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Investigating Bioactive Compounds from *Parkia biglobosa* Stem Bark for theTreatment of Elephantiasis: A Virtual Screening and Drug Design Approach

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ABSTRACT

Elephantiasis (L*ymphatic filariasis*) is a neglected tropical disease that causes severe swelling and disability. Current treatments such as albendazole are useful but limited by side effects and drug resistance, so there is a need for new, safer therapies. In this study, the stem of *Parkia biglobosa* (African locust bean tree), a plant widely used in African traditional medicine, was examined for bioactive compounds. The present study investigated the phytochemical composition and bioactivity of *Parkia biglobosa* stem essential oil and extract. GC-MS analysis revealed major constituents including 2-amino-6-methylbenzoic acid (29.82%), 2,4-di-tert-butylphenol (20.40%), 9,10-methanoanthracen-11-ol (5.31%), α-phellandrene (4.48%), and pentacosane (4.79%). Drug-likeness evaluation using SwissADME indicated one Lipinski's rule violation, attributed to the high molecular weight of certain constituents. Antioxidant activity was assessed using FRAP, DPPH, and ABTS assays. The essential oil exhibited strong ABTS scavenging activity (average 86.78%), while the stem extract showed concentration-dependent potency in the DPPH assay (95.28% at 100 mg/ml). Both samples demonstrated weak ferric reducing activity in the FRAP assay. Molecular docking further revealed favorable binding interactions of selected phytochemicals with protein 8E4F, suggesting potential therapeutic relevance. These findings highlight *Parkia biglobosa* stem essential oil and extract as promising sources of natural antioxidants with drug-like properties, warranting further pharmacological exploration.

KEYWORDS: Bioactive compounds, *Parkia biglobosa,* Elephantiasis, Drug design, Virtual screening.

1. INTRODUCTION

Elephantiasis also known as lymphatic filariasis, is a neglected tropical disease caused by parasitic filarial worms such as *Wuchereriabancrofti*, *Brugia malayi*, and *Brugia timori*. The disease is transmitted through the bites of infected mosquitoes, primarily *Culex*, *Anopheles*, and *Aedes* species. First recorded in ancient Egyptian texts and later documented in ancient India, elephantiasis is characterized by severe swelling of limbs and genitals due to lymphatic obstruction caused by the parasites.

Parkia biglobosa, commonly referred to as the African locust bean tree, is a multipurpose tree native to sub-Saharan Africa, particularly in savannah regions of West Africa. It belongs to the family Fabaceae (Leguminosae) and is widely known for its food, medicinal, and economic value. Traditionally, the seeds are fermented to produce a local condiment called "dawadawa" or "iru," widely used in Nigerian and Ghanaian cuisine. However, beyond the seeds, other parts of the tree, including the bark, stem, leaves, and pods, have shown great potential in traditional medicine.

Numerous studies have been conducted to evaluate the pharmacological and phytochemical properties of *Parkia biglobosa*: Odeyemi et al. (2015) reported antimicrobial activity in stem bark extracts against *Staphylococcus aureus* and *Escherichia coli*. Akinmoladun et al. (2014) found flavonoids, saponins, tannins, alkaloids, and glycosides in ethanolic and aqueous extracts of the plant's stem and roots. Ogunmoyole et al. (2018) assessed antioxidant potential of methanolic extracts of the root and stem, demonstrating significant radical scavenging activities. Adedapo et al. (2011) showed anti-inflammatory and analgesic activity in aqueous extracts from the bark and leaves. Adebayo et al. (2019) analyzed essential oil compositions using GC-MS and identified compounds such as alpha-pinene, linalool, eugenol, and caryophyllene in the volatile fractions of the leaves and bark. Ajaiyeoba et al. (2003**)** confirmed antifungal properties of the root and bark against *Candida albicans* and dermatophytes. Balogun et al. (2020) explored the immunomodulatory effects of the stem extracts on lymphocyte proliferation and cytokine expression. Ezekwesili-Ofili et al. (2021**)** investigated the hepatoprotective effects of methanolic extracts in Wistar rats with paracetamol-induced liver damage.

Despite these findings, there is a paucity of comprehensive studies combining cold maceration, rotary evaporation, hydro distillation, andGC-MS to examine the volatile profile of the **s**tem of *Parkia biglobosa*. This project aims to fill that research gap by using an integrated approach. Additionally, this project is driven by the hypothesis that the phytochemicals derived from the stem bark of *Parkia biglobosa* may offer therapeutic relevance in the management or potential cure of elephantiasis, a neglected tropical disease caused by lymphatic filarial parasites. The investigation into its phytochemical constituents may pave the way for future pharmaceutical applications against lymphatic filariasis.

2. MATERIALS AND METHODS

2.1 Reagent and Materials

Methanol, ethyl acetate, n-hexane, distilled water, ice block, beaker, round-bottom flask, measuring cylinder, funnel, retort stand, Clevenger apparatus, rotary evaporator, bucket, keg, cotton wool, muslin cloth, GC-MS, MOE, CHEMDRAW, UCSF Chimera, Plip, SWISSADME.

2.2 Plant Collection and Preparation

Fresh stem samples of Parkia biglobosa were collected in February 2025 from a forest in Ibarapa Local Government Area, Oyo State, Nigeria. The plant was authenticated by Dr. Odewo at the Forestry Research Institute of Nigeria (FRIN). Samples were air-dried under shade for four weeks, then ground into coarse powder. A total of 2515 g of the powder was extracted with methanol and ethyl acetate (4 L each) at room temperature for five days with intermittent agitation. Extracts were filtered and concentrated under reduced pressure at 40°C using a rotary evaporator.

2.3 Hydro distillation

Essential oil was obtained from 40 g of powdered sample using a Clevenger-type apparatus for 45 minutes (in two portions) and stored under refrigeration.

2.4 GC–MS Analysis

Samples were analyzed using an Agilent 8890 GC coupled with a 5795 MS. Helium (99.999%) served as the carrier gas on an HP-5MS column (30 m × 0.320 mm, 0.25 µm). The oven temperature was programmed from 80°C (2 min) to 240°C at 12°C/min (held 6 min). A 1 µL sample was injected, and compound identification was performed using the NIST library and retention times.

2.5 Ligand and Protein Preparation

Ligands were drawn and optimized in ChemDraw and exported for docking. The target protein (PDB ID: 8E4F) was retrieved from the Protein Data Bank and prepared in Chimera by removing water molecules, adding hydrogens, and defining active sites.

2.6 Molecular Docking and Interaction Analysis

Docking was performed using MOE software. Binding affinities were evaluated using London dG and GBVI/WSA dG scoring functions. Top poses were analyzed, and interactions were profiled using PLIP to identify hydrogen bonds, hydrophobic interactions, and other key contacts.

2.7 ADMET Prediction and Candidate Selection

Pharmacokinetic properties were predicted using SwissADME. Compounds were prioritized based on docking scores, interaction profiles, and drug-likeness for further validation.

2.8 Antioxidant Assays

(a). FRAP Assay: Ferric reducing antioxidant power was determined using the method of Sharmaet al. (2024). Extract (200 µL) was mixed with 3.0 mL FRAP reagent, incubated for 10 min, and absorbance measured at 593 nm. Results were expressed as µmol Fe^{2+} equivalents/g extract.

(b). DPPH Assay: DPPH scavenging activity was evaluated using the method of Khalid et al. (2023). Sample (1 mL, 1 mg/mL) was mixed with 4 mL DPPH solution (30 mg/L), incubated for 30 min in the dark, and absorbance read at 520 nm.

(c). ABTS Assay: ABTS scavenging activity was determined using the method of Gulcin et al. (2024). Sample (1 mL) was added to 4 mL ABTS solution, incubated for 6 min in the dark, and absorbance measured. Inhibition (%) for DPPH and ABTS was calculated as:

$$\frac{Absorbance\ of\ control - Absorbance\ of\ sample}{Absorbance\ of\ control}\ x\ 100$$

3. RESULTS AND DISCUSSION

3.1 Results

The GC–MS analysis revealed a diverse range of metabolites, including aromatic acids, terpenoids, hydrocarbons, esters, fatty acids, and sulfur-containing compounds. These constituents varied in their retention times and relative percentage compositions, suggesting a complex mixture of volatile and semi-volatile metabolites. The essential oil contained twenty-one (21) identifiable compounds. Among these, 2-amino-6-methylbenzoic acid (29.82%) and 2,4-di-tert-butylphenol (20.40%) were the predominant constituents, accounting for nearly half of the total composition. Other notable compounds include alpha-phellandrene (4.48%), pentacosane (4.79%), and eucalyptol (4.31%), which have been reported in literature for their antioxidant, antimicrobial, and anti-inflammatory properties. The presence of long-chain alkanes such as octacosane, hexacosane, and docosane, as well as fatty acids and esters, further highlights the chemical diversity of the extract.

This compositional profile is significant as it reflects the potential pharmacological properties of Parkia biglobosa stem essential oil, with phenolic and terpenoid compounds likely contributing to its antioxidant and therapeutic activities.

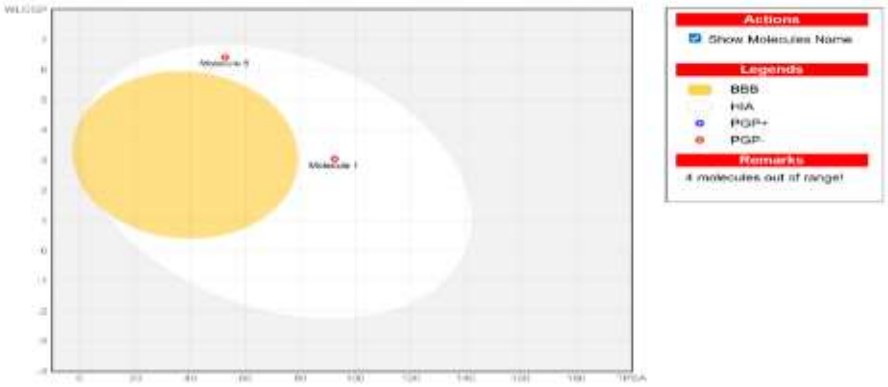
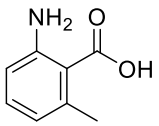
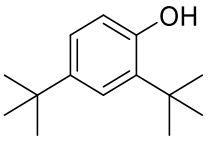


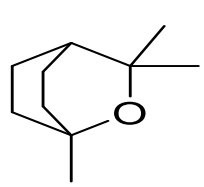
Figure 1: Boiled-Egg Model Illustrating Gastrointestinal Absorption (HIA) and Blood–Brain Barrier (BBB) Permeation of the Test Molecules.



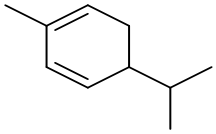
2-amino-6-methylbenzoic acid



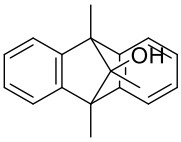
2,4-di-tert-butylphenol



Eucalyptol



alpha-phellandrene



9,10,-Methanoanthracen-11-ol,9,10-dihydro-9,10,11-trimethyl

pentacosane

Figure 2: Structures of the Constituents of the Essential Oil
The structures above are the chemical structures of major constituents identified in the essential oil.

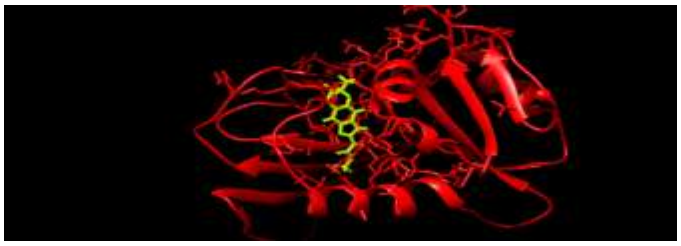


Figure 3: Binding interaction of Albendazole with Protein (8E4F) active site.

Figure 4: Binding interaction of Octacosane with Protein (8E4F) active site.

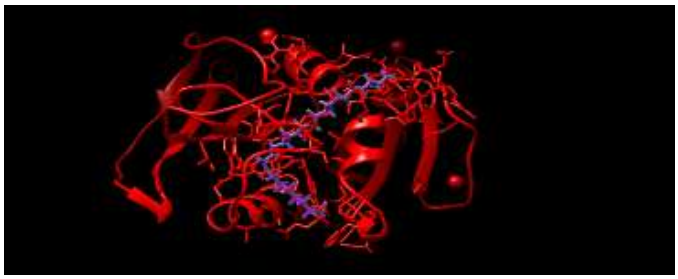


Figure 5: Binding interaction of Hexacosane with Protein (8E4F) active site.

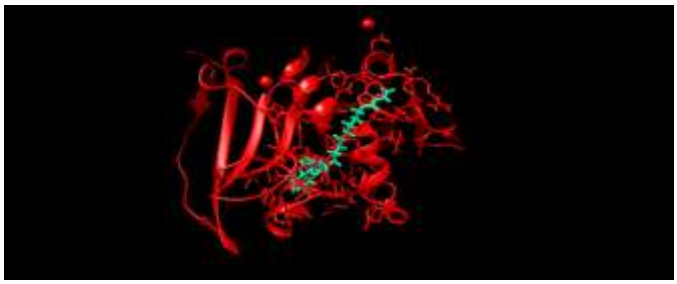


Figure 6: Binding interaction of Carbonic acid, eicosyl vinyl ester with Protein (8E4F) active

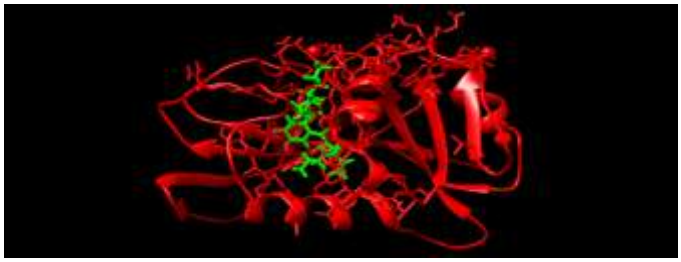


Figure 7: Binding interaction of 1,2-Benzenedicarboxylic acid, bis(2-propylpentyl) ester with Protein (8E4F) active site.

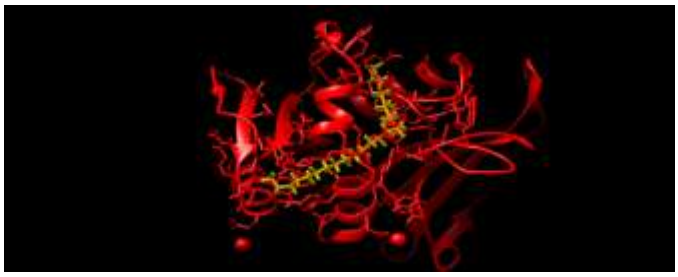


Figure 8: Binding interaction of Pentacosane with Protein (8E4F) active site.

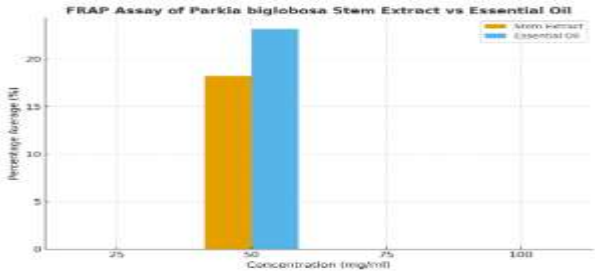


Figure 9: FRAP Assay of *Parkia biglobosa* stem Extract vs Essential Oil

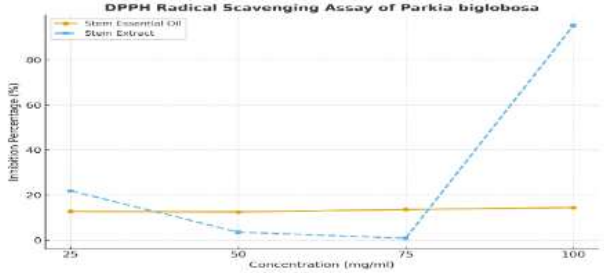


Figure 10: DPPH Radical Scavenging Assay of *Parkia biglobosa* Stem Extract vs Essential Oil

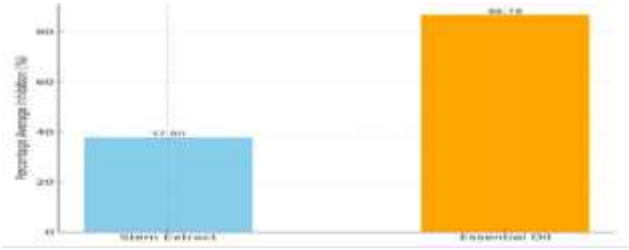


Figure 11: ABTS Scavenging Assay of *Parkia biglobosa* Stem Extract vs Essential

Table 1: Percentage composition of Essential oil of stem of Parkia biglobosa

S/N	Constituents	Chemical formular	KOVAT Index	Retention time (Min)	Percentage composition (%)
1.	Trans-2-methyl-3-propyloxirane	$C_6H_{12}O$	-	3.38	2.47
2.	2-Amino-6-methylbenzoic acid	$C_8H_9NO_2$	-	3.46	29.82
3.	Alpha-phellandrene	$C_{10}H_{16}$	-	4.15	4.48
4.	1-Methyl-3-(1-methylethyl)-benzene	$C_{10}H_{14}$	1010	4.43	2.20
5.	Limonene	$C_{10}H_{16}$	-	4.48	2.46
6.	Eucalyptol	$C_{10}H_{18}O$	1030	4.55	4.31
7.	9,10-Methanoanthracen-11-ol,9,10-dihydro-9,10,11-trimethyl	$C_{18}H_{18}O$	-	5.46	5.31
8.	Dodecanal	$C_{12}H_{24}O$	-	9.40	2.06
9.	Eicosane	$C_{20}H_{42}$	-	10.34	1.62
10.	2,4-Di-tert-butylphenol	$C_{14}H_{22}O$	-	10.64	20.40
11.	Dodecanoic acid	$C_{12}H_{24}O_2$	1580	11.17	1.75
12.	Octacosane	$C_{28}H_{58}$	-	12.56	2.31
13.	Hexacosane	$C_{26}H_{54}$	-	12.98	1.81
14.	Docosane	$C_{22}H_{46}$	-	14.55	2.45
15.	Pentacosane	$C_{25}H_{52}$	-	14.92	4.79
16.	1-Hexadecanethiol	$C_{16}H_{34}S$	-	15.42	1.75
17.	1,2-Benzenedicarboxylic acid, bis(2-propylpentyl) ester	$C_{24}H_{38}O_4$	-	15.61	3.15
18.	Eicosane	$C_{20}H_{42}$	-	16.52	1.61
19.	Carbonic acid, eicosyl vinyl ester	$C_{23}H_{44}O_3$		16.88	1.86
20.	Octacosane	$C_{28}H_{58}$	-	17.00	1.81
21.	Sulfurous acid, 2-ethylhexyl hexyl ester	$C_{14}H_{30}O_3S$	-	17.27	1.60
	Total				**100**

Table 2: Constituents with top-ranked binding energies compared to standard drug

S/N	Molecules	Binding energy(kcal/mol)
1.	Albendazole	-6.7578
2.	Octacosane	-9.3733
3.	Hexacosane	-9.1402
4.	Carbonic acid, eicosyl vinyl ester	-8.9437
5.	1,2-Benzenedicarboxylic acid, bis(2propylpentyl) ester	-8.8271

6.	Pentacosane	-8.7618

Table 3: Protein-Ligand interaction between target protein and tested ligands

Ligand	Hydrogen Bond Interactions	Hydrophobic Interactions	Key Residues Involved	Binding Characteristics
Albendazole (Standard)	2 (ILE-10A: 2.78 Å, ILE-114A: 2.15 Å)	4 (ILE-19A, LYS-57A, VAL-58A, TYR-120A)	Polar+ hydrophobic residues	Strong and specific binding due to combined hydrogen bonds and hydrophobic stabilization.
Octacosane	None	8 (ALA-12A, ILE-19A, PHE-36A, LYS-57A, VAL-58A, LYS-79A, LEU-122A, VAL-145A)	Predominantly hydrophobic residues	Extensive hydrophobic interactions, stable fit but lacks polar specificity.
Hexacosane	None	6 (ALA-12A, PHE-36A ×3, LEU-69A, VAL-145A)	PHE-36A (repeated), VAL-145A	Hydrophobic-driven stabilization, less versatile than octacosane.
Carbonic acid, eicosyl vinyl ester	None	4 (PHE-36A, LYS-57A, LEU-77A, LYS-79A)	Non-polar and basic residues	Stable hydrophobic binding but less extensive than hydrocarbons.
1,2-Benzenedicarboxylic acid, bis(2-propylpentyl) ester	None	10 (ALA-12A, ILE-19A, PHE-36A ×2, LYS-57A ×2, ILE-62A, LEU-69A, VAL-145A ×2)	Multiple hydrophobic residues	Highest number of hydrophobic contacts, suggesting strongest binding among phytochemicals.
Pentacosane	None	6 (PHE-36A, LYS-57A, LEU-77A, LYS-79A, GLU-118A, VAL-145A)	Hydrophobic + GLU-118A	Moderate hydrophobic stabilization, similar to hexacosane.

Table 4: Drug-likeness Predictions of Selected Compounds Computed by SwissADME

S/N	Chemical formular	Molecular weight (g/mol)	TPSA (Å²)	LogP (Consensus)	GI Absorption	BBB Permeant	P-gp substrate	Lipinski violation
1	$C_{12}H_{15}N_3O_2S$	265.33	92.31	2.29	High	No	No	0
2	$C_{28}H_{58}$	394.76	0.00	10.81	Low	No	Yes	1
3	$C_{26}H_{54}$	366.71	0.00	10.09	Low	No	Yes	1
4	$C_{23}H_{44}O_3$	368.59	35.53	7.73	Low	No	No	1
5	$C_{24}H_{38}O_4$	390.56	52.60	6.16	High	No	No	1
6	$C_{25}H_{52}$	352.68	0.00	9.72	Low	No	Yes	1

Table 5: Ferric Reducing Antioxidant Power (FRAP) Assay of Parkia biglobosastem bark essential oil

Concentration mg/ml	Blank	Absorbance sample	Percentage average
25	0.268	0.260	
50	0.268	0.535	23.21

75	0.268	15.1816
100	0.268	31.2391

Table 6: DPPH Radical Scavenging Assay of Parkia biglobosastem essential oil

Concentration mg/ml	Blank	Absorbance sample	Inhibition percentage
25	1.180	1.029	12.80
50	1.180	1.032	12.54
75	1.180	1.019	13.64
100	1.180	1.009	14.49

Table 7: ABTS [2,2'-azino - bis (3-ethylbenzothiazoline-6-sulfonic acid)] Scavenging activityof Parkia biglobosa stem Essential Oil

Concentration mg/ml	Blank	Absorbance sample	Inhibition percentage
25	1.337	0.214	83.99
50	1.337	0.216	83.84
75	1.337	0.162	87.88
100	1.337	0.115	91.40
Percentage Average			**86.78**

Table 8: Ferric Reducing Antioxidant Power (FRAP) Assay of Parkia biglobosaroot Extract

Concentration mg/ml	Blank	Absorbance sample	Percentage Average
25	0.268	0.268	
50	0.268	0.356	18.22
75	0.268	15.6487	
100	0.268	20.7871	

Table 9: DPPH Radical Scavenging Assay of Parkia biglobosastem Extract

Concentration mg/ml	Blank	Absorbance sample	Percentage Average
25	0.268	0.268	
50	0.268	0.356	18.22
75	0.268	15.6487	
100	0.268	20.7871	

Table 10: ABTS [2,2'-azino-bis (3-ethylbenzothiazoline-6-sulfonic acid)] Scavenging activityof Parkia biglobosa stem Extract

Concentration mg/ml	Blank	Absorbance sample	Inhibition percentage
25	1.780	1.334	25.06
50	1.780	1.121	37.02

75	1.780	1.003	43.65
100	1.780	0.971	45.45
Percentage Average			**37.80**

3.2 Discussion

3.2.1 Essential Oil

From Table 1 above, the most abundant compound detected from the GC-MS analysis was 2-amino-6-methylbenzoic acid (29.82%), an aromatic carboxylic acid derivative. Aromatic acids and related nitrogen-containing derivatives are known to contribute to antimicrobial and pharmacological properties in plant extracts (Akpuaka et al.,2013). Another highly abundant constituent was 2,4-di-tert-butylphenol (20.40%), a phenolic antioxidant commonly reported in essential oils and plant-derived fractions. This compound has been documented to exhibit strong antioxidant, antimicrobial, and anti-inflammatory activities (Gao et al., 2011). The high proportions of these two compounds suggest that they may account for much of the extract's potential bioactivity.

3.2.2 Molecular docking result

The molecular docking study provided insights into the binding affinities of phyto-constituents identified from Parkia biglobosa stem extract in comparison with the standard drug albendazole. Binding energy values (ΔG) are critical indicators of the strength and stability of ligand–protein interactions, with more negative values reflecting stronger binding potential.

Among the analyzed molecules as shown in Table 2 above, long-chain alkanes such as Octacosane (–9.3733 kcal/mol), Hexacosane (–9.1402 kcal/mol), Docosane (–8.5759 kcal/mol), and Pentacosane (–8.7618 kcal/mol) exhibited the highest binding affinities, surpassing the reference albendazole (–6.7578 kcal/mol). Similarly, Carbonic acid, eicosyl vinyl ester (–8.9437 kcal/mol) and 1,2-Benzenedicarboxylic acid, bis(2-propylpentyl) ester (–8.8271 kcal/mol) also demonstrated strong binding interactions, suggesting that they may contribute significantly to the bioactivity of the extract.

3.2.3 Protein-Ligand interaction profile

The protein-ligand interaction results from Table 3 highlight the nature of interactions between the target protein and the tested ligands (Albendazole and selected phytochemicals). The interactions involve both hydrogen bondingandhydrophobic contacts, which are critical for stabilizing ligand binding within the protein active site as shown in figure 4.2 above.

3.2.4 UCSF Chimera

Molecular docking using UCSF Chimera revealed that Albendazole (Figure 3), the standard drug, formed stable hydrogen bond and hydrophobic interactions with the protein (8E4F) active site, serving as a reference. Among the phytochemicals, Octacosane, Hexacosane, and Pentacosane (Figure 4–8) mainly showed hydrophobic interactions due to their hydrocarbon chains, suggesting weaker binding affinity. In contrast, Carbonic acid, eicosyl vinyl ester and 1,2-benzenedicarboxylic acid ester exhibited stronger interactions through polar and aromatic groups, indicating better potential activity. Overall, the results suggest that the polar and aromatic constituents of Parkia biglobosa essential oil may contribute more significantly to bioactivity than the straight-chain hydrocarbons, which aligns with earlier reports on plant-derived bioactive compounds (Kumar et al., 2021; Zaki et al., 2022).

3.2.5 ADME Prediction and Pharmacological Evaluation

The predicted properties of the tested compounds are summarized in Table 4, and their distribution in the BOILED-Egg model is illustrated in Figure 1 above. The diagram represents the BOILED-Egg predictive model, which is widely applied in drug discovery to evaluate the likelihood of compounds being absorbed in the gastrointestinal tract and/or crossing the blood–brain barrier (BBB). The two

descriptors plotted are WLOGP (lipophilicity, y-axis) and Topological Polar Surface Area (TPSA, x-axis), both of which strongly influence molecular pharmacokinetics.
The yellow region corresponds to the BBB-permeable space, indicating compounds that are likely to cross into the central nervous system. The white region represents the optimal space for human intestinalabsorption (HIA), highlighting compounds expected to show favorable oral bioavailability. Each molecule is plotted as a circle, with the outline color denoting P-glycoprotein (P-gp) interaction:
Red outline (PGP-) indicates molecules that are not substrates of P-gp, meaning they are not actively effluxed from cells. Blue outline (PGP+), which does not appear here, would denote molecules that are subject to P-gp efflux, potentially lowering absorption or distribution.
significantly reduce its potential as a drug candidate.

The Boiled-Egg model demonstrates that Molecule 5 is a strong candidate for CNS-active drug design, while Molecule 1 has potential for systemic (non-CNS) applications with good intestinal absorption. The four out-of-range compounds highlight possible limitations in bioavailability, requiring optimization.

3.2.6 FRAP Assay of Parkia biglobosa Stem Extract vs. Essential Oil

The ferric reducing antioxidant power (FRAP) of Parkia biglobosa stem extract and essential oil is illustrated in Figure 9. Both samples exhibited relatively low and inconsistent percentage values compared to the ABTS and DPPH assays. The stem extract recorded 18.22% inhibition at 50 mg/ml, with no substantial activity at other concentrations, while the essential oil showed 23.21% inhibition at 50 mg/ml, also with weak or negligible values across the remaining concentrations.

These results suggest that neither the stem extract nor the essential oil demonstrated strong ferric reducing ability under the tested conditions.

3.2.7 DPPH Radical Scavenging Assay of Parkia biglobosa Stem Extract vs. Essential Oil

As shown in Figure 10, the stem essential oil showed consistently low inhibition values (12.80 –14.49%) across concentrations, indicating relatively weak radical scavenging potential in the DPPH system. In contrast, the stem extract displayed variable activity, with very low inhibition at 50–75 mg/ml (3.61% and 0.92%, respectively), but a sharp increase to 95.28% inhibition at 100 mg/ml. This suggests that the antioxidant effect of the extract may be concentration-dependent, becoming highly active at higher doses, whereas the oil remains weak in this assay.

These results highlight that the DPPH assay response differs from the ABTS assay, where the oil was dominant. Such differences are often attributed to the polarity of antioxidant compounds and the solubility of radicals in the assay medium (Molyneux et al. 2004; Prior et al., 2005). Hence, while the essential oil performed better in the ABTS assay, the extract demonstrated stronger radical scavenging activity in the DPPH assay at higher concentrations.

3.2.8 ABTS Scavenging Activity of Parkia biglobosa Stem Extract and Essential Oil

The bar chart (Figure 2) compares the average percentage inhibition of Parkia biglobosa stem extract and essential oil in the ABTS assay. The results show that the stem extract exhibited a moderate antioxidant activity with 37.80% average inhibition, while the essential oil displayed a significantly higher activity with 86.78% average inhibition. This suggests that the essential oil contains more potent or higher concentrations of radical-scavenging phytochemicals compared to the crude extract.

These findings are consistent with studies where essential oils, rich in monoterpenes and phenolic compounds, generally demonstrate stronger ABTS radical scavenging activities than polar extracts (Brand-Williams et al., 1995; Re et al., 1999). Thus, the essential oil of Parkia biglobosa shows greater potential as a natural antioxidant source compared to its stem extract.

4. CONCLUSION

This study demonstrated that *Parkia biglobosa* stem harbors diverse phytochemicals with significant pharmacological potential against lymphatic filariasis. Virtual screening revealed that long-chain hydrocarbons and ester derivatives exhibited stronger binding affinities to the filarial protein 8E4F than

albendazole, the current standard drug. Interaction profiling highlighted the predominance of hydrophobic contacts, while ADMET analysis identified a subset of compounds with acceptable oral bioavailability and drug-likeness. Additionally, antioxidant assays confirmed the therapeutic relevance of the plant by demonstrating free radical scavenging activity. Collectively, these findings validate the ethnomedicinal use of *Parkia biglobosa* stem bark and provide a computational basis for the development of novel anti-filarial agents. Future work should focus on in vitro validation, toxicity studies, and structural optimization of the lead compounds to enhance their efficacy and pharmacokinetic properties.

5. RECOMMENDATIONS

The promising phytochemicals identified in *Parkia biglobosa* stem bark through docking and ADMET predictions should be isolated and subjected to laboratory-based in vitro and in vivo studies to confirm their anti-filarial efficacy and safety.

Compounds such as octacosane, hexacosane, pentacosane, and ester derivatives with strong binding affinities should undergo structural modifications to reduce excessive lipophilicity and improve solubility for enhanced pharmacological performance.

Since albendazole remains a standard treatment, combined therapy with *Parkia biglobosa* phytochemicals should be investigated to evaluate potential synergistic effects, reduced drug resistance, and minimized side effects.

Comprehensive toxicological studies are needed to evaluate long-term safety, potential mutagenicity, and cytotoxicity of the bioactive compounds before clinical applications.

Variations in phytochemical composition due to geography, season, or extraction methods should be addressed by developing standardized extraction protocols to ensure reproducibility and therapeutic consistency.

The identified compounds should be incorporated into larger virtual screening and cheminformatics pipelines, exploring derivatives and analogues that may yield more potent anti-filarial candidates.

Government and research institutions should support phytomedicine research on *Parkia biglobosa* and other African medicinal plants, as they provide cost-effective and culturally acceptable alternatives for managing neglected tropical disease.

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