

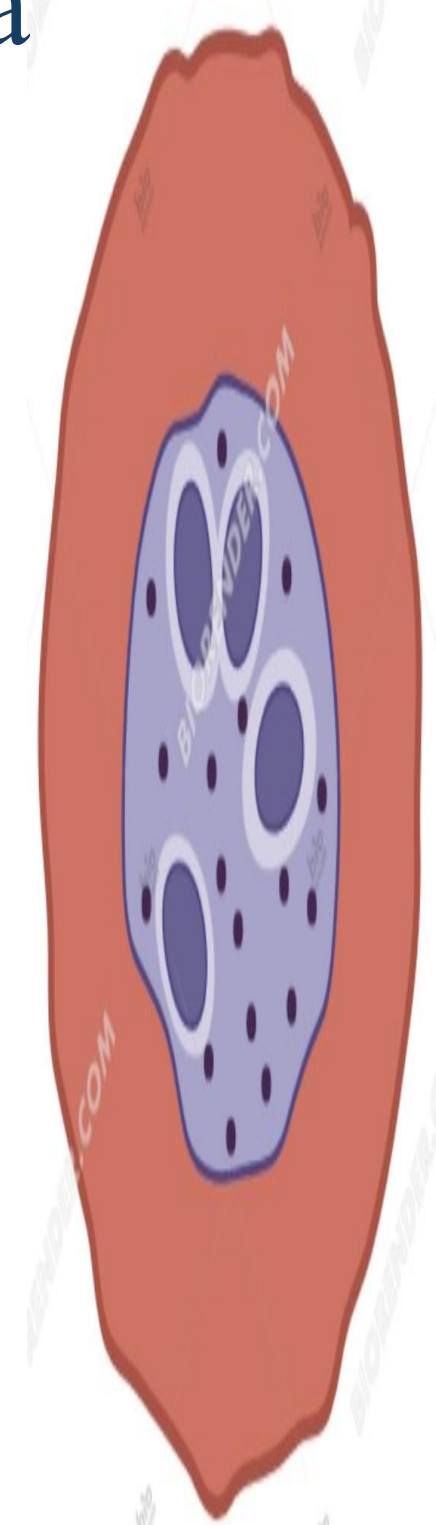


? INTRODUCTION

Malaria remains a global health challenge, especially in Sub-Saharan Africa

PfPKG plays a critical role in parasite survival and represents a promising anti-malarial drug target

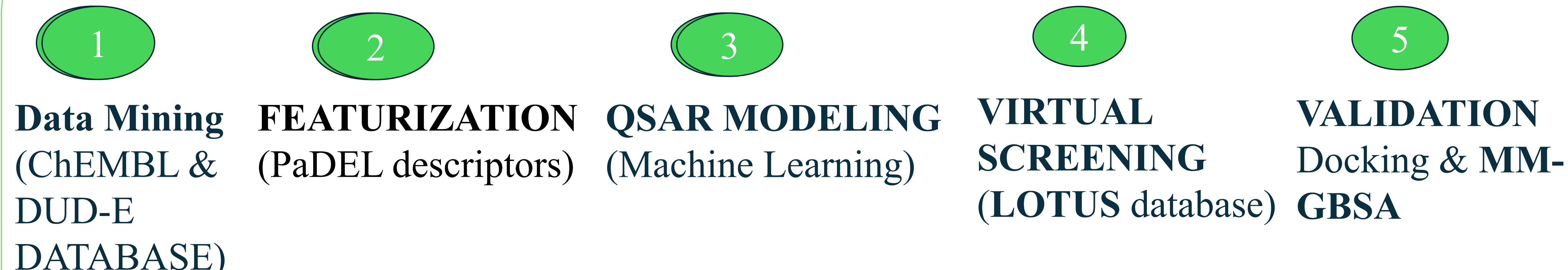
This study focuses on **UN SDG 3 (Good Health and Wellbeing)** by leveraging computational tools to discover novel antimalarials from natural resources



🎯 OBJECTIVES

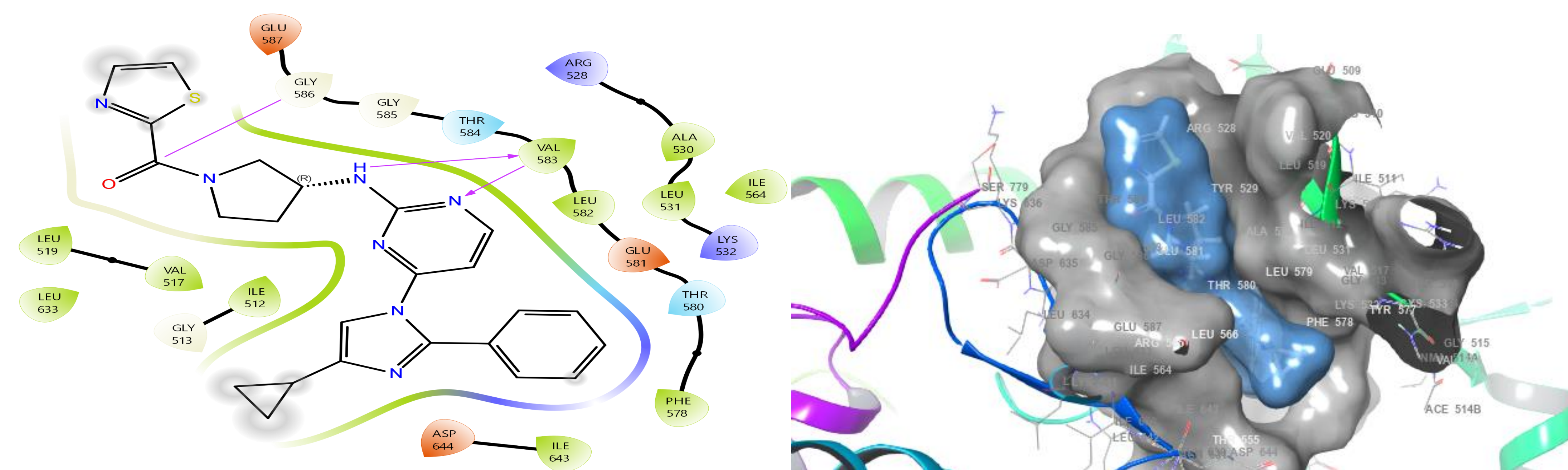
- Build a predictive QSAR model for PfPKG inhibitors
- Identify novel antimalarial leads from the LOTUS database
- Validate binding stability using Docking and **MM-GBSA**

⚙️ METHODOLOGY WORKFLOW



Tools & Platform: Python, PaDEL, Scikit-learn, Schrodinger Maestro, AdmetLab

🏆 LEAD INTERACTION (Best Lead: LTSOO95215)



Docking Score
-9.785 kcal/mol

MM-GBSA
-90.96 kcal/mol

Binding Mode
Stable & Favorable



ACKNOWLEDGEMENTS

We acknowledge the use of open-access databases (ChEMBL, DUD-E, LOTUS) and computational resources that made the research possible

📈 RESULTS: QSAR AND SCREENING

METRIC	VALUE
Training R ²	0.967
Test R ²	0.84
Identified Hits (pIC ₅₀ > 6)	496 candidates
Best Docking Score (kcal/mol)	-10.662
ADMET Prediction	Favorable

★ KEY FINDINGS

- A robust QSAR model was developed with high predictive power
- Virtual screening of natural products database yielded 496 promising hits
- Lead compound LTSOO95215 exhibited strong binding affinity (-9.785 kcal/mol) and favorable ADMET properties
- This work supports the discovery of novel PfPKG inhibitors from natural products and contributes to malaria drug discovery aligned with **UN SDG 3**

🏰 CONCLUSION

This study successfully integrated QSAR modeling, virtual screening, and docking analysis to identify potent PfPKG inhibitors. The identified hits provide valuable starting points for future **Molecular Dynamics (MD)** to evaluate long-term binding stability, followed by experimental validation as antimalarial drug candidates