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Antibacterial Potential and Molecular Docking Analysis of Phytochemicals from Moringa oleifera and Zingiber officinale Against Escherichia coli

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ABSTRACT

Background: Infectious diseases remain a major cause of mortality globally, particularly in developing countries. The increasing resistance of bacteria such as Escherichia coli to conventional antimicrobial agents necessitates the exploration of plant-derived alternatives.

Methods: The antibacterial activities of Moringa oleifera leaves and Zingiber officinale rhizomes were assessed against E. coli isolates using agar well diffusion and broth dilution methods to determine zones of inhibition, minimum inhibitory concentration (MIC), and minimum bactericidal concentration (MBC). In silico molecular docking was performed using Maestro software to evaluate the binding affinity of phytochemicals with key E. coli target proteins, including DNA gyrase B, dihydropteroate synthase, enoyl acyl carrier protein reductase, FIMH adhesin, and ParE topoisomerase IV.

Results: Moringa and ginger extracts showed antibacterial activity at concentrations ≥200 mg/ml, with Moringa exhibiting a stronger effect. MICs were 200 mg/ml for Moringa and 400 mg/ml for Ginger, while MBCs were 400 mg/ml and 800 mg/ml respectively. Docking results revealed high binding affinities of compounds such as Shogasulfonic C, 5-Hydroxyhexahydrocurcumin (ginger), and Quercetin-3-O-malonylglucoside, Rutin, Nicotiflorin, Chlorogenic acid (moringa), suggesting potential interactions with bacterial enzymes involved in replication, adhesion, and metabolism.

Conclusion: The study confirmed the antibacterial potential of Moringa and Ginger extracts against E. coli, supported by both in vitro and molecular docking evidence. These findings support the potential development of plant-based antimicrobials for managing resistant infections.
Keywords: Antibacterial compound, Escherichia coli, Moringa oleifera, molecular docking, Zingiber officinale

1. INTRODUCTION

More than half of all human deaths in tropical nations such as Nigeria are caused by infectious disease such as septicemia, urinary tract infections, neonatal meningitis and so on [1]. E .coli is a normal flora of the human large intestine and normally colonizes an infant's gastrointestinal tract within 40 hours of birth, through food or water. Despite being a normal flora, it is one of the major causative agents for urinary tract infections (UTI) and abdominal diseases [2, 3]. Antibacterial agents that have been used to treat infections are no longer effective as they used to at

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the beginning of the twentieth century [4]. This is because pathogenic organisms, such as E. coli have developed gradual resistance overtime to common antibiotics. Recent studies have confirmed a short life expectancy of novel antimicrobial agents being made owing to the rapid and extensive emergence of resistance. Hence there is a need to search for new natural products from medicinal plants [4]. Plants have been used as valuable sources of natural products for preserving human health and well-being since time immemorial [5]. In turn natural products have been used to treat skin infection, malaria, urinary tract infection, diabetes, wound infection, anemia and so on. Some plants have been indicated by researchers to contain many constituents such as tannins, alkaloids, essential oils, phenols and flavonoids among others which are responsible for various pharmacological activities and could serve as sources for antimicrobial production [6]. Over the last few years, attention has been drawn to the use of "multipurpose'' plants (M. oleifera Lam). M. oleifera is a highly valued plant, found in many tropics and subtropics. It belongs to one of the 14 species of the family Moringaceae, which is native to India, Africa, and Arabia. All parts of Moringa tree are edible and have been utilized by humans for its amazing array of medicinal and high nutritional values [7]. Ginger (Z. officinale) is a perennial herb which grows from underground rhizomes. There are over 90 species of Ginger. The rhizome of ginger is responsible for its characteristic slightly hot, citrus-like taste and it contains medicinal properties. This herb belongs to the family Zingiberaceae. Fresh ginger has been used in the treatment of nausea, asthma, coughs, loss of appetite and rheumatism, fever, swelling, dysentery, diarrhea and soreness. Hence, the medicinal plants highlighted for this study are investigated for possible antibacterial activity on E. coli. This would make a significant contribution to Nigerian traditional medicine [8]. Molecular docking is an important step in identifying novel compounds of therapeutic interest. Molecular docking virtual screening is widely employed and plays a significant role when predicting the binding orientation and affinities of two molecules when bound together to form a stable complex. More so, calculated docking could be in the form of dock score, which is the arithmetic way of estimating the strength of binding between docked compounds once the docking is accomplished [9, 10]. This study extends from in-vitro antibacterial activity of M. oleifera leaves and rhizomes Z. officinale, to molecular docking of compounds in those plants against drug target of E. coli as the test bacteria. The compounds that were isolated from medicinal plants were theoretically studied via docking methods and ligand interactions [9, 11, 12, 13, 14, 15]. The antibacterial activity of the two plants was limited to extraction using ethanol as solvent. The continual emergence of antibiotic resistance in E.coli to existing antimicrobial agents has become a global public health problem, thus posing threats to the effective treatment of E. coli infections and significantly affecting the global economy. This resistance could be attributed to inappropriate use of commercial drugs. Antibiotic resistance also leads to prolonged hospital stay, higher medical costs, and increased mortality. The high cost and undesirable side effects of some conventional drugs is barrier in the effective treatment of infectious diseases. Hence, there is an increased need to search for alternative source of drugs such as medicinal plants which could be used in the treatment of infectious diseases. Without immediate action, a period of time where common infections can again kill would be headed for. Serious food poisoning, urinary tract infections, diarrhea, neonatal meningitis or death can be caused by E. coli. Bacterial infections are usually treated with antimicrobial agents and since resistance has been reported to conventional drugs, it is very important to search for novel drugs. About 80% of individuals from developed countries use conventional medicine, which have compounds derived from medicinal plants. Easy availability, known exhibition of minimum side effects, and cost effectiveness have made it a wonderful source of antimicrobial agents. Much of the current research works have been driven towards obtaining natural antimicrobial molecules from medicinal plants in order to overcome or avoid multi drug resistance [4]. The study aimed at evaluate the in vitro antibacterial activity of the leaves and rhizome extracts of Moringa and Ginger respectively on E. coli, and to validate the use of medicinal plants as potential drug candidates by molecular docking analysis, determine the antibacterial activity of M. oleifera and Z. officinale (Ginger) on Escherichia coli, to compare the antibacterial activities of M. oleifera and Z. officinale with conventional antibiotic, Ciprofloxacin against the selected bacteria, determine the minimum inhibitory and minimum bactericidal concentration of M. oleifera and Z. officinale against the selected bacteria and to determine lead compounds as novel antibacterial agent in the treatment of infections caused by E. coli.

2. MATERIALS AND METHODS

2.1 Materials

2.1.1 Biological Materials

Rhizome, Leaves, Plant extracts, E. coli

2.1.2 Chemical and Reagents

Water, nutrient agar, ciprofloxacin, infusion, MacConkey agar, ethanol, Dimethyl sulphoxide

2.1.3 Equipment and other materials
Refrigerator Mortar and pestle, wooden spoon, airtight containers, knife, oven, Whatman no. 1 filter paper

2.2 Methods
2.2.1 Collection of Samples
The study was conducted in Afe Babalola University Ado-Ekiti, Ekiti State, Nigeria. Ado Ekiti is situated in southwest Nigeria and it is the state capital of Ekiti state. Leaves of M. oleifera were bought from a market in Kaduna state. Rhizomes of ginger used in the study were bought from a market in Ado-Ekiti, Ekiti State.

2.2.2 Ethical Clearance
Ethical approval to carry out this work in Afe Babalola University was sought and obtained from the Ethics and Research Committee of the College of Medicine and Health Sciences of Afe Babalola University Ado-Ekiti, Ekiti State (ABUADHREC/25/05/2023/174).

2.2.3 Collection of Test Organisms
Five isolates of E. coli were collected from the Medical Microbiology Laboratory of Afe Babalola university multisystem teaching hospital, Ado-Ekiti [16]. The bacteria isolates were inoculated in nutrient agar slants then it was transported in sterile condition to the medical laboratory in College of Medicine and Health sciences and preserved in a refrigerator at 40C until it was ready to be used. The conventional antibiotic used in this study was Ciprofloxacin infusion.

2.2.4 Sample Preparation
Healthy and uninfected Moringa leaves were collected. The leaves were washed and cleansed thoroughly under running tap water; air dried for 4 days then oven dried at 600C. With the aid of a mortar and pestle, the dried leaves were homogenized to fine powder. Different sterile airtight containers were used to store the powdered form of the leaves until when needed [17]. Ginger rhizomes were washed to remove debris, peeled and diced using a laboratory knife. On drying trays, they were spread then kept in an oven for 8 days at 600C. The dried samples were grinded with a mortar and pestle before extraction [18].

2.2.5 Confirmation of the Test Organisms
The isolates were sub-cultured on MacConkey agar. After 24 hours incubation at 370C, the isolates were confirmed using cultural, morphological and biochemical characteristics. [19, 20].

2.2.6 Ethanol Extraction of Moringa Leaves and Ginger Rhizomes
Extraction of Moringa leaves and rhizome of ginger were done using maceration method. The 20 grams of dried Moringa leaves was macerated in 200ml of 95% ethanol for 72 hours at room temperature with intermittent shaking. The extract was filtered using Whatman no. 1 filter paper, and the marc (extraction residue) was extracted again using the same method and solvent until the extraction was finished. The ethanol was extracted by placing the filtrate in a hot air oven at 450C until evaporation took place [17, 21]. Ethanolic ginger extract was prepared by dissolving 20 grams of grounded ginger in 400 mls of 95% ethanol and left at room temperature for 72 hours. Filtration was done with the aid of Whatman no. 1 filter paper to obtain a clear solution. The ethanol was extracted by placing the filtrate in a hot air oven at 450C until evaporation took place then stored in a refrigerator until ready for use [22].

2.2.7 Percentage Yield of Extract
The yield of extraction is a measure of how effective a solvent is at extracting specific components from a starting material the extract residue after solvent extraction was weighed, and the percentage was obtained using the following formula:

Yield of extract % = weight of extract recovered×100/ weight of dried powder [23].

2.2.8 Extract Reconstitution
The moringa and ginger extracts were dissolved in Dimethyl sulphoxide (DMSO) after solvent evaporation [17, 18]. Stock solutions of the Z. officinale and M. oleifera extracts were prepared by aseptically weighing 0.8g of the extract and dissolving in 2ml of Dimethyl sulphoxide (DMSO) respectively to make a 40% (400mg/ml) solution. Different

working concentrations (200, 100, 50, 25 mg/ml) of Z. officinale and M. oleifera ethanol extracts were prepared from the stock solution [17, 24].

2.2.9 In-Vitro Antibacterial Assay

2.2.9.1 Preparation of Bacteria Inoculum

Bacteria suspension was prepared and compared with the 0.5McFarland Standard (108 CFU/ml) to matched the required concentration [19].

2.2.9.2 Antibacterial Activity of Moringa and Ginger Using Agar Well Diffusion Method

Agar well diffusion method was used to evaluate the in vitro antibacterial activity of Moringa and Ginger. Muller Hinton agar was poured in sterile petri dishes and allowed to solidify. 1ml of the inoculated peptone water was poured on the solidified agar then was spread all over the surface of the agar using the pour plate method. Each well was filled with 60 microliter of the extracts. The plates were placed on the leveled bench for 30 minutes for pre-diffusion of extract to occur. Ciprofloxacin infusion was used as positive control while DMSO was used as negative control. The plates were incubated aerobically at 370C for 24 hours. Zone of inhibition (mm) was recorded as an indication of sensitivity of the organisms to the extract [25, 26].

2.2.9.3 Determination of Minimum Inhibitory Concentration (MIC)

Minimum Inhibitory Concentration, the lowest concentration of the rhizomes of Z. officinale and M. oleifera leaves extract that inhibited growth of test organisms were determined using the broth dilution method. 8 tubes were set up. 2ml of nutrient broth were also added to each tube except the first tubes which served as the neat, 2ml of each of the various extracts in the different test tubes were added, and serially diluted out to various concentrations ranging from 800 to 6.25mg/ml. A 20µl of each test organism was inoculated into each of the test tubes and incubated at 370C for 24 hours. Lowest concentration of extract to show no growth (turbidity) was recorded as the MIC [19].

2.2.9.4 Minimum Bactericidal Concentration (MBC)

A 20µl of bacterial culture from the first tube after the MIC, the MIC and all tubes before the MIC were sub cultured on to nutrient agar and incubated at 370C for 24 hours. The lowest concentration of the extract that showed no growth was recorded as the MBC [19].

2.2.10 Molecular Docking

Maestro 9.3 (Schrodinger 2018) docking suite was used in ligand preparation, protein preparation, receptor grid formation and ligand docking against different E. coli specific proteins that have been documented as potential and conventional drug targets. The target proteins were selected by searching for proteins either implicated in disease conditions or part of the life cycle of E. coli. The following proteins were used for this work, DNA gyrase B (PDB ID: 6F86), Dihydropteroate synthase (PDB: 1AJ0), Enoyl acyl carrier protein reductase (5CG1), FIMH (PDB: 4XO8), Par E topoisomerase IV (PDB: 1S16), and the crystal structures were downloaded from the protein data bank. The chemical structures of the phytocompounds were obtained from PubChem databases. The files were saved in 2D SDF format. Phytocompounds of M. oleifera and Z. officinale respectively were docked against active sites of the respective proteins. The protein and ligand files were opened on Maestro and the proteins and ligands preparation were done using standard protocol [27].

2.2.10.1 Ligand Selection and Preparation

One hundred and nine and eighty-four phyto-compounds of Moringa and Ginger were used for this study respectively. They were obtained from published literature and used in the generation of a library of compounds. The phyto-compounds for each plant were copied to the project table then prepared using the LigPrep interface in Schrondinger with an OPL3 force field, at neutral pH. Desalt, and tautomers were automatically selected on the ligprep interface and only one stereoisomer of the ligands were generated each. It was necessary to ligand prep in order to convert the 2D structures of the ligands to 3D structures [28].

2.2.10.2 Protein Selection and Preparation

X-ray crystallized three-dimensional structure of the target proteins were retrieved from the protein data bank. A selected protein was copied onto the project table of maestro. It was then highlighted for preparation. The 3D structure was viewed with Maestro interface and prepared using protein preparation wizard. The protein was first preprocessed. Hydrogen was added, and het state was generated during the preprocessed stage. The protein was optimized, water molecules were removed and lastly, the protein was minimized so that it conformed to the maestro suite [28].

2.2.10.3 Glide Grid Preparation
After protein and ligand preparation, the grid was developed. This was carried out with the receptor grid generation tool in maestro which defined the area round the active sites in terms of co-ordinates x, y and z [28].

2.2.10.4 Extraction of Reference Compound
The co-crystalized ligand was extracted to make the active site accessible for new compound. It was also redocked for validation for which the docking score was used to compare the test ligands [28].

2.2.10.5 Ligand Docking
The docking analysis was accomplished using a ligand docking tool on Maestro. The prepared libraries of ligands (phyto-compounds) were docked into the active site of the target proteins. The ligands were treated as flexible while the protein receptors were treated as rigid. The ligand docking was set at extra precision (XP). Docking analysis was carried out on the test and control co-crystallized ligands to search for the best-docked conformation between ligand and protein. The conformation with the most favorable (least) free binding affinity (docking score) was selected for analyzing the interactions between the target receptor and ligands [29, 28].

2.3 Statistical Analysis
Antimicrobial activity of extracts using zone of inhibition assay were measured by mean ± SD. Bar chats were generated using Microsoft Excel. The heat maps were analyzed using GraphPad Prism software version 8

3. RESULTS
3.1 Percentage Yield Extract of Moringa and Ginger
The percentage yield was 20g (11.3%) and 20g (2%) for Moringa and Ginger extracts respectively. M. oleifera leaves had the highest yield compared to that of Ginger.

3.2 In Vitro Antibacterial Activity of Moringa and Ginger
The antibacterial activity of the extracts showed different zones of inhibition. Ethanol extract of Moringa and Ginger inhibited growth respectively only at concentrations of 400mg/ml and 200mg/ml. The results of their activity were shown in Table 1and 2 and Figure 1 and 2 respectively. At concentrations of 100mg/ml and 50mg/ml, no zones of inhibition were observed. The mean zones of inhibition for Moringa leaves ranged from 7.0±0.0 to 15±5.0 mm at 400mg/ml and 4.0±0.0 to 9±0.0 mm at 200 mg/ml, while mean zones of inhibition at 400mg/ml for Ginger rhizomes ranged from 3.0±0.0 to 13±1.0 mm and at 200mg/ml ranged from 4±0.0 to 7.5±1.5 mm against E. coli. M. oleifera showed a better inhibition effect on the growth of E. coli than Z. officinale. Ciprofloxacin inhibited all the bacteria tested.

Table 1: Mean zone of inhibition of Moringa ethanol extract at concentrations of 400 and 200mg/ml respectively and Ciprofloxacin zone of inhibition.

Moringa	400 mg/ml	200 mg/ml	200mg/100ml
Organism	Mean±SD	Mean±SD	CIP
E.coli I	0	0	26
E.coli II	15	8.5	30
E.coli III	12	7.5	34
E.coli IV	10	9	24
E.coli V	7	4	20

Table 2: Mean zones of inhibition for ginger ethanol extract at 400 mg/ml and 200 mg/ml concentrations, compared with ciprofloxacin.

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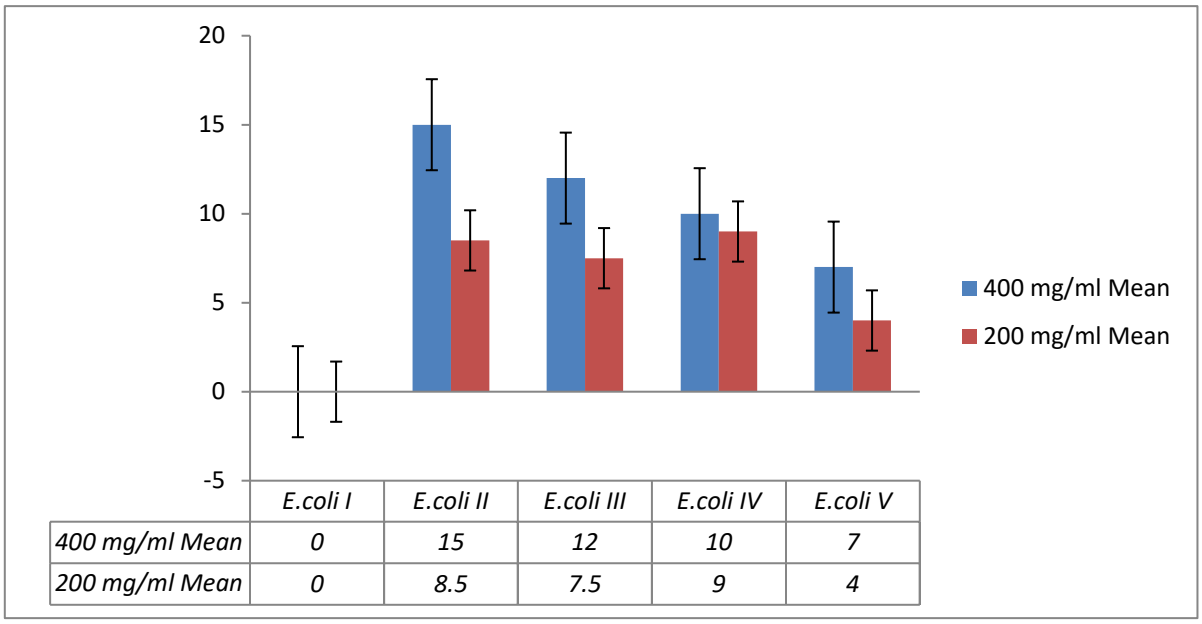
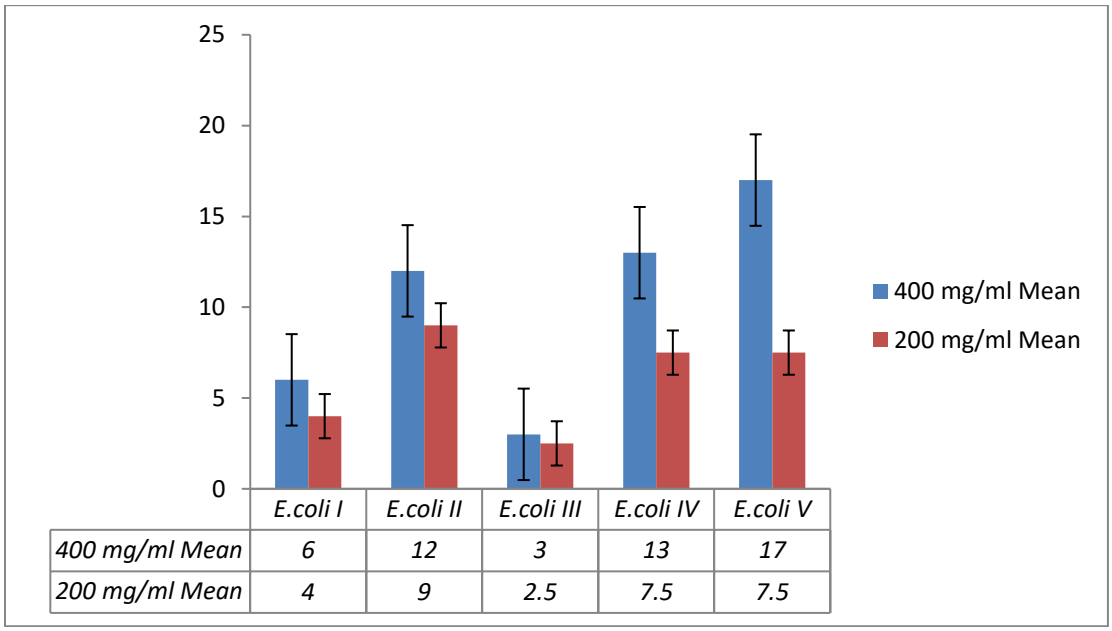
Ginger	400 mg/ml	200 mg/ml	200mg/100ml
Organism	Mean±SD	Mean±SD	CIP
E.coli I	6	4	26
E.coli II	12	9	30
E.coli III	3	2.5	34
E.coli IV	13	7.5	24
E.coli V	7	7.5	20



	E.coli I	E.coli II	E.coli III	E.coli IV	E.coli V
400 mg/ml Mean	0	15	12	10	7
200 mg/ml Mean	0	8.5	7.5	9	4

Figure 1: Mean zone of inhibition (mm) of ethanolic Moringa extract.



	E.coli I	E.coli II	E.coli III	E.coli IV	E.coli V
400 mg/ml Mean	6	12	3	13	17
200 mg/ml Mean	4	9	2.5	7.5	7.5

Figure 2:Mean zone of inhibition (mm) of ethanolic Ginger extract

3.3 Minimum Inhibitory Concentration of Moringa, Ginger and Standard antibiotic

E. coli isolate I, showed no zone of inhibition using the agar well method when tested against M. oleifera ethanolic leaf extracts hence only isolates II-V were further subjected to two antibacterial sensitivity tests while all E. coli isolates on testing with ethanolic ginger extract showed zone of inhibition hence all five isolates were further subjected to two antibacterial sensitivity tests. Table 3 and 4 show values of the MIC and MBC of Moringa and Ginger ethanolic extract respectively. Moringa MIC and MBC values of 200mg/ml and 400mg/ml were recorded for isolates II-V respectively while Ginger MIC and MBC values were found to be 400 mg/ml and 800 mg/ml respectively for isolates II-V.

Table 5 shows the MIC and MBC values of the control drug, Ciprofloxacin. The MIC and MBC values for the drug ranged from 6.25-50 mg/ml and 12.5-100 mg/ml.

Table 3: The Minimum Inhibitory Concentration (MIC) and Minimum Bactericidal Concentration (MBC) of Ethanolic Moringa extract against E. coli

Moringa	MIC(mg/ml)	MBC(mg/ml)
E. coli II	200	400
E. coli III	200	400
E. coli IV	200	400
E. coli V	200	400

Table 4: The Minimum Inhibitory Concentration (MIC) and Minimum Bactericidal Concentration (MBC) of Ethanol Ginger extract against E. coli

Ginger	MIC(mg/ml)	MBC(mg/ml)
E. coli I	0	0
E. coli II	200	800
E.coli III	200	800
E.coli IV	200	800
E.coli V	200	800

Table 5: The Minimum Inhibitory Concentration (MIC) and Minimum Bactericidal Concentration (MBC) of Ciprofloxacin against E. coli

Ciprofloxacin	MIC(mg/ml)	MBC(mg/ml)
E.coli I	12.5	50
E.coli II	6.25	12.5
E.coli III	12.5	25
E.coli IV	50	100
E.coli V	12.5	50

3.4 Molecular Docking of Moringa and Ginger Compounds

Molecular docking was performed in order to estimate the binding affinity of one hundred and nine and eighty-four phytocompounds of Moringa and Ginger respectively with 5 different receptors. The chance of ligand to be an effective drug increases with decrease of binding energy.

3.4.1 Heat Map of Moringa and Ginger Compounds

Figure 3 shows the heat map of the Eighty-four ginger compounds including reference standards while figure 4 shows the heat map of one hundred and nine moringa compounds including reference standards. This map represents the affinity of the ligands across all five receptors used. The red color indicates positive values, the white mark indicates that there was no binding of the ligand at the receptor pockets, the dark green regions signify values towards zero from the negative point. The less intense green color indicates the docking score with minimum binding energy. The compound with minimum binding energy that shows light green color indicate the activity of a compound across all receptors. Shogasulfonic C, 5-hydroxyhexahydrocurcumin, hexahydrocurcumin and chlorogenic acid, coumaroylquinic acid, neochlorogenic acid from Ginger and Moringa heat maps were shown to have activity across

all the receptors.

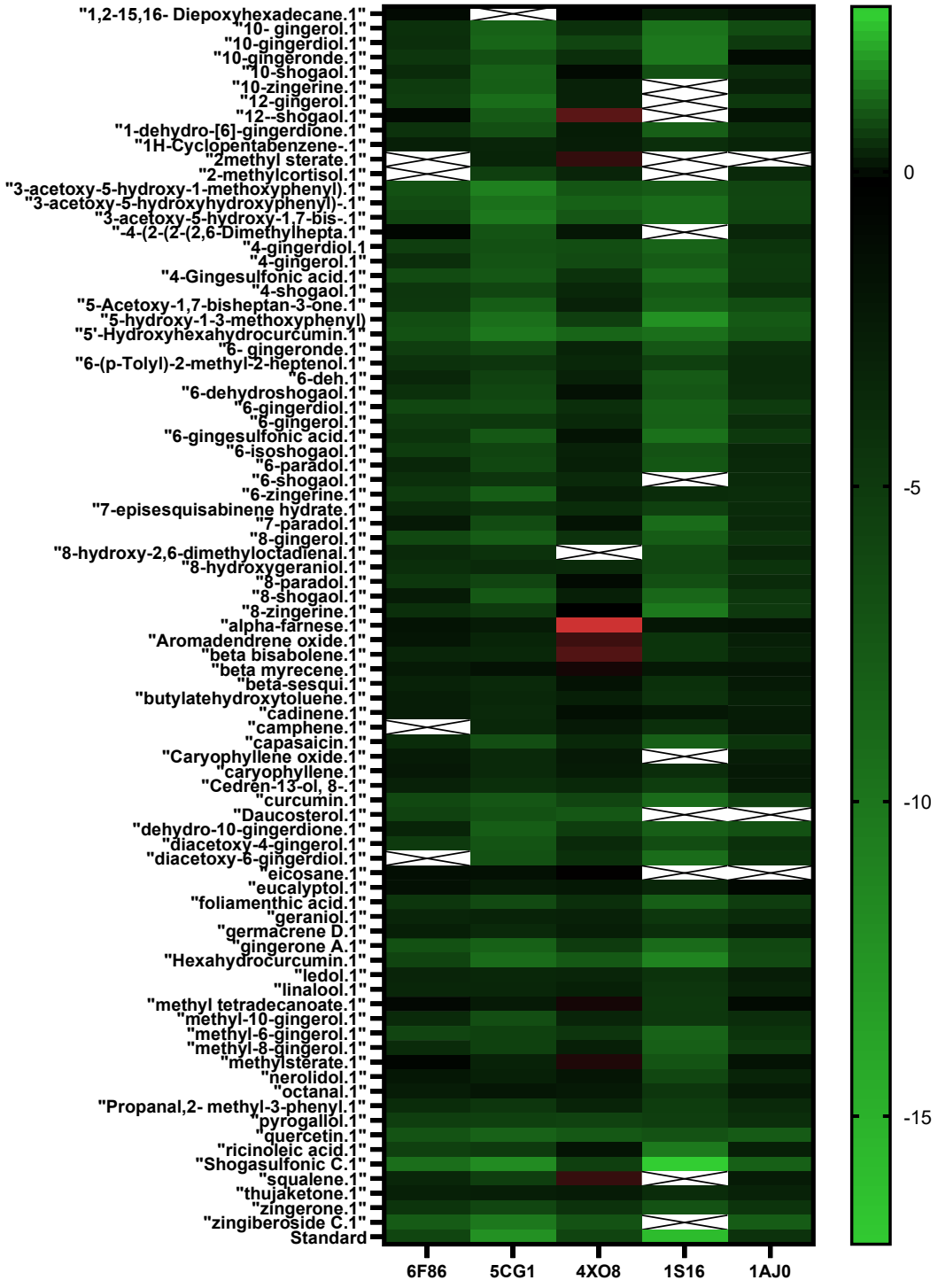


Figure 3: Heat map for Ginger compounds

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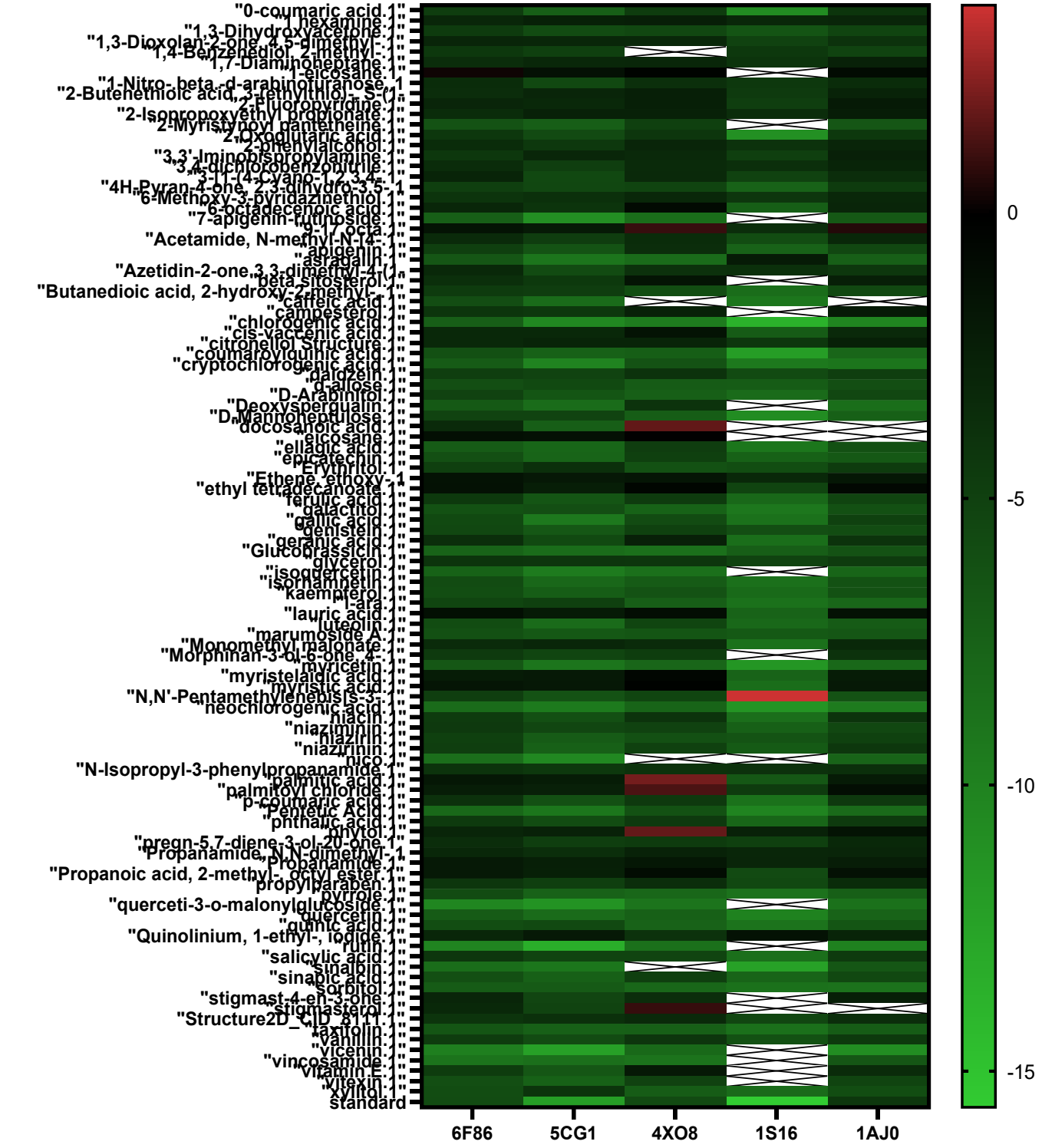


Figure 4: Heat map for Moringa compounds

3.4.2 Docking Scores of Moringa and Ginger Compounds with DNA Gyrase B

The values of all Moringa compounds docked to DNA gyrase B ranged from 0.251 to -10.247 kcal/mol. The values of all the docked Ginger compounds ranged from -0.44 to -9.202 kcal/mol while the docking score of best ten selected Moringa and Ginger compounds with DNA gyrase B were shown in figures 5 and 6 respectively. The docking score of the reference compound 4-(4-bromanylpyrazol-1-yl)-6-(ethylcarbamoylamino)-(N)-pyridin-3-yl-pyridine-3-carboxamide (CWW) was -5.77 kcal/mol. The selected compounds of Moringa had docking scores ranging from -7.5 (isoquercetin) to -10.1 (Quercetin-3-o-malonylglucoside) kcal/mol. Selected compounds of ginger showed minimum binding energy ranging from -6.03 (Diacteoxy-6-gingerdiol) to -9.2 (Shogasulfonic C) kcal/mol.

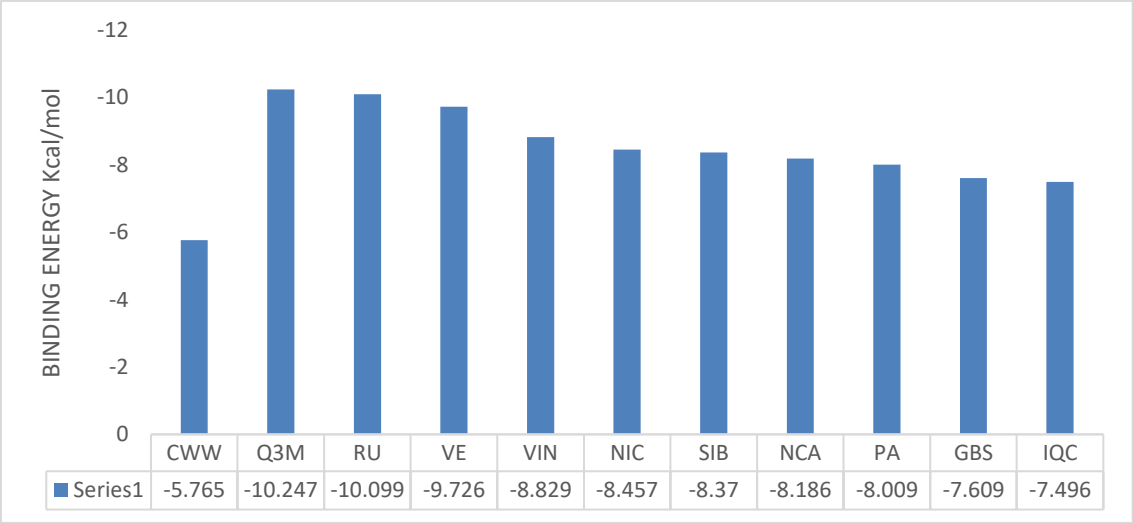


Figure 5: Docking score of selected Moringa compounds with DNA gyrase B

KEYS: CWW- 4-(4-bromanylpyrazol-1-yl)-6-(ethylcarbamoylamino)- (N) –pyridin-3-yl-pyridine-3-carboxamide Q3M- Quercetin-3-o-malnylglucoside, RU- Rutin, VE- Vicenin, VIN- Vincosamide, NIC- Nicotiflorin, SIB- Sinalbin, NCA- Neochlorogenic acid, PA-Pentetic acid, GBS-Glucobrassicin, IQC- Isoquercetin.

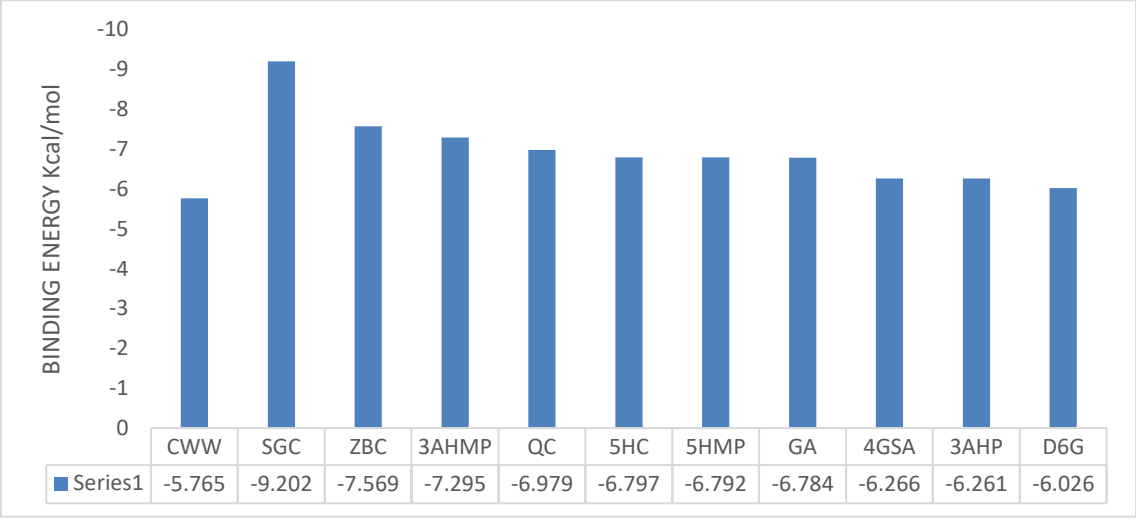


Figure 6: Docking score of selected Ginger compounds with DNA gyrase B

KEYS: CWW- 4-(4-bromanylpyrazol-1-yl)-6-(ethylcarbamoylamino)- (N) –pyridin-3-yl-pyridine-3-carboxamide SGC- Shogasulfonic C, ZBC- Zingiberoside C, 3AHMP- 3-acetoxy 5-hydroxy-1-(4-hydroxy-3-methoxyphenyl), QC- Quercetin, 5HC- 5-Hexahydrocurcumin, 5HMP- 5-hydroxy-1-(4-hydroxy-3-methoxyphenyl), GA- Gingerone A, 4GSA- 4-Gingesulfonic acid, 3AHP- 3-acetoxy-5-hydroxy-1-(4-hydroxyphenyl), D6G- Diacteoxy-6-gingerdiol.

3.4.3 Docking Scores of Moringa and Ginger Compounds with Enoyl ACP Reductase

The docking score of ten best selected Moringa and Ginger compounds were given in figure 7 and 8 respectively. The values of all Moringa compounds docked to Enoyl ACP reductase ranged from -1.265 to -13.318 kcal/mol while the values of all the docked Ginger compounds ranged from -1.347 to -12.11 kcal/mol. The docking score of the reference compound Nicotinamide Adenine Dinucleotide (NAD) gave binding energy of -12.1 kcal/mol. Selected compounds of Moringa showed docking score with minimum binding energy ranging from -9.21(gallic acid) to -13.3 (rutin) kcal/mol. Selected ginger compounds showed docking score with minimum binding energy ranging from -8.47 (10-gingerdiol) to -11.6 (shogasulfonic C) kcal/mol.

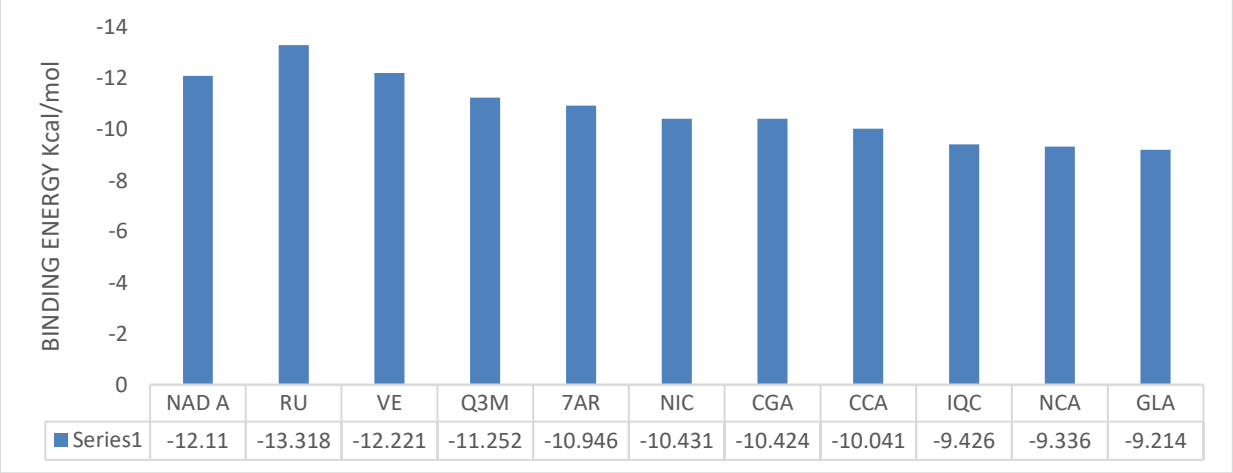


Figure 7: Docking score of selected Moringa compounds with Enoyl ACP reductase
KEYS: Nicotinamide Adenine Dinucleotide (NAD), RU-Rutin, VE-Vicenin, Q3M-Quercetin-3-o-malonylglucoside, 7AR- 7-apigenin-rutinoside, NIC-Nicotiflorin, CGA-Chlorogenic acid, CCA- Cryptochlorogenic acid, IQC-Isoquercetin, NCA- Neochlorogenic acid, GLA- Gallic acid.

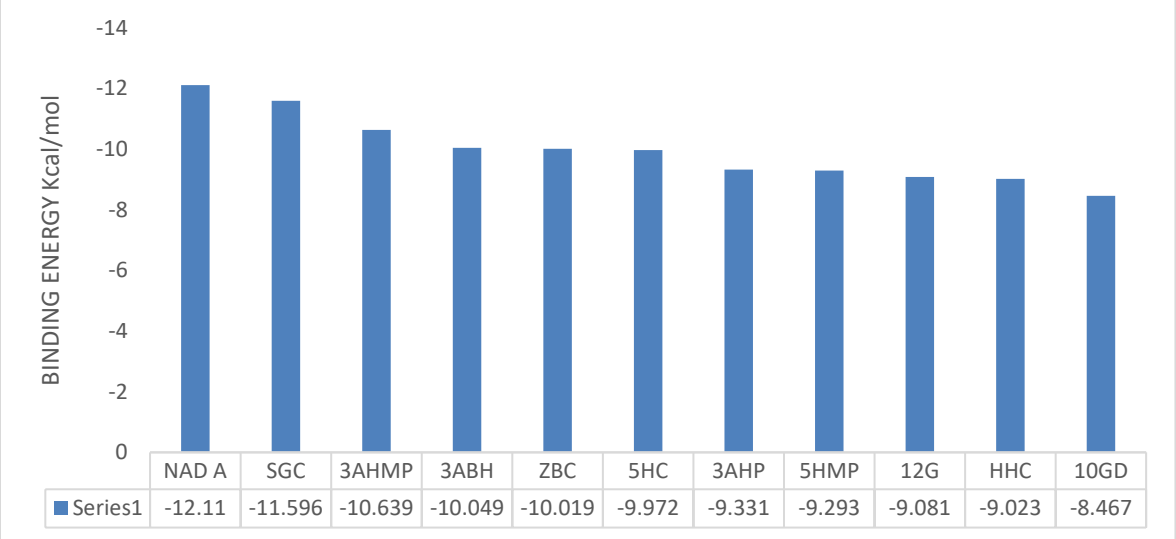


Figure 8: Docking score of selected Ginger compounds with Enoyl ACP reductase
KEYS: NAD- Nicotinamide Adenine Dinucleotide (NAD), SGC-Shogasulfonic C, 3AHMP- 3-acetoxy 5-hydroxy-1-(4-hydroxy-3-methoxyphenyl), 3ABH- 3-acetoxy-5-hydroxy-1,7,-bis(4-hydroxy), ZBC- Zingiberoside C, 5HC- 5-hydrohexahydrocurcumin, 3AHP- 3-acetoxy-5-hydroxy-1-(4-hydroxyphenyl), 5HMP- 5-hydroxy-1-(4-hydroxy-3-methoxyphenyl, 12G- 12-Gingerol, HHC- Hexahydrocurcumin, 10GD- 10-gingerdiol.

3.4.4 Docking Scores of Moringa and Ginger Compounds with FIMH Adhesin

The docking score of selected Moringa and Ginger compounds were shown in figure 9 and 10 respectively. The values of all Moringa compounds docked to FIMH adhesin ranged from 2.026 to -10.342 kcal/mol while the values of all the docked Ginger ligands ranged from 2.614 to -8.427 kcal/mol. The docking score of the reference compound (heptylesteralpha-D-mannopyranoside (KGM) gave binding energy of -5.717 kcal/mol. Selected Moringa compounds gave minimum binding energy of ranging from -8.202 (asragalin) to -10.3 (Nicotiflorin) kcal/mol. Selected Ginger compounds showed minimum binding energy ranging from -6.473 (4-gingerdiol) to -8.427 (5-hydrohexahydrocurcumin) kcal/mol.

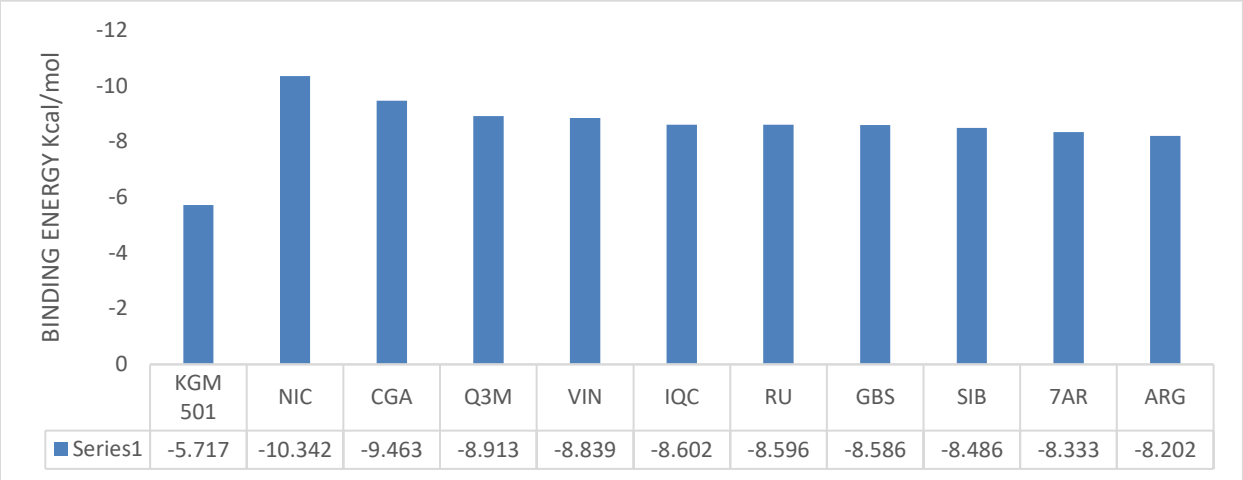


Figure 9: Docking score of selected Moringa compounds with FIMH adhesin

KEYS: KGM-heptylesteralpha-D-mannopyranoside, NIC-Nicotiflorin, CGA- Chlorogenic acid, Q3M-Quercetin-3-o-malonylglucoside, VIN- Vincosamide, IQC- Isoquercetin, RU- Rutin, GBS- Glucobrassicin, SIB-Sinalbin, 7AP- 7-apigenin-rutinoside, ARG- Asragalin.

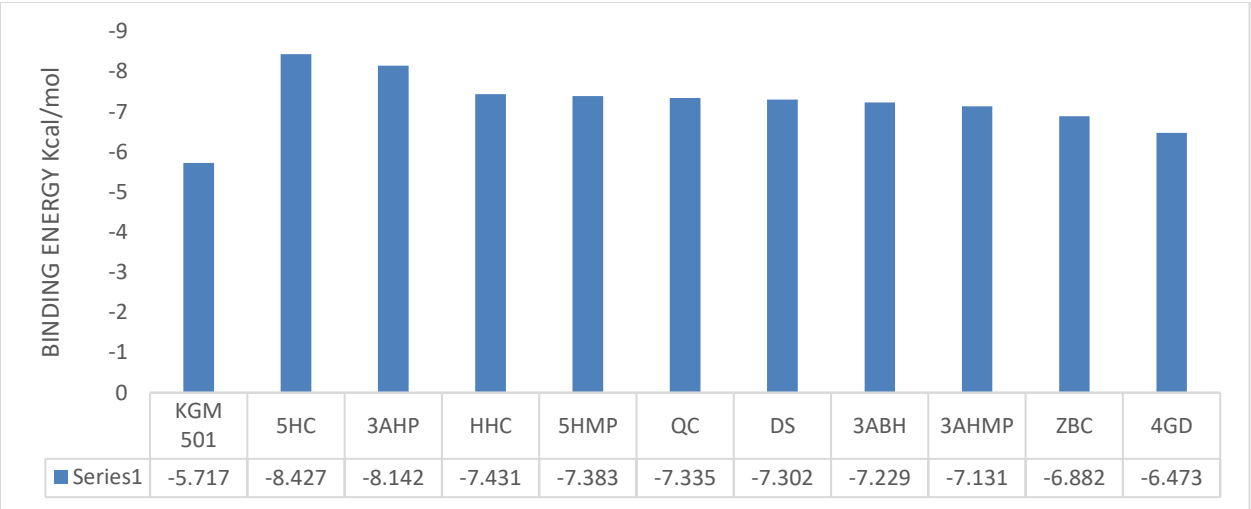


Figure 10: Docking score of selected Moringa compounds with FIMH adhesin

KEYS: KGM-heptylesteralpha-D-mannopyranoside, 5HC- 5-hydroxyhexahydrocurcumin, 3AHP- 3-acetoxy-5-hydroxy-1-(4-hydroxyphenyl), HHC- Hexahydrocurcumin, 5HMP- 5-hydroxy-1-(4-hydroxy-3-methoxyphenyl, QC-Quercetin, DS-Daucosterol, 3ABH- 3-acetoxy-5-hydroxy-1,7,bis(4-hydroxy), 3AHMP- 3-acetoxy 5-hydroxy-1-(4-hydroxy-3-methoxyphenyl), ZBC- Zingeroside C, 4GD- 4- Gingerdiol.

3.4.5 Docking Scores of Moringa and Ginger Compounds with Par E Subunit DNA Topoisomerase IV

The values of all Moringa compounds docked to Par E topoisomerase IV ranged from 3.605 to - 15.637 kcal/mol while the values of all the docked Ginger ligands ranged from -1.883 to -17.036 kcal/mol. The docking score of selected Moringa and Ginger compounds were shown in figure 11 and12respectively. The docking score of the reference compound phosphoaminophosphoric Acid-Adenylate (ANP) gave binding energy of -15.64 kcal/mol. Selected Moringa compounds had docking scores ranging from -9.951 (quercetin) to -13.59 (Chlorogenic acid) kcal/mol. Selected Ginger compounds had docking scores ranging from -9.45 (6-gingesulfonic acid) to -17.04 (Shogasulfonic C) kcal/mol.

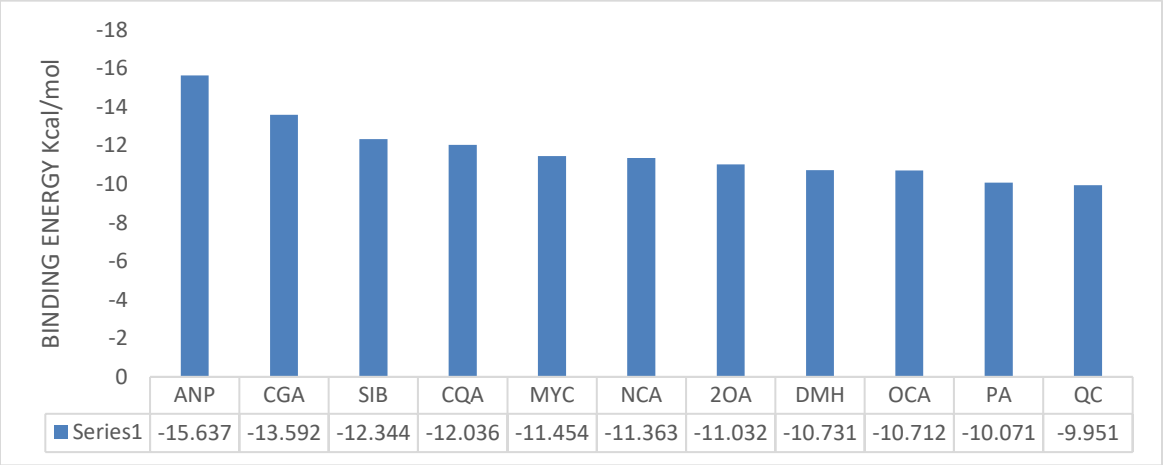


Figure 11: Docking score of selected Moringa compounds with Par E topoisomerase IV

KEYS: ANP-phosphoaminophosphoric Acid-Adenylate, CGA- Chlorogenic acid, SIB- Sinalbin, CQA-Coumaroylquinic acid, MYC- Myricetin, NCA- Neochlorogenic acid, 2OA- 2-oxoglutarc acid, DMH- D-Mannoheptulose, OCA- O-Coumaric acid, PA-Pentetic acid, QC- Quercetin.

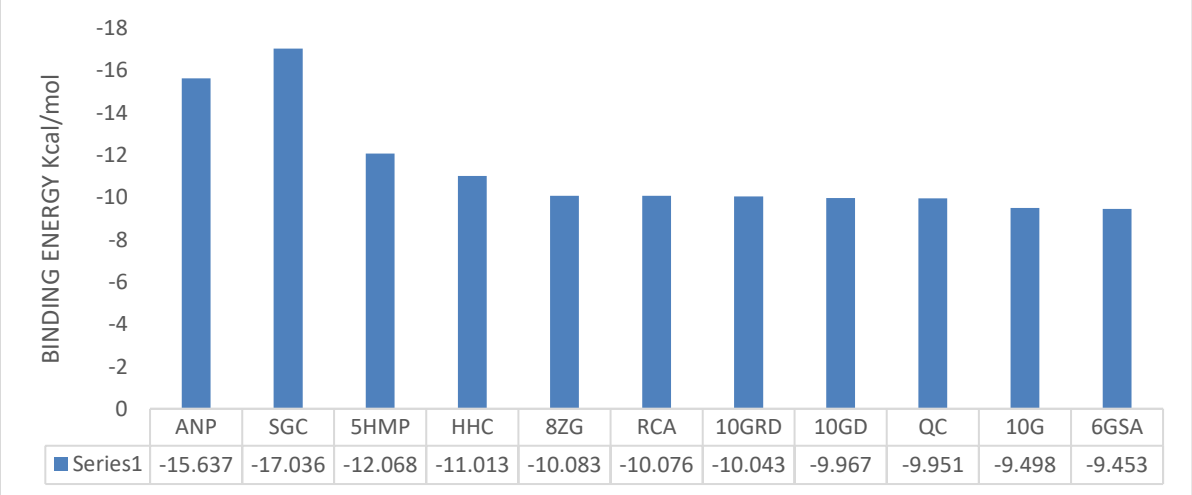


Figure 12: Docking score of selected Ginger compounds with Par E topoisomerase IV

KEYS: ANP-phosphoaminophosphoric Acid-Adenylate, SGC-Shogalsulfonic C, 5HMP- 5-hydroxy-1-(4-hydroxy-3-methoxyphenyl), HHC- Hexahydrocurcumin, 8ZG- 8-Zingerine, RCA-Ricinoleic acid, 10GRD- 10- Gingeronde, 10GD- 10- Gingerdiol, QC-Quercetin, 10G- 10-Gingerol, 6GSA- 6-gingesulfonic acid.

3.4.6 Docking Scores of Moringa and Ginger Compounds with Dihydropteroate Synthase

The values of all Moringa compounds docked to dihydropteroate synthase ranged from 0.617 to -10.77 kcal/mol while the values of all the docked Ginger compounds ranged from -0.68 to -7.983 kcal/mol. The docking score of selected Ginger and Moringa compounds were shown in figure 13 and 14 respectively. The docking score of the reference compound sulfanilamide (SAN) gave binding energy of -4.197 kcal/mol. Selected Moringa compounds were found to have minimum binding energy ranging from -7.94 (Myricetin) to -10.77 (Vicenin) kcal/mol. Selected Ginger compounds were found to have minimum binding energy ranging from -5.927 (Gingerone A) to -7.983 (Shogasulfonic C) kcal/mol.

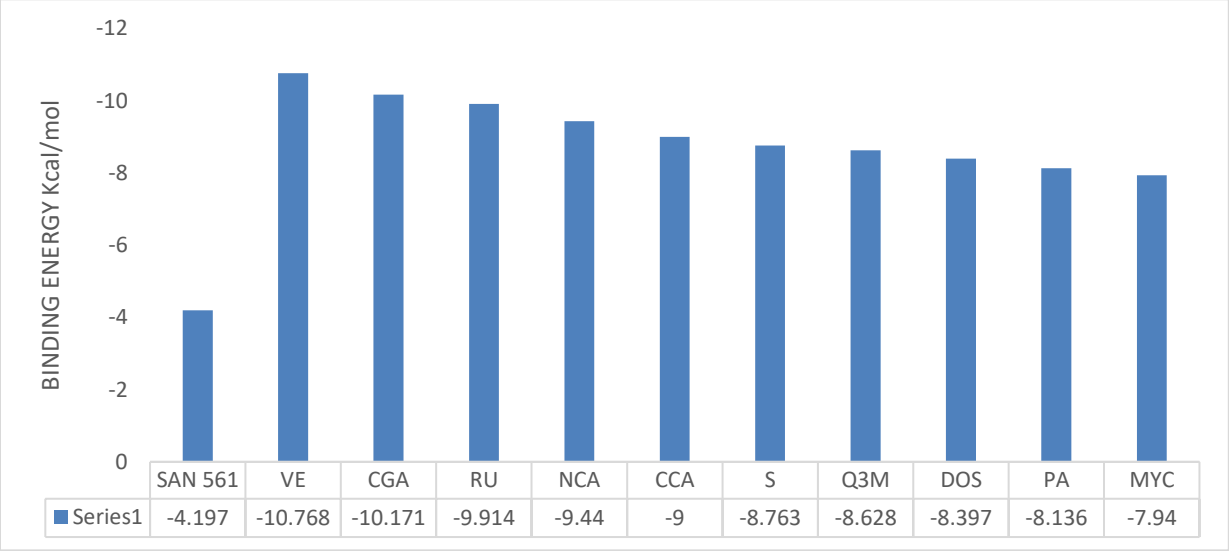


Figure 13: Docking score of selected Moringa compounds with for Dihydropteroate synthase

Keys: SAN- sulfanilamide, VE-Vicenin, CGA- Chlorogenic acid, RU- Rutin, NCA- Neochlorogenic acid, CCA-Cryptochlorogenic acid, S- Sorbitol, Q3M- Quercetin-3-o-malonylglucoside, DOS- Deoxyspergualin, PA-Pentetic acid, MYC-Myricetin

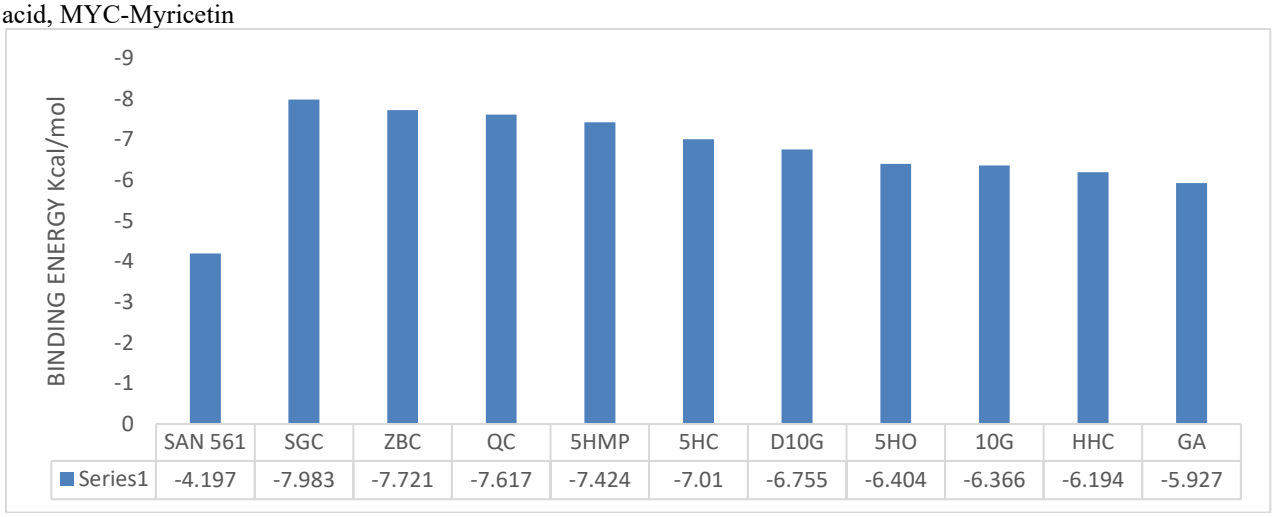


Figure 14: Docking score of selected Ginger compounds with Dihydropteroate synthase

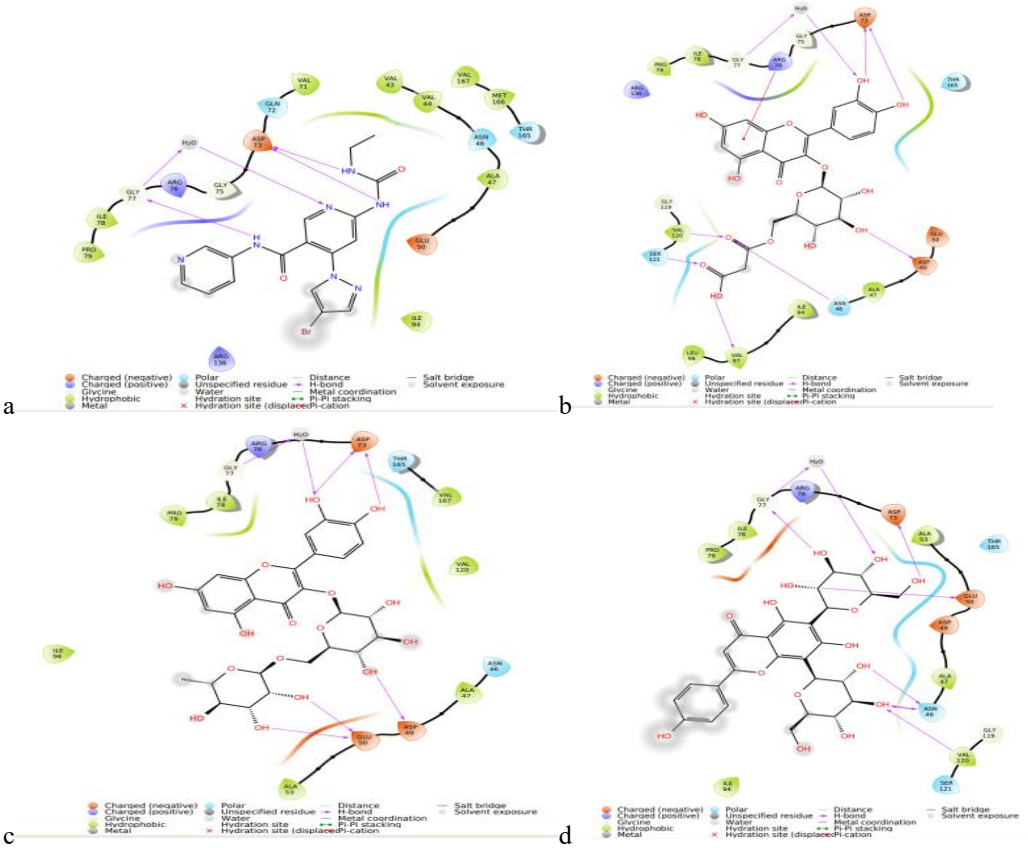
Keys: SAN- sulfanilamide, SGC- Shogasulfonic C, ZBC-Zingiberoside C, QC- Quercetin, 5HMP- 5-hydroxy-1-(4-hydroxy-3-methoxyphenyl), 5HC- 5-Hydrohexahydrocurcumin, D10G- Dehydro-10-gingerdione, 5HO- 5-acetoxy-1,7-bis(4-hydroxy-3-methoxyphenyl) heptan-3-one, 10G-10-gingerol, HHC-Hexahydrocurcumin, GA-Gingerone A

3.5 Selected Ligand Interaction

Figures 15-24, shows the interaction between the reference compounds and best five compounds of Moringa and Ginger respectively with proteins of the target organism. The compounds shown in these figures were found to exhibit several molecular interactions (hydrogen bond, pi-pi stacking, hydrophobic interaction) with their respective target proteins and were considered to be responsible for antibacterial activity of the compounds.

3.5.1 Ligand Interaction of Moringa with DNA Gyrase B

The interaction of the reference compound (CWW) with DNA gyrase B was shown in figure15a. Hydrogen bonds were formed with amino acid residues glycine (GLY) 77, aspartic acid (ASP)73. Hydrophobic bonds were formed with valine (VAL71), isoleucine (ILE94), alanine (ALA47), proline (PRO79), ILE78, VAL43, VAL44, VAL167, methionine (MET166). Figure 15b-f showed the interaction of selected Moringa compounds with DNA gyrase B respectively. Quercetin-3-o-malonylglucoside in figure 15b showed hydrogen bond interaction with amino acid residues VAL97, asparagine (ASN) 46, serine (SER)121, VAL120, ASP49, GLY77, ASP73. Pi-pi interaction was formed with ARG76 and hydrophobic bonds were formed with PRO79, ILE78, ILE94, ALA47 similar to the reference compound (CWW).Rutin in figure 15c, showed hydrogen bond interaction with amino acid residues GLU50, ASP49, ASP73. Hydrophobic bonds were formed with PRO79, ILE78, ALA47 similar to the reference compound (CWW).
Vicenin in figure 15d showed hydrogen bond interaction with amino acid residues GLY77, ASP73, glutamic acid (GLU) 50, ASN46, VAL120. Hydrophobic bonds were formed with ILE94, ALA47, PRO79, ILE78 similar to the reference compound (CWW).
Vincosamide in figure 15e demonstrated hydrogen bond interaction with amino acid residues glycine (GLY) 77, ASN46, serine (SER) 121, ILE94. Hydrophobic bonds were formed with ILE94, ALA47, ILE78, PRO79 similar to the reference compound (CWW).
Nicotiflorin in figure 15f showed hydrogen bond interaction with amino acid residues VAL97, aspartic acid (ASP) 49, asparagine (ASN) 46, ASP73. Pi-pi stacking interaction was shown with ARG76. Hydrophobic bonds were formed with PRO79, ILE78, ALA47, ILE94 similar to the reference compound (CWW).



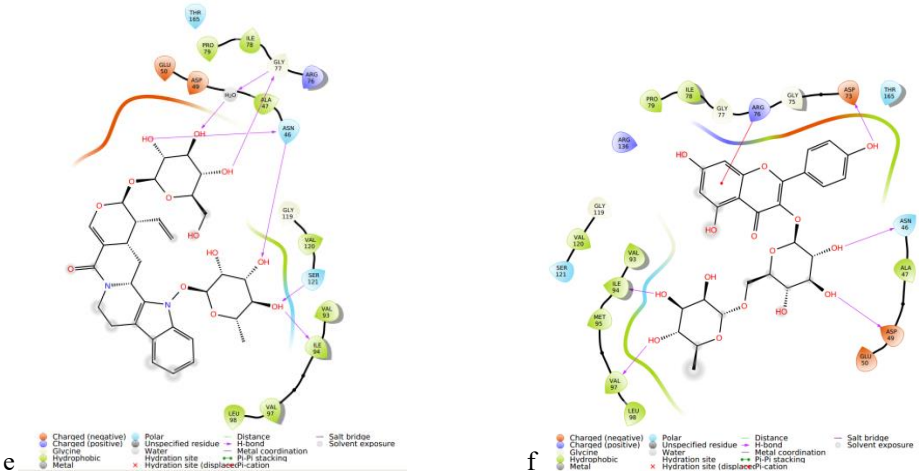


Figure 15: Ligand Interaction of Moringa compounds with DNA Gyrase B
Ligand Interaction with DNA gyrase B (a) CWW (b) Quercetin-3-o-malonylglucoside (c) Rutin (d) Vicenin (e) Vincosamide (f) Nicotiflorin. The amino acid residues with negative charge are shown in red, positive charge in velvet, polar in cyan, hydrophobic bonds in green, undefined residues in grey. Hydrogen bond interaction are shown as pink-arrow, pi-pi stacking as green line and pi-cation as red line.

3.5.2 Ligand Interaction of Ginger with DNA Gyrase B

The interaction of the reference compound (CWW) with DNA gyrase B was shown in figure 16a. Hydrogen bonds were formed with amino acid residues glycine (GLY)77, aspartic cid (ASP)73. Hydrophobic bonds were formed with valine (VAL71), isoleucine (ILE94), alanine (ALA47), proline (PRO79), ILE78, VAL43, VAL44, VAL167, methionine (MET166).

Figure 16b-f showed the interaction of selected ginger ligands with DNA gyrase B respectively. Shogasulfonic C in figure 16b, formed hydrogen bonds with amino acid residues ASP73, GLY77, ASN46, VAL120, SER121, ILE94. Hydrophobic bonds were formed with ILE94, PRO79, ILE78, ALA47 similar to the reference compound (CWW).
Zingiberoside C in figure 16c was formed hydrogen bonds with amino acid residues ASN46, VAL97, ASP73. Hydrophobic bonds were formed with ILE94, ALA47, PRO79, ILE78 similar to the reference compound (CWW).
3-acetoxy-5-hydroxy-1-(4-hydroxy-3-methoxyphenyl in figure 16d showed hydrogen bond with amino acid residues VAL120, ASN46, ASP73, GLY77. Hydrophobic bonds were formed with PRO79, ILE78, ALA47, ILE94 similar to the reference compound (CWW).

Quercetin in figure 16e demonstrated hydrogen bond interaction with amino acid residues ASN46, ASP73, VAL71. Hydrophobic bonds were formed with amino acid residues PRO79, ILE78, ILE94, VAL43, ALA47, VAL71, MET166, VAL167 similar to the reference compound (CWW).
5-hydroxyhexahydrocurcumin in figure 16f demonstrated interaction with amino acid residues ASN46, VAL120, ASP73, GLY77. Hydrophobic bonds were formed with ALA47, ILE94, PRO79, ILE78 similar to the reference ligand (CWW).

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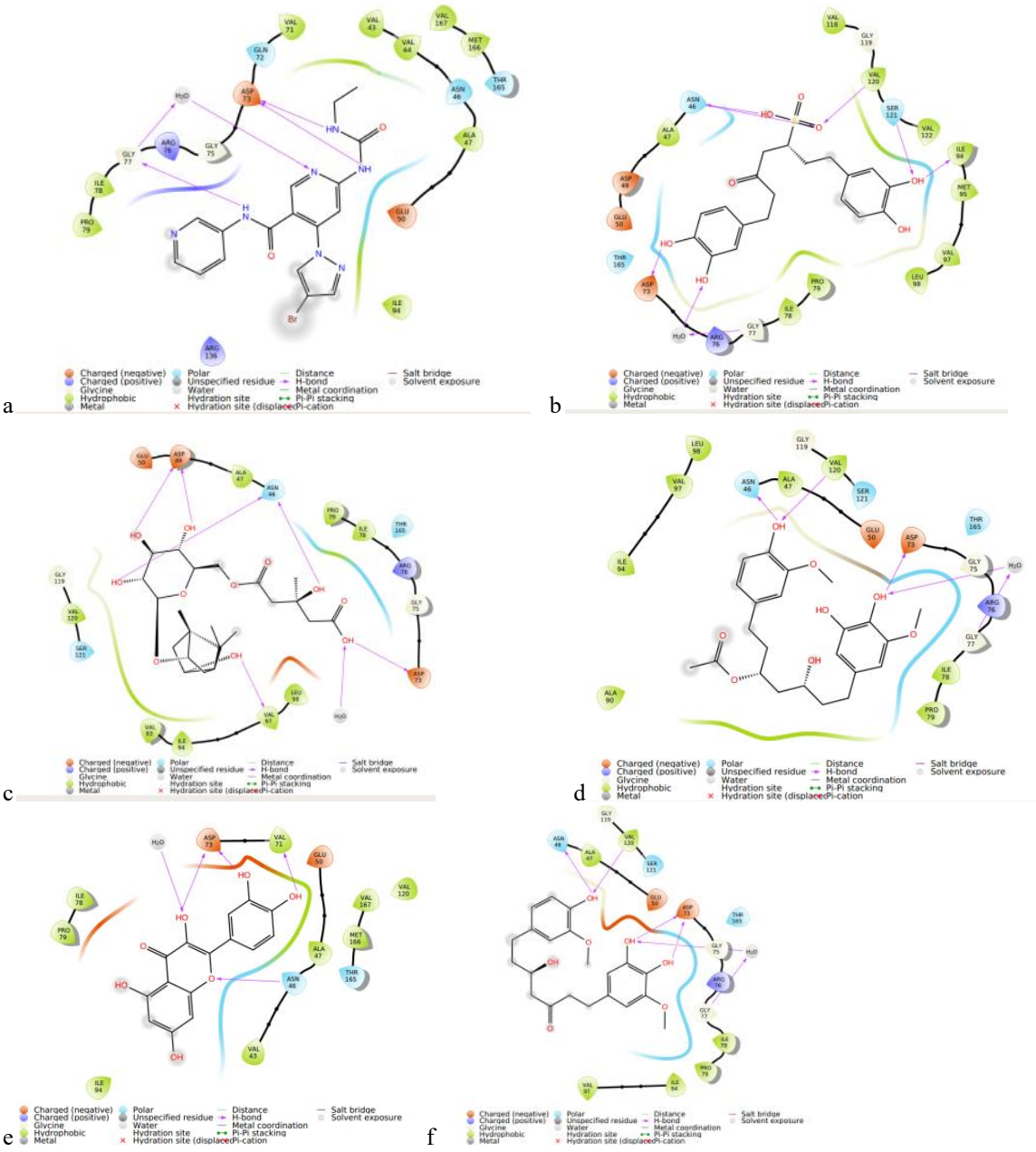


Figure 16: Ligand Interaction of Ginger compounds with DNA Gyrase B
Ligand Interaction with DNA gyrase B (a) CWW (b) shogasulfonic C (c) Zingeberoside C (d) 3-acetoxy-5-hydroxy-1-(4-hydroxy-3-methoxyphenyl (e) Quercetin (f) 5-hydroxyhexahydrocurcumin The amino acid residues with negative charge are shown in red, positive charge in velvet, polar in cyan, hydrophobic bonds in green, undefined residues in grey. Hydrogen bond interaction are shown as pink-arrow, pi-pi stacking as green line and pi-cation as red line.

3.5.3 Ligand Interaction of Moringa with Enoyl Acyl Carrier Protein Reductase

In Figure 17a, reference compound (NAD) interacted with amino acid residues (VAL65, ASP64, GLN40, SER19, ILE20, ALA21, SER91, TYR156, ILE192) of Enoyl ACP reductase and hydrophobic bonds were formed with amino acid residues ILE192, PRO191, ALA189, tyrosine (TYR) 146, leucine (LEU) 144, MET159, tyrosine (TYR) 156, ILE92, phenylalanine (PHE) 92, ALA21, ILE20, ALA15, LEU44, ILE119, ALA66, VAL65, cysteine (CYS) 63.

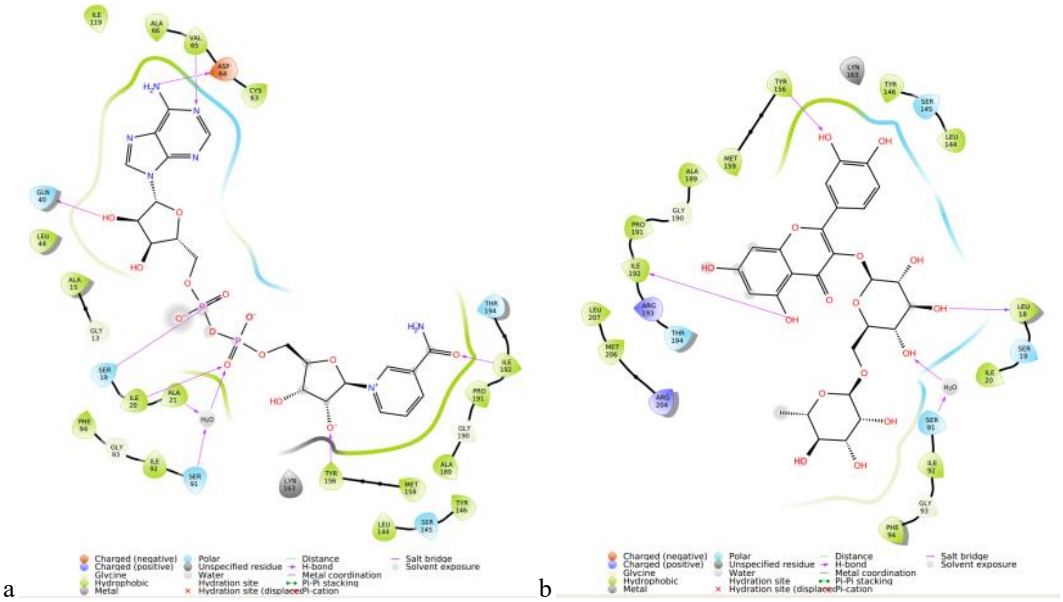
In figure 17b, Rutin from Moringa showed interaction with amino acid residues (ILE192, TYR156, LEU18, SER91) to form hydrogen bonds. Hydrophobic bonds with amino acid residues were formed ILE92, ILE20, ILE192, PRO191, MET159, TYR156, TYR146, LEU144 similar to the reference compound (NAD).

Vicenin in figure 17c interacted with amino acid residues to form hydrogen bond (SER91, GLY93, GLN40, GLY13, LEU18, ALA189. Hydrophobic bonds with amino acid residues were also formed ILE92, LEU144, TYR146, PRO191, ILE192, ILE20, ALA15, LEU44 similar to the reference compound (NAD).

In figure 17d, Quercetin-3-o-malonylglucoside showed interaction with amino acid residues (ILE192, TYR156) and formed hydrogen bonds. Hydrophobic bonds were formed with amino acid residues ILE192, PRO191, MET159, TYR156, ILE92, ALA21, ILE20, LEU144, TYR146 similar to the reference compound (NAD).

Figure 17e, showed 7-apigenin-rutinoside interacted with amino acid residues SER145, ILE20, GLN40, SER91, GLY93for hydrogen bond formation. Pi-pi stacking interaction was shown with TYR146. Hydrophobic bonds were formed with ILE192, PRO191, TYR146, LEU144, ILE20, ILE92, LEU44, ALA15 similar to the reference compound (NAD).

In figure 17f, Nicotiflorin interacted with amino acid residues LYN163, GLY190, ILE20, LEU18, SER91, GLN40) for hydrogen bond formation. Hydrophobic bonds were formed with ILE92, ALA15, ILE20, PRO191, ILE192, TYR156, TYR146, LEU144 similar to the reference compound (NAD).



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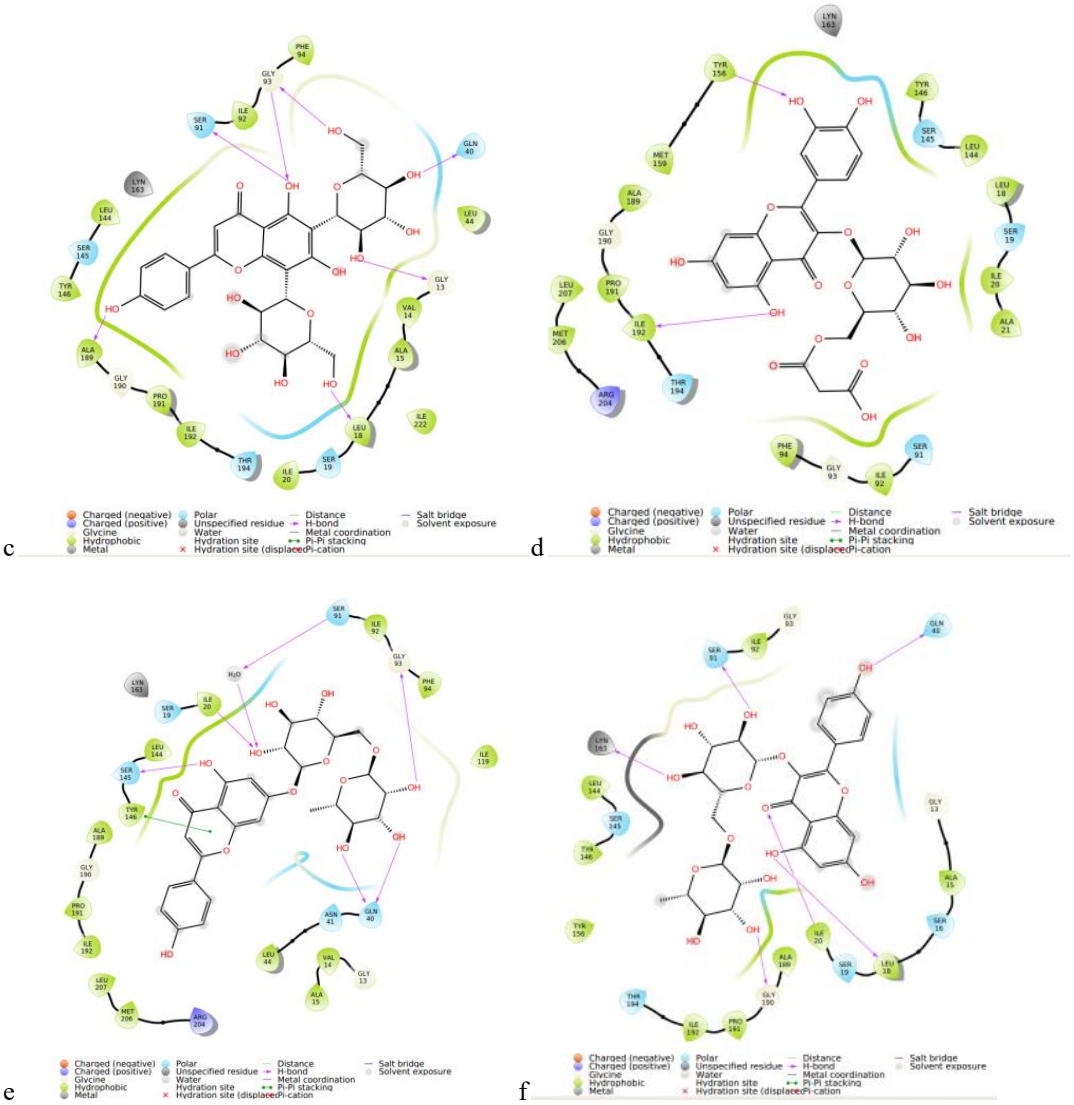


Figure 17: Ligand Interaction of Moringa compounds with Enoyl ACP Reductase
Interaction with Enoyl ACP reductase (a) NAD (b) Rutin (c) Vicenin (d) Quercetin-3-o-malonylglucoside (e) 7-apigenin-rutinoside(f) Nicotiflorin. The amino acid residues with negative charge are shown in red, positive charge in velvet, polar in cyan, hydrophobic bonds in green, undefined residues in grey. Hydrogen bond interaction are shown as pink-arrow, pi-pi stacking as green line and pi-cation as red line.

3.5.4 Ligand Interaction of Ginger with Enoyl Acyl Carrier Protein Reductase

In Figure 18a, reference compound (NAD) interacted with amino acid residues (VAL65, ASP64, GLN40, SER19, ILE20, ALA21, SER91, TYR156, ILE192) of Enoyl ACP reductase and hydrophobic bonds were formed with amino acid residues ILE192, PRO191, ALA189, tyrosine (TYR) 146, leucine (LEU) 144, MET159, tyrosine (TYR) 156, ILE92, phenylalanine (PHE) 92, ALA21, ILE20, ALA15, LEU44, ILE119, ALA66, VAL65, cysteine (CYS) 63.

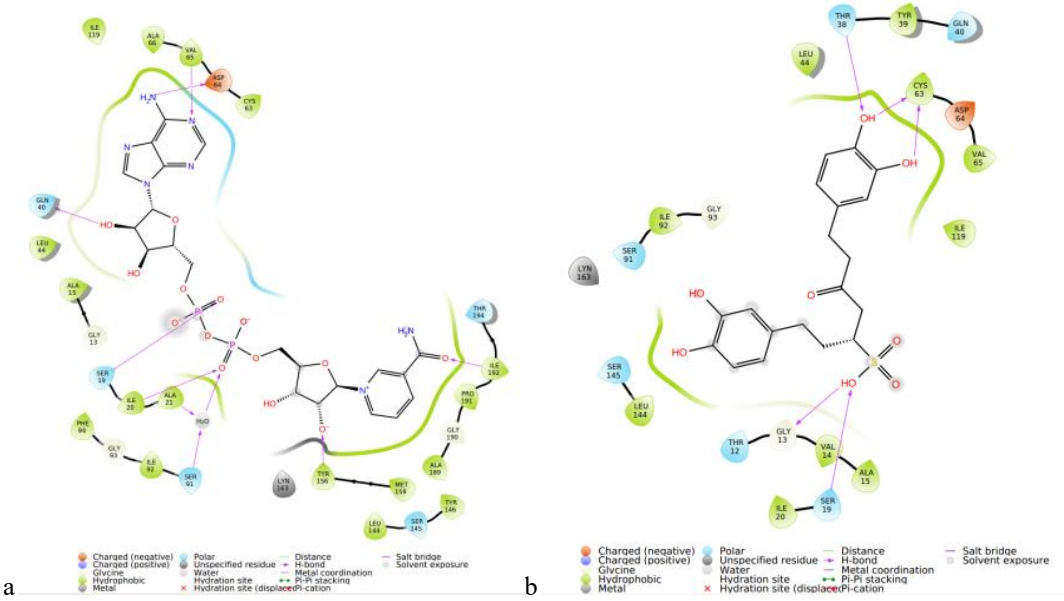
Figure 18a-f showed the interaction of Ginger compounds with Enoyl ACP reductase respectively. Figure 18b represented interaction of Shogasulfonic C with amino acid residues (SER19, GLY13, THR38, CYS63) in which hydrogen bonds were formed. Hydrophobic bond was formed by interaction between amino acid residues LEU44, CYS63, VAL65, ILE119, ILE20, ALA15, LEU144, similar to the reference compound (NAD).

Figure 18c represented interaction of 3-acetoxy-5-hydroxy-1-(4-hydroxy-3-methoxyphenyl) with amino acid residues (CYS63, THR38, GLY13, SER19) in which hydrogen bonds were formed. Hydrophobic bonds were formed with amino acid residues TYR156, MET159, ILE20, ALA15, LEU44, VAL65, CYS63 similar to the reference compound (NAD).

Figure 18d represented interaction of 3-acetoxy-5-hydroxy-1,7,-bis(4-hydroxy) with amino acid residues GLY93, SER19, GLY13, CYS63, THR38 in which hydrogen bonds were formed. Hydrophobic bonds were formed with amino acid residues VAL65, CYS63, ALA15, LEU44, ILE20, LEU144, TYR146, TYR156, MET159 similar to the reference compound (NAD).

Figure 18e represented interaction of Zingiberoside C amino acid residues (TYR156, SER145, LYN163, ILE192, ILE20, LEU18, GLY13, SER19) and hydrogen bonds were formed. Hydrophobic bonds were formed with amino acid residues MET159, TYR156, LEU144, TYR146, ILE20, ILE192, PRO191 similar to the reference compound (NAD).

5-hydroxyhexahydrocurcumin interacted with amino acid residues GLY93, LYN163, CYS63, THR38, GLY13in figure 18f and hydrogen bonds were formed. Hydrophobic bonds were formed with amino acid residues VAL65, CYS63, ALA15, VAL48, LEU44, ILE20, LEU144, TYR146, TYR156, MET159, ILE92 similar to the reference compound (NAD).



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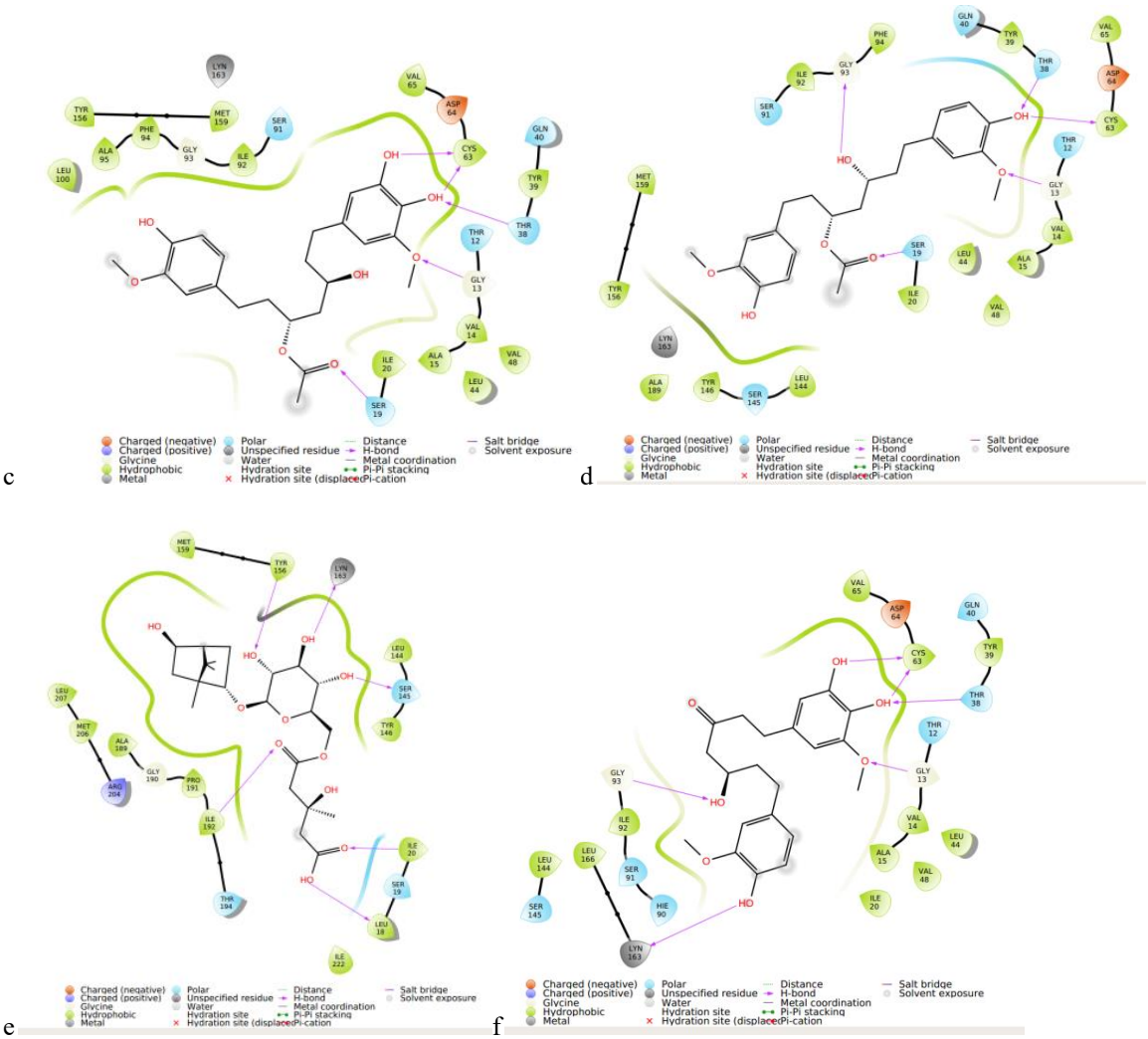


Figure 18 Ligand Interaction of Ginger compounds with Enoyl ACP Reductase
Interaction with Enoyl ACP reductase (a) NAD (b) Shogasulfonic C (c) 3-acetoxy-5-hydroxy-1-(4-hydroxy-3-methoxyphenyl) (d) 3-acetoxy-5-hydroxy-1,7,-bis(4-hydroxy (e) Zingiberoside C (f) 5-hydrohexahydrocurcumin. The amino acid residues with negative charge are shown in red, positive charge in velvet, polar in cyan, hydrophobic bonds in green, undefined residues in grey. Hydrogen bond interaction are shown as pink-arrow, pi-pi stacking as green line and pi-cation as red line.

3.5.5 Ligand Interaction of Moringa with FIMH Adhesin
The interaction of reference compound (KGM) with FIMH adhesin was shown in figure 19a. Hydrogen bond interaction with amino acid residues GLY14, PHE1, ASP140, GLN133, ASP54, ASP47. Hydrophobic interaction with amino acids ILE13, PHE142, TYR137, PHE1, ILE52, TYR48 were shown.

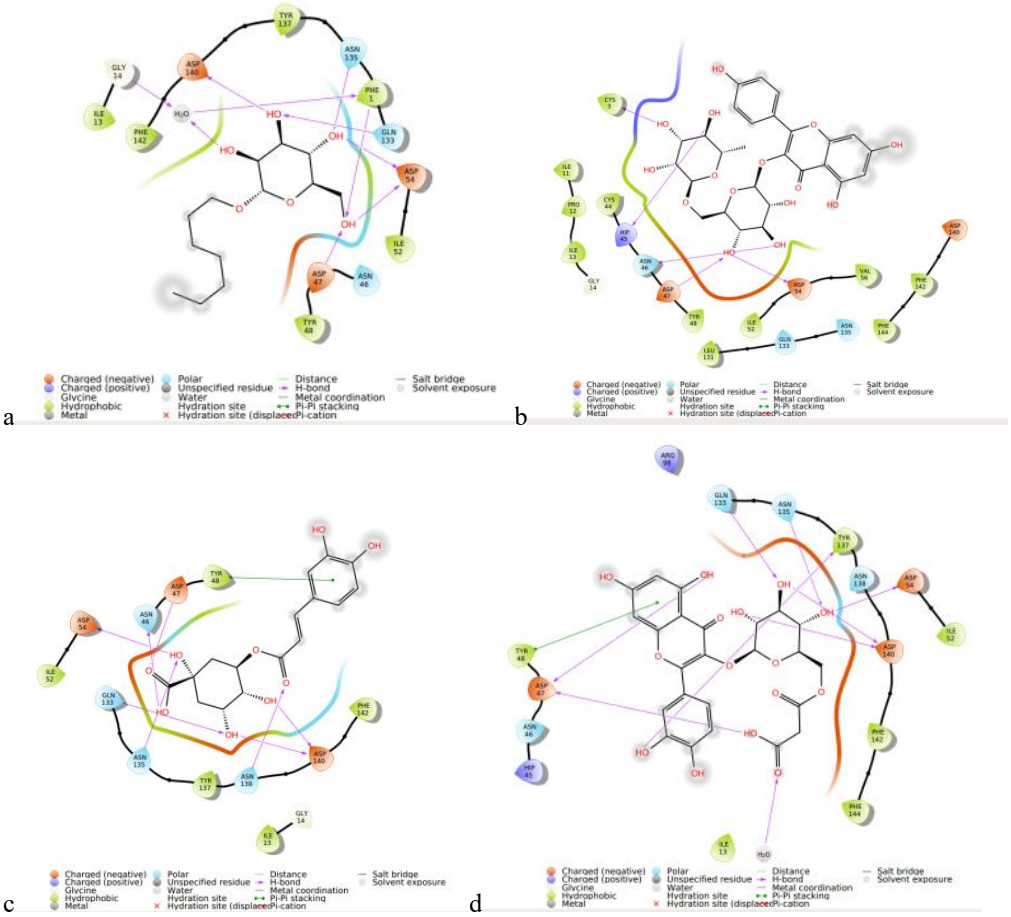
Figure 19b-f showed interaction of selected Moringa compounds with FIMH adhesin receptor respectively. Nicotiflorin in figure 19b was shown to interact with amino acid residues CYS3, HIP45, ASN46, ASP47, ASP54 and formed hydrogen bonds. Hydrophobic bond interactions were demonstrated with ILE13, TYR48, ILE52, PHE 142 similar to the reference compound (KGM).

Chlorogenic acid in figure 19c, was shown to interact with amino acid residues ASP54, GLN133, ASN135, ASN46, ASP47, ASN138, ASP140 forming hydrogen bonds. Pi-pi stacking interaction with TYR48 was shown. Hydrophobic bonds interaction was demonstrated with PHE142, ILE13, TYR137, ILE52, TYR48 similar to the reference ligand (KGM).

Quercetin-3-o-malonylglucoside in figure 19d was showed hydrogen bond interaction with amino acid residues ASP47, ASP140, GLN133, ASN135, TYR137, ASP54. Pi-pi stacking interaction with TYR48 was shown. Hydrophobic bonds interaction was demonstrated with TYR48, ILE13, TYR137, PHE142, ILE52 similar to the reference ligand (KGM).

Vincosamide in figure 19e showed hydrogen bond interactions with amino acid residues ASP47, ASP54, ASN135, GLN133, ASP140. Hydrophobic bond interaction with PHE142, ILE13, TYR137, TYR48, ILE52 similar to the reference compound (KGM).

Isoquercetin in figure 19f showed hydrogen bond interaction with amino acid residues ASP140, TYR137, GLN133, ASN135, ASP54, ASP47. Pi-pi stacking interaction with TYR48 was shown. Hydrophobic bonds interaction was demonstrated PHE142, ILE13, TYR137, TYR48, ILE52 similar to the reference compound (KGM).



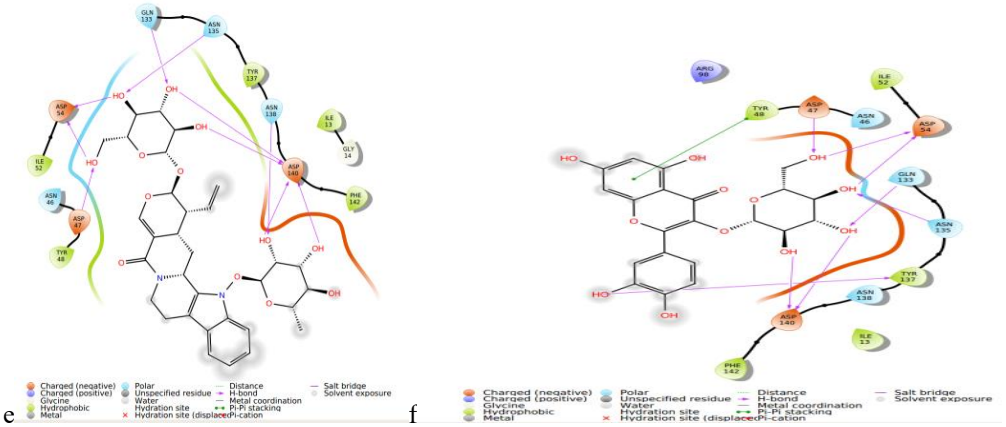


Figure 19: Ligand Interaction of Moringa compounds with FIMH Adhesin
Ligand Interaction with FIMH adhesin (a) KGM (b) Nicotiflorin (c) Chlorogenic acid (d) Quercetin-3-o-malonylglucoside (e) Vincosamide (f) Isoquercetin. The amino acid residues with negative charge are shown in red, positive charge in velvet, polar in cyan, hydrophobic bonds in green, undefined residues in grey. Hydrogen bond interaction are shown as pink-arrow, pi-pi stacking as green line and pi-cation as red line.

3.5.6 Ligand Interaction of Ginger with FIMH Adhesin

Figure 20a-f showed interaction of selected ginger compound with FIMH adhesin respectively.The interaction of reference compound (KGM) with FIMH adhesin was shown in figure 20a. Hydrogen bond interaction with amino acid residues GLY14, PHE1, ASP140, glutamine (GLN) 133, ASP54, ASP47. Hydrophobic interaction with amino acids ILE13, PHE142, TYR137, PHE1, ILE52, TYR48 were shown. 5-hydrohexahydrocurcumin in figure 20b, showed hydrogen bond interaction with amino acid residues ASP47, CYS3, HIS45, ASP54, ASN135. Pi-pi stacking interaction was shown with TYR137 and hydrophobic bonds were formed with ILE52, TYR137, PHE142, TYR48 similar to the reference compound (KGM).

3-acetoxy-5-hydroxy-1(4-hydrophenyl) in figure 20c, showed hydrogen bond interaction with amino acid residues TYR137, ASP54, ASP47, CYS3, HIP45. Pi-pi stacking interaction with TYR48 was shown. Hydrophobic bonds were formed with TYR48, ILE52, PHE142, TYR137 similar to the reference compound (KGM).

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In Figure 20d, Hexahydrocurcumin exhibited hydrogen bond interactions with amino acid residues CYS3, ASP54, ASN135, HIP45, and ASP47. It also formed π–π stacking interactions with TYR137, and hydrophobic interactions with ILE52, CYS3, VAL56, PHE144, CYS44, PHE142, TYR48, ILE13, and TYR137, closely resembling the binding pattern of the reference compound (KGM).

In Figure 20e, 5-hydroxy-1-(4-hydroxy-3-methoxyphenyl) demonstrated hydrogen bonding with ASP54, HIP45, ASP47, CYS3, ASN135, and GLN133, while hydrophobic interactions were observed with TYR137, TYR48, ILE13, PHE142, and ILE52, also showing similarity to the reference compound (KGM).

: In Figure 20f, Quercetin exhibited hydrogen bond interactions with amino acid residues HIP45, CYS3, ASP47, ASP54, and ASP140. Additionally, it formed hydrophobic interactions with TYR137, PHE142, ILE13, TYR48, and ILE52, mirroring the interaction pattern of the reference compound (KGM).

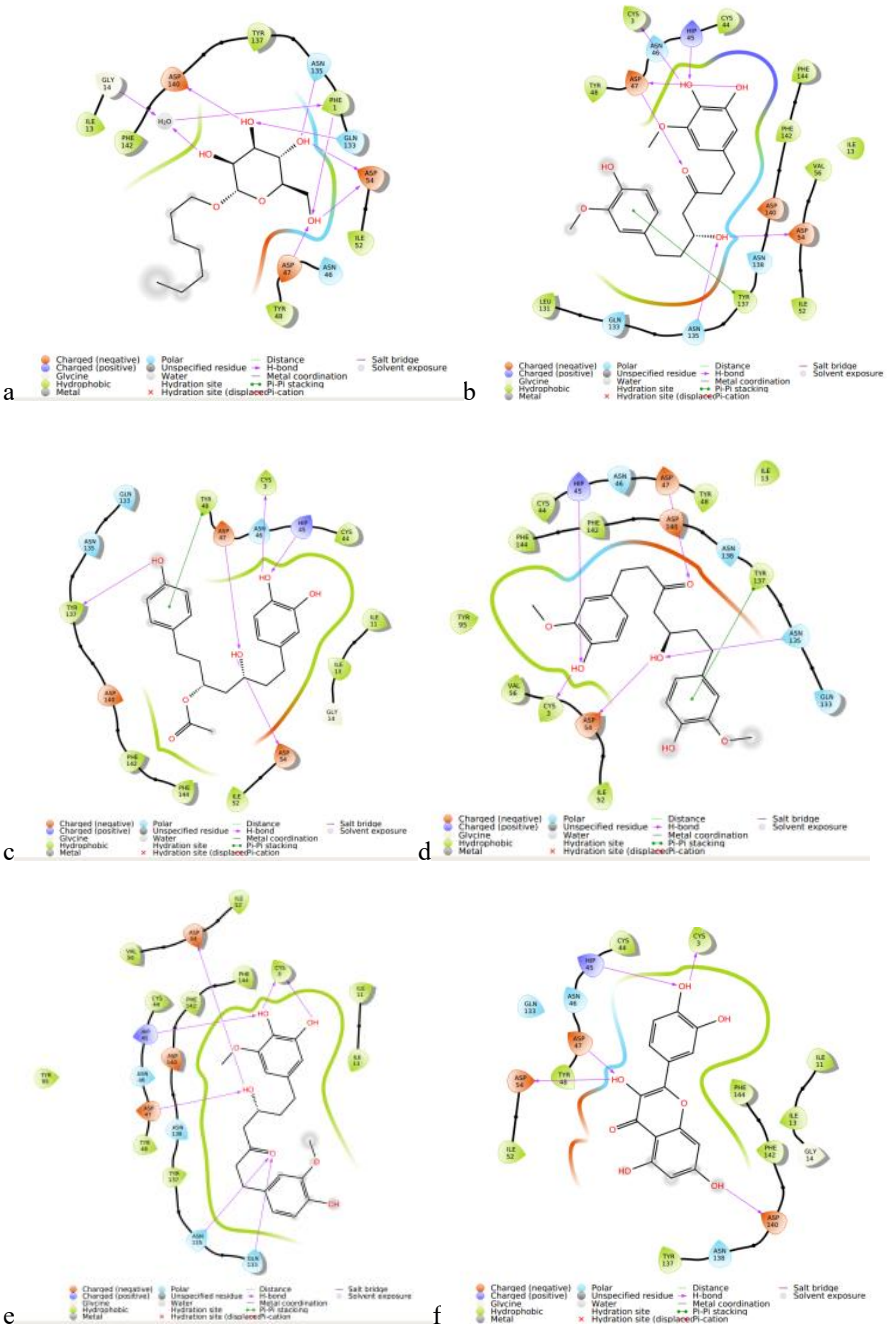


Figure 20: Ligand Interaction of Ginger compounds with FIMH Adhesin
Ligand Interaction with FIMH adhesin (a) KGM (b) 5-hydrohexahydrocurcumin (c) 3-acetoxy-5-hydroxy-1(4-hydrophenyl) (d) Hexahydrocurcumin (e) 5-hydroxy-1-(4-hydroxy-3-methoxyphenyl) (f) Quercetin. The amino acid residues with negative charge are shown in red, positive charge in velvet, polar in cyan, hydrophobic bonds in green, undefined residues in grey. Hydrogen bond interaction are shown as pink-arrow, pi-pi stacking as green line and pi-cation as red line.

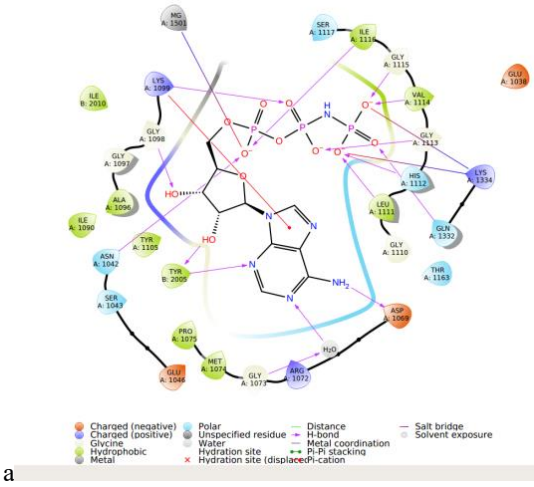
2.5.7 Ligand Interaction of Moringa with Par E Topoisomerase IV

In Figure 21a, the reference compound (ANP) exhibited hydrogen bond interactions with amino acid residues GLY1073, ASP1069, TYR2005, ASN1042, GLY1098, ILE1116, GLY1115, VAL1114, GLY1113, HIS1112, LEU1111, and GLN1332 of ParE topoisomerase IV. A π–π stacking interaction was observed with LYS1099, while hydrophobic interactions were formed with ILE2010, ALA1096, ILE1090, TYR1105, TYR2005, PRO1075, MET1074, LEU1111, VAL1114, and ILE1116.

In Figure 21b, Chlorogenic acid from Moringa adopted a binding conformation within the ParE topoisomerase IV active site by forming hydrogen bonds with GLU1046, GLY1073, GLY1098, ILE1116, GLY1115, VAL1114, GLY1113, HIS1112, and LEU1111. Hydrophobic interactions were noted with TYR1105, ALA1096, ILE1090, ILE1116, VAL1114, LEU1111, and TYR2005, similarly to the reference compound (ANP).

In Figure 21c, Sinalbin interacted with ParE topoisomerase IV by forming hydrogen bonds with ASN1042, ASP1069, GLY1073, and TYR2005. A π–π stacking interaction was observed with MG1501, and hydrophobic interactions were formed with LEU1111, ALA1096, ILE1090, VAL1114, ILE1116, TYR2005, and TYR1105, mimicking the binding profile of ANP.

In Figure 21d, Coumaroylquinic acid from Moringa exhibited stable binding within the ParE topoisomerase IV active site through hydrogen bonds with GLY1098, ILE1116, GLY1115, VAL1114, HIS1112, LEU1111, LYS1334, ASN1042, and ASP1069. Hydrophobic interactions were identified with TYR1105, ALA1096, ILE1090, ILE1116, VAL1114, LEU1111, MET1074, and TYR2005, comparable to the reference compound (ANP). In Figure 21e, Myricetin interacted within the binding site of ParE topoisomerase IV by forming a hydrogen bond with GLY1098 and a π–π stacking interaction with LYS1099. Additionally, it formed hydrophobic interactions with LEU1111, ILE1090, VAL1114, ILE1116, TYR2005, MET1074, and TYR1105, similar to the reference compound (ANP).
In Figure 21f, Neochlorogenic acid engaged the ParE topoisomerase IV active site by forming hydrogen bonds with GLY1113, ASP1069, and ILE1116. Hydrophobic interactions were also observed with ALA1096, MET1074, TYR1105, LEU1111, VAL1114, ILE1116, ILE1090, and TYR2005, closely resembling the interaction profile of ANP.



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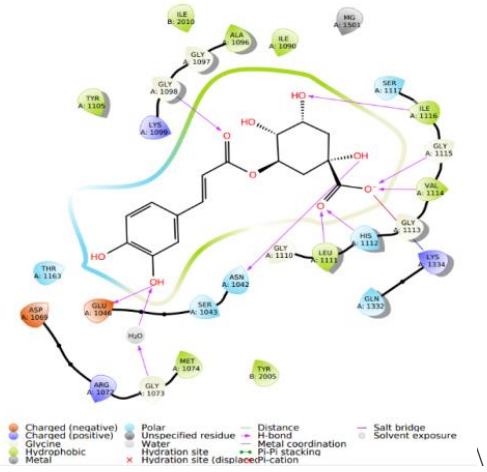

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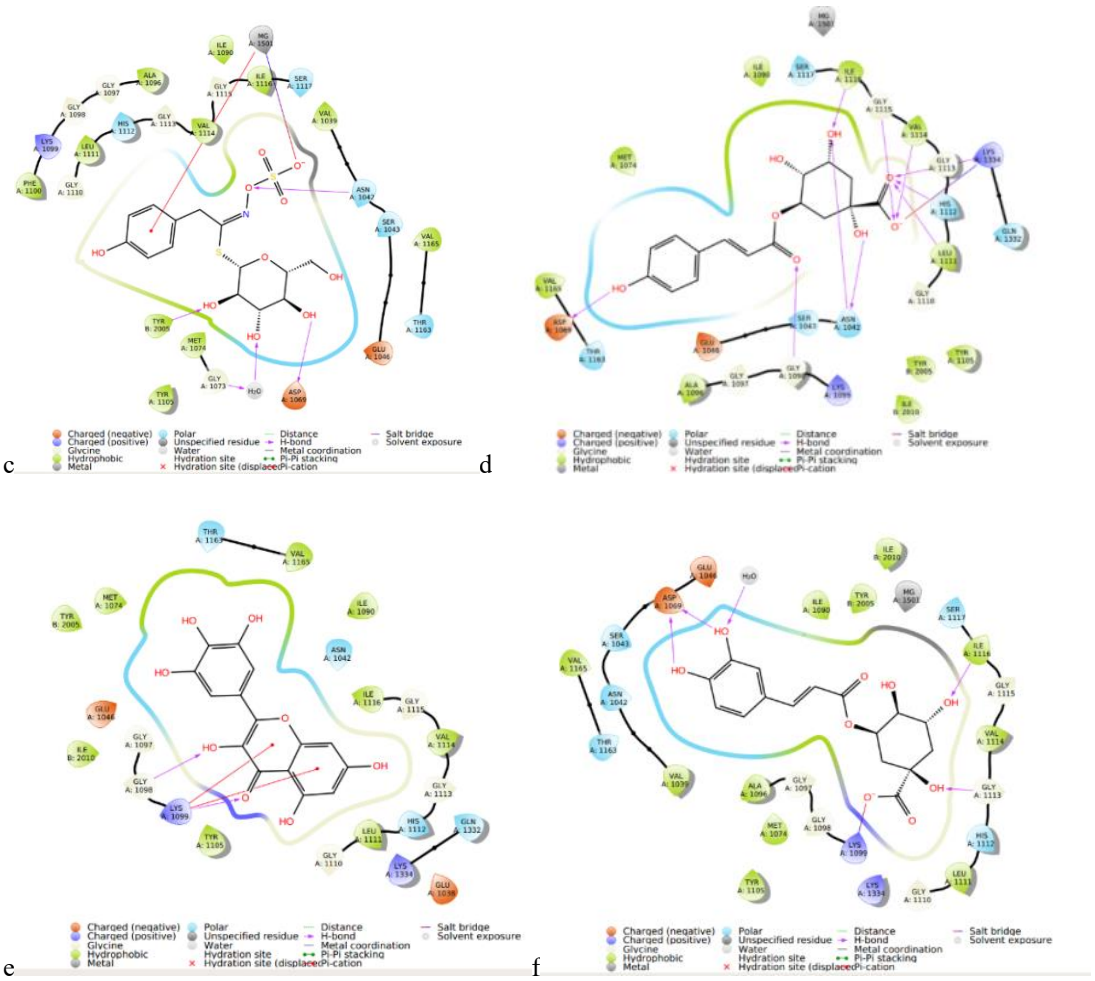


Figure 21: Ligand Interaction of Moringa compounds with Par E Topoisomerase IV
Ligand Interaction with Par E topoisomerase IV (a) ANP (b) Chlorogenic acid (c) Sinalbin (d) Coumaroylquinic acid (e) Myricetin (f) Neochlorogenic acid. The amino acid residues with negative charge are shown in red, positive charge in velvet, polar in cyan, hydrophobic bonds in green, undefined residues in grey. Hydrogen bond interaction are shown as pink-arrow, pi-pi stacking as green line and pi-cation as red line.

2.5.8 Ligand Interaction of Ginger with Par E Topoisomerase IV

In Figure 22a, the reference compound (ANP) formed hydrogen bonds with the amino acid residues GLY1073, ASP1069, TYR2005, ASN1042, GLY1098, ILE1116, GLY1115, VAL1114, GLY1113, HIS1112, LEU1111, and GLN1332 of ParE topoisomerase IV. A π–π stacking interaction was observed with LYS1099, while hydrophobic interactions were formed with ILE2010, ALA1096, ILE1090, TYR1105, TYR2005, PRO1075, MET1074, LEU1111, VAL1114, and ILE1116.

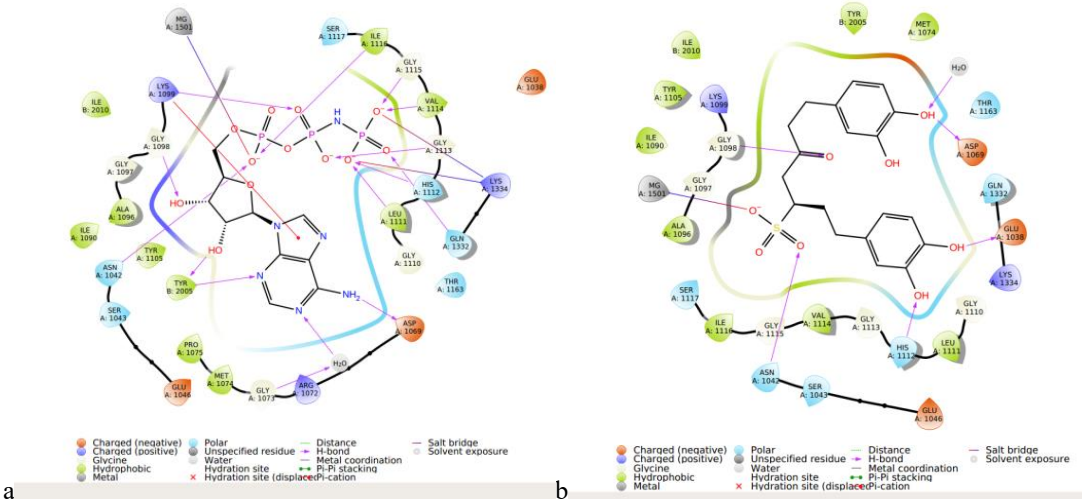
In Figure 22b, Shogasulfonic C from Ginger exhibited favorable binding within the active site by forming hydrogen bonds with ASN1042, GLY1098, HIS1112, and GLU1038. Hydrophobic interactions were observed with TYR1105, ILE1090, ALA1096, ILE1116, VAL1114, LEU1111, MET1074, and TYR2005, similar to those of the reference compound (ANP).

In Figure 22c, 5-hydroxy-1-(4-hydroxy-3-methoxyphenyl) adopted a stable conformation within the ParE topoisomerase IV binding site by forming hydrogen bonds with ASN1042, TYR2005, HIS1112, LEU1111, and ASP1069, as well as a π–π stacking interaction with LYS1099. Hydrophobic interactions were noted with TYR1105,

TYR2005, PRO1075, MET1074, ILE1090, ALA1096, LEU1111, VAL1114, and ILE1116, in a pattern similar to ANP.

In Figure 22d, Hexahydrocurcumin showed stable interaction within the binding pocket of ParE topoisomerase IV by forming hydrogen bonds with TYR1105, GLY1073, ASP1069, HIS1112, LEU1111, and GLY1098, along with a π–π stacking interaction with LYS1099. Hydrophobic bonds were formed with ILE1090, ALA1096, LEU1111, VAL1114, ILE1116, MET1074, TYR1105, and PRO1075, consistent with ANP binding.

In Figure 22e, 8-Zingerine demonstrated orientation within the ParE topoisomerase IV binding site by forming hydrogen bonds with TYR2005, VAL1039, MET1074, PRO1075, ALA1096, ILE1068, VAL1067, VAL1165, ILE1116, VAL1114, LEU1111, ILE2010, TYR1105, ILE1090, and LEU1091. π–π stacking interactions were observed with LYS1099 and ARG1072. Hydrophobic interactions included ILE1090, ALA1096, LEU1111, VAL1114, ILE1116, MET1074, TYR1105, PRO1075, TYR2005, and ILE1068, aligning closely with the ANP binding profile.
In Figure 22f, Ricinoleic acid interacted with the ParE topoisomerase IV binding site by forming hydrogen bonds with TYR1105, LYS1099, GLY1115, VAL1114, and HIS1112. Hydrophobic interactions were recorded with ILE1090, ALA1096, LEU1111, VAL1114, ILE1116, TYR2005, MET1074, and TYR1105, comparable to those of the reference compound (ANP).



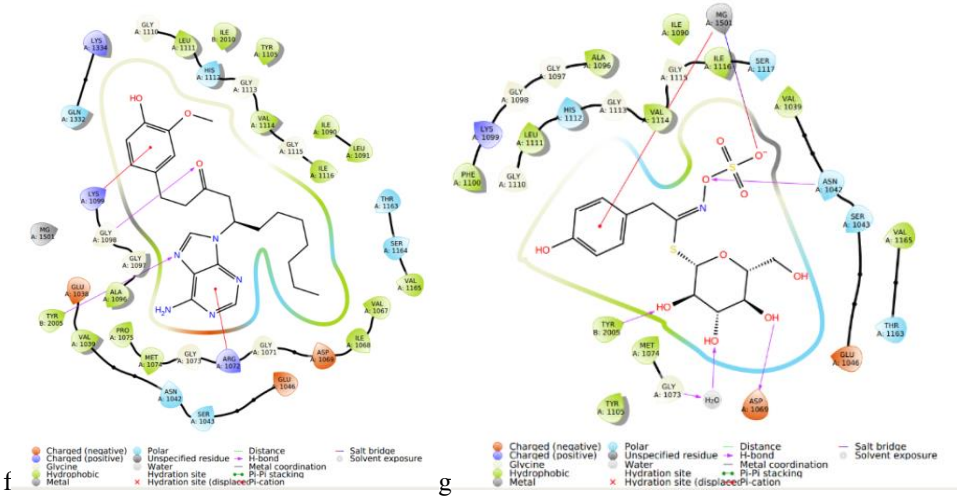


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Figure 22: Ligand Interaction of Ginger compounds with Par E Topoisomerase IV
Ligand Interaction with Par E topoisomerase IV (a) ANP (b) Shogasulfonic C (c) 5-hydroxy-1-(4-hydroxy-3-methoxyphenyl)(d) Hexahydrocurcumin (e) 8-zingerine (f) Ricinoleic acid. The amino acid residues with negative charge are shown in red, positive charge in velvet, polar in cyan, hydrophobic bonds in green, undefined residues in grey. Hydrogen bond interaction are shown as pink-arrow, pi-pi stacking as green line and pi-cation as red line.

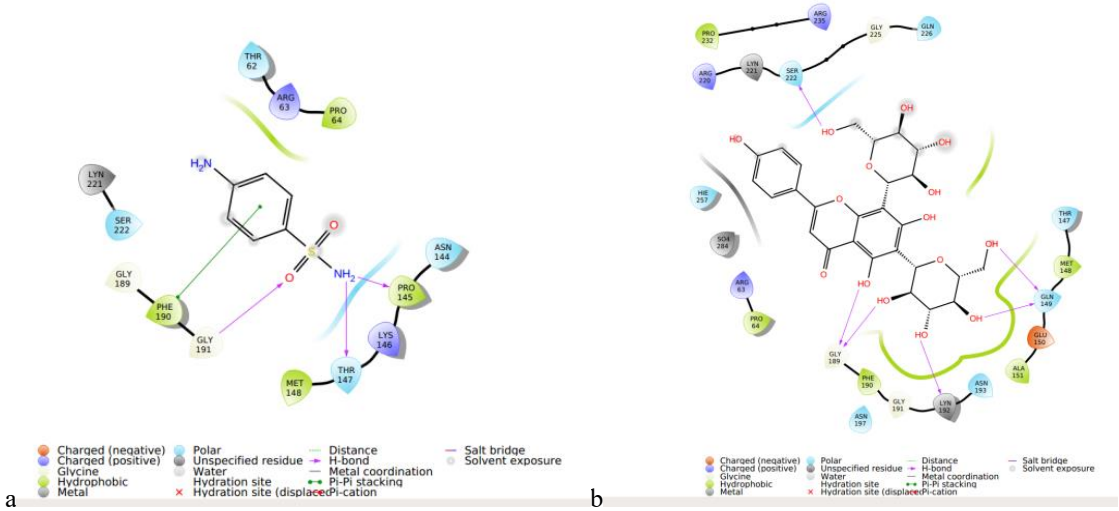
2.5.9 Ligand Interaction of Moringa Compounds with Dihydropteroate Synthase
The interaction of the reference compound (SAN) with dihydropteroate synthase is illustrated in Figure 23a. Hydrogen bonds were formed with the amino acid residues GLY192, TYR147, and PRO145, while a π–π stacking interaction was observed with PHE190. Hydrophobic interactions involved PHE190, PRO64, MET148, and PRO145.

Figures 23b–f display the interactions of various Moringa-derived ligands with dihydropteroate synthase:
Vicenin (Figure 23b) formed hydrogen bonds with SER222, GLY189, LYS192, and GLN149, and hydrophobic interactions with PRO64, PHE190, and MET148, similar to the reference compound (SAN).

Chlorogenic acid (Figure 23c) demonstrated hydrogen bonding with LYS192, GLY189, and THR147, along with hydrophobic interactions involving PRO145, PHE190, and PRO64, reflecting a binding pattern comparable to SAN.
Rutin (Figure 23d) established hydrogen bonds with SER222, GLN226, THR62, PRO64, and GLN149, and π–π stacking with PHE190. Hydrophobic interactions were formed with PRO145, PHE190, and PHE64, consistent with the interaction profile of SAN.

Neochlorogenic acid (Figure 23e) formed hydrogen bonds with LYS192, GLY189, GLN149, and THR62, and hydrophobic interactions with PRO64, PRO145, MET148, and PHE190, aligning closely with the reference compound's interactions.

Cryptochlorogenic acid (Figure 23f) engaged in hydrogen bonding with GLY189, GLN149, THR147, SER222, and GLY191, and exhibited π–π stacking with PHE190. Hydrophobic bonds were formed with PRO64, PHE190, MET148, and PRO145, mirroring those of SAN.


Charged (negative)
Charged (positive)
Glycine
Hydrophobic
Metal
Polar
Unspecified residue
Water
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Hydration site (displaced
Distance
H-bond
Metal coordination
Pi-Pi stacking
Pi-cation
Salt bridge
Solvent exposure

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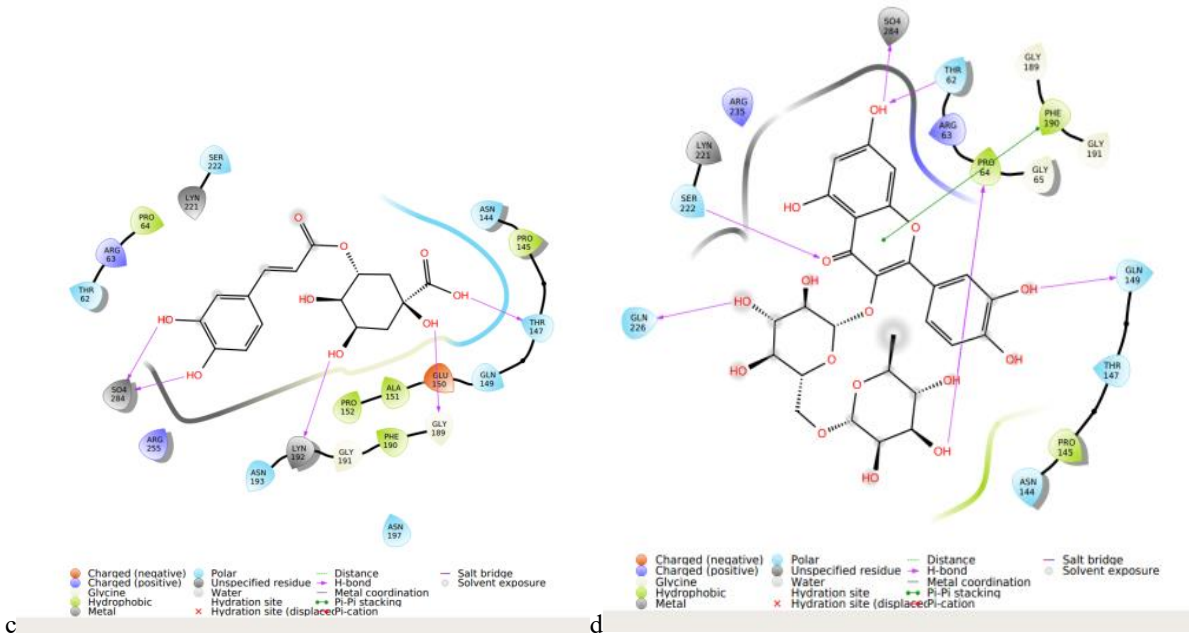
Charged (negative)
Charged (positive)
Glycine
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Metal
Polar
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Pi-Pi stacking
Pi-cation
Salt bridge
Solvent exposure

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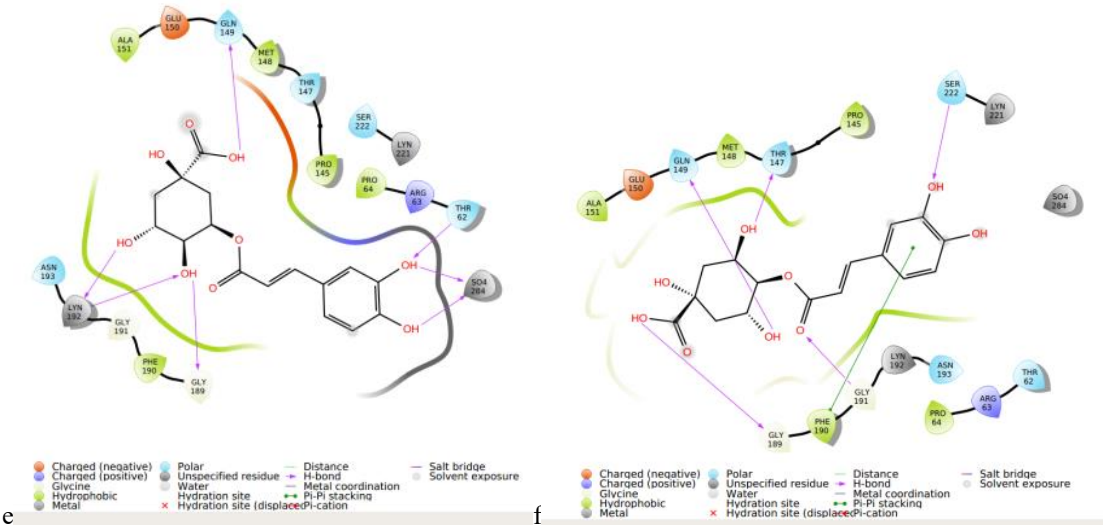

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Figure 23: Ligand Interaction of Moringa compounds with Dihydropteroate Synthase
Ligand Interaction with dihydropteroate synthase (a) SAN (b) Vicenin (c) Chlorogenic acid (d) Rutin (e) Neochlorogenic acid (f) Cryptochlorogenic acid. The amino acid residues with negative charge are shown in red, positive charge in velvet, polar in cyan, hydrophobic bonds in green, undefined residues in grey. Hydrogen bond interaction are shown as pink-arrow, pi-pi stacking as green line and pi-cation as red line.

2.5.10 Ligand Interaction of Ginger Compounds with Dihydropteroate Synthase
The interaction of the reference compound (SAN) with dihydropteroate synthase is illustrated in Figure 24a. Hydrogen bonds were formed with amino acid residues GLY192, TYR147, and PRO145, while π–π stacking was observed with PHE190. Hydrophobic interactions involved PHE190, PRO64, MET148, and PRO145.

Figures 24b–f depict the binding interactions of selected Ginger compounds with dihydropteroate synthase:
In Figure 24b, Shogasulfonic C formed hydrogen bonds with SER222, PRO145, and GLY189, and hydrophobic interactions with PHE190, PRO145, and PRO64, resembling the interaction pattern of SAN.

In Figure 24c, Zingiberoside C formed hydrogen bonds with GLY191, GLY189, and THR62. Hydrophobic interactions were observed with PHE190, PRO64, PRO145, and MET148, consistent with SAN.

In Figure 24d, Quercetin interacted via hydrogen bonds with THR62 and GLN142, and formed π–π stacking with PHE190. Hydrophobic interactions involved PHE190, PRO145, and PRO64, similar to the reference compound.

In Figure 24e, 5-hydroxy-1-(4-hydroxy-3-methoxyphenyl) formed hydrogen bonds with SER222, GLN149, and ASN144. Hydrophobic interactions with PHE190, PRO145, and PRO64 mirrored those of SAN.

In Figure 24f, 5-hydroxyhexahydrocurcumin interacted through hydrogen bonds with GLY189 and ASN144, while forming hydrophobic interactions with PHE190, PRO145, and PRO64, consistent with the reference compound.

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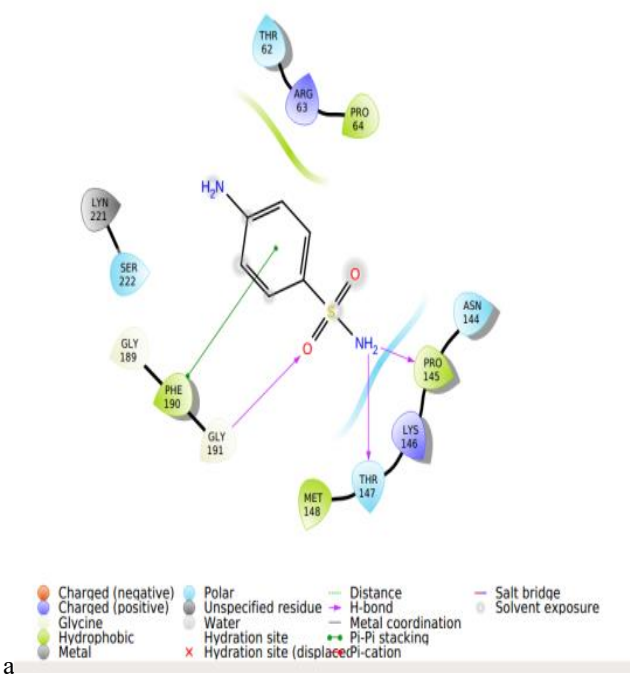

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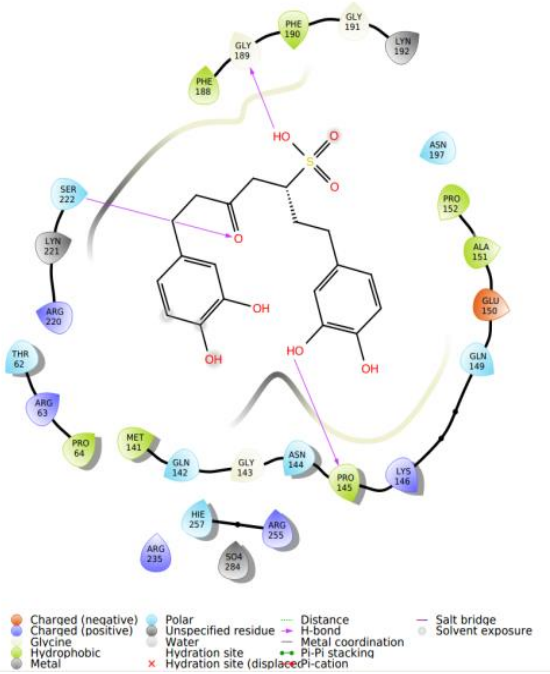

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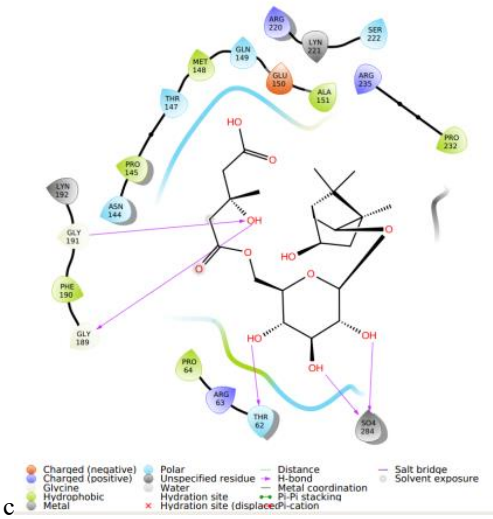

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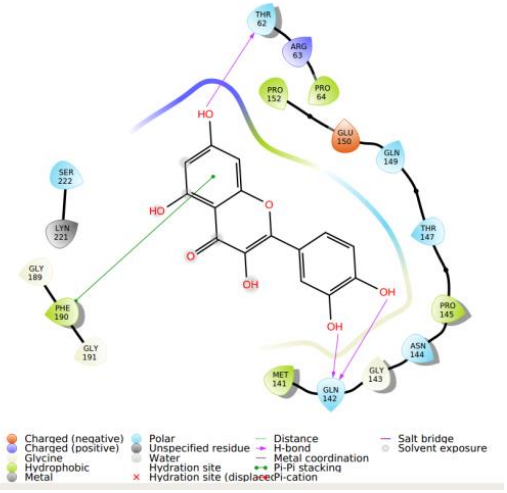

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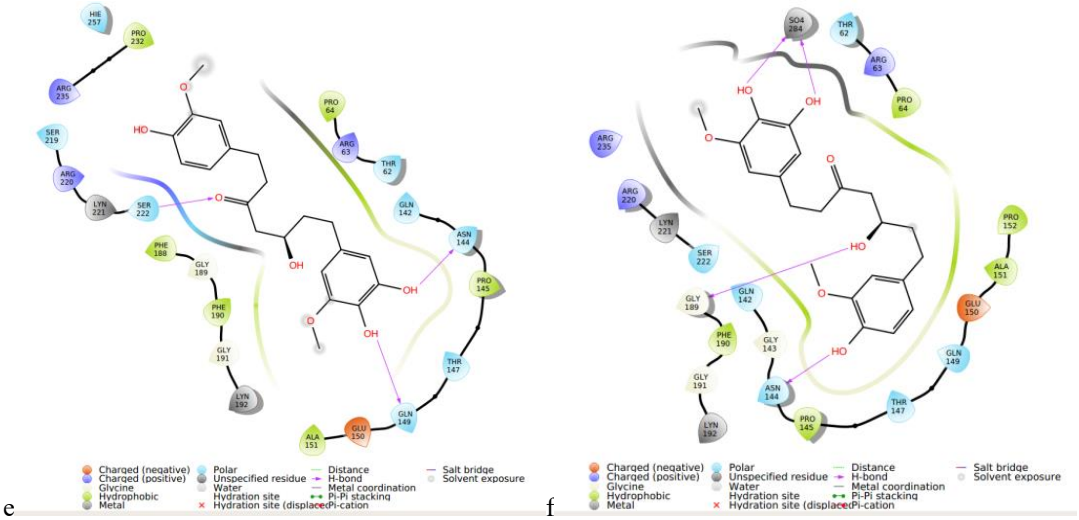

Figure 24: Ligand Interaction of Ginger compounds with Dihydropteroate Synthase
Ligand Interaction with dihydropteroate synthase (a) SAN (b) Shogasulfonic C (c) Zingeberoside C (d) Quercetin (e) 5-hydroxyhexahydrocurcumin (f) 5-hydroxyhexahydrocurcumin. The amino acid residues with negative charge are shown in red, positive charge in velvet, polar in cyan, hydrophobic bonds in green, undefined residues in grey. Hydrogen bond interaction are shown as pink-arrow, pi-pi stacking as green line and pi-cation as red line.

4. DISCUSSION

This study investigated the antibacterial activity of Moringa oleifera (Moringa) and Zingiber officinale (Ginger) extracts against E. coli, with the goal of identifying potential compounds for drug development. Our findings demonstrate that both Moringa and Ginger possess antibacterial properties against E. coli. The minimum inhibitory concentration (MIC) for Moringa was found to be 200 mg/ml, while Ginger had an MIC of 400 mg/ml. Furthermore, the minimum bactericidal concentration (MBC) was determined to be 400 mg/ml for Moringa and 800 mg/ml for Ginger. These results align with previous studies highlighting the antibacterial efficacy of M. oleifera leaves and Z. officinale against E. coli [31, 32, 33]. In comparison, the conventional antibiotic Ciprofloxacin exhibited a broader zone of inhibition than both plant extracts. This enhanced activity is likely due to Ciprofloxacin being a more purified and concentrated antibacterial agent [17, 30, 16, 34]. While the antibacterial activity of these plants is evident, the precise mechanisms are not yet fully understood [35]. Conventional antimicrobial agents typically act through five main mechanisms: inhibiting cell wall synthesis, protein synthesis, cell membrane function, nucleic acid synthesis, or metabolic pathways (e.g., folic acid synthesis). These inhibitions occur through specific interactions with bacterial proteins. To identify novel medicinal compounds and understand their mechanisms, molecular docking was employed. This technique allows for the prediction of how compounds interact with specific target proteins within E. coli. We selected five E. coli receptors crucial for the organism's survival and pathogenicity, including those involved in adhesion, replication, folic acid synthesis, and fatty acid synthesis. The docking studies revealed that several compounds from Moringa and Ginger interacted effectively with the active sites of these target receptors, similar to reference compounds. The key findings are detailed as follows: Dihydropteroate Synthase Inhibition (Folic Acid Synthesis): This enzyme is vital for folic acid metabolism and pyrimidine synthesis [37]. Shogalsulfonic C from Ginger and Vicenin from Moringa showed top docking scores of -7.983 kcal/mol and -10.768 kcal/mol, respectively. These scores are significantly better than the reference compound (SAN) at -4.197 kcal/mol, indicating that these two lead ligands form more stable receptor-ligand complexes. This suggests that Shogalsulfonic C and Vicenin can effectively inhibit Dihydropteroate synthase and could serve as alternatives to conventional sulfonamide drugs [37]. This aligns with research where Dihydropteroate synthase from E. coli was inhibited by ethyl Iso-allocholate from medicinal rice [37]. DNA Gyrase B Inhibition (Bacterial Replication): DNA gyrase B is a crucial protein for E. coli replication. Shogalsulfonic C from Ginger and Quercetin-3-o-malonylglucoside from Moringa achieved peak docking scores of -9.202 kcal/mol and -10.247 kcal/mol, respectively. Compared to the reference compound (CWW) at -5.765 kcal/mol, these two compounds demonstrate strong potential to inhibit DNA gyrase B, making them suitable replacements for Ciprofloxacin [38]. Similar inhibition of this receptor by compounds like Myricetin and Taxifolin has been reported [39]. Enoyl Acyl Carrier Protein Reductase (FabL) Inhibition (Fatty Acid Synthesis): FabL is the

final enzyme in E. coli's fatty-acid biosynthetic pathway and is a promising drug target. Shogalsulfonic C from Ginger and Rutin from Moringa exhibited high docking scores of -11.596 kcal/mol and -13.318 kcal/mol, respectively. These scores surpass the reference compound (NAD) at -12.11 kcal/mol, indicating that these compounds can effectively inhibit Enoyl ACP reductase and potentially replace conventional drugs like Triclosan. This finding is consistent with studies where Benzotriazole (A1) inhibited this protein [40]. FIMH Adhesin Inhibition (Bacterial Adhesion): FIMH adhesin is an adhesion protein that enables E. coli to adhere to host cells. 5-hydrohexahydrocurcumin from Ginger and Nicotiflorin from Moringa yielded the highest docking scores of -8.427 kcal/mol and -10.342 kcal/mol, respectively. These are superior to the reference compound (KGM) at -5.717 kcal/mol, suggesting that these two compounds can actively inhibit FIMH adhesin and are promising novel antibacterial agents. This aligns with research on FIMH adhesin inhibition for E. coli-caused urinary tract infections [41]. Par E Subunit DNA Topoisomerase IV Inhibition (DNA Replication): The Par E subunit of DNA topoisomerase IV, containing ATP binding pockets, is critical for DNA replication. Shogalsulfonic C from Ginger and Chlorogenic acid from Moringa recorded impressive peak docking scores of -17.036 kcal/mol and -13.592 kcal/mol, respectively. These are better than the reference compound (ANP) at -15.637 kcal/mol, indicating that these two compounds can effectively inhibit DNA topoisomerase IV E subunit and could serve as replacements for fluoroquinolone drugs. This is consistent with studies where Chlorogenic acid inhibited the Main-protease of SARS-CoV-2 [42, 43].

5. CONCLUSION

Our comprehensive study not only validates the traditional use of Moringa and Ginger as antimicrobial agents against E. coli but also identifies specific compounds within them—such as Shogalsulfonic C, Vicenin, Quercetin-3-o-malonylglucoside, Rutin, 5-hydrohexahydrocurcumin, Nicotiflorin, and Chlorogenic acid—that exhibit strong potential as novel antibacterial drug candidates. These compounds demonstrate promising interactions with key E. coli proteins, suggesting diverse mechanisms of action that could be leveraged in the development of new treatments for a wide range of infections. The identification of these potent compounds from natural sources like Moringa and Ginger opens up exciting avenues for addressing the growing challenge of antimicrobial resistance. These findings have several practical applications: Firstly the lead compounds identified, such as Shogalsulfonic C and Vicenin, can serve as scaffolds for designing and synthesizing novel antibacterial agents with improved efficacy and reduced side effects. Secondly, given the increasing resistance to conventional antibiotics, these natural compounds could lead to alternative therapeutic options for E. coli-related infections, particularly those affecting the urinary tract, gastrointestinal system, and other body parts. This research also supports the potential for integrating natural products into modern medicine, offering a sustainable source for drug discovery. It highlights the value of traditional knowledge in identifying promising medicinal plants and finally by providing effective natural alternatives, this work could help decrease the overuse of synthetic antibiotics, thereby contributing to the global effort to combat antibiotic resistance. Future research should focus on the in vitro and in vivo validation of the identified lead compounds, including toxicity assessments and further elucidation of their precise mechanisms of action and pharmacokinetics to pave the way for clinical trials.

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Author contributions

AJF, JH, and ASB conceptualised the study. AJF, ASB, JH and OOB designed the study. AJF, JH, AEH and ACC participated in the bench work and data collection. AJF, JH, EAH, ACC, OOB and THZ, ASB performed the data analysis; AJF, JH, ASB, and OOB interpreted the data. ASB, JH, and AJF prepared the first draft of the manuscript, which was reviewed by JH, EAH, ASB, AJF, ACC, THZ and OOB. All the authors contributed to the development of the final manuscript and also approved its submission for publication.

Conflicts of interest

None to declare

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