, suggest strong inhibitory interactions with the studied targets. Pharmacokinetics properties obtained from SwissADME and ADMETlab 3.0 showed that almost all the compounds exhibited a more balanced pharmacokinetic profile, characterized by good predicted permeability, satisfactory free fraction, and limited toxicity.

Conclusion

The integration of docking results and ADMET predictions thus highlights promising candidatesf or their favorable pharmacokinetic balance, as well as for their strong structural affinity toward the protein targets. These findings provide a rational basis for further experimental studies to confirm the antimalarial potential of compounds derived from *Cylicodiscus gabunensis.*

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