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Profiles and Molecular Docking Simulations of Potential Bioactive Compounds Found in Ginger (*Zingiber officinale*), Garlic (*Allium sativum*) and Chili Pepper (*Capsicum anuum*) Extracts

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ABSTRACT

This study uses molecular modeling to examine how bioactive compounds from ginger, garlic, and chili peppers interact with key pest proteins. Biopesticides offer a cost-effective and environmentally friendly alternative for pest control, particularly beneficial for farmers in sub-Saharan Africa. Five treatments (0g/l, 3g/l, 7.5g/l, 12g/l and 15g/l) of a biopesticide mixture (ginger, garlic and chili pepper in the ratio of 1:1:1) were applied on tomato (*Solanum lypercicum*) plants to control aphid (*Aphis gossypii*) infestation. Results from these applications showed that the treatment 15g/l most effectively controled aphid infestation on tomato (*Solanum lypercicum*) plants. HPLC-DAD-MS analysis identified four major bioactive compounds: 6-gingerol and 6-shogaol (from ginger), allicin (from garlic), and capsaicin (from chili peppers). These compounds were tested as ligands against three critical pest target proteins: PERK (Protein Kinase R-like Endoplasmic Reticulum Kinase, PDB ID: 4X7K), TRPV (Transient Receptor Potential Vanilloid, PDB ID: 7LPE), and SARS-CoV-2 Main Protease (PDB ID: 6Y2E). Targeting these receptors provides an eco-friendly approach to disrupting pest survival, behavior, and disease transmission in agriculture. Molecular docking simulations, conducted using the Molecular Operating Environment (MOE), evaluated binding affinities and interactions. Among the tested compounds, capsaicin exhibited the strongest affinity across all modeled receptors, with its interaction with PERK-4X7K yielding the most favorable binding energy of -8.2 ± 0.2 kcal/mol. Further analysis of drug-like and ADME properties revealed that capsaicin's larger molecular size (305.15 g/mol), high total polar surface area (TPSA), high lipophilicity, and low water solubility contribute to its bioactivity. These findings underscore capsaicin's potential as a natural pest control agent, supporting its role in sustainable agriculture.

Keywords: biopesticides, capsaicin, gingerols, shogaols, allicin, molecular docking

INTRODUCTION

Ginger is found in the Zingiberaceae family comprising about 53 genera and a total of over 1200 species.[1] It is widely distributed in the tropical region of Asia, Africa, and America. These plants are taxonomically characterized as perennial, aromatic, tuberous and non-tuberous rhizomes.[2] The rhizome is the main part of the plant which is economically important and a rich source of effective phytoconstituents for biological activities.[2, 3]Ginger (*Zingiber officinale* Rosc.) is one of the most popular species belonging to this family, China, Thailand, Vietnam, India, and Indonesia are considered to be center of origin. It has been mainly utilized as a food seasoning ingredient [4] and medicinal resource particularly for treating diseases related to inflammation and oxidative stress.[5–9] For its wide range of health functionality, the presence of higher concentration of phenolic derivatives plays an important role. [6, 9–11] Over the last three decades, extensive studies have been conducted to understand the detailed chemical composition and biological activities of normal ginger. Phenolic acids, diarylheptanoids, terpenoids, and flavonoids were reported to exist in ginger rhizomes.[11,12] Gingerol and shogaol related derivatives are the principal medicinally active components contributing to the characteristic pungent flavour of ginger together with essential oil major component, zingerone.[12, 13] Gingerols and gingerdiols have

demonstrated many anti-fungal properties. The maturation state, environment, cultivar, and processing steps are major factors to influence the biosynthesis and concentration of the chemical composition in the rhizomes.[14]

Garlic (*Allium sativum L.*) belongs to the family Alliaceae containing more than 800 species. Garlic is a perennial plant grown for its bulbs. The bulb is covered with membranous skin and encloses up to 20 edible bulblets called cloves. The genus *Allium* is widely cultivated over the warm-temperate and tropical regions in Africa, America, Asia and Europe. Garlic is commonly used as a kitchen spice and a flavouring agent. Garlic has also been used as a medicine such as in maintaining stamina, clearing the respiratory tract from coughing and phlegm, maintaining healthy hair and skin, relieving nausea, treating toothache, treating insect and snake bites, preventing infections and reducing obesity.[15,16] Phytochemical screening has shown that garlic contains allicin, flavonoids, phenols, and terpenoids. Allicin (sulphur containing compounds) has shown many antimicrobial and pest repelling properties. The aphid (*Aphis gossypii*) can be controlled by garlic treatments on cotton plants.[17] Beyond its well documented strong antibacterial properties, allicin also shows toxic effects towards fungal cells and is able to inhibit spore germination and hyphal growth *in vivo* and *in vitro*. Some efforts have been made to utilize this activity and develop allicin for application in medical therapy and agricultural plant protection.[18]

Chili peppers (*Capsicum anuum*) are annual plants found in the Solanaceae family with more than 40 species, cultivated worldwide for their fruits.[19] These fruits are economically important for their varying sizes, shapes and colours. In addition to spicing food chili peppers have been shown to contain antioxidants and immune boosters. Excessive consumption of chili peppers leads to stomach irritations. Capsaicin and its derivatives have been identified as phytochemicals in chili peppers. Capsaicin (phenolic amide) produces a burning sensation when it comes in contact with the eyes, skin and mucous membranes.[20]It has been shown to have antibacterial properties, [21] and a bio- repellant to insect pests.[22]

Botanical pesticides, derived from plants, are gaining traction as eco-friendly alternatives to synthetic pesticides. Analyzing these biopesticides requires a combination of research skills, experimental techniques, and specialized equipment to ensure efficacy and safety in agricultural applications. The main bioactive compounds of ginger, garlic and chili peppers have mostly been exploited medically but their use against pests is still under study. Insect transient receptor potential vanilliod channels (TRPV) have been identified as potential targets of insecticides.[23] Against the above background, the objectives of this study were to; (1) evaluate the effect of biopesticide treatments (ginger, garlic and chili pepper mixtures) on aphids and profile potential bioactive compounds using IR and HPLC-MS techniques, (2) use molecular docking simulations to highlight important physico-chemical properties of the potential bioactive ligands.

Materials and Methods

Biopesticide preparation

The biopesticide consisted of 500g each of ginger rhizome, garlic cloves and chili pepper fruits, purchased from the Yaounde Central market (fig.1). The peeled garlic cloves were dried together with the ginger and chili pepper fruits under a shade at 25°C. The dried ginger, garlic and chili pepper were then ground separately to powder (using a Samsung blender 1000 W).

Fig.1. A= Ginger rhizome, B= Garlic cloves C= chili pepper fruit

Five treatments of biopesticide composed of ginger, garlic and chili pepper in the ratio of 1:1:1 were prepared according to table 1.

Table 1: Treatment description of varying concentrations of ginger, garlic and chili pepper.

Treatment	Description
T_0 (control)	0g ginger powder + 0g garlic powder+ 0g chili pepper powder dissolved in 1litre of water =0g/l
T_1	1g ginger powder + 1g garlic powder+ 1g chili pepper powder dissolved in 1litre of water =3g/l
T_2	2.5g ginger powder + 2.5g garlic powder + 2.5g chili pepper powder dissolved in 1litre of water =7.5g/l
T_3	4g ginger powder + 4g garlic powder + 4g chili pepper powder dissolved in 1litre of water =12g/l
T_4	5g ginger powder + 5g garlic powder + 5g chili pepper powder dissolved in 1litre of water =15g/l

Planting material: One month old tomato (*Solanum lycopersicum*) plant seedlings were used.

Experimental site: the field trials were conducted on an experimental farm at Nkong- Bibega, Mbankomo sub-division Centre region, Cameroon, located at latitude 3°49′52.54″N and longitude 11°27′15.79″E and 714m above sea level. The area is characterized as a humid rainforest zone and the soil is clay loam. The total annual rainfalls for 2023 was 1802.8 mm while the total rainfalls during the period of experimentation (March to June 2023) was 1730.2mm.

Experimental design

The experimental design was a randomized complete block design (RCBD) with 3 replications. The site was divided into 3 blocks. Each block was further divided into 5 experimental plots. Each experimental plot measured 4m x 3m with plant spacing of 0.5m giving 48 tomato plants per plot.

Planting and biopesticide applications

One month old *Solanum lycopersicum* plant seedlings were placed in holes of depth 10cm. One week after planting, five treatments (0g/l, 3g/l, 7.5g/l, 12g/l and 15g/l) of the biopesticide mixture were applied twice a week, on the leaves of *Solanum lycopersicum* plant seedlings.

Aphid scouting and aphid scores

After planting, scouting for aphids was done once per week for a period of 10 weeks. The aphid count score data was recorded in table 2.

Extraction of bioactive compounds

500g each of ginger rhizome, garlic cloves and chili peppers fruits were crushed (using a Samsung blender 1000 W) separately in 500ml of an extraction solvent (Water /methanol solvent (50v/v)). Each homogenous mixture was filtered by vacuum filtration. The Extracts obtained were then stored at -20 ºC in a refrigerator.

IR spectrum interpretation

PekinElmer spectrum infrared version 10.6.1 was used to identify the characteristic functional groups in the extract components. A small quantity (5 mg) of the extract was dispersed in dry potassium bromide (KBr). The mixture was thoroughly mixed in a mortar and pressed at pressure of 6 bars within 2 min to form a KBr thin disc. Then the disc was placed in a sample cup of a diffuse reflectance accessory. The sample was scanned from 4000 - 400 cm^{-1}.

Determination of purity:

The purity of extract was determined by HPLC analysis.

Qualitative determination of bioactive compounds using HPLC-DAD-(HR) ESI-MS

Sample preparation

Aqueous preparation extracts were separately dissolved in HPLC grade methanol in a concentration of 5 mg/ml then filtrated through a syringe-filter-membrane. Aliquots of 5 µl were injected into the LC-DAD/MS Dionex Ultimate 3000 HPLC, used for performing the analyses.

HPLC-MS conditions

High resolution mass spectra were obtained with an OTOF Spectrometer equipped with a HRESI source and a UV-vis absorbance detector. The spectrometer was operated in positive mode (mass range: 100-1500, with a scan rate of 1.00 Hz) with automatic gain control to provide high-accuracy mass measurements within 2 ppm deviation using Na Formate as calibrant. Mass spectra were simultaneously acquired using electrospray ionization in the positive ionization mode. The following parameters were used for experiments: spray voltage of 4.5 kV, capillary temperature of 200°C. Nitrogen was used as sheath gas (10 l/min). The spectrometer was attached to an Ultimate 3000 (Thermo Fisher, USA) HPLC system consisting of LC-pump, UV traces were measured at 215, 218, 254, 280 and 330 nm and UV spectra-Diode Array Detector-(DAD) were recorded between 190 and 600 nm, autosampler (injection volume 5 □l) and column oven (35,0 °C). The separations were performed using a Synergi MAX-RP 100A (50x2 mm, 2.5µ particle size) with a H2O (+0.1% HCOOH) (A)/acetonitrile (+0.1% HCOOH) (B) gradient (flow rate 500 µL/min). Samples were analyzed using a gradient program as follows: 95% A isocratic for 1.5min, linear gradient to 100 % B over 6 min, after 100% B isocratic for 2min, the system returned to its initial condition (90 % A) within 1 min and was equilibrated for 1 min.

Identification of peaks

Identification of all constituents was performed by HPLC-DAD-MS/MS analysis and by comparing the UV, MS spectra and MS/MS fragmentation of the peaks in the samples with those of data reported in the literature of Scifinder database.

Molecular Docking Methods

In this study, the interactions between the 4 ligands (Allicin, Capsaicin, Gingerol and Shogaol) and 3 pest protein targets (PERK-4X7K,TRPV-7LPE and SARS-6Y2E) were modeled using two major docking tools: AutoDock Vina and the Molecular Operating Environment (MOE).15-17 The USCF Chimera tool Dock Prep was used to refine the receptor molecules by removing solvents, fixing non-standard residues, adding hydrogens, and assigning Gasteiger charges.15-17 AutoDock Vina software was then employed to perform a global search of the best bound complexes, which were then ranked and scored based on favorable hydrophobic, hydrogen bond, and van der Waals interactions. This was performed using the protein and ligand coordinates along with a search volume box with size 25 Å x 22 Å x 32 Å centered around the binding sites of target proteins. The proteins and ligands were rigid during the docking, and the complexes with root-mean square deviations (RMSD) less than 1.0 Å were clustered according to their energy of binding. The docked complexes with the lowest binding energies were then extracted for further analysis.

The Molecular Operating Environment (MOE) software was also used to characterize the interaction affinity between the ligands and protein receptors. Each optimized ligand was uploaded into an MOE window, subjected to 3D protonation and energy minimization, and saved in a molecular database (MDB) file for docking. The crystal structures for each receptor were uploaded into MOE, and prepared for docking using the QuickPrep feature of MOE as described by Al-Karmalawy and Khattab.15,18,19 This involved the addition of hydrogens in appropriate geometries, removal of solvent molecules, and minimization of the structure to relax atomic clashes and correct protein issues. The docking simulation was done using the 2 MOE default forcefields (CHARMM27 and Amber10: EHT), with atoms tethered 8 Å around the active site, allowing for enhanced flexibility of site molecules during the docking process. The docking site was selected as receptor atoms, the ligand placement methodology with triangle matcher, and the London dG scoring function to estimate the free energy of binding. The refinement methodology was adjusted as Induced Fit, with a scoring function based on GBVI/WSA dG to select the 5 best poses out of 30 for each ligand/receptor system.[24]

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RESULTS

Aphid score counts

Results from the record of aphid score counts after 10 weeks of observations are summarized in table 2. The treatments 12g/l and 15g/l were more effective in controlling aphid infestations compared to the control (0g/l).

Table 2: Record of aphid count Score

	Weeks after planting									
Treatments	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
T_0 (0g/l)	None	Very Light	Very Light	Light	Medium	Heavy	Heavy	Heavy	Heavy	Heavy
T_1 (3g/l)	None	Very Light	Very Light	Very Light	Light	Light	Light	Medium	Light	Light
T_2 (7.5g/l)	None	Very Light	Very Light	Very Light	Very Light	Very Light	Very Light	Very Light	Very Light	Very Light
T_3 (12g/l)	None	Very Light	Very Light	Very Light	Very Light	None	Very Light	None	None	None
T_4 (15g/l)	None	Very Light	none	Very Light	None	None	None	None	None	None

KEY: None= No aphids present, Very Light= 1-3 aphids found on plants, Light= Large family of aphids on a few plants, Medium= Aphids are found on numerous plants, Heavy= Numerous aphids on most plants and leaves show much curling

IR Spectra

The results from our IR spectra analysis are illustrated in fig 2, while table 3 defines the different functional groups found in the test samples.

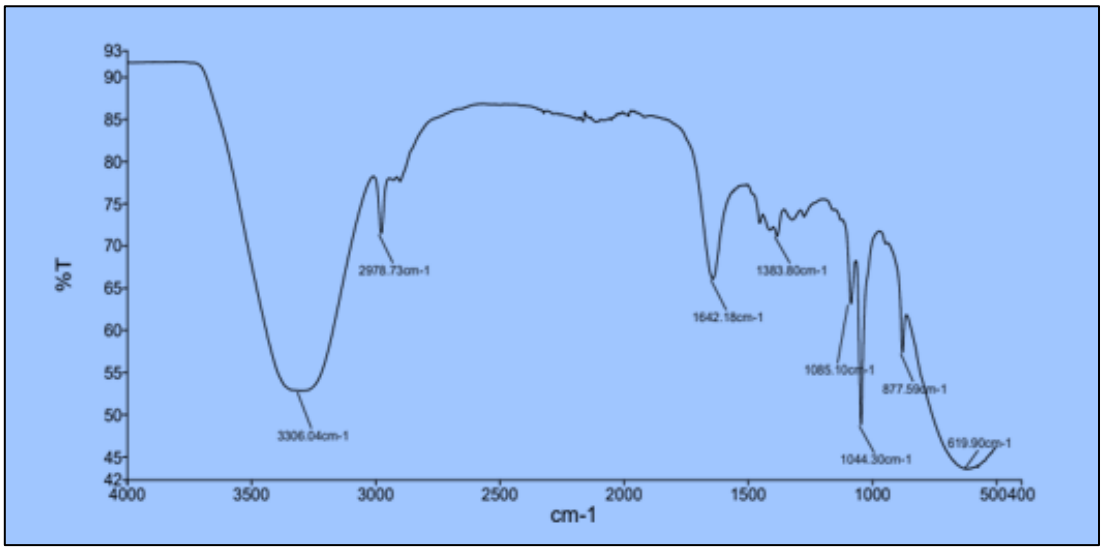

Fig. 2: IR spectra of mixture (ginger, garlic and chili pepper) extract

Table 3: IR Interpretation

Sr No	Functional group	Theoritical peaks (cm^{-1})	Practical peaks (cm^{-1})
1	C-H(stretch)	2700-3300	2978.73
2	C-O(stretch)	900-1300	1085.80, 1044.30
3	O-H(stretch)	3000-3700	3306.04
4	C=O (stretch)	1600-1900	1642.18

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HPLC Spectra

The HPLC chromatograms for the different test samples are illustrated in fig. 3(blank), fig. 4. (ginger extract), fig.5 (garlic extract), fig.6 (chili pepper extract) and fig.7(mixture of ginger, garlic and chili pepper extracts).

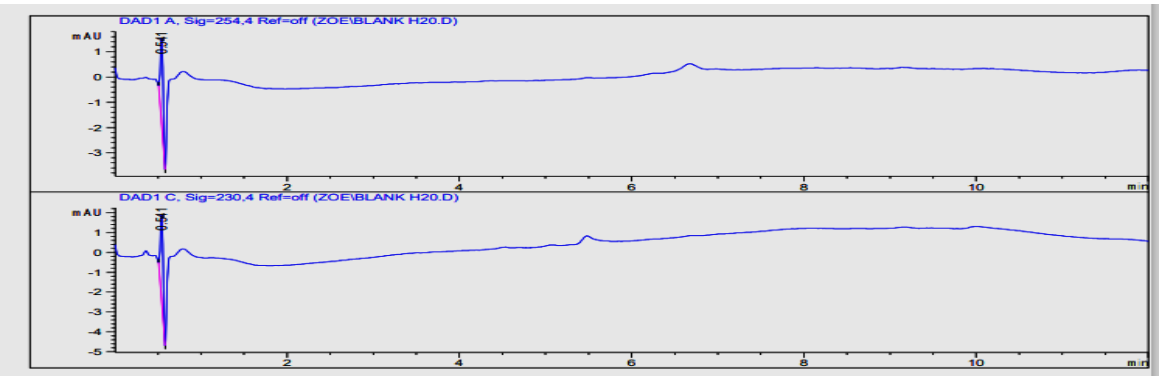

Fig. 3: HPLC profile of blank (water)

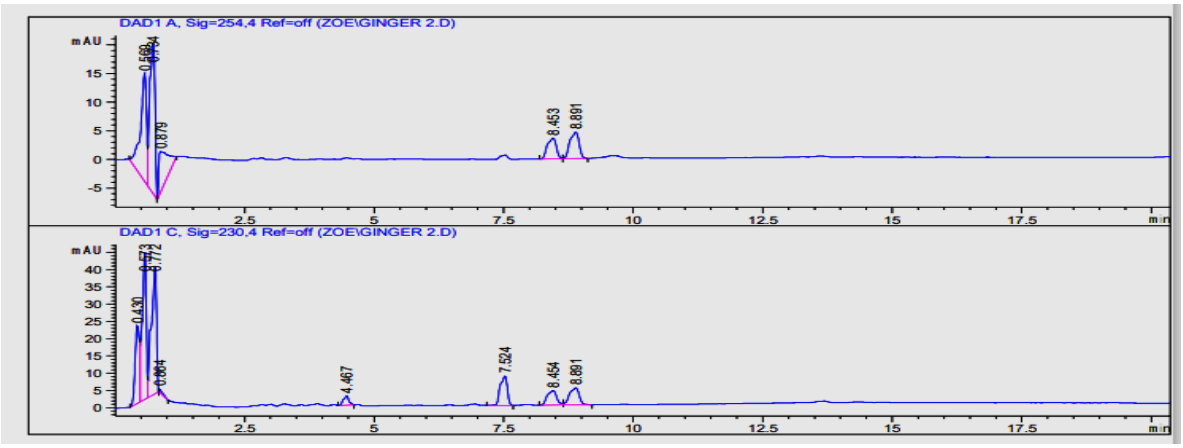

Fig. 4: HPLC profile of ginger extract

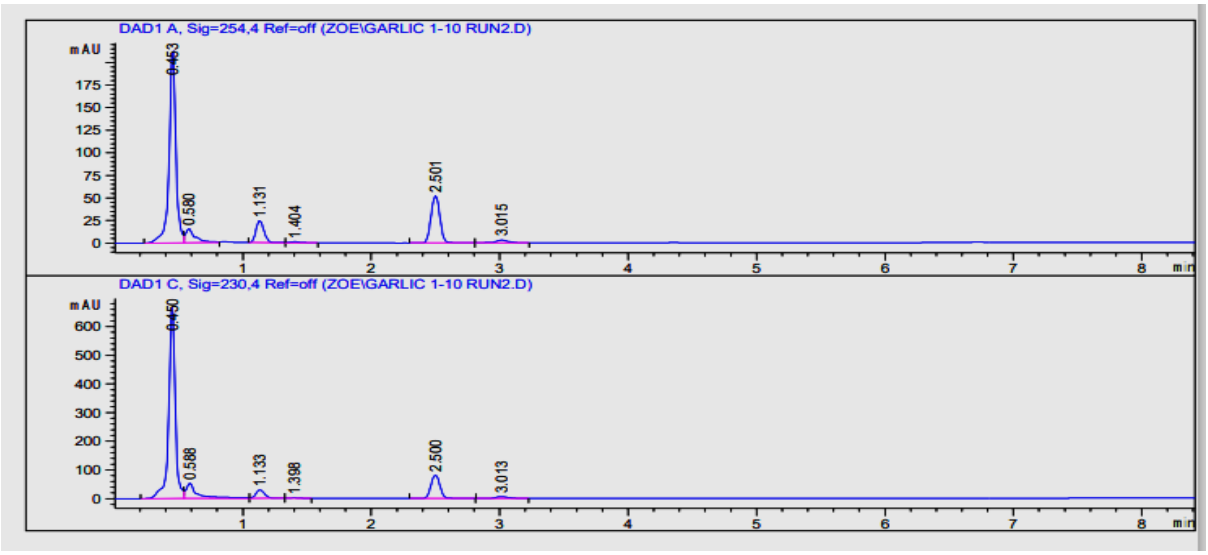

Fig. 5: HPLC profile of garlic extract

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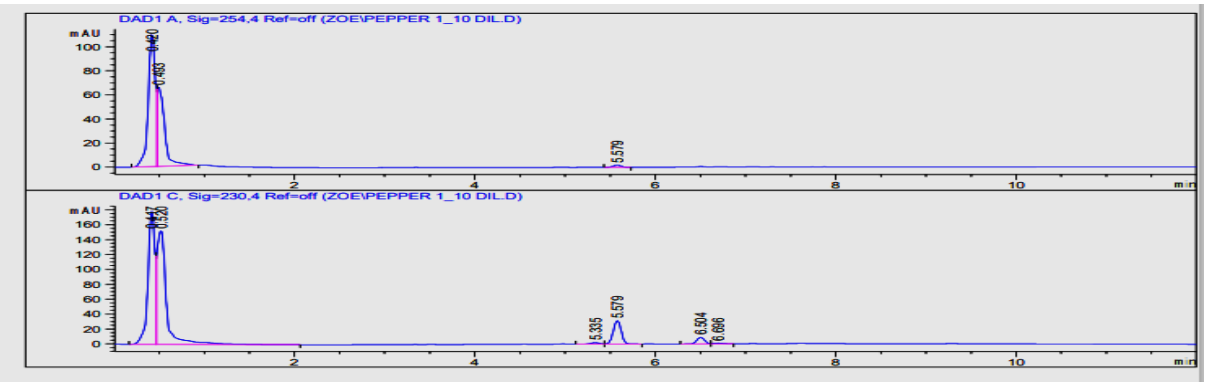

Fig. 6: HPLC profile of chili pepper extract

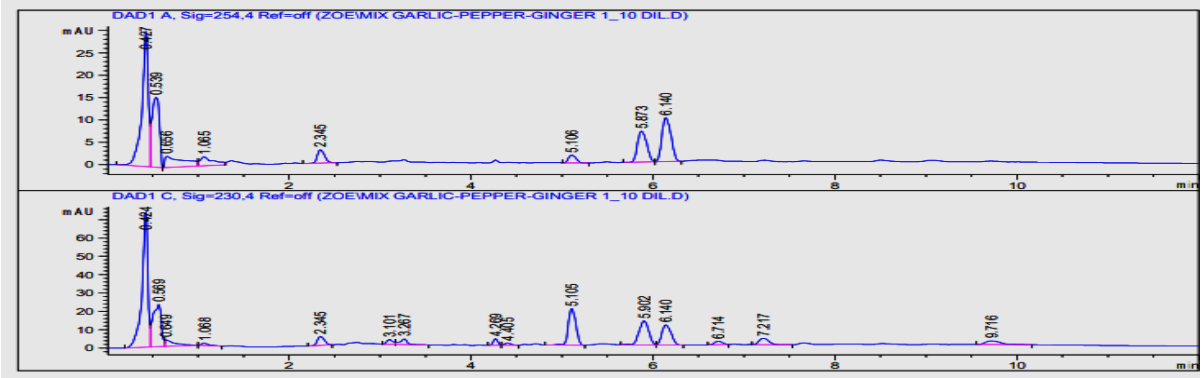

Fig. 7: HPLC profile of mixture (ginger, garlic and chili pepper extracts)

The different bioactive components identified by HPLC-DAD-MS/MS analysis are summarized in table 4, while fig.8 illustrates the postulated structures of these bioactive compounds.

Table 4: Spectra analyses

	Rt (min)	$[M+H]^+$			UV, λ_{max} (nm)	Formula	Metabolites
		Exp.	Calcd.	Δ(*ppm*)			
01	2.501	162.1690	162.1557	2.4	210 270 335	$C_6H_{10}OS_2$	Diallythiosulfinate (allicin) Isomer 1
02	3.013				214 270 335		Diallythiosulfinate (allicin) Isomer 2
03	5.579	305.1585	305.1552	2.1	214 270 335	$C_{18}H_{27}NO_3$	8-methyl-N-vanillyl-6 nonenamide(capsaicin) (Isomer 1)
04	6.504				214 270 339		8-methyl-N-vanillyl-6 nonenamide(capsaicin) (Isomer 2)
05	6.696				214 270 335		8-methyl-N-vanillyl-6 nonenamide(capsaicin) (Isomer 3)
06	8.453	294.1169	294.1133	0.8	210 270 335	$C_{17}H_{26}O_4$	6-gingerol
07	8.891	276.2161	276.2166	1.6	218	$C_{17}H_{24}O_3$	6-Shogaol

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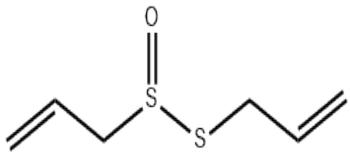
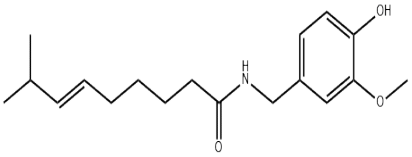
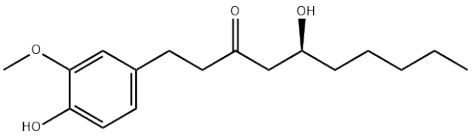


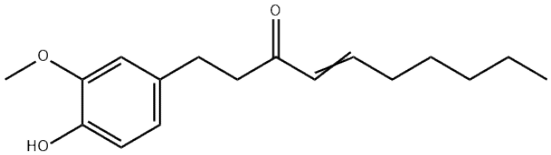
A. Allicin ($C_6H_{10}OS_2$)



B. Capsaicin ($C_{18}H_{27}NO_3$)



C. 6- Gingerol ($C_{17}H_{26}O_4$)



D. 6- Shogaol ($C_{17}H_{24}O_3$)

Fig. 8: Structures of Allicin (A), Capsaicn (B), 6-Gingerol (C), 6-Shogaol (D)

Binding Energy of Bioactive Ligands

To estimate the affinity and viability of bioactive compounds as potential biopesticide agents, 12 docking simulations between 4 ligands and the 3 target receptors were performed using AutoDock Vina and MOE. For each docked system, 3 high affinity complexes were analyzed for key binding domains and contact residues responsible for interactions. The binding affinities of the bioactive ligands (allicin, capsaicin, 6-gingerol and 6-shogaol) and target receptors (PERK-4X7K,TRPV-7LPE and SARS-6Y2E) are represented in fig. 9.

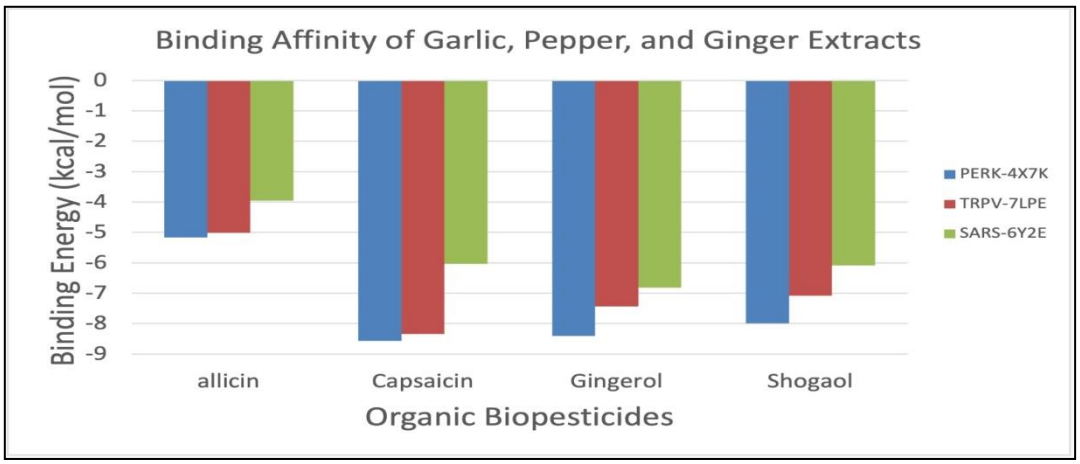
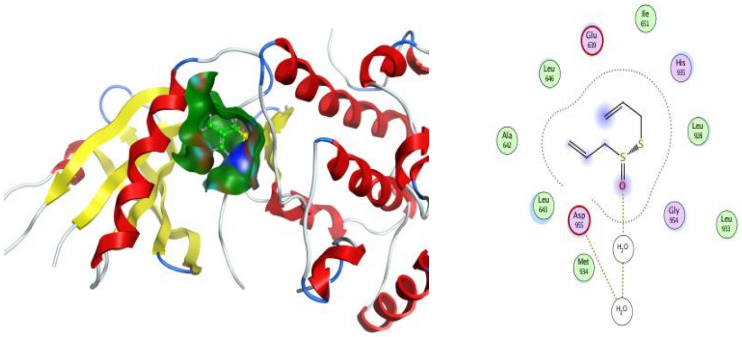


Fig. 9: Binding affinity of garlic, pepper and ginger extracts

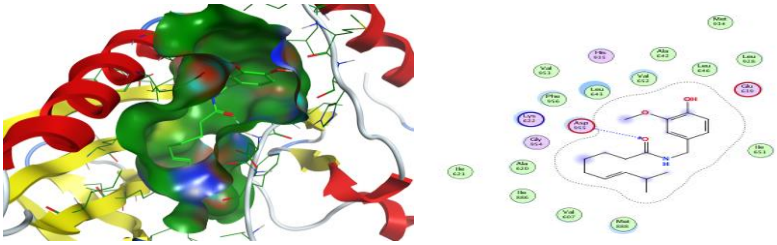
Ligand – PERK interactions

Ligand – PERK interactions are illustrated in fig. 10 (Allicin complex with PERK), fig. 11 (Capsaicin complex with PERK), fig. 12 (Gingerol complex with PERK) and fig.13 (Shagaol complex with PERK).



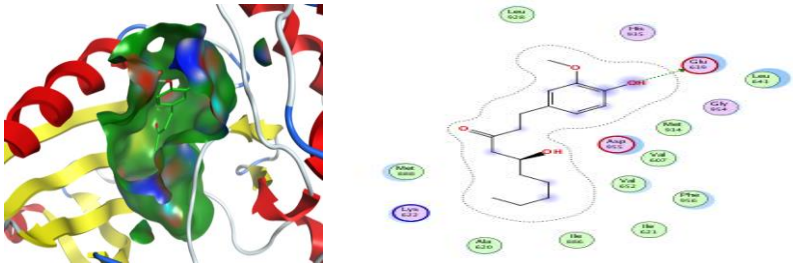
Ligand	Receptor	Interaction	Distance	E (kcal/mol)
O 3	O HOH 1362 (A)	H-acceptor	2.84	-2.9

Fig. 10: Allicin complex with PERK



Ligand	Receptor	Interaction	Distance	E (kcal/mol)
O 1	N ASP 955 (A)	H-acceptor	2.84	-4.1

Fig. 11: Capsaicin complex with PERK



Ligand	Receptor	Interaction	Distance	E (kcal/mol)
O 4	OE2 GLU 639 (A)	H-donor	2.72	-3.4

Fig. 12: Gingerol complex with PERK

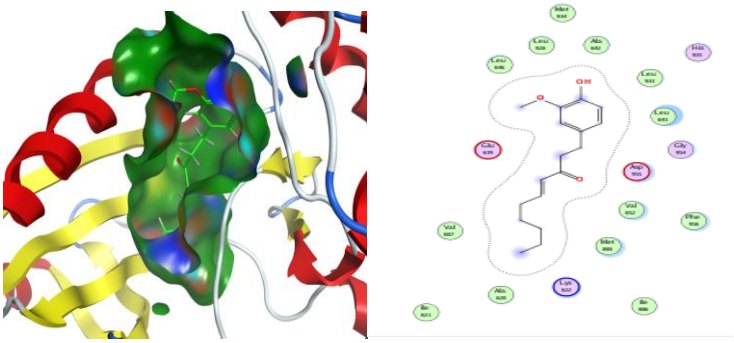


Fig. 13: Shagaol complex with PERK

Drug-like and ADME (Absorption, Distribution, Metabolism and Excretion) properties

Further analysis of drug-like and ADME properties revealed that gingerol had the highest H-bond interactions with target proteins (fig. 14), while capsaicin's larger molecular size (305.15 g/mol) (fig.15) high total polar surface area (TPSA) (fig. 16) high lipophilicity (fig. 17), and low water solubility (fig. 18) contribute to its bioactivity.

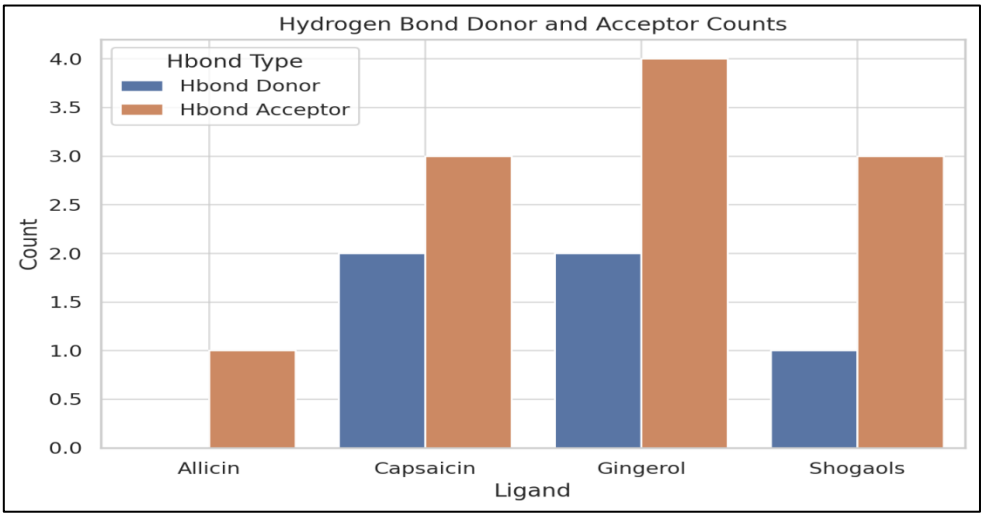


Fig. 14: Pesticide-like properties of Ligands

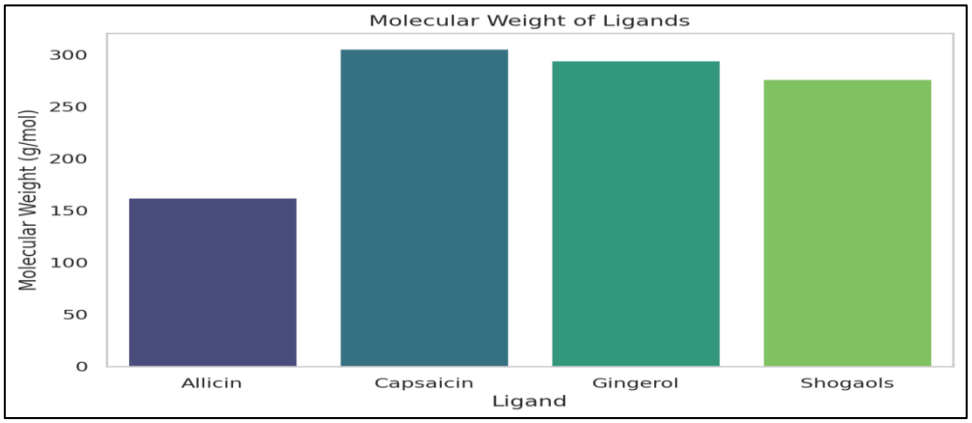


Fig. 15: Molecular weights of Ligands

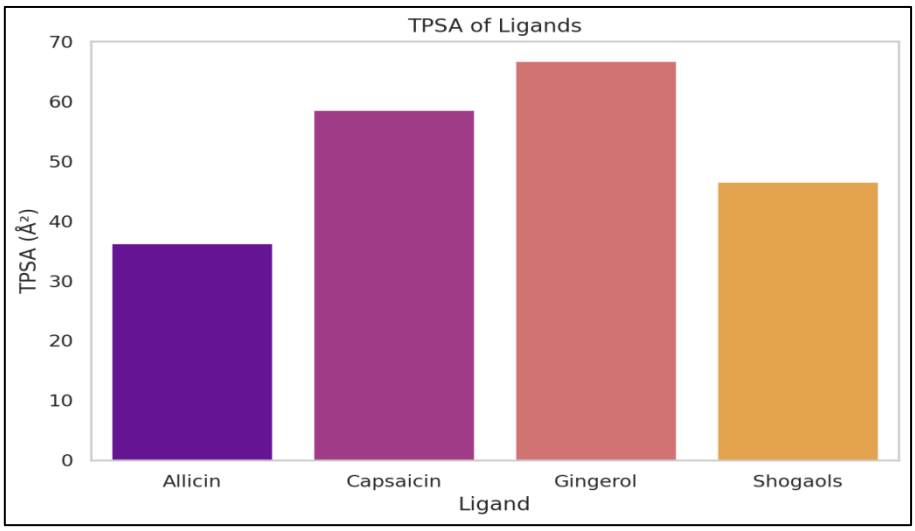


Fig. 16: Total polar surface area (TPSA) of Ligands

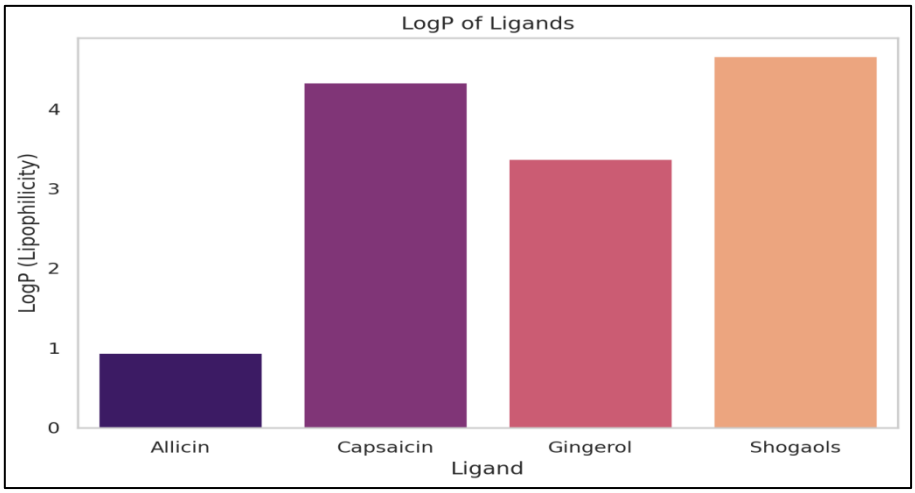


Fig. 17: Lipophilicity of Ligands

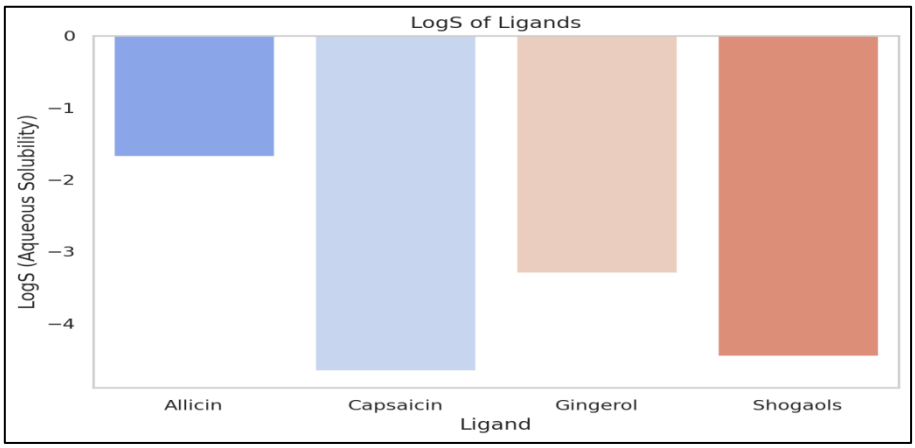


Fig. 18: Aqueous Solubility of Ligands

DISCUSSION

Biopesticide treatments of 12g/l and 15g/l were the more effective than the other treatments in controlling aphid infestation on tomato (*Solanum lypersicum*) plants, agreeing with results from Magwenya *et al.*, 2016 [17] who also showed that different concentrations of garlic extracts control aphid infestations on cotton plants. IR spectrum results from the mixture (ginger, garlic and chilli pepper) identified C-H, C-O, O-H and C=O functional groups. Similarly Gaikwad *et al*.,2017 [25] used Fourier transform infrared (FTIR) to identify these functional groups in gingerol extracts. The IR spectrum results did not clearly identify N-H, and S-S functional groups in our extract mixtures, maybe because the bioactive compounds were not in their pure form. High-performance liquid chromatography coupled with electrospray ionization tandem mass spectrometry (HPLC–ESI-MS/MS) has shown better sensitivity for identification of bioactive compounds from ginger rhizomes.[12,14] Our HPLC-DAD-MS/MS analysis revealed 6-gingerols and 6-shogaols in the ginger rhizomes. These results are concordant with those of Gelila *et al.*, 2019,[26] who used UPLC-DAD-QTOF-MS to detect 18 phenolic acids including 6-gingerols and 6-shogaols. Diallythiosulfinate (allicin) was detected in our garlic cloves, similarly C. Malaphong *et al*., 2022 [27] used a simple and rapid HPLC method coupled to DAD to determine S-allyl-L-cystein in black garlic cloves. Results from our HPLC chromatograms also showed the presence of capsaicin in chili pepper, agreeing with results obtained by Zeid *et al.*, 2011 [28] who used HPLC-DAD to detect capsaicin and dihydrocapsaicin in different peppers.

The binding affinity scores from the 12 docking simulations indicated that capsaicin displayed the strongest hydrogen bonding interactions with protein kinase RNA-like endoplasmic kinase (PERK-4X7K) receptors and an estimated binding energy of -8.2 ± 0.2 kcal/mol. Capsaicin also showed very strong interactions with transient receptor potential vanilloid (TRPV-7LPE) receptors(binding energy of -8.1 ± 0.2 kcal/mol) . The high molecular weight (300.15) of capsaicin coupled to its high total polar surface area (TPSA) could account for multiple contact sites with receptors, enhanced by strong hydrogen bond interactions. Meanwhile the relatively high lipophilicity and low aqueous solubility of capsaicin indicated by our results, contributes to its bioavailability and bioactivity in the phospholipid bilayer membranes of insect pests. Concordantly Sonya *et al*., 2015 [20] highlighted that transient receptor potential vanilloid subtype 1 (TRPV1) is a heat-sensitive ion channel also involved in pain sensation, and is the receptor for capsaicin, the active ingredient of hot Chili peppers. They further simulated strong molecular docking interactions between capsaicin and TRPV1. According to Z. Huang *et al*., 2023, [23] chordotonal organs are miniature sensory organs present in insects. Chordotonal organs depend on transient receptor potential (TRP) channels. Transient receptor potential vanilloid (TRPV) channels are the only TRPs identified that can act as targets of insecticides. By binding with TRPV channels, insecticides targeting the chordotonal organs trigger the inflow of calcium ions, resulting in abnormal function of the chordotonal organ to achieve the goal of eliminating pests.

Our molecular docking simulation also showed very strong binding affinity scores between the 2 ligands (6-gingerol and 6- shagaol) and 2 target pest protein receptors(PERK-4X7K and TRPV-7LPE) .Similarly to capsaicin, 6-gingerol and 6-shagaol recorded relatively high molecular weights (294.11 and 276,21 respectively) coupled to high total polar surface areas (TPSA).6-Gingerol recorded the highest hydrogen acceptor count (4.0) while 6-shogaol showed a high hydrogen acceptor count of 3.0. The above 2 molecular physical factors coupled to hydrogen interactions could account for multiple contact sites with the receptors, thereby enhancing strong interactions as depicted by the results. In addition 6-gingerol and 6-shagaol portrayed high lipophilicity and low aqueous solubility values, suggesting fluid interactions with pest proteins in the phospholipid bilayer membranes. Similarly [29]showed that 6-shogaol induces apoptosis in human hepatocellular carcinoma cells in relation to caspase activation and endoplasmic reticulum(ER) stress signaling. Their proteomic analysis revealed that ER stress was accompanied by 6-shogaol-induced apoptosis in hepatocellular carcinoma cells. 6-shogaol affected the ER stress signaling by regulating unfolded protein response (UPR) sensor PERK and its downstream target eIF2a. G.Andersen *et al*, 2023 [30] showed that 6-Gingerol facilitates CXCL8 Secretion and ROS Production in Primary human neutrophils by targeting the TRPV1 Channels.

Among the 4 ligands, allicin recorded the lowest binding affinity scores with all 3 target protein (PERK-4X7K, TRPV-7LPE and SARS-6Y2E) receptors. This could be explained by the fact that allicin had the least molecular weight (162.16) coupled to a low total polar surface surface area (TPSA) thereby reducing its contact sites with the 3 target receptors. In addition the pesticide-like properties of the 4 ligands indicated that allicin had no hydrogen bond donor counts, and the least hydrogen acceptor count (1.0).Further justifying its low interaction with the 3 target protein receptors. Allicin was also the most aqueous soluble and the least lipophilic amongst the 4 ligands tested. These 2 molecular physical factors suggests a low bioavailability of allicin in pest systems and a high risk of leaching in soils. However several authors have demonstrated that allicin has antimicrobial and antifungal properties. According to J. Borlinghaus *et al*., 2014 [18] allicin is physiologically active in microbial, plant and mammalian cells. In a dose-dependent manner allicin can inhibit the proliferation of both bacteria and fungi or kill cells outright, including antibiotic-resistant strains like methicillin-resistant *Staphylococcus aureus* (MRSA).

CONCLUSION

Gingerol shogaol, allicin and capsaicin are natural bioactive products found in ginger, garlic and chilli peppers respectively. The good ADME properties of capsaicin could account for its bioactivity, suggesting further research. Our results have shown interesting roles of these bioactive compounds as potential biopesticides. This makes the concept of farmers being able to "grow their own" plant protection in an environmentally friendly manner attractive, particularly in subsistence agriculture where the cost of commercial preparations may be prohibitive. The results from this work hopefully provides some scientific literature for interested scientists in biopesticide formulations.

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CONFLICTS OF INTERESTS

The authors have not declared any conflict of interests.

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