



IDENTIFICATION OF POTENTIAL ANTI-MALARIA LEAD COMPOUND FROM SELECTED PLANTS IDENTIFIED

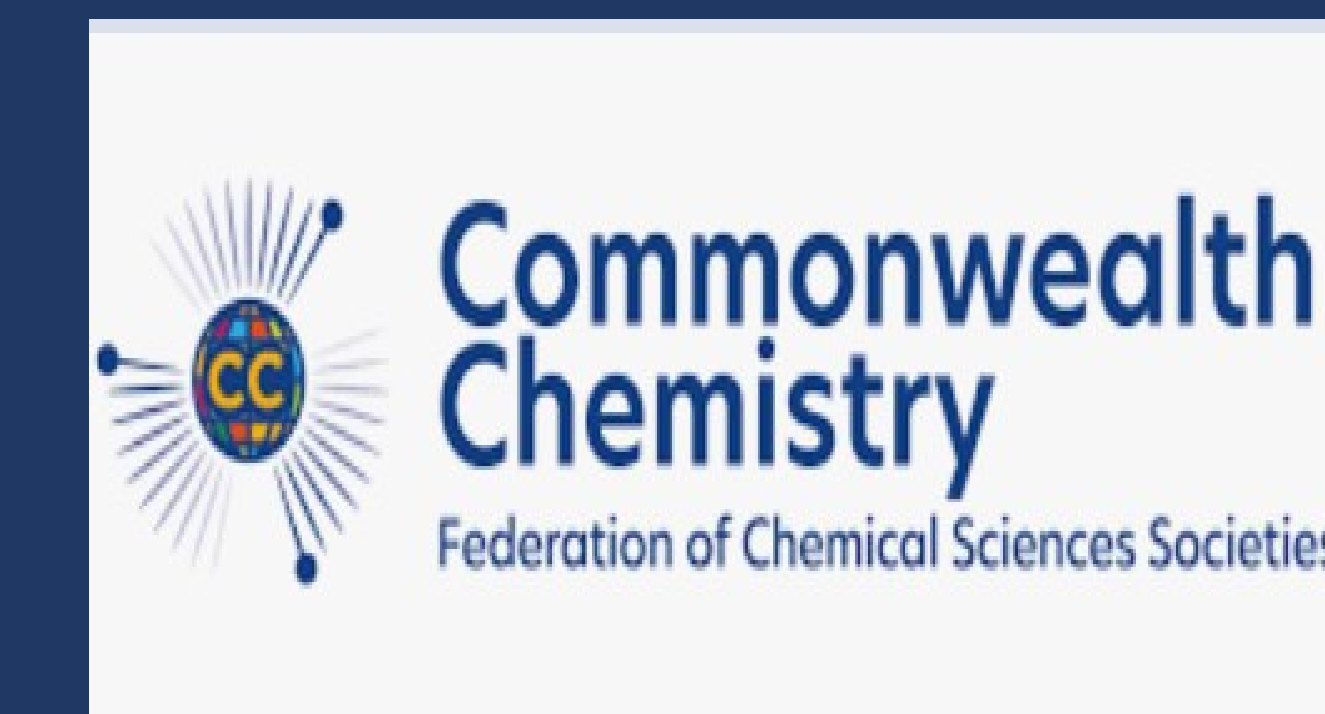
PHYTOCHEMICALS: A COMPUTER-AIDED DRUG DESIGN (CADD) STUDY

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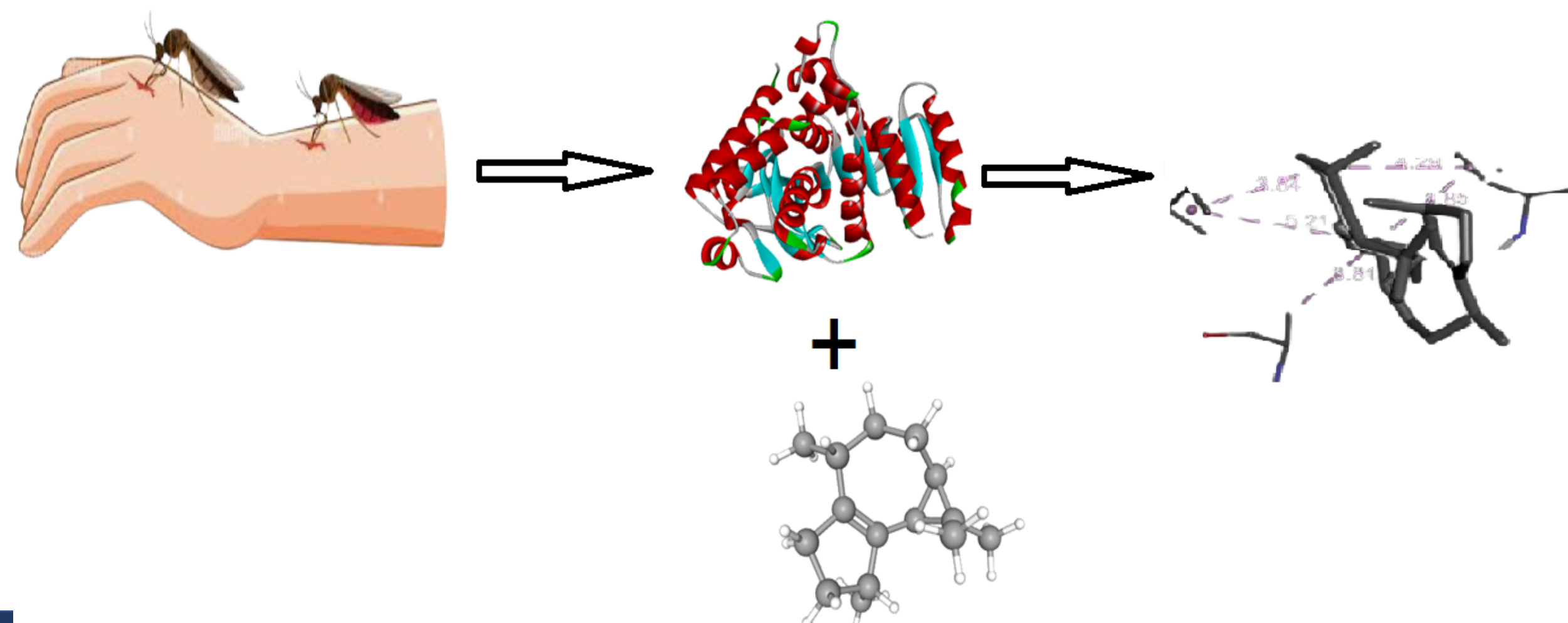
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GRAPHICAL ABSTRACT



METHODS

Retrieval of 131 bioactive compounds of the selected plants and pfLDH enzyme from databases

ADMET, bioavailability and drug likeness Screening using ADMETlab3.0 and SwissADME databases

Molecular Docking

Post docking analysis

RESULTS

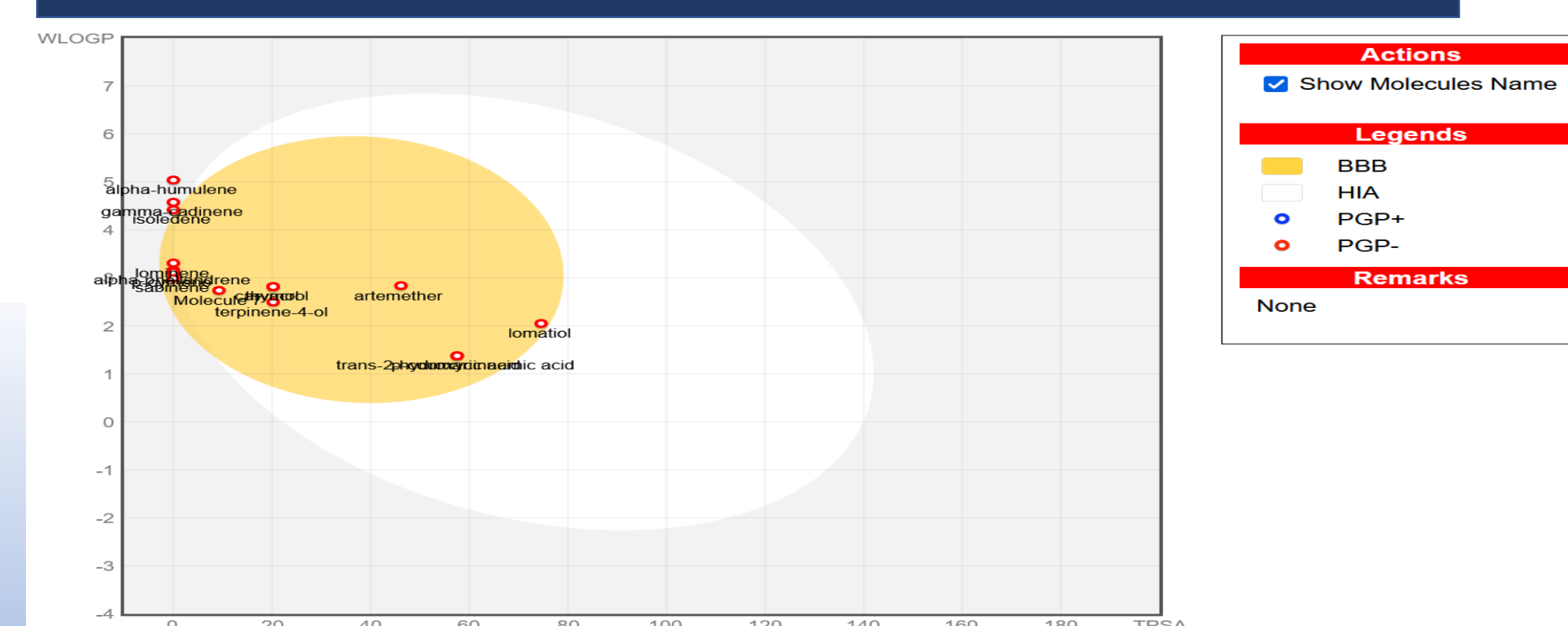


Figure 1: Schematic of assessment prediction of gastrointestinal absorption (HIA), Brain permeant (BBB) using BOILED-Egg

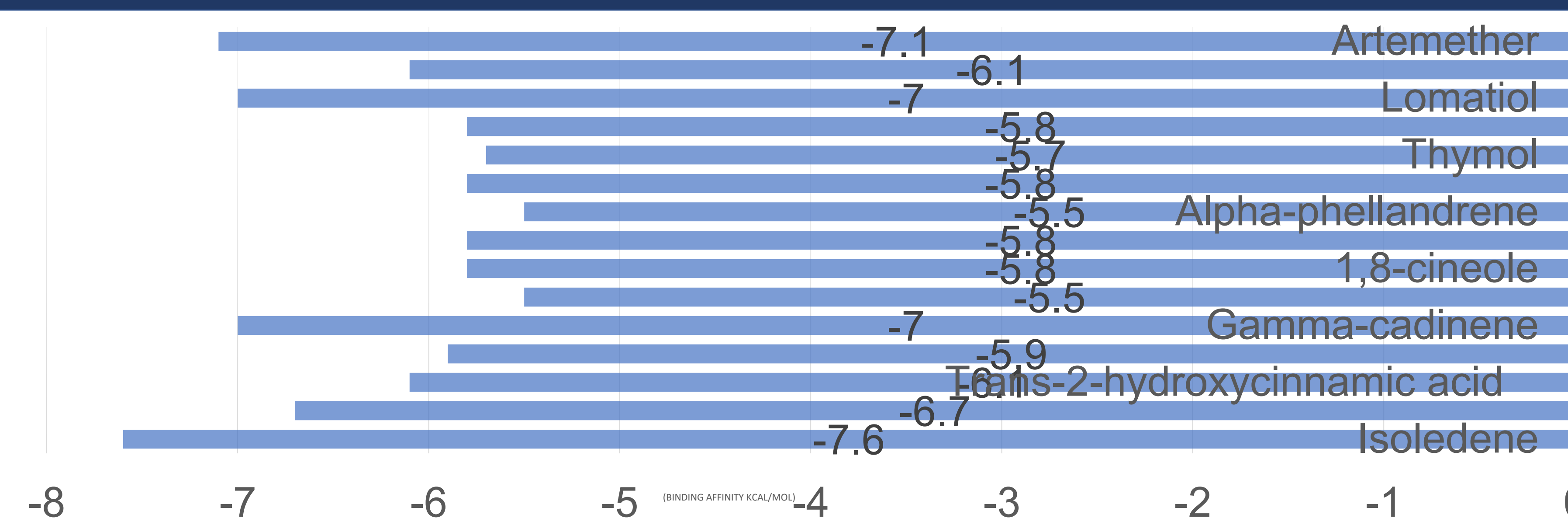


Figure 2: Bar chart showing the binding affinity values (kcal/mol) of each docked ligand to pfLDH

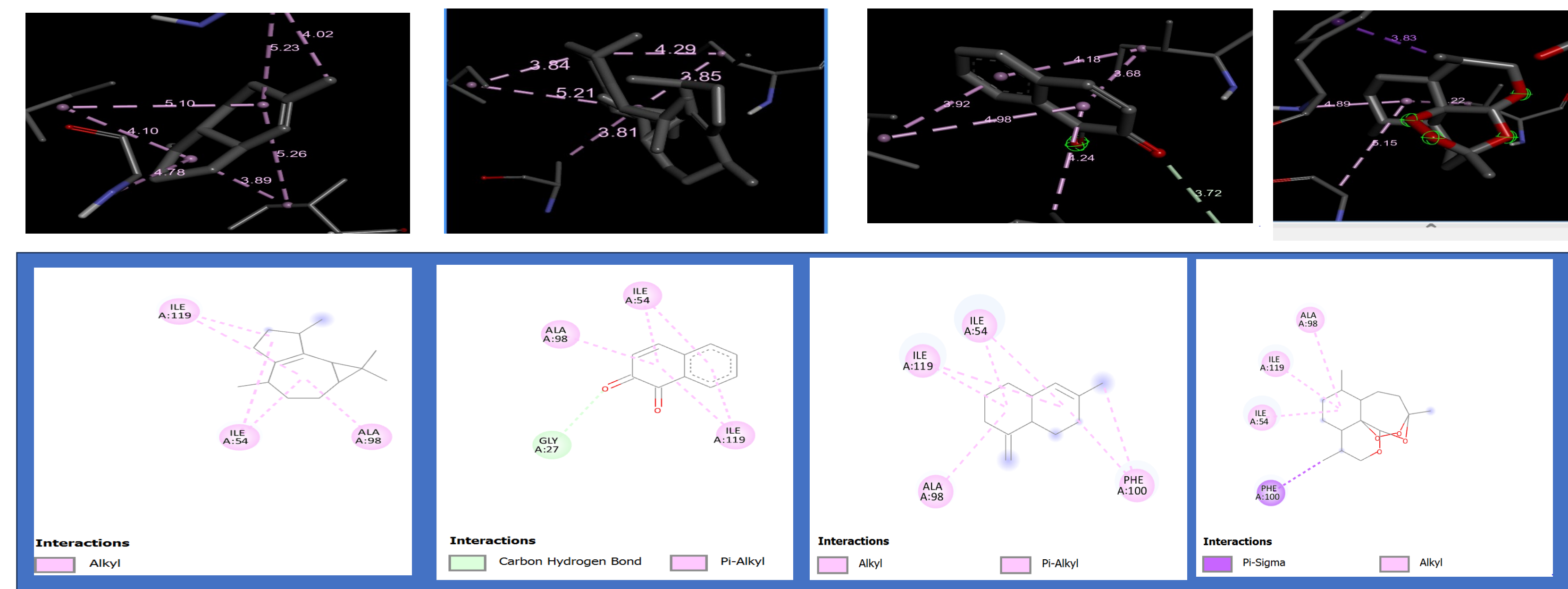


Figure 3: Interaction mapping of 1LDG receptor with isoledene, gamma-cardinene, lomatol and Artemether

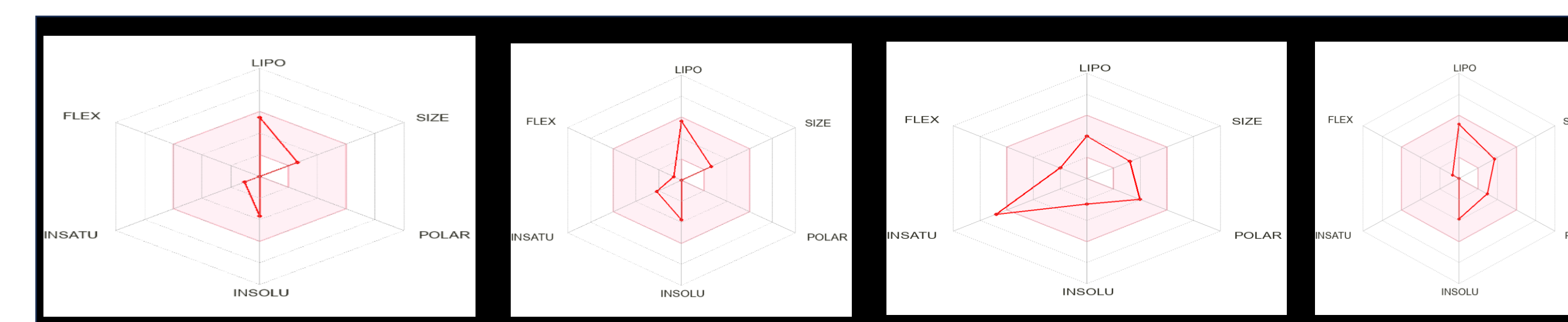


Figure 4: Oral-bioavailability

CONCLUSION

- Isoledene: Best hit (-7.6 kcal/mol), stronger than artemether (-7.1 kcal/mol). Limitation: Suboptimal pharmacochemical properties (optimization required)
- Other leads: Gamma-cardinene and Lomatol (-7.0 kcal/mol each). Strengths: Good drug-likeness, ADMET, interactions
- Further steps required
 - molecular modelling to improve isoledene
 - Molecular dynamics to test stability
 - Derivatization to enhance efficacy

REFERENCES

1. Arhin, A. O., Frimpong, R. B., Acheampong, K. 2023. A double bootstrap data envelopment analysis model for evaluating malaria spending efficiency in Sub-Saharan Africa, Healthcare Analytics 3, 100137.
2. Fu, L., Shi, S., Yi, J., Wang, N., He, Y., Wu, Z., Peng, J., Deng, Y., et al. ADMETlab 3.0: an updated comprehensive online ADMET prediction platform enhanced with broader coverage, Accessed on 24 November 2024.
3. WHO. 2024, Strategy to respond to antimalarial drug resistance in Africa <https://www.who.int/publications/item/9789240060265>, accessed January 30, 2024.

INTRODUCTION

Malaria is a severe, and deadly disease caused by single-celled protozoa of the genus *Plasmodium*. *Plasmodium falciparum* is responsible for the greatest number of deaths and clinical cases in the tropics. Moreover, its infection can lead to serious complications affecting the brain, lungs, kidneys and other organs. It is transmitted through infected female *Anopheles* mosquito to uninfected person. Several antimalaria drugs have been employed over years in the control of the disease.

Why the need for novel antimalaria therapeutic agents?

- Prevalence of antimalaria drug resistance
- Antimalaria drugs with minimal toxicity

AIM

To investigate the activities of the phytochemicals identified in *Ocimum grattissimum*, *Citrus aurantifolia* and *Gossypium barbadense* against *Plasmodium falciparum* lactate dehydrogenase (pfLDH) enzyme.