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Molecular Network Mapping of Anti-Plasmodial Biomolecules in *Dialium lopense* Wood By-Products

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Objectives

- Residues from *Dialium lopense*, traditionally used in Gabon for malaria treatment, represent a potential economic resource for the forestry industry.
- To identify the solvent phase and characterize bioactive compounds found in *Dialium lopense* tissues against *Plasmodium falciparum*.
- A detailed analysis was conducted using molecular networking and LC-MS/MS to investigate the wood samples.
- Bioactive compounds were predominantly extracted in the ethanol-water phase. Ultrasonic extracts from bark, sapwood, and heartwood showed IC50 values of 7.97 ± 1.11, 1.14 ± 0.44, and 4.92 ± 2.49 µg/mL, respectively, against *Plasmodium falciparum* strains.

Introduction

- In Central Africa, legal logging has become more selective due to stricter timber quality standards on international markets.
- The number of harvested species is decreasing, with species such as *Aucoumea klaineana* suffering from low regeneration capacity.
- Local sawmills often produce low yields, and the by-products are frequently burned or left abandoned in the forest.
- Some *Dialium* species regenerate well and possess promising wood properties, making them strong candidates for sustainable forest management and efficient use of forest
- African trees are rich in secondary metabolites with significant bioactivity, offering potential for treating diseases such as malaria.
- Malaria still affects over 247 million people, particularly in tropical Africa, with growing *Plasmodium falciparum* resistance to current treatments.
- There is an urgent need to discover new bioactive compounds to overcome this resistance and effectively combat the parasite.
- *Dialium* species contain various compounds, such as steroids, polyphenols, terpenoids, and flavonoids, with antimalarial properties identified in several studies.
- There is a notable gap in research on by co-product residues from *Dialium* and other forest species as sources of bioactive compounds.
- This study investigates the potential of *Dialium lopense* forest residues, utilizing a molecular network approach to identify antiplasmodial compounds in their hydroethanolic and Dichloromethan extracts.

Materials and Methods

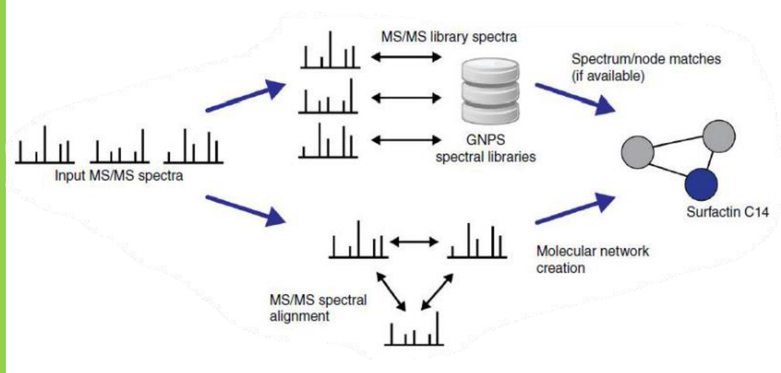

Figure 1: Molecular network stages

Plasmodium assay

•*Antiplasmodium Testing:* Cultures of chloroquine-sensitive *Plasmodium falciparum* (3D7) were grown in red blood cells (A+ or O+), using RPMI 1640 medium enriched with supplements. Extracts were diluted and tested alongside artemisinin as a positive control.

•*Assessment Method:* After a 48-hour incubation, parasite growth was measured through SYBR Green fluorescence, with readings taken at specific excitation and emission wavelengths using a FlexStation system.

•*Data Analysis:* Each test was repeated three times, and the minimum inhibitory concentration (MIC) values were calculated from the results of these experiments.

Results

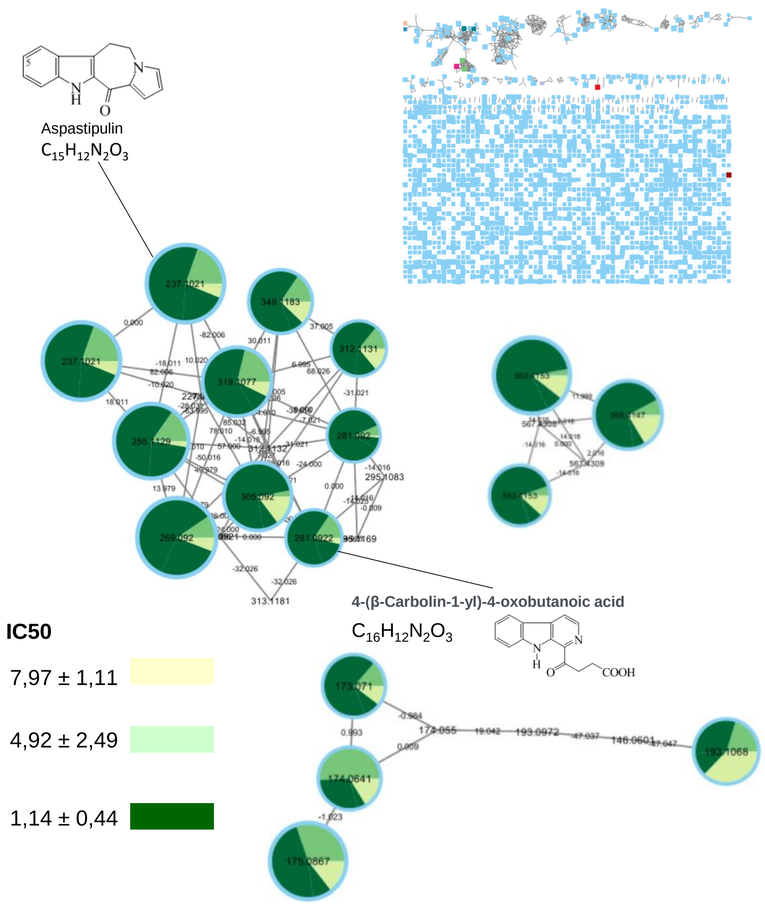

Figure 2: Clusters in the molecular network representing the most effective antiplasmodials compounds.

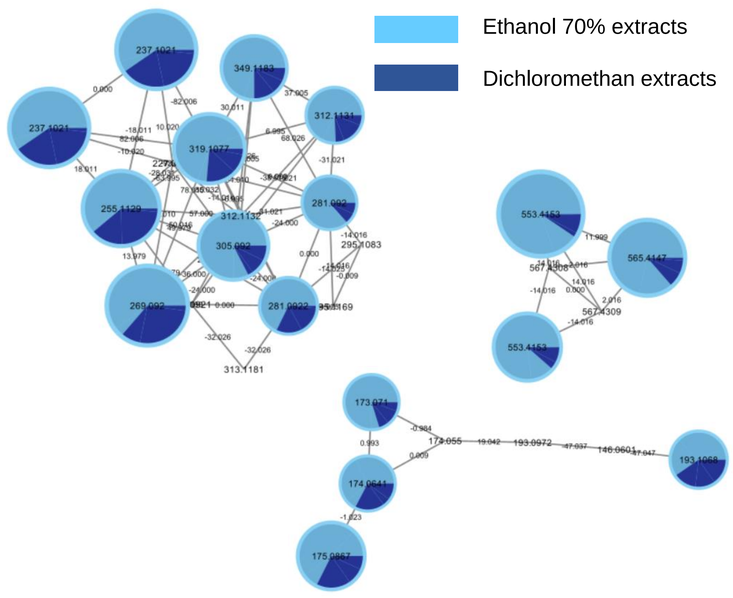

Figure 3: Antiplasmodial compounds localised in polar and apolar phase.

Results

- Several biomolecules derived from *Dialium lopense* co-products have demonstrated promising antiplasmodial activity.
- Two alkaloids were putatively identified: 4-(β-Carbolin-1-yl)-4-oxobutanoic acid and aspastipuline.
- Several compounds did not match the GNPS databases, potentially indicating the presence of novel biomolecules.
- The antiplasmodial compounds were primarily extracted from the polar phase.

Conclusions

Wood co-products from *Dialium lopense* represent a promising pharmaceutical resource, particularly as a source of antiplasmodial biomolecules. The novel compounds present in this species may be effectively extracted using polar solvents, offering potential for further research into their medicinal properties. These findings suggest that the valorization of these co-products could lead to innovative applications in drug discovery, particularly in combating malaria.

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Acknowledgements

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