IN SILICO IDENTIFICATION OF ANTIMALARIAL PHYTOCHEMICALS FROM *CASSIA ABBREVIATA OLIV*

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INTRODUCTION

Malaria is a mosquito-borne disease that has affected over 100 countries and territories and is one of the most fatal diseases that causes an more than of 435 000 deaths [1].
Plasmodium Falciparum is one of the most prevalent yet deadliest malarial parasite in Sub Saharan Africa.
Natural Products such as the *Cassia Abbreviata Oliv* that are traditionally used for treatment of Malaria in countries like Zimbabwe [2].

Cassia Abbreviata Oliv phytochemicals are potential Inhibitors of Plasmodium falciparum target proteins.

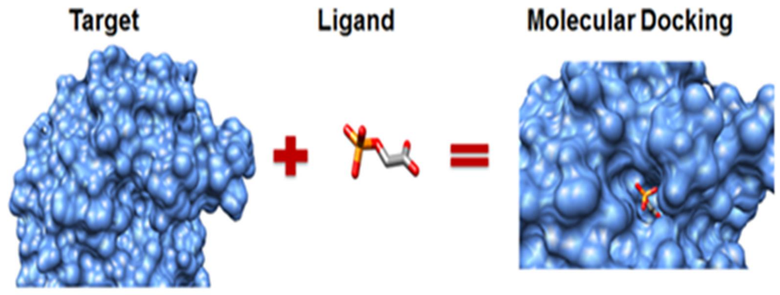


Fig 1: Example of protein and compound binding into a lock and key target-ligand pair.

Extraction and characterization of *Cassia Abbreviata Oliv* Compounds resorted in literature.

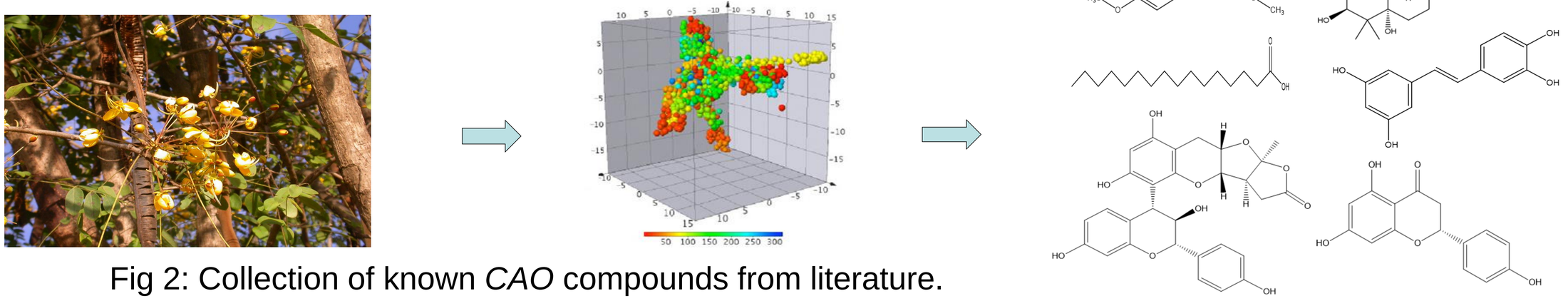


Fig 2: Collection of known *CAO* compounds from literature.

Use of Machine learning model for identification of *Plasmodium Falciparum* protein target.

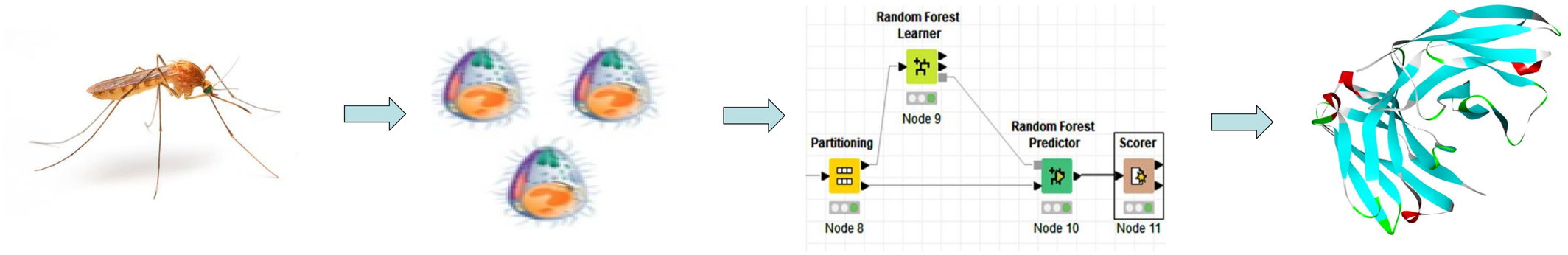


Fig 3: A machine learning model generated from *Plasmodium Falciparum* data found in ChEMBL database was used to identify targets that bind to *Cassia Abbreviata Oliv* phytochemicals.

Binding pocket analysis and Target protein after molecular docking of *CAO* compounds.

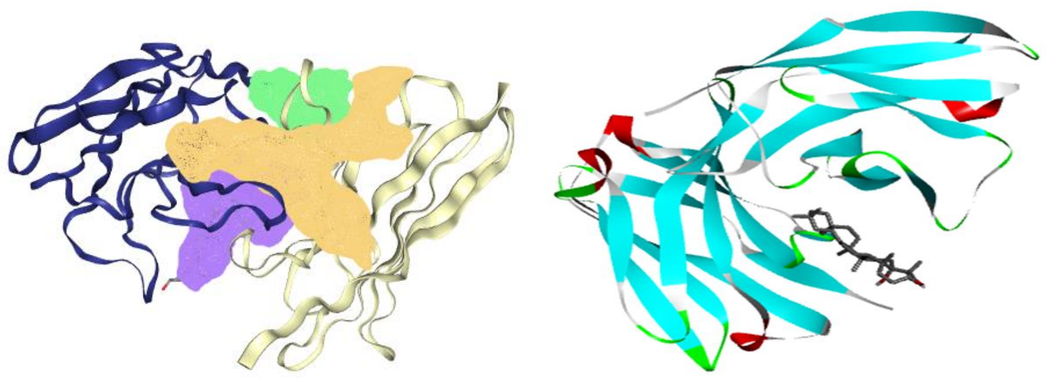


Fig 4: Protein binding pockets and Protein-ligand pair

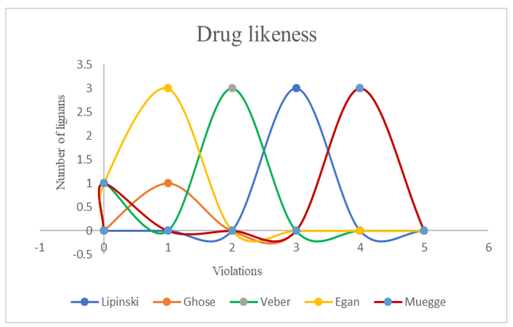
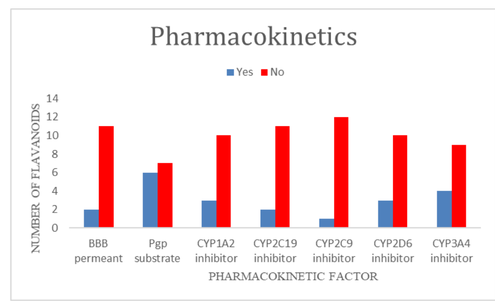


Fig 6:Pharmacokinetic studies show that 8 compounds are bioactive according to Lipisnki's rules.

Fig 5:70% of the phytochemicals showed drug-like properties meaning they have therapeutic potential



CONCLUSION

6 compounds i.e. 4 flavonoids and 2 terpenoids after molecular docking and interaction analysis, proved to be potential antimalarial phytochemicals that target a specific protein of the *Plasmodium falciparum*.

REFERENCES.

[1]Cragg, G. M. & Newman, D. J. 2013. doi.org/10.1016/j.bbagen.2013.02.008. PMID 23428572 Biochim. Biophys. Acta - Gen. Subj. 1830, 3670–3695.
[2]Atanas G. Atanasov S, Sergey B. Zotchev, Verena M. Dirsch. 2021. doi 10.1038/s41573-020-00114-z . PMID 33510482 Nat. Rev. Drug Discov. 20, 200–216.

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INTRODUCTION

- Malaria remains a global health burden with an estimation of more than 600 000 deaths and 241 million cases as of 2020,
- *Plasmodium Falciparum*, the most prevalent malaria causing parasite is resistant to nearly all currently available anti-malarials.
- *Cassia Abbreviata Oliv* common herb traditionally in the treatment of Malaria in Zimbabwe [2].

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Experimental methods

Results and Discussion

Conclusion