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Isolation, Characterization and *In Silico* Molecular Docking Studies of Two Terpenoids from *Strychnos innocua* (Delile) Root Bark for Antibacterial Properties

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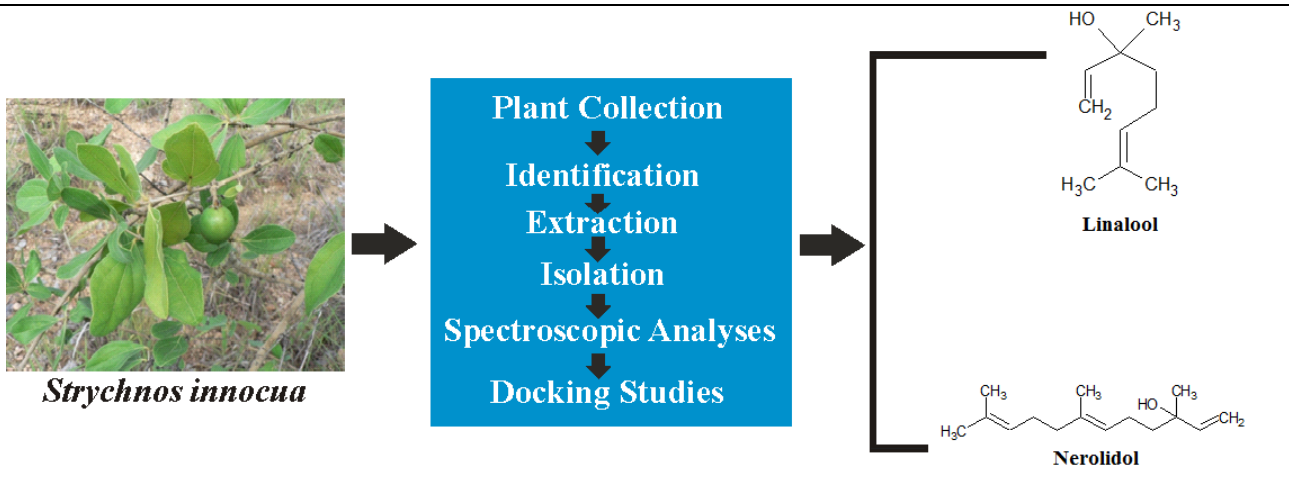
ABSTRACT

Terpenoids are definite secondary metabolites with active therapeutic components that contribute to plants' medicinal potential. *Strychnos innocua* is a *Loganiaceae* family medicinal plant found in various African countries. This study reports the isolation, characterization, and molecular docking analyses of Linalool (**1**) and Nerolidol (**2**) from ethyl acetate root bark extract of *S. innocua*. Their structures were validated using mass spectrometry, nuclear magnetic resonance (1D and 2D NMR), and compared with literature data. This is a novel report of terpenoids isolated from *S. innocua* root bark. An *in silico* docking examination revealed the binding energies of Linalool with the binding sites of *Staphylococcus aureus* pyruvate carboxylase (PDB: 3HO8) and *Pseudomonas aeruginosa* virulence factor regulator (PDB: 2OZ6) were -4.7 and –5.6 kcal/mol, respectively. Furthermore, the binding energies of Nerolidol with the binding sites of *S. aureus* and *P. aeruginosa* were -5.8 and -6.9 kcal/mol, respectively. Compared to ciprofloxacin (standard drug), which showed binding energies of -6.6 and -8.7 kcal/mol, respectively. This study concluded that Linalool and Nerolidol are abundant in the root bark of *S. innocua*. At the same time, docking results revealed that the compounds had moderate interactions with *S. aureus* and *P. aeruginosa*, exhibiting antibacterial effects.

GRAPHICAL ABSTRACT



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Introduction

Terpenoids have found useful therapeutic applications in medicine [1]. While antidysentery, antidiarrhea, antidiabetes, antihypertension, analgesic, anti-inflammatory, antibacterial, antibiotic, antiseptic, and antioxidant activities are some of the biological applications of terpenoids [2]. On the other hand, various additional phytochemicals such as flavonoids, alkaloids, and steroids have also been shown to possess active therapeutic components, which reports show exhibit favorable medicinal properties [3].

Plants are the primary source of bioactive compounds, and the plant kingdom holds many therapeutic development potentials [4]. Linalool has been demonstrated to possess antibacterial, antifungal, anticancer, anti-inflammatory, and antioxidant activities, while several *in vivo* studies have proven Linalool's pharmacological importance [5]. On the other hand, Nerolidol is sesquiterpene alcohol with a flowery odor found in several plants. Researchers have examined its therapeutic properties, which might have favorable influences on human health [6].

The antimicrobial activity of natural compounds derived from plants has been studied utilizing various *in vitro*, *in vivo*, and computational methods. Docking is one of these methods that have received widespread applications in developing antimicrobial drugs [7]. Researchers have also recently employed computational approaches to explore the effects of drugs and vitamins on the human body [8-15]. Ciprofloxacin, a standard antibiotic used to treat various bacterial infections, respiratory tract infections, and urinary tract infections, is significant in treating *S*. *aureus* and *P*. *aeruginosa* [16].

Strychnos innocua is a *Loganiaceae* plant with a straight stem that may reach a height of 18 meters. It has a trunk diameter varying from 7 to 40 cm and many branches. Its leaves are usually simple. However, they have a rounded base in rare instances. *S*. *innocua* is found in several countries, including Sudan, Malawi, Cameroon, Uganda, and Nigeria. The plant's root is used to cure gonorrhoea, and a fresh infusion of the plant's root is used to heal snake bites. [17,18]. Kaduna State is one of the Nigerian states where the plant is commonly harvested.

Chemical compositions and antimicrobial evaluations of *S. innocua* root bark extracts have been studied and published in the literature [19–21]. However, there is a paucity of information concerning the isolation of compounds from *S*. *innocua* root bark extracts. This study isolated, characterized and docked two terpenoids, Linalool (**1**), Nerolidol (**2**) from the root bark of *S*. *innocua*. This is a novel report of Linalool and Nerolidol isolated from the plant's root bark.

Materials and Methods

Plant collection and extraction

The plant of *S*. *innocua* was collected from the wild in Kaduna State, Nigeria, identified and authenticated in the Department of Biological Sciences at ABU, Zaria by Mr. Namadi Sunusi, where V/N – 01884 is the herbarium voucher number. The root bark of *S*. *innocua* was dried under shade. Subsequently, it was then crushed to a fine powder. The powder (i.e., pulverized sample, 2 kg) was extracted using the maceration technique with analytical grade solvents, such as n-hexane, ethyl acetate, and methanol, respectively, in increasing polarity, as reported by [19-22].

General experimental procedure

On GC 7890B, MSD 5977A, Agilent Tech, GC-MS of the isolated compounds was performed. Both 1D and 2D NMR spectra were determined on the Varian–Vnmrs 400 MHz spectrometer in ppm (the chemical shift), while chloroform ($CdCl_3$) was the solvent used.

Reagents and chemicals used

The reagents and chemicals used in this study are all analytical grade JDH (methanol, chloroform, ethyl acetate, and n-hexane).

Column chromatography and isolation

Many spots were revealed by thin-layer chromatography (TLC) analysis of the ethyl acetate extract using several solvent systems. The extract (30 g) was combined with 60-120 mesh silica gel and dried before being transferred to a column (size, 5 cm × 60 cm) parked with silica gel and n-hexane. The column was eluted using a suitable solvent system (n-hexane: Ethyl acetate) with increasing polarity (n-hexane 100 %, 9:1, 8:2, 7:3, 6:4, 1:1, 4:6, 3:7, 2:8, 1:9, and 100 % Ethyl acetate) at a flow rate of 1 drop/sec and two hundred and sixty one (261) 50 mL collections. A pre-coated TLC plate was used to monitor these collections with a spraying reagent (Methanol: Glacial Acetic Acid: Sulphuric Acid: P-anisaldehyde at a ratio of 85: 10: 5: 0.l mL), yielding twenty-four fractions (F1-F24). A small amount of F17 was subjected to preparative thin-layer chromatography. The TLC was scraped and placed in a beaker. Chloroform solvent was added, the mixture was filtered, the filtrate was evaporated, and one spot was observed on the TLC plate. This was an isolated Compound **1** (Rf value: 0.24), with a yield value of 32 mg. Furthermore, fractions 8 and 9 were combined to get 2.9 g, mixed with Silica Gel, and left to dry. It was transferred to a column packed with silica gel and eluted with 100 % n-hexane (twenty collections of 10 mL) and a 9:1 n-hexane: Ethyl acetate gradient mixture (forty collections of 10 mL). The flow rate was 1 drop per 5 seconds. The collections were monitored using a pre-coated TLC plate, which yielded eight subfractions (FF1-FF8). Compound **2** was isolated on FF6 using preparative thin-layer chromatography (Rf = 0.23). The yield of **2** was 28 mg.

Docking studies

An i*n silico* docking study was performed on ligands, (isolated compounds and Ciprofloxacin) with target receptors (PDB: 3HO8 and 2OZ6) downloaded from (www.rcsb.org). ChemDraw professional 16.0 was used to generate the ligands two-dimensional (2D) structure, which was then converted to three-dimensional (3D) geometrical optimization using Spartan 20v.1.1/2020. The target receptors in three-dimensional form were prepared using Discovery Studio Visualizer software v.21.1.0.20298, saved in the PDB file format, and uploaded to Pyrx software for docking. The docking output was shown in Discovery Studio with the binding score to examine the protein-ligand interactions [23, 24].

Results and Discussion

Compound **1** (32 mg) was obtained as pale oil. The mass spectrum (Figure 1) of **1** indicated molecular ion peaks at *m/z* 154 and fragment ions *m/z* 136, *m/z* 121, *m/z* 93, *m/z* 71, *m/z* 55, *m/z* 43, and *m/z* 27 suggesting its molecular formula to be $C_{10}H_{18}O$. The NMR spectra data (Table 1) of **1** were very similar to the literature for Linalool with ^{1}H NMR (Figure 2) displaying δ_H for two allylic methyl protons (δ_H 1.63 H-8 and 1.76 H-9), two olefinic methine protons (δ_H 5.19 H-6 and 5.91 H-2), two methylene protons (δ_H 1.37 H-4 and 2.01 H-5), and one olefinic methylene, methyl and hydroxyl protons (δ_H 5.33 H-1, 0.90 H-10, and 4.76 -OH). The ^{13}C NMR (Figure 3) and DEPT displayed 10 carbon signals for two methylene groups (δ_C 22.52 C-5 and 43.87 C-4), two quaternary carbons (δ_C 75.68 C-3 and 131.96 C-7), three olefinic carbons (δ_C 108.65 C-6, 120.17 C-1, and 145.25 C-2), and three methyl groups (δ_C 17.53 C-8, 24.95 C-9, and δ_C 29.83 C-10).

Compound **2** (28 mg) was obtained as a pale yellow oil. The mass spectrum (Figure 4) of **2** indicated fragment ion peaks at *m/z* 204,

representing a loss of H_2O from molecular ions at *m/z* 222, and fragment ions *m/z* 189, *m/z* 175, *m/z* 161, *m/z* 136, *m/z* 121, *m/z* 107, *m/z* 93, *m/z* 69, *m/z* 55, and *m/z* 41 suggesting its molecular formula to be $C_{15}H_{26}O$. The NMR spectra data (Table 2) of **2** were very similar to the literature for Nerolidol with ^1H NMR (Figure 5), displaying δ_H for four methylene protons (δ_H 1.36 H-4, 2.00 H-5, 2.33 H-8, and 2.35 H-9), one olefinic methylene protons (δ_H 5.40 H-1), three allylic methyls (δ_H 1.50 H-12, 1.60 H-14, and 1.73 H-13), one methyl protons (δ_H 0.94 H-15), three olefinic methine protons (δ_H 5.15 H-6, 5.15 H-10, and 6.00 H-2), one hydroxyl proton (δ_H 4.54 -OH) The ^{13}C NMR (Figure 6) and DEPT displayed 15 carbon signals for three quaternary carbons (δ_C 73.72 C-3, 133.45 C-11, and 135.67 C-7), three allylic methyl carbons (δ_C 15.49 C-14, 17.46 C-13, and δ_C 25.21 C-12), one methyl carbon (δ_C 29.31 C-15), Four methylene carbons (δ_C 22.91 C-5, 27.43 C-9, 39.38 C-8, and 43.10 C-4), three olefinic methine carbons (δ_C 122.53 C-10, δ_C 124.75 C-6, and 145.44 C-2), and one olefinic methylene (δ_C 110.54 C-1).

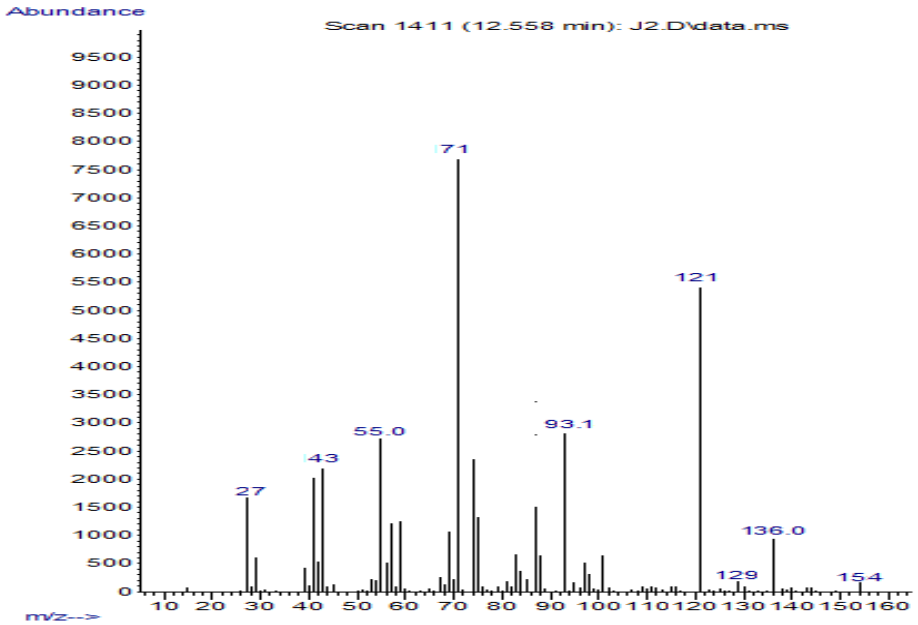

Figure 1. Mass Spectrum for Linalool

Table 1. The NMR (400 MHz) Data of Linalool

	Linalool			Literature Data [25]		
Position	**^1H (ppm)**	**^{13}C (ppm)**	**DEPT**	**^1H (ppm)**	**^{13}C (ppm)**	**DEPT**
C-1	5.33 (d, 2H)	120.17	CH_2	5.23 (d, 2H)	124.27	CH_2
C-2	5.91 (t, 1H)	145.25	CH	5.94 (m, 1H)	144.97	CH
C-3		75.68	C		73.40	C
C-4	1.37 (t, 2H)	43.87	CH_2	1.38 (m, 2H)	41.99	CH_2
C-5	2.01 (q, 2H)	22.52	CH_2		22.73	CH_2
C-6	5.19 (t, 1H)	108.65	CH	5.19 (m, 1H)	111.61	CH
C-7		131.96	C		131.83	C
C-8	1.63 (s, 3H)	17.53	CH_3		17.62	CH_3
C-9	1.76 (s, 3H)	24.95	CH_3		25.62	CH_3
C-10	0.90 (s, 3H)	29.83	CH_3		27.76	CH_3
OH	4.76 (s, 1H)			4.75 (s, 1H)		

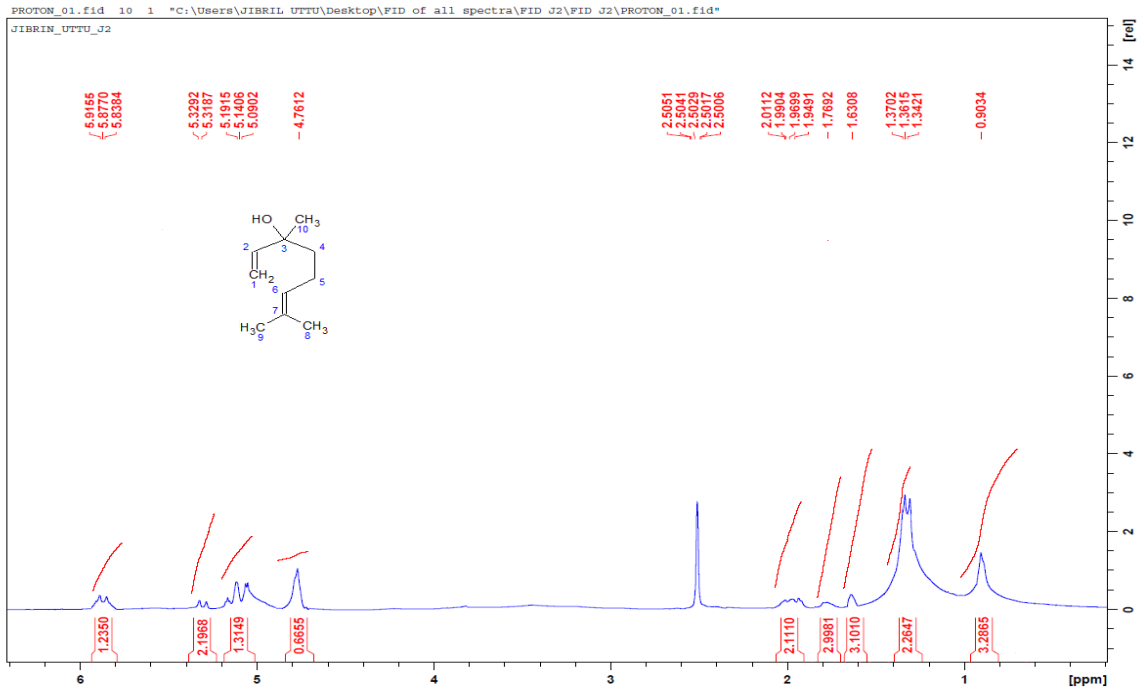

Figure 2. ^{1}H NMR Spectrum for Linalool

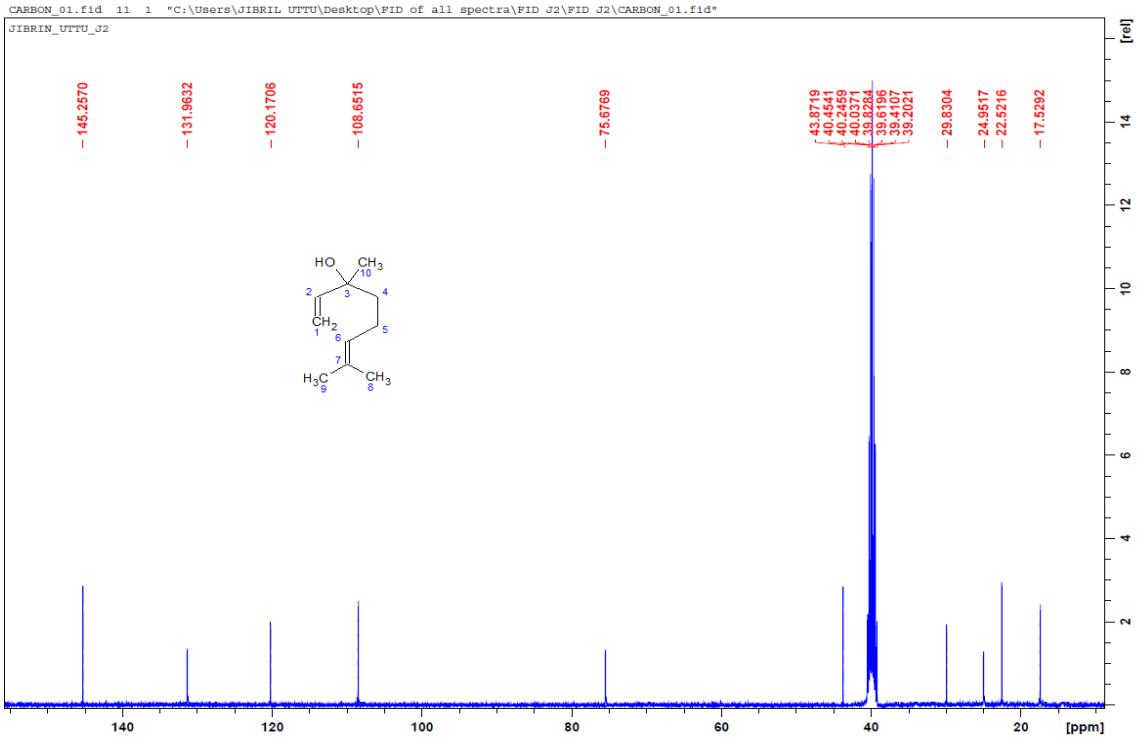

Figure 3. ^{13}C NMR Spectrum for Linalool

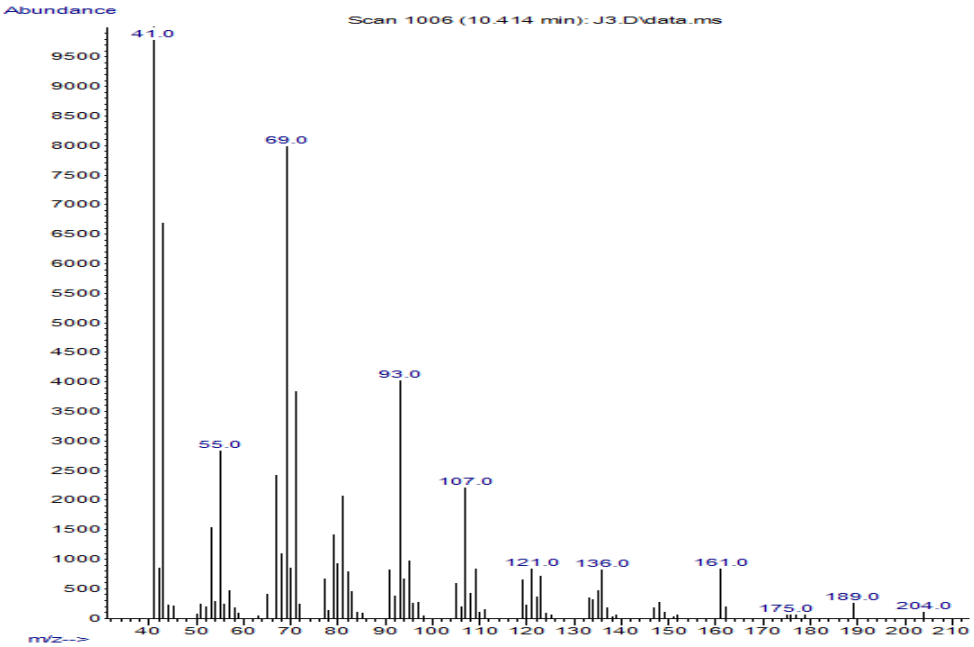

Figure 4. Mass Spectrum for Nerolidol

Table 2. The NMR (400 MHz) Data of Nerolidol

	Nerolidol			Literature Data [26]		
Position	**^{1}H (ppm)**	**^{13}C (ppm)**	**DEPT**	**^{1}H (ppm)**	**^{13}C (ppm)**	**DEPT**
C-1	5.40 (d, 2H)	110.54	CH_2	5.23 (d, 2H)	112.00	CH_2
C-2	6.00 (m, 1H)	145.44	CH	5.90 (m, 1H)	145.40	CH
C-3		73.72	C		73.80	C
C-4	1.36 (m, 2H)	43.10	CH_2		42.00	CH_2
C-5	2.00 (m, 2H)	22.91	CH_2		23.10	CH_2
C-6	5.15 (m, 1H)	124.75	CH	5.17 (m, 1H)	124.65	CH
C-7		135.67	C		135.90	C
C-8	2.33 (m, 2H)	39.38	CH_2		40.00	CH_2
C-9	2.35 (m, 2H)	27.43	CH_2		27.00	CH_2
C-10	5.15 (m, 1H)	122.53	CH	5.17 (m, 1H)	124.62	CH
C-11		133.45	C		131.70	C
C-12	1.50 (s, 3H)	25.21	CH_3		26.00	CH_3
C-13	1.73 (s, 3H)	17.46	CH_3	1.67 (s, 3H)	18.00	CH_3
C-14	1.60 (s, 3H)	15.49	CH_3	1.59 (s, 3H)	16.30	CH_3
C-15	0.94 (s, 3H)	29.31	CH_3	1.27 (s, 3H)	28.20	CH_3
OH	4.54 (s, 1H)					

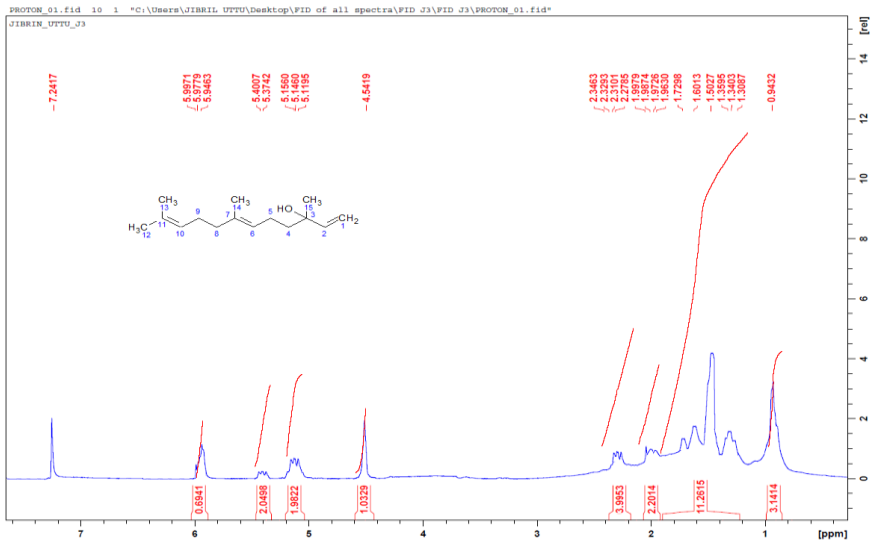

Figure 5. ^{1}H NMR Spectrum for Nerolidol

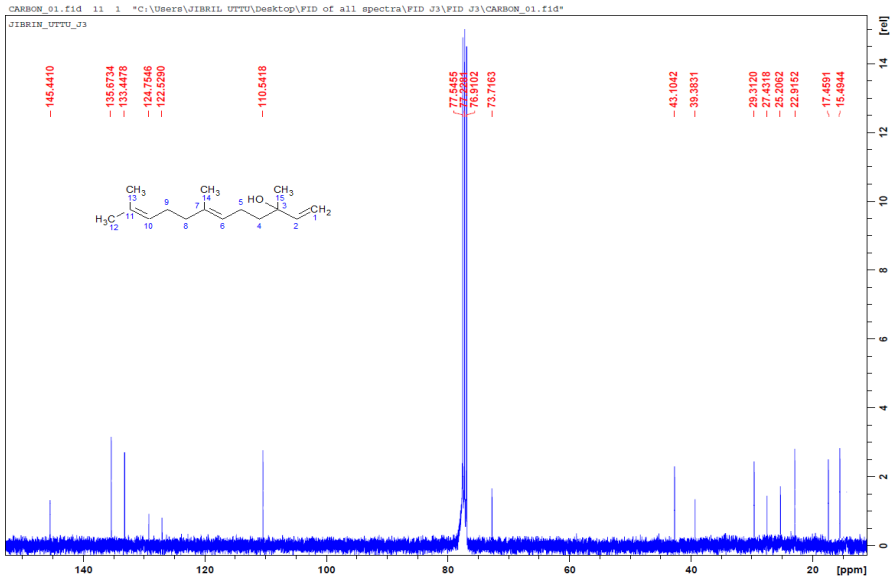

Figure 6. ^{13}C NMR Spectrum for Nerolidol

The presence of terpenoids was verified in the phytochemical analysis of the ethyl acetate extract, and the extract demonstrated *in vitro* antibacterial activity against *S. aureus*, *B. subtilis*, and *P. aeruginosa* [21]. This bolsters the therapeutic value of medicinal plants [27-29]. Linalool and Nerolidol were isolated from the extract using chromatographic separation, and their structures were identified using spectroscopic analysis and compared to previously published data [30,31].

Linalool is an acyclic monoterpenoid found in many plant species [32]. It is also a component of essential oils in various plant species and has demonstrated improved antibacterial action against *Salmonella typhimurium* in nanoemulsions [33]. Nerolidol, commonly known as peruviol, is sesquiterpenoid alcohol with antibacterial, antioxidant, and other

pharmacological effects. The antibiofilm properties of Nerolidol were also studied, with the findings indicating its therapeutic efficacy [34].

The compounds' interactions with the target receptors (PDB: 3HO8 and 2OZ6) were investigated using molecular docking and compared to ciprofloxacin (standard drug). Table 3 reveals that the binding scores of the compounds with *S. aureus* pyruvate carboxylase 3HO8 (receptor) are all moderately comparable to ciprofloxacin. Though the binding energy of Nerolidol (-5.8 kcal/mol) is higher than that of Linalool (-4.7 kcal/mol), their interactions with the receptor are shown in Figures 7 and 8, respectively. Ciprofloxacin's binding energy was -6.6 kcal/mol, and its interaction is shown in Figure 9.

Table 4 shows that Linalool and Nerolidol binding scores with the *P. aeruginosa* virulence factor regulator 2OZ6 (receptor) are also moderately comparable to ciprofloxacin. Nerolidol has higher binding energy (-6.9 kcal/mol) than Linalool (-5.6 kcal/mol). Their interactions with the receptor are shown in Figures 10 and 11, respectively. Ciprofloxacin's binding energy was -8.7 kcal/mol, and its interaction with the receptor is shown in Figure 12.

Table 3. Binding Energy Results of the Isolated Compounds/Ciprofloxacin with Target Receptor (PDB: 3HO8)

Ligands	Binding Score (Kcal/mol)	Protein Interaction	Types of Interaction	Bond Distance Å
Linalool (1)	-4.7	VAL404	Alkyl	4.90
		PRO410	Alkyl	4.65
		LYS518	Alkyl	5.75
		LYS518	Alkyl	4.13
		LEU926	Alkyl	4.96
		TYR923	Pi-Alkyl	5.47
		TYR923	Pi-Alkyl	5.45
		TYR923	Pi-Alkyl	4.83
		TYR400	Pi-Alkyl	5.26
		TYR400	Pi-Alkyl	5.05
		TYR400	Pi-Alkyl	4.23
		PHE932	Pi-Alkyl	4.69
		PHE409	Pi-Alkyl	5.29
		PHE409	Pi-Alkyl	4.79
Nerolidol (2)	-5.8	VAL404	Alkyl	4.46
		LYS518	Alkyl	4.79
		PRO418	Alkyl	4.68
		PRO418	Alkyl	4.32
		PHE409	Pi-Alkyl	5.18
		TYR400	Pi-Alkyl	4.80
		TYR923	Pi-Alkyl	5.05
Ciprofloxacin	-6.6	PRO410	Pi-Sigma	3.70
		PHE934	Pi-Alkyl	5.28
		PHE409	Pi-Alkyl	5.12
		PRO410	Pi-Alkyl	5.06
		LYS518	Alkyl	4.14
		PRO410	Alkyl	5.15
		ASN403	Conventional Hydrogen bond	2.73

Table 4. Docking Results of the Isolated Compounds/Ciprofloxacin with Target Receptor (PDB: 2OZ6)

Ligands	Binding Score (Kcal/mol)	Protein Interaction	Types of Interaction	Bond Distance Å
Linalool (1)	-5.6	LEU59	Alkyl	4.33
		LEU59	Alkyl	4.60
		LYS119	Alkyl	4.94
		ARG116	Alkyl	4.74
		ARG116	Alkyl	4.32
		ARG116	Alkyl	3.71
		ILE44	Alkyl	3.87
		LEU68	Alkyl	4.51
		ILE44	Alkyl	4.23
		VAL79	Alkyl	5.23
		ALA77	Alkyl	4.49
		GLU67	Conventional Hydrogen bond	2.35
Nerolidol (2)	-6.9	LEU68	Alkyl	4.59
		LEU68	Alkyl	4.62
		LEU68	Alkyl	3.94
		ALA77	Alkyl	4.47
		ARG75	Alkyl	4.58
		ILE25	Alkyl	3.92
		VAL79	Alkyl	4.92
		ILE44	Alkyl	3.72
		ARG116	Alkyl	4.91
		LEU59	Alkyl	5.06
		LEU59	Alkyl	4.88
		ARG116	Alkyl	3.64
		ARG116	Alkyl	4.72
		LYS119	Alkyl	4.17
		LYS119	Alkyl	4.46
		GLY66	Conventional Hydrogen bond	2.16
Ciprofloxacin	-8.7	GLU57	Pi-Anion	4.48
		ILE44	Pi-Sigma	3.99
		ALA77	Carbon Hydrogen Bond	2.52
		LEU68	Alkyl	4.76
		ALA77	Alkyl	5.14
		ALA77	Alkyl	4.72
		ILE56	Alkyl	4.42
		ALA77	Alkyl	4.72
		ARG116	Pi-Alkyl	4.84
		LEU68	Pi-Alkyl	5.43
		ILE44	Pi-Alkyl	4.16
		THR120	Conventional	2.37
		GLY66	Hydrogen bond	2.37

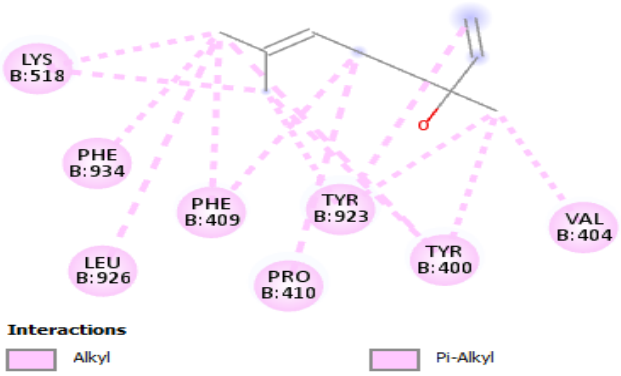

Figure 7. 2D Interaction of Linalool with crystal structure of *S. aureus* (PDB: 3HO8)

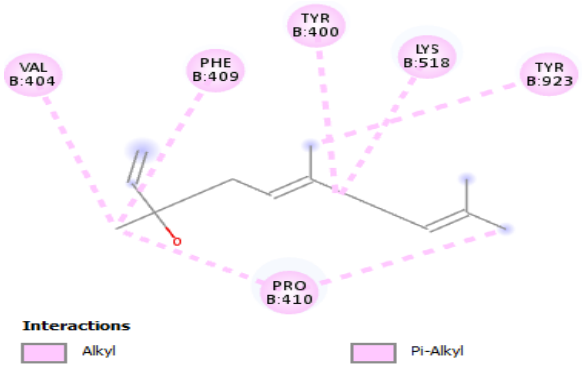

Figure 8. 2D Interaction of Nerolidol with crystal structure of *S. aureus* (PDB: 3HO8)

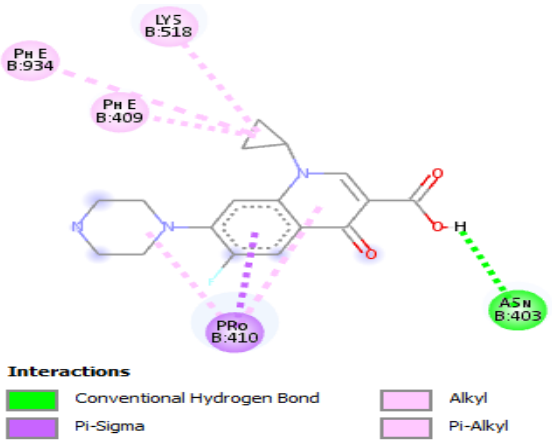

Figure 9. 2D Interaction of Ciprofloxacin with crystal structure of *S. aureus* (PDB: 3HO8)

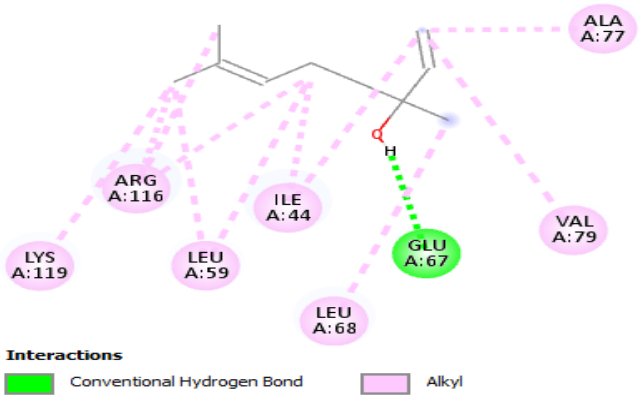

Figure 10. 2D Interaction of Linalool with crystal structure of *P. aeruginosa* (PDB: 2OZ6)

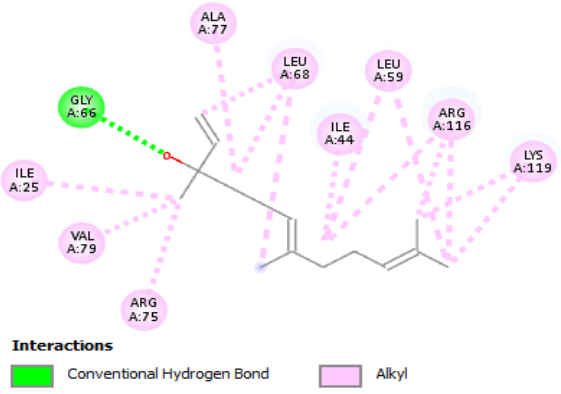

Figure 11. 2D Interaction of Nerolidol with crystal structure of *P. aeruginosa* (PDB: 2OZ6)

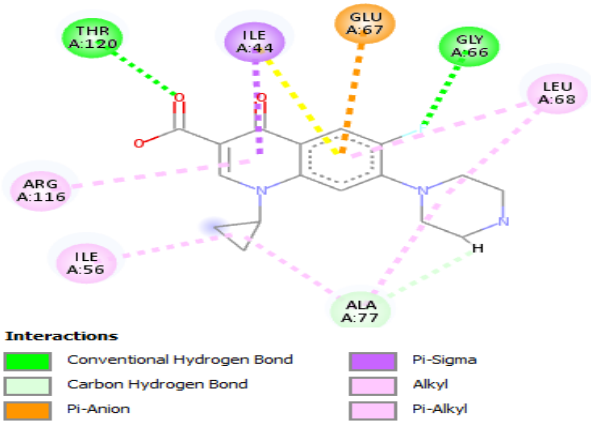

Figure 12. 2D Interaction of Ciprofloxacin with crystal structure of *S. aureus* (PDB: 2OZ6)

Conclusion

Column chromatography was utilized to isolate two compounds (Linalool and Nerolidol) from *S. innocua* root bark, and their structures were determined using MS and NMR spectroscopy. Linalool and Nerolidol demonstrated moderate binding scores (-4.7 and -5.8 kcal/mol respectively) with the binding sites of *S. aureus* (PDB: 3HO8) compared to Ciprofloxacin (-6.6 kcal/mol). Furthermore, their binding energies of -5.6 and -6.9 kcal/mol with *P. aeruginosa* (PDB: 2OZ6), were also comparable to ciprofloxacin (-8.7 kcal/mol). These moderate binding energies, found that Linalool and Nerolidol might be potential antibacterial agents.

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Disclosure statement

The authors declare no competing interests.

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