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Research Article

Molecular interactions of Gas Chromatography – Mass Spectrometry (GC-MS) and HPLC Characterization of *Alstonia Boonei* and *Ficus Exasperata* Leaves Methanol Extracts

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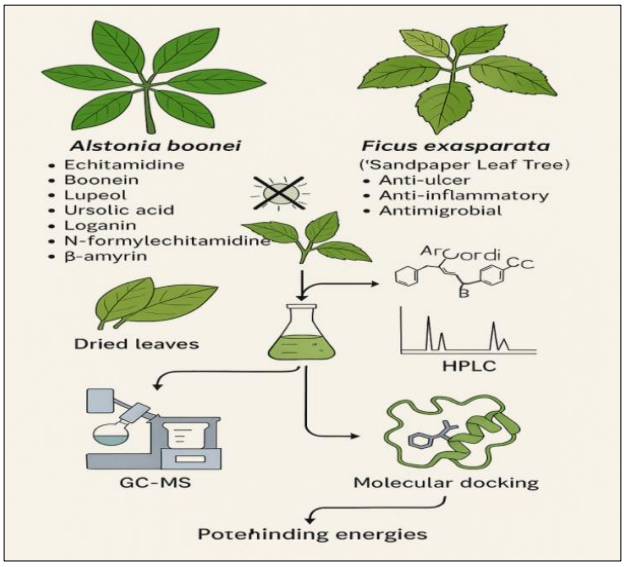
Abstract: *Alstonia boonei* is a well-known plant whose components are high in bioactive chemicals such echitamidine, boonein, lupeol, ursolic acid, loganin, N- formylechitamidine and b-amyrin, with triterpenoids and alkaloids accounting for a large fraction of the total bioactive compound while *Ficus exasperata Vahl. (F. exasperata*) sometimes known as "Sandpaper Leaf Tree" because of the coarse surface of its leaves, is utilized for the management of various diseases, and as a result, research supporting traditional uses are expanding According to reports, *F. exasperata* leaves have anti-ulcer, oxytocin inhibiting, anticonvulsant, antinociceptive, antipyretic, anti-inflammatory, antimicrobial, anxiolytic, hypolipidemic, anti-candidal, insecticidal, hypoglycemic, and pesticidal propertie. The leave of *Ficus exasperata'* and *Alstonia boonei* were dried in a laboratory environment devoid of direct sunlight till completely dry, after which they were extratec using methanol and then rotaroy evaporated to collect the extracts. Both the GC-MS and HPLC analyses revealed the presence of some biochemically useful hydrocarbons while the molecular docking results revealed the potential usefulness of some of these compounds as medicinal compounds as a result of the binding energies.

Keywords: Gas chromatography, molecular interaction, Ficus, Astonia, methanol

Graphical Abstract



Graphical Abstract Description

The graphical abstract visually summarizes the core findings of this study. It illustrates the experimental design, showing the process from pre-test through post-test outcomes. Using simple icons and directional arrows, the diagram highlights the advanced analytical tools for predictive prescriptive models that significantly boost research efficiently.

1. Introduction

Humans have relied on plants for survival throughout history. Due to its structural features, it may be used as a primary food source, as well as a building material and weapon. It can also be used as a source of medication[1]. *Ficus exasperata Vahl.* (*F. exasperata*) sometimes known as "Sandpaper Leaf Tree" because of the coarse surface of its leaves, is utilized for the management of various diseases, and as a result, research supporting traditional uses are expanding [2]. According to reports, *F. exasperata* leaves have anti-

ulcer, oxytocin inhibiting, anticonvulsant, antinociceptive, antipyretic, anti-inflammatory, antimicrobial, anxiolytic, hypolipidemic, anti-candidal, nsecticidal, hypoglycemic, and pesticidal properties [3], [4], [5]. *Alstonia boonei* (*A. boonei*) is a well-known plant whose components are high in bioactive chemicals such echitamidine, boonein, lupeol, ursolic acid, loganin, N- formylechitamidine and b-amyrin, with triterpenoids and alkaloids accounting for a large fraction of the total bioactive compound [6]. The specific objective of this research was to analyze and characterize the composition of crude methanol leaf extract using GC-MS and HPLC.

1.1 Objective of the study

The objectives of this research were to analyze the qualitative and quantitative phytochemical constituents of the crude methanol leaf extract of *F. exasperata and A. boonei* and to analyze and characterize the composition of crude methanol leaf extract using GC-MS and HPLC as well as the molecular interactions of some compounds

1.2 Organization

This article is organized into the following sections: Section 1 presents the introduction and objective of the study. Section 2 provides a review of related work and literature. Section 3 outlines the methodologies

2. Related Work

Almost every early drug discovery came from the natural product sciences [7[. Most countries have used herbal medicines for treatment since ancient times and continue to do so now [8]. Plant-based traditional medical approaches, as well as a decade of beliefs and observations, have shaped the evolution of contemporary medicine [9]. As a result, *A. boonie* has been added to the African Pharmacopoeia as an anti-malaria medication [10]. A cold infusion of *Alstonia* bark extract is administered orally to children to treat round worm, thread worm, and other intestinal parasites [11]. Because of the rough surface of its leaves, *F. exasperata* Vahl., commonly known as the "Sandpaper Leaf tree," is increasingly being utilized for a variety of diseases, and as a result, research supporting traditional claims are emerging [12]. Infusions of the leaves are used to treat gastrointestinal issues in Guinea. Coughs, ulcers, colics, anxiety disorders, epileptic seizures, hypertension, arthritis, arthritis, cancer, intestinal discomfort, and wounds are all treated with the leaves [13].

3. Methodology

3.1 Materials:

Ficus exasperata and *Alstonia boonei* leaves were obtained from various locations around the University of Benin in Benin, Nigeria. Dr. Henry Adewale Akinobosun of the University of Benin's in PBB Department identified the leaves with the voucher numbers $UBHF_{319}$ and $UBHA_{319}$, respectively. The leaves were then washed and dried.

3.2 Preparation of Plant Extract:

Ficus exasperata' and *Alstonia boonei* leaves were shade dried till completely dry. The dried leaf samples were grinded into powdered specimens and kept in an airtight container. At room temperature, a known amount of powdered plant samples was extracted in known quantities of 100% methanol for seventy two hours. The sample mixtures were filtered using Whatman filter paper (No. 1) and the filtrate was evaporated to dryness using a rotary evaporator. The final yield was kept in an airtight container and stored in the refrigerator at 4 degrees Celsius.

3.3 Gas Chromatography-Mass Spectrometry (GC-MS) Analysis:

The methyl esters of plant extracts were analyzed using a GC-MS-TQQQ instrument with a column measuring 30 mm x 250 m x 0.25 m including helium being the mobile phase. The analyte volume, 1µl and set pressure was 10.97 pounds per square inch (psi). The oven was preheated for 0.5 minutes before being left at 70°C incubated for 5 minutes. The total runtime lasted 73 minutes period. The MS transfer tube was kept at 325 degrees celsius. The electron ionization mode was used with a source temperature of 250^{o}C and a 70eV ionization energy. The starting mass was 20 amu while the end mass was 650amu for the scan time in 200 ms, The total Ion Count (TIC) of the system was used for evaluation of the compound(s) identification. The compounds and thier spectra were synchromized in line with the data base of the NIST R.S. L, with a Match Factor (MF) of ≥ 700 being satisfactory. The peak area of the GC was utilized for the estimation of the relative percentage of the chemicals detected.

3.4 High Performance Liquid Chromatography (HPLC) Screening:

The Method employed was HPLC with UV Detector. The Column is the uBondapak C18 (µBondapak C18 columns are general purpose, silica-based, reversed-phase C18 columns that are based on 10 µm particle technology). The Carrier was Acetonitrile/Water in ratio 70:30. 10g sample was extracted with acetonitrile, extract was stabilized with ethyl acetate and made up to 25ml in standard flask. 5ul injected

3.5 Molecular docking experiments to determine binding affinities:

Molecular docking calculations were performed using Autodock Vina [14]. The modelled structure of APC and Kras and elucidated compounds were loaded into the *AutoDock Vina software*, and docking parameters were retrieved from the log. *File*. The various ligand conformations were viewed using the *Discovery Studio software* and snapshots were taken using the *Windows 10 snipping tools*.

4. Results and Discussion

The Total Ion Chromatogram (TIC) and the various components of *Alstonia boonei* leaves that were identified

using GC-MS (Gas Chromatography – Mass Spectrometry are shown in figure 4.1 and Table 4.4 respectively. The pharmacological functions, properties as well as structures (figure 4.2) of some of the identified compounds were also stated.

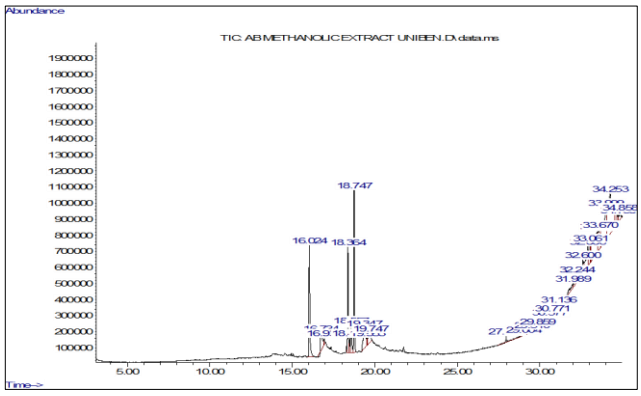


Figure 1: TIC (Total Ion Chromatogram) of Methanol extract of *Alstonia boonei* leaves using GC-MS

The result from the profiling shows that a total of ten compounds were identified. These includes Hexadecanoic acid, methyl ester, n-Hexadecanoic acid, Octadecanoic acid; (5) trans-13-Octadecenoate, Phytol, Methylated stearate, Oleic Acid, cis-11 Octadecenoic acid, Eicosanoate.

Table 1. List of identified phytocompounds of methanol leaf extract of *Alstonia boonei* using GC-MS

Compound	**Formula**	**Mol.W (g/mol)**	**R.T (Min)**	**Area (%)**
Hexadecanoic acid, methyl ester	$C_{17}H_{34}O_2$	270	15.99	8.41
n-Hexadecanoic acid	$C_{6}H_{32}O_2$	256	16.70	29.33
9-Octadecenoic acid, methyl ester	$C_{19}H_{36}O_2$	296.5	18.37	5.45
Methyl stearate	$C_{19}H_{38}O_2$	298.5	18.76	9.72
Oleic acid	$C_{18}H_{34}O_2$	282	19.16	18.95
Octadecanoic acid	$CC_{18}H_{36}O_2$	284	19.55	28.14

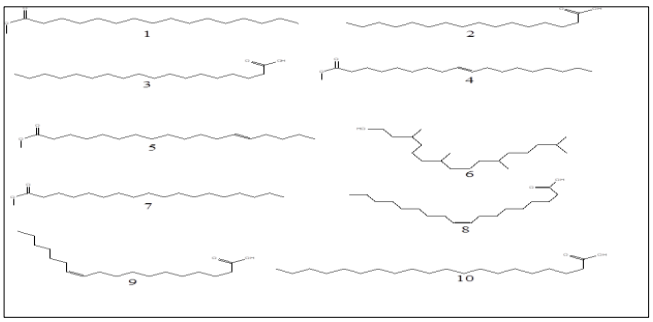


Figure 2: Structure of compounds identified from methanol extract of *A. boonei leaf*:

(1) Hexadecanoic acid, methyl ester; (2) n-Hexadecanoic acid; (3) Octadecanoic acid; (4) 9-Octadecenoic acid, methyl ester; (5) trans-13-Octadecenoic acid, methyl ester; (6) Phytol; (7) Methyl stearate; (8) Oleic Acid; (9) cis-11 Octadecenoic acid; (10) Eicosanoic acid

The Total Ion Chromatogram (TIC) and the various components of *Ficus exasperata* leaves that were identified using GC-MS (Gas Chromatography – Mass Spectrometry are shown in figure 4.3 and Table 4.5 respectively. The pharmacological functions, properties as well as structures (figure 4.4) of some of the identified compounds were also stated.

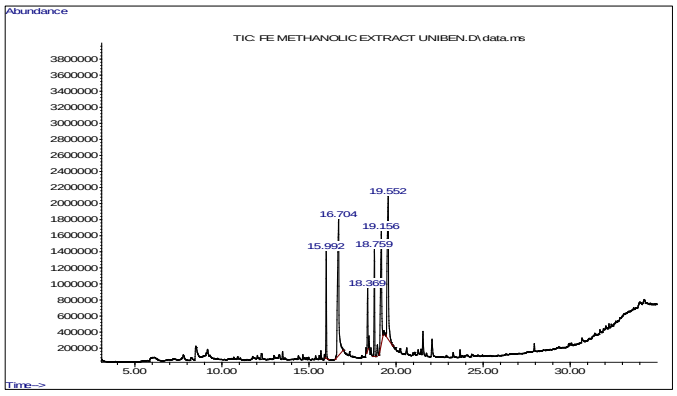


Figure 3: TIC (Total Ion Chromatogram) of Methanol extract of *Ficus exasperata* leaves using GC-MS

The result from the profiling shows that a total of six compounds were identified. These includes Hexadecanoic acid, methyl ester, n-Hexadecanoic acid, 9-Octadecenoic acid, methyl ester, Methyl stearate, Oleic Acid and Octadecanoic acid were identified.

Table 2: List of Identified phytocompounds of methanolic leaf extract of *Ficus exasperata* using G.C-M.S

Compound	**Formula**	**Mol.Wt (g/mol)**	**R.T (Min)**	**Area (%)**
Hexadecanoic acid, methyl ester	$C_{17}H_{34}O_2$	270	16.02	8.92
n-Hexadecanoic acid	$C_{6}H_{32}O_2$	256	16.74	2.41
Octadecanoic acid	$C_{18}H_{36}O_2$	284	16.93	0.59
9-Octadecenoic acid, methyl ester	$C_{19}H_{36}O_2$	296.5	18.36	6.32
trans-13-Octadecenoic acid, methyl ester	$C_{19}H_{36}O_2$	296.5	18.46	1.04
Phytol	$C_{20}H_{40}O$	296.5	18.56	2.40
Methyl stearate	$C_{19}H_{38}O_2$	298.5	18.75	9.84
Oleic Acid	$C_{18}H_{34}O_2$	282	19.35	3.75
cis-11 Octadecenoic acid	$C_{18}H_{34}O_2$	282.5	19.55	0.64

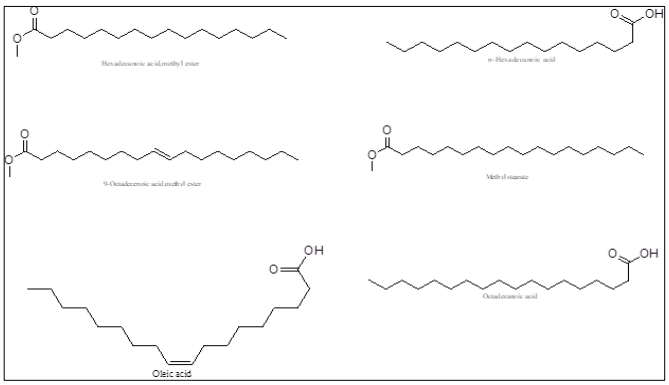


Figure 4: Structure of compounds identified from methanol leaf extract of *F. exasperata*

(1) Hexadecanoic acid, methyl ester; (2) n-Hexadecanoic acid; (3) 9-Octadecenoic acid, methyl ester; (4) Methyl stearate; (5) Oleic Acid (6) Octadecanoic acid

High Performance Liquid Chromatography (HPLC) Characterization of Methanol Leaf Extracts of *Alstonia Boonei* and *Ficus Exasperata*

The HPLC-fingerprint and secondary metabolites identified from methanol leaf extract of *A. boonei* are shown in figure 5 and table 3 respectively. The pharmacological functions, properties as well as structures of some of the identified compounds were also stated.

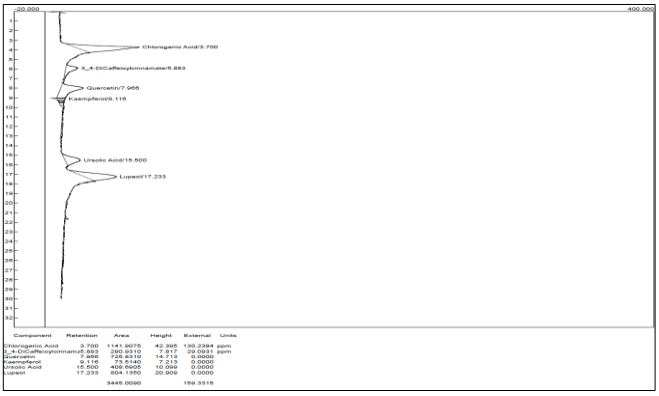
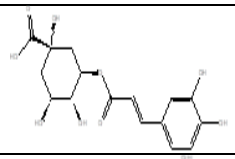
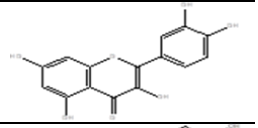
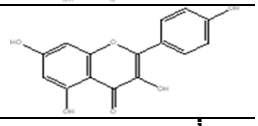
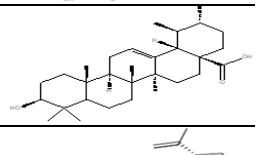
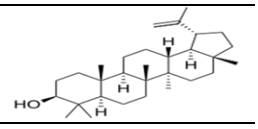


Figure 5: HPLC Fingerprint of methanol leaf extract of *A. boonei* The fingerprint shows that a total of five compounds namely chlorogenic acid, quercetin, kaempferol, ursolic acid and lupeol were identified

Table 3: Secondary metabolites identified from methanol extract of *A. boonei* leaf using HPLC

Name of Compound	Mol. Formular	MW (g/mol)	Structure
Chlorogenic acid	$C_{16}H_{18}O_9$	354.3	
Quercetin	$C_{15}H_{10}O_7$	302.22	
Kaempferol	$C_{15}H_{10}O_6$	286.2	
Ursolic acid	$C_{30}H_{48}O_3$	456.7	
Lupeol	$C_{30}H_{50}O$	426.7	

The HPLC-fingerprint and secondary metabolites identified from methanol leaf extract of *Ficus exasperata* are shown in figure 6 and table 4 respectively. The pharmacological functions, properties as well as structures of some of the identified compounds were also stated.

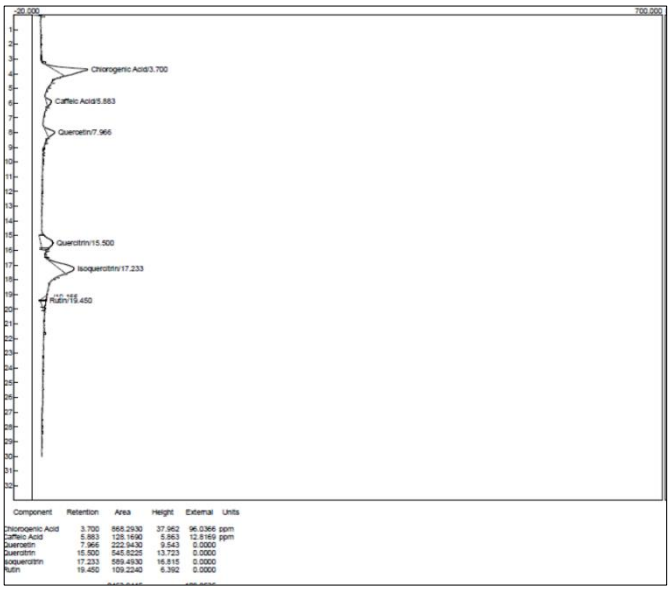
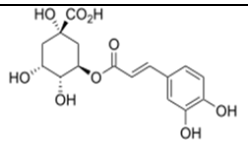
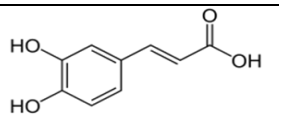
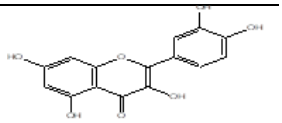
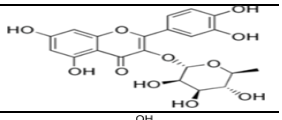
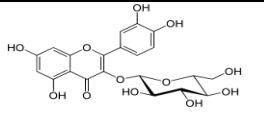
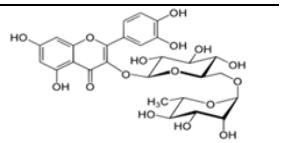
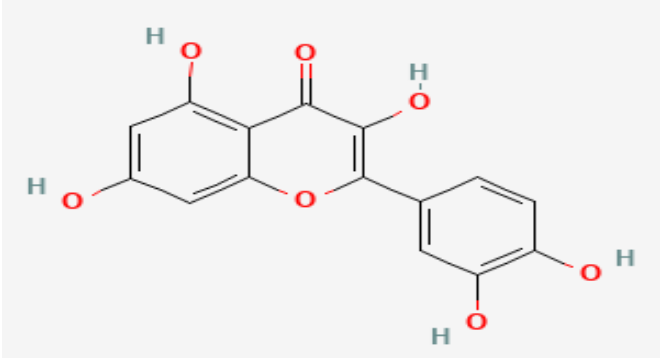


Figure 6: HPLC Fingerprint of methanol leaf extract of *F. exasperata* The fingerprint shows that a total of six compounds namely chlorogenic acid, caffeic acid, quercetin, quercitrin, isoquercitrin and rutin were identified

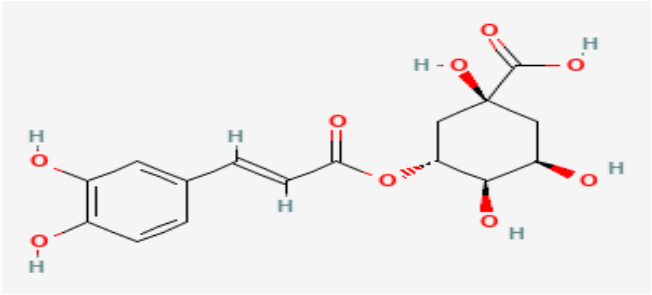
Table 4: Secondary metabolites identified from methanol extract of *F. exasperata* leaf using HPLC

Name of Compound	Mol. Formula	MW (g/mol)	Structure
Chlorogenic acid	$C_{16}H_{18}O_9$	354.3	
Caffeic acid	$C_9H_8O_4$	180.2	
Quercetin	$C_{15}H_{10}O_7$	302.2	
Quercitrin	$C_{21}H_{20}O_{11}$	448.4	
Isoquercitrin	$C_{21}H_{20}O_{12}$	464.4	
Rutin	$C_{27}H_{30}O_{16}$	610.5	

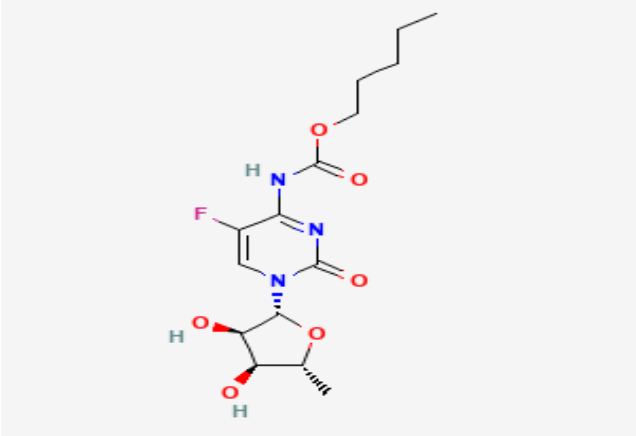
HPLC-Identified Phyto-Compounds and Standard Drugs Used in *In silico* Studies



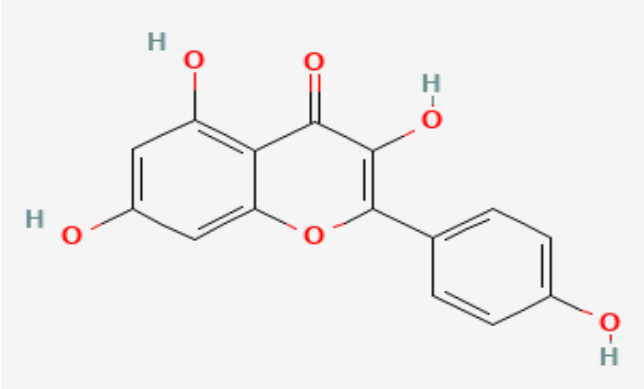
Quercetin ($C_{15}H_{10}O_7$)



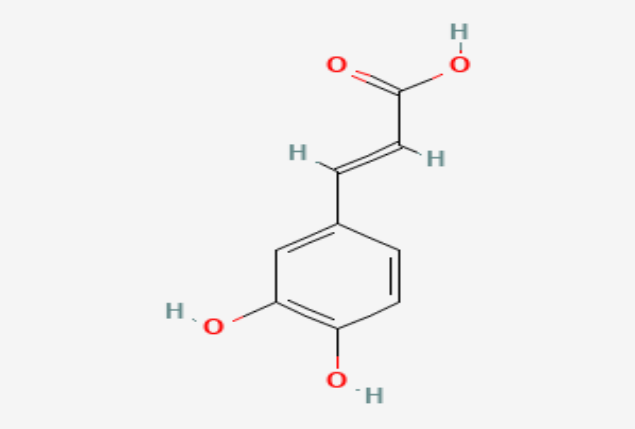
Chlorogenic Acid ($C_{16}H_{18}O_9$)



Capecitabine ($C_{15}H_{22}FN_3O_6$)



Kaempferol ($C_{15}H_{10}O_6$)



Caffeic Acid ($C_9H_8O_4$)

5-Fluorouracil ($C_4H_3FN_2O_2$)

Figure 7. 2D structures of quercetin, kaempferol, chlorogenic acid, caffeic acid, capecitabine and 5-fluorouracil

Molecular Interaction of Phyto-compounds with KRAS and APC Proteins Using Molecular Docking Techniques

The Docking procedure revealed the appropriate positions and orientations that were energetically and geometrically favoured when the pyto-compounds (quercetion, kaempferol, chlorogenic acid and caffeic acid) bound to both KRAS and APC binding site. The strength of the protein-ligand complex is related to the intermolecular interactions between the binding partners and the best proses were selected based on the root mean square deviation (RMSD) and affinity energy. Literature has it that RMSD < 2.0 Å corresponds to good docking solutions while binding energies of -6kcal/mol to -14kcal/mol are considered as a good binding energy for intermolecular interaction. The results has shown in the table 5 and figures below revealed that all the selected chemical constituent in both *A. boonei* and *F. exasperata* showed binding energy ranging from -5.7 kcal/mol to -9.1 kcal/mol and RMSD values of 0.000 (check appendix). The higher negative values is an indication of a high binding interaction of the chemical constituent with the amino acid residues in the binding sites of KRAS and APC thereby forming a stabilized complex. The compounds, quercetin and kaempferol showed the highest binding energy (-9.1 kcal/mol.) with KRAS and this proved that they formed the most stable complex with KRAS when compared to other compounds and standard drugs. The ligand chlorogenic acid showed the highest binding energy (-7.5 kcal/mol.) with APC

and this proved that they formed the most stable complex with APC when compared with other compounds and standard drugs. Also, the results indicated that hydrogen bond from the hydroxyl phenol group and other interactions ranging from van der waal, carbon-hydrogen bond, Pi-Sigma, Pi-Pi stacking etc. contributed significantly to the stability of the ligand-protein complexes.

Table 5: Selected Models Based on Binding Affinity and Ligand-Amino Acid Interactions.

Compound	**Binding Affinity (Kcal/mol) for KRAS**	**Ligand-Amino Acid Interactions**	**Binding Affinity (Kcal/mol) for APC**	**Ligand-Amino Acid Interactions**
Quercetin (Model 1)	-9.1	Ser145, Asp119, Ala146, Lys147, Lys117, Glu31	-7.1	Ser546, Asn550, Thr506, Phe510
Kaempferol (Model 1)	-9.1	Ala146, Phe28, Lys147, Lys117, Ala18	-6.9	Arg549. Asn594, Trp593, Trp553
Chlorogenic Acid (Model 1)	-7.5	Asn116, Lys117, Lys147, Tyr32, Phe28, Ala146, Ala18	-7.5	Trp553, Arg549, Asn594, Ser590, Glu633
Caffeic Acid (Model 1)	-6.8	Gly13, Lys16, Tyr32, Ala18, Glu31	-5.7	Trp593, Ala597
Capecitabine (standard drug) (Model 1)	-7.1	Asp30, Ser17, Tyr32, Lys16	-6.9	Asn550, Gln542, Ser546, Ser587, Arg549, Phe510 Trp553
5-Fluorouracil (standard drug) (Model 1)	-7.3	Asp33, Tyr32, Thr35, Lys16, Val29, Lys117, Gly13 Ser17.	-6.0	Ser678, Thr675, His715, Met717, Arg640

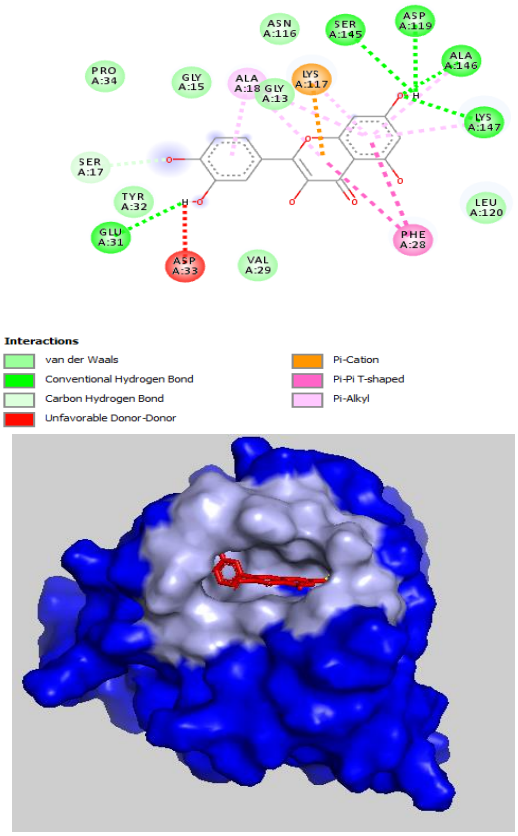


Figure 8: 2D and 3D structure of quercetin illustrating the intermolecular interactions at the binding site of KRAS

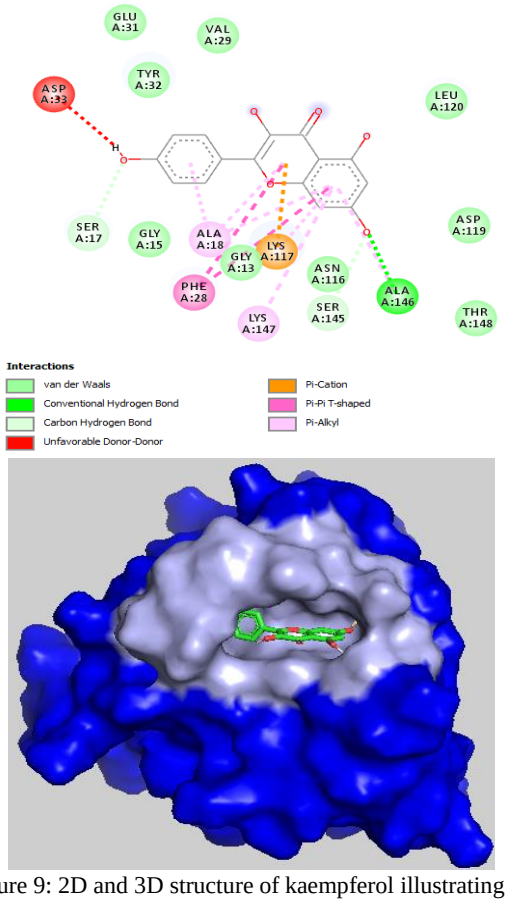


Figure 9: 2D and 3D structure of kaempferol illustrating the intermolecular interactions at the binding site of KRAS

When the pytocompounds (quercetion, kaempferol, chlorogenic acid, and caffeic acid) were docked to the binding site of both KRAS and APC proteins, the docking process revealed the optimal locations and orientations that were energetically and geometrically preferred. The strength of the protein-ligand complex is proportional to the intermolecular interactions between the binding partners, and the best candidates were based purely on the root mean square deviation (RMSD) and affinity energy [15]. According to the literature, RMSD 2.0 correlates to good docking solutions [16], whereas binding energies ranging from -6kcal/mol to -14kcal/mol are regarded good binding energies for intermolecular interaction [17]. According to the findings of this investigation, all of the selected phytoconstituents in both plants had binding energies ranging from -5.7 kcal/mol to -9.1 kcal/mol with RMSD values of 0.000. The higher the negative value, the stronger the phytoconstituent's binding affinity with the residues of amino acids in the binding sites of KRAS and APC proteins, generating a stable complex. When compared to other compounds, the ligands quercetin and kaempferol had the highest binding energy (-9.1 kcal/mol.) with KRAS, indicating that they formed the most stable complex with KRAS. When compared to other compounds, chlorogenic acid had the highest binding energy (-7.5 kcal/mol.) with the APC protein, indicating that it formed the most stable complex with the protein. The hydrogen bond from the hydroxyl phenol group, as well as additional interactions such as van der waal, carbon-hydrogen bond, Pi-Sigma, Pi-Pi stacking, and so on, were found to contribute significantly to the stability of the ligand-protein complexes. All of the phytoconstituents examined reacted strongly with the corresponding protein motifs and are likely to be useful as DMH antagonists. This observed high binding energies obtained during molecular docking which is higher than that of the standard drugs (5-Flouracil and Capecitabine) would be due to the strong hydrophobic interactions between the phytochemical ligands and the protein motifs-APC and kras. The resulting in-silico computational results must be validated by further in vivo and in vitro anticarcinogenic research

5. Conclusion

The current study may have confirmed that the methanol leaf extracts of *A. boonei* and *F. exasperata* could contain beneficial phyto-constituents with antioxidant capabilities and are relatively safe when used at the prescribed level. The existence of polyphenolic and phenolic acid substances such as quercetin, kaempferol, chlorogenic acid, and caffeic acid, as well as other pharmacologically beneficial chemicals with therapeutic qualities thus enhanced their viabilities and use as medicinal plants.

Author's Statements Disclosures: The authors declare that the study is original, has not been submitted elsewhere, and is accurate to the best of their knowledge. No part of this manuscript has been plagiarized, and all sources of data have been appropriately credited.

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