

Original Article

Isolation, Structural Elucidation and Anti-inflammatory Studies (In-vitro & in-silico) on the Fruit Extract of *Sarcocephalus latifolius* (Sm) BruceHassan Braimah Yesufu^{1*}, Cletus Anes Ukwubile^{2*}, Hananiya Hamza Milagawanda¹, Abdulqadir Bukar Bababe¹¹Department of Pharmaceutical and Medicinal Chemistry, Faculty of Pharmacy, University of Maiduguri, Nigeria.²Department of Pharmacognosy, Faculty of Pharmacy, University of Maiduguri, Maiduguri, Nigeria.

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ABSTRACT

The quest for novel therapeutic agents from natural sources has led to a burgeoning interest in medicinal plants, particularly those used in traditional medicine. *S. latifolius*, a member of the Rubiaceae family, has attracted attention due to its diverse phytochemical composition and documented medicinal properties. The Plant material was extracted with ethanol (Soxhlet method) and then fractionated with n-hexane. The fractions (n-hexane and residual aqueous) were evaluated via in-vitro assays (DPPH assay, Egg albumin and Histamine). The most active fraction (n-hexane) was subjected to GC-MS analysis and further isolation protocol. The results showed moderate to good free radical scavenging potential with IC₅₀= 0.33 (n-hexane) and IC₅₀= 0.55 (residual aqueous) when compared to the standard ascorbic acid IC₅₀= 0.56. Also, higher inhibition of histamine induced inflammation (In-vitro) was recorded by the extracts at 200 mg and 400 mg while inhibition of the egg-albumin induced inflammation (in-vitro) was recorded at 200 mg when compared to the standard drug (acetic acid). The binding potential of the compounds to the Pro-inflammatory receptor used (TNF- α 1) showed favorable interaction and inhibition of the Pro-inflammatory cytokine. The isolated compound (nauclyne) which hitherto has been reported from other parts of the plant except the fruit also showed good binding affinity to the inflammatory receptor. Our study showed that the isolation and structural elucidation of phytochemicals from *S. latifolius* fruits revealed a complex tapestry of bioactive compounds with significant therapeutic potential. Hence, the need for clinical trials to substantiate the traditional uses of *S. latifolius* and explore its full pharmacological potential.

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Abbreviations

SLET: *Sarcocephalus latifolius* ethanol; NHE: *n*-hexane extract; AQS: Aqueous extract; DPPH: 1,1-diphenyl-2-picrylhydrazine; TNF α 1: TNF-alpha 1; BBB: Blood Brain Barrier; CHCl₃: Chloroform; MeOH: Methanol; 1D-NMR: 1 Dimensional Nuclear Magnetic Resonance; 2D-NMR: 2-Dimensional Nuclear Magnetic Resonance; HSQC: Heteronuclear Single Quantum Correlation; H¹H: Cosy-Proton-Proton Correlation Spectroscopy; HMBC: Heteronuclear multiple bond correlation; MET: Methionine; ASP: L-aspartate; PHE: L-Phenylalanine; ARG: L-arginine; THR: L-Threonine; ALA: L-Alanine; ILE: L-isoleucine; GLU: L-glutamine.

Introduction

Sarcocephalus latifolius, a significant member of the Rubiaceae family, is renowned for its rich phytochemical profile and potential therapeutic applications. This evergreen shrub, primarily found in tropical regions of Africa, particularly in the medicinal practices of traditional medicine, has been a subject of extensive phytochemical investigations. *S. latifolius* is reported to have a wide range of medicinal properties and its medicinal uses vary from one traditional setting to another; common traditional uses include fever, pain, dental caries, septic mouth, malaria, hypertension, dysentery, diarrhea, and diseases of the central nervous system such as epilepsy [1, 2, 3]. The aqueous extract of leaves of the plant has been used as a remedy for diabetes in Northern Nigeria [4]. The anticonvulsant, anxiolytic and sedative properties of *S. latifolius* roots decoction [2] has already been reported as well as the antihypertensive and laxative activities [5]. Inflammation is a complex physiological response that plays a vital role in the body's defense mechanism against pathogens and injury. However, chronic inflammation is implicated in various diseases, including arthritis, cardiovascular diseases, and cancer [6]. The search for effective anti-inflammatory agents from natural sources has gained traction, particularly among traditional medicinal plants. Recent advancements in computational biology, particularly molecular docking, have paved the way for a deeper understanding of the interactions between bioactive compounds derived from *S. latifolius* and biological targets [7, 8]. The isolation of bioactive compounds, especially from the fruit, and also establishing the anti-inflammatory potential of fruit extracts from *S. latifolius*, highlighting their mechanisms of action, and implications for therapeutic applications served as a propellant for this research.

Materials and Methods

All chemicals and reagents used were of Analar grade (Riedel-de Hën, Sigma-Aldrich, Fluka, Germany). The silica gel for column chromatography was of mesh size (60-120G, Merck®, Germany) and that of thin layer chromatography (TLC) was Kieselgel 60 G (Merck®) made to the thickness of 0.25mm, precoated aluminium TLC plate {20×20cm} (Merck® Germany) Sephadex LH-20 for column chromatography (Pharmacia, Biotech, Sweden). Methanol, *n*-hexane, chloroform, ethyl acetate, distilled water.

Methods

Plant Collection, Extraction and Fractionation

S. latifolius fruit were randomly sampled from different branches of the tree from Gaya in Hong L.G.A of Adamawa State. The plant material was authenticated by a plant taxonomist in the Department of Biological Sciences, University of Maiduguri. The samples were washed, air-dried under shade in the laboratory, then pulverized into coarse powdered form using wooden mortar and pestle. A voucher specimen (UMM/FPH/RUA/002) was prepared and deposited in the Department of Pharmacognosy Herbarium Laboratory University of Maiduguri. Dried grounded fruits of *S. latifolius* (1.5 kg) was extracted in a Soxhlet apparatus using 95% ethanol. The extraction was carried out at boiling temperature for six (6) hours. The yield was labeled SLET and stored at 4°C until required.

Two hundred grams (200 g) of SLET was dissolved in water and partitioned successively with solvents of increasing polarities and tested for biological activity. Fractions with the best activity were then subjected to isolation and further purification.

Isolation and purification

Column and Thin layer Chromatography (CC & TLC) were adopted in line with standard procedures [9, 10], for the separation and purification of compounds from the promising fractions, this consist of open column guided by TLC and fractions with similar/same R_f values were pooled together. The eluting solvents (mobile phase) were applied from top through the column starting with less polar solvent that elute less polar compounds to the most polar solvent which elute polar compounds, and also in ratio combination CHCl₃: MeOH (100:0 to 0:100) in increasing polarity respectively. Semi-purified compounds were further separated by re-chromatographing on smaller columns and then preparative TLC. The structure(s) of

compounds were determined using GCMS for the most active fraction while the isolated compound was analyzed with spectroscopic tools such as 1D, 2D-NMR, UV, IR and mass spectroscopic analysis.

In-vitro studies

Evaluation of anti-inflammatory

Anti-inflammatory effects were assessed using the inhibition of albumin denaturation assay, as described by [11] The reaction suspension (5 mL) contained 1 mL of the extract (1 mg/mL), 3.8 mL of phosphate buffered saline (PBS, pH 6.4), and 0.2 mL of aqueous solution containing 1% bovine albumin. After incubation for 15 minutes at 37°C in a water bath, the reaction mixture was heated to 70 °C for 5 min. After cooling, the absorbance at 660 nm was measured using UV-vis spectrophotometer. Histamine and egg-albumin were used as negative control, and phosphate buffer solution was used as positive control. The following formula was used to compute the % inhibition of protein denaturation:

$$\% \text{ Inhibition of protein denaturation} = 100 \times \frac{1-A_2}{A_1}$$

Where, A1 is the absorption of the control sample and A2 is the absorption of the test sample.

Evaluation of antioxidant activity

The assay was carried out in line with modified method [12] 1.0 g of the extract was dissolved in 10ml ethanol. The solutions were transferred to test tubes in order to

obtain the stock solutions of 100, 50, 25, 12.5 and 6.25 µg /mL concentrations respectively; and the total volume was adjusted to 3 mL with distilled ethanol. Later, 1 mL of DPPH stock solution was added to each sample medium. After incubating in the dark for 30 min at 25°C, the absorbance values were measured at 517nm using UV spectrophotometer. 3mL ethanol was used in the detection with 1 mL of DPPH solution as a control. The decreased absorbance indicated the amount of DPPH solution remained after the free radical-scavenging activity. Calculations on the DPPH and that of the standard antioxidant compound ascorbic acid (vitamin C) were performed according to the following equation:

$$\% \text{ Inhibition of DPPH} = \frac{AC-AS}{AC} \times 100$$

Statistical analysis

Data was expressed as means ± SD (n = 3). Regression analysis was also employed for determining the inhibition concentration at 50 percent radical scavenging.

Results

Percentage yield of extract

Exactly 90 g of the crude ethanol fruit extract of *S. latifolius* was obtained. After fractionating with solvents of different polarity, ethyl acetate extract showed the highest yield of 32 g (35.5%) The yield and percent yield are shown in Table 1 below.

Table 1: Percentage yield and colour.

Fractions	Weight(g)	Yield %	Colour
Ethyl acetate	32	35.5	Dark brown
Hexane	30	33.3	Oily reddish brown
Residual Aqueous	24	26.6	Dark Brown

DPPH assay

The *In-vitro* DPPH Assay was carried on the least and most polar fraction (n-hexane and residual aqueous) as shown in Table 2. The percent inhibition was higher in

the non-polar (n-hexane) fraction (57-67 %) than the polar (residual aqueous) fraction (40-56 %). The Inhibitory concentration is as shown in Table 2 and Figure 1a-c.

Table 2: Antioxidant Activity of *Sarcocephalus latifolius* extract (IC₅₀).

Plant extract	IC ₅₀
<i>n</i> -hexane (NHE)	0.33
Residual Aqueous (RAE)	0.55
Ascorbic acid	0.56

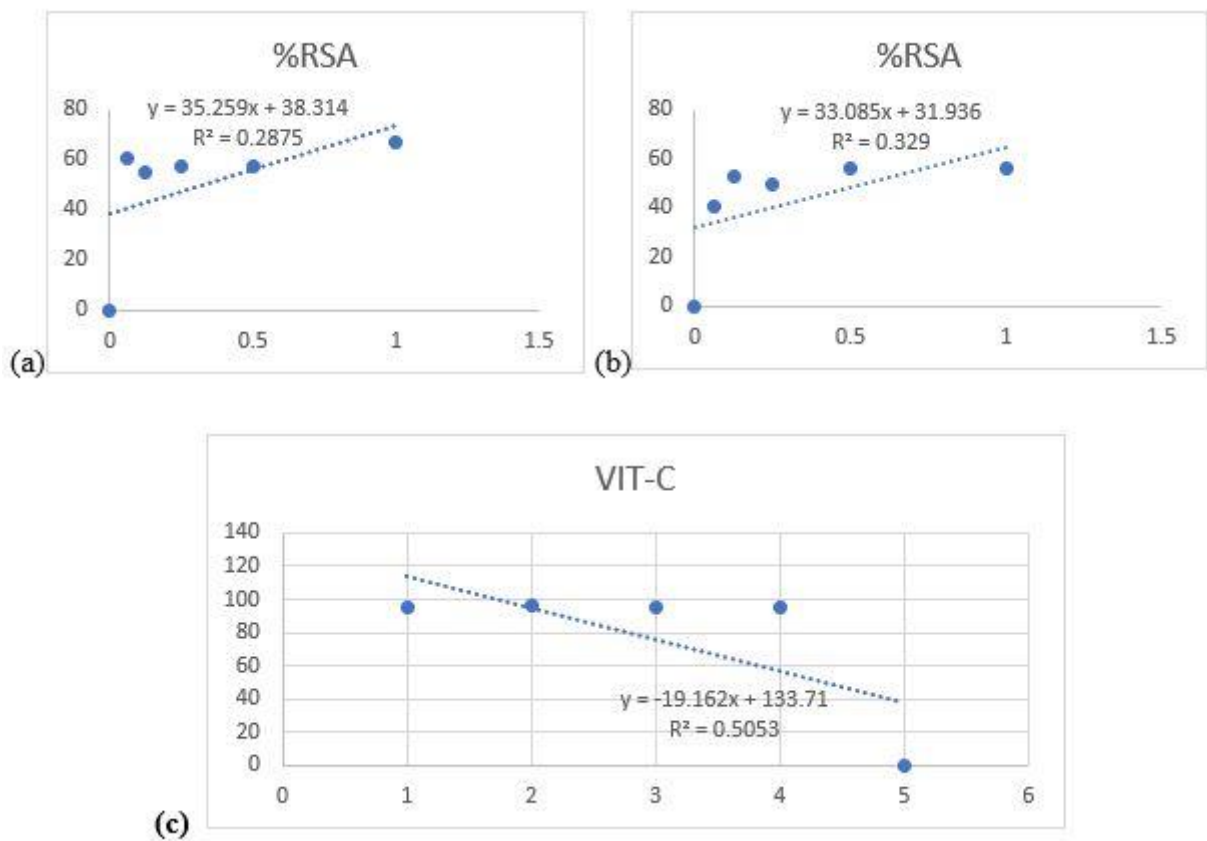


Figure 1: IC₅₀ determination by regression analysis for (a) n-hexane (b) residual aqueous (c) ascorbic acid in-vitro DPPH assay.

In-vitro anti-inflammatory assay

The in-vitro anti-inflammatory assay was conducted on two fractions (NHE and AQE) with better inhibition

recorded in the polar fraction for the egg albumin induced inflammation while the non- polar fraction was higher in the histamine induced inflammation as shown in Figure 2a &b.

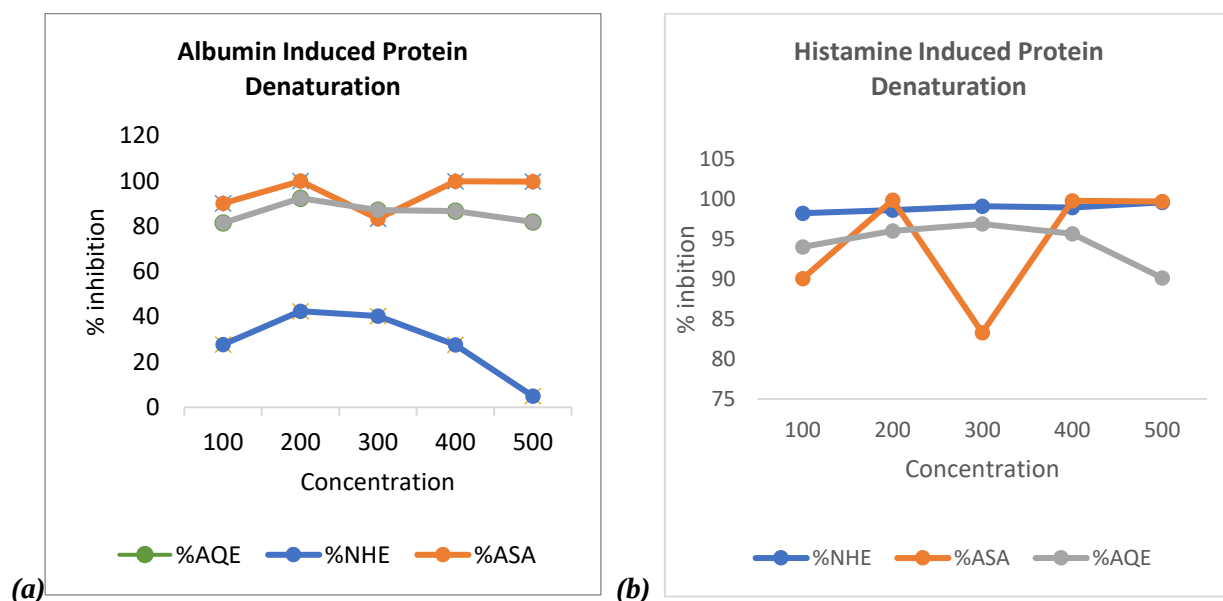


Figure 2: Comparison curve of Acetylsalicylic acid (ASA), n-hexane (NHE) and Residual Aqueous (AQE) fractions of *S. latifolius* Fruit.

Isolation and purification of *S. latifolius* fruit

The n-hexane fraction (30 g) was divided into two (2) portions. 5 g was used for GC-MS analysis while 25 g was run on column and purified with TLC and

Sephadex LH-20. 33 eluates were obtained from columns, Spots with similar retention factor were pooled, re-run on smaller columns until single spots emerged on TLC. Findings from GC-MS analysis and TLC profile are in Table 3 and Fig. 3.

Table 3: GC-Mass Profile of chemical constituents of *Sarcocephalus latifolia*.

S. No.	Compound	RT	%Peak Area	Mol. wt	Quality (%)
1	1-Docosene	18.386	1.69	308.6	92
2	4-dodecene	36.913	0.08	168.32	95
3	Oleic acid	36.069	0.22	282.5	93
4	Methylstereate	32.954	0.40	298.5	95
5	Ethyl, 10-(2-iodophenyl) Undecanoate	19.531	0.07	416.3	90
6	Linoleic acid ethylester	35.443	0.12	308.5	93
7	14-methyloctadecanoic acid	32.470	2.00	298.5	90
8	2-methyl-Z,Z-3,13-Octadecadienol	36.368	0.14	266.5	92
9	Dodecylacrylate	23.718	4.82	240.38	91
10	Tetradecanoic acid, methylester	25.979	0.51	242.40	93
11	Ethyl-13-methyltetradecanoate	28.177	0.12	270.50	92
12	Ethyl-9-hexadecanoate	29.856	1.35	282.5	98
13	Hexane decanoic acid	30.369	88.5	284.5	99

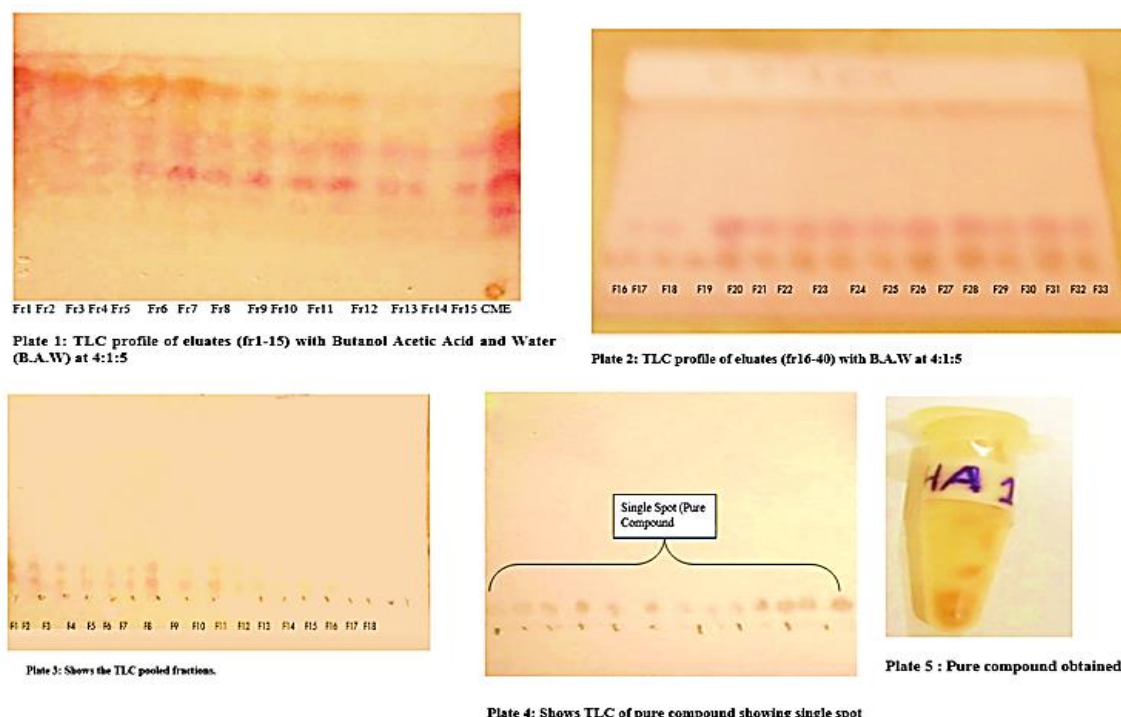
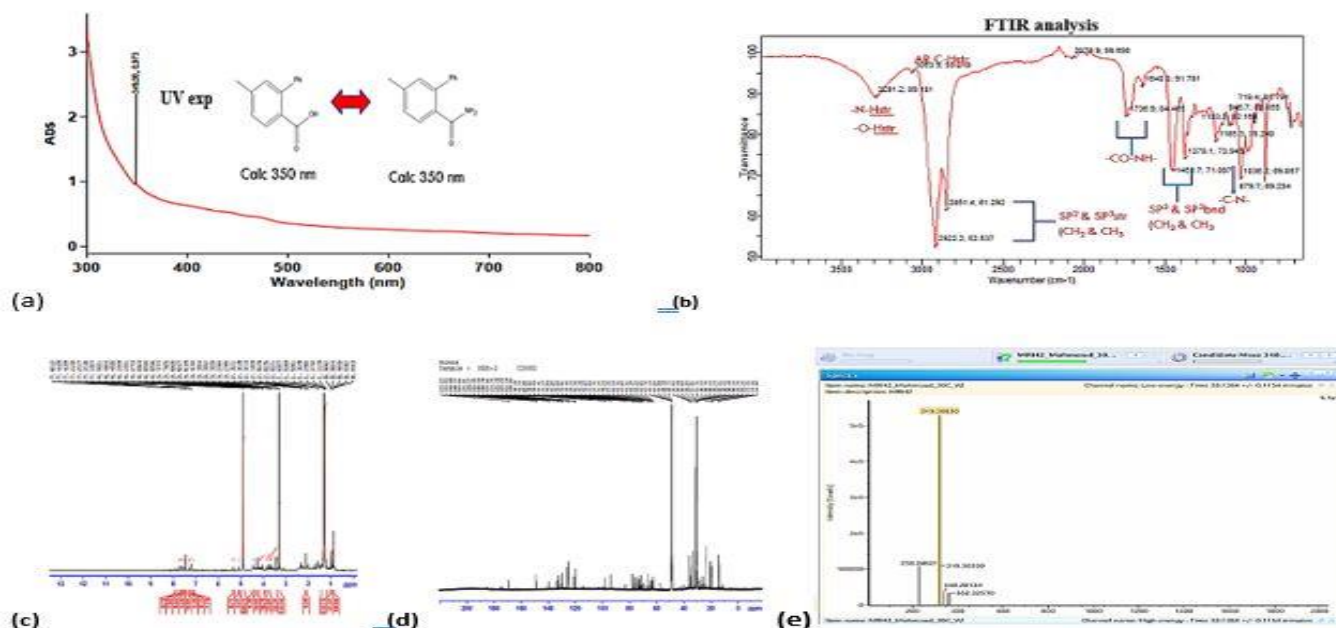


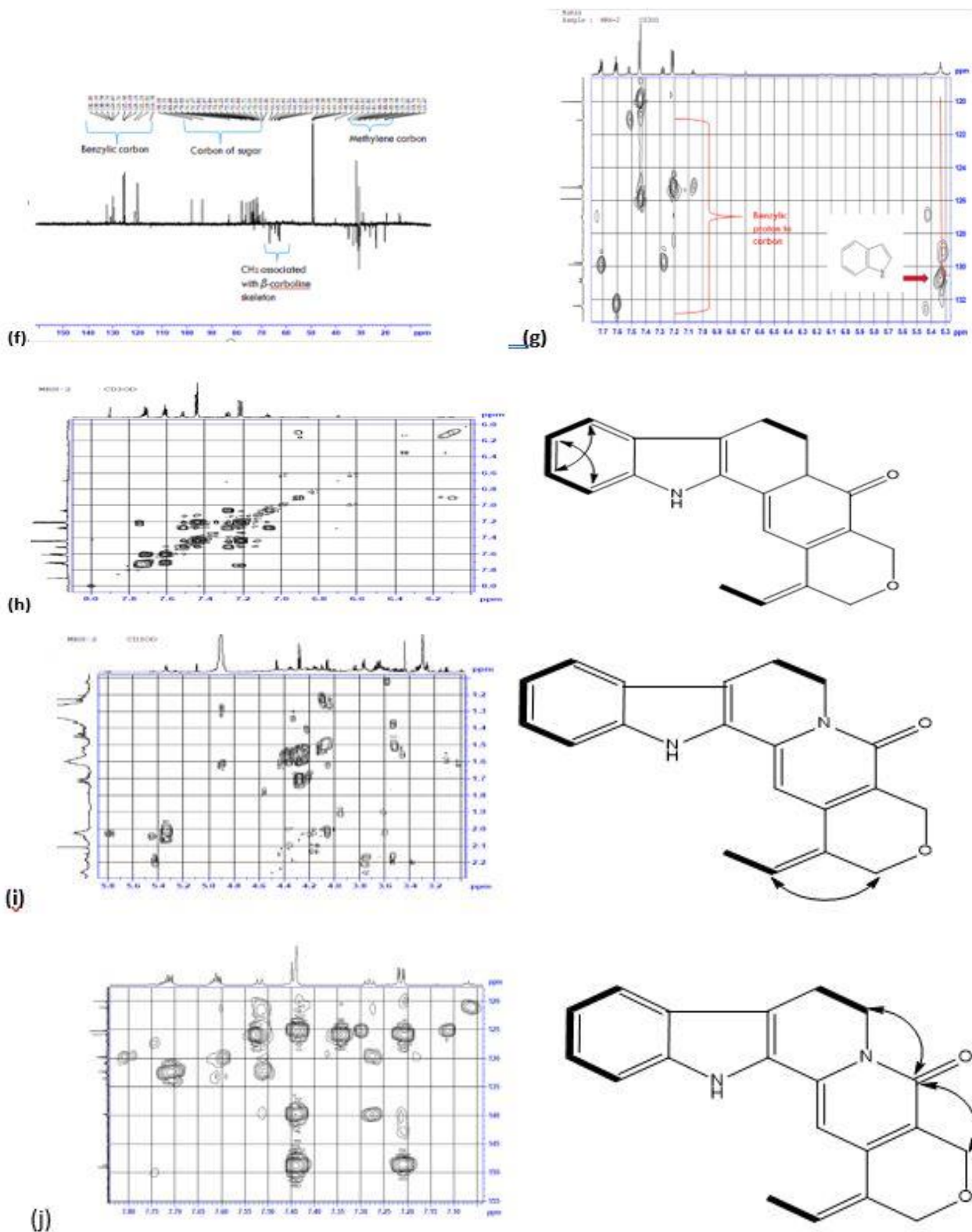
Figure 3: Plates showing the TLC Profile of *S. latifolius* fruit.

Chemical characterization of *S. latifolius* fruit

The pure compound (HA-1) was analyzed using spectrophotometric tools such as UV, IR, and NMR and MS as shown in figure 4. The UV showed absorbance for a substituted benzene at 349 nm while the IR revealed functional groups such as the amide and carbonyl vibrational frequencies. 1D NMR showed chemical shift pattern consistent with an indole moiety

and Mass spectrum showed an abundant peak at 318 mass to charge ratio (m/z). A 2D NMR data analyses conducted showed interactions between proton-proton (HSQC, H-H COSY) and proton-carbon (HMBC) as shown in figure 4. Further identification was conducted with data comparison with previously isolated compound with similar data from other sources as shown in Table 4.





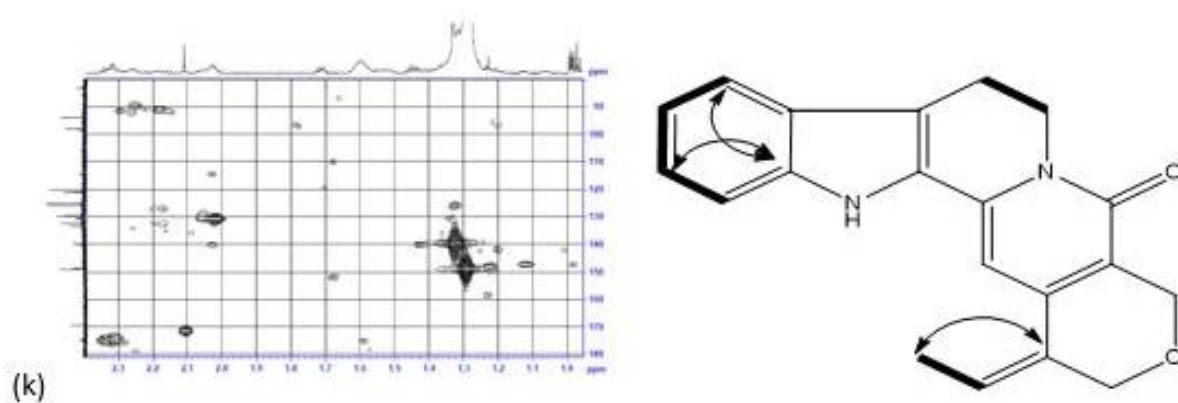


Figure 4: Characterization of HA-1 using UV, IR and 1D&2D Proton and Carbon NMR (a) UV Spectra of HA-1 a peak at λ max. at 349 nm (b) FITR spectra of compound HA-1 (c) ^1H -NMR of compound HA-1 (d) ^{13}C -NMR of compound HA-1 (e) MS spectrum of HA-1 (f) DEPT NMR of compound HA-1 (g) HSQC of compound HA-1 (h) H-H COSY of compound HA-1 (i) H-H COSY of compound HA-1 (j) HMBC of compound HA-1 (k) HMBC of compound HA-1.

Table 4: Comparison of data obtained from HA-1 with Literature data.

	$^1\text{H}(\text{dH, Hz})$	$^{13}\text{C}(\text{dC})$	$^1\text{H}(\text{dH, Hz})$	$^{13}\text{C}(\text{dC})$
NH-1	7.89.9.72	-	7.92(s)	
2	-	127.4	-	125.9
3	-	137.9	-	132.8
4	4.03(m)	40.7	4.39(t)	40.15
5	4.59(m)			
6	2.96(m)	19.5	3.12(t)	19.47
7	-	114.4	-	114.7
8	-	125.6	-	125.2
9	7.48(d)	119.5	7.49(d)	120.0
10	7.10(dd)	120.5	7.07(m)	121.1
11	7.21(dd 73.82)	124.7	7.22(m)	125.1
12	7.33(d.8.2)	111.9	7.45(d)	114.3
13	-	138.5	-	139.8
14	6.32(s)	102.0	7.73(s)	98.20
15	-	136.6	-	133.6
16	-	125.7	-	125.9
17	4.36(d)	58.9	4.46(d)	62.7
18	1.46(d. 6.6)	14.6	0.99(s)	14.46
19	5.76(q. 6.6)	125.9	-	129.8
20	-	148.0	-	148.8

Citation: Yesufu HB, Ukwubile CA, Milagawanda HH, et al. Isolation, Structural Elucidation and Anti-inflammatory Studies (In-vitro & in-silico) on the Fruit Extract of *Sarcocephalus latifolius* (Sm) Bruce. *J Pharm Res Sci Technol* 2024; 8(2): 181. doi: [10.31531/jprst.1000181](https://doi.org/10.31531/jprst.1000181)

21	4.18(d)	66.6	4.28(d)	66.6
22	-	163.1	-	169.6

¹H/ ¹³C IN LIT; Sook et al. [13]

¹H/ ¹³C IN Compound HA-1

In-silico studies on *S. latifolius* fruit

The compounds obtained from GCMS and NMR analyses were investigated for their Pharmacokinetic properties as shown in Table 5. Also, the binding interactions of the compounds to the inflammatory

cytokine receptor (TNF- α) was reported in Table 6. Interestingly, the pure isolate (HA-1) which was identified as Naucline exhibited the best ligand-receptor interaction as shown in Figure 5. Other ligand-receptor interaction is captured in the supplementary data.

Table 5: Pharmacokinetic properties of constituents from *n*-hexane fraction of *S. latifolius* fruit.

S. No.	Compound ID	Formula	HBA (≤ 10)	HBD (≤ 5)	Mol LogP (≤ 15)	BBB	CYPD26/CYP1A2	GI ABSP	Drug likeness ($V \geq 4.15$)
1	74138	C ₂₂ H ₄₄	0	0	7.67	No	No/Yes	Low	≥ 4.15
2	5364443	C ₁₂ H ₂₄	0	0	5.25	No	No/Yes	Low	≥ 4.15
3	445639	C ₁₈ H ₃₄ O ₂	2	1	4.57	No	No/Yes	High	≥ 4.15
4	8201	C ₁₉ H ₃₈ O ₂	2	0	4.91	No	No/Yes	High	≥ 4.15
5	3037234	C ₁₉ H ₂₂ IO ₂	2	0	5.33	No	No/Yes	High	≥ 4.15
6	5282184	C ₂₀ H ₃₆ O ₂	2	0	-	-	-	-	-
7	5312308	C ₁₉ H ₃₈ O ₂	2	1	4.91	No	No/Yes	High	≥ 4.15
8	5283306	C ₁₈ H ₃₄ O	1	1	4.68	No	No/Yes	High	≥ 4.15
9	75084	C ₁₅ H ₂₈ O ₂	2	0	3.84	Yes	No/Yes	High	0
10	31284	C ₁₅ H ₃₀ O ₂	2	0	3.94		No/Yes	High	0
11	71380066	C ₁₇ H ₃₄ O ₂	2	0	4.44	Yes	No/Yes	High	≥ 4.15
12	5364759	C ₁₃ H ₃₄ O ₂	2	0	4.57	Yes	No/Yes	High	≥ 4.15
13	12366	C ₁₈ H ₃₆ O ₂	2	0	4.67	No	No/Yes	High	≥ 4.15
14	102193811	C ₂₀ H ₄₈ N ₂ O ₂	2	1	2.51	Yes	No/Yes	High	0

Table 6: Docking score and residues involved in receptor-Ligand interaction.

S. No.	Compound ID	$\Delta G_{\text{binding}}$ (kcal mol)	Amino acid residue	Binding Interaction
1	CID 74138	-3.3	ILE 90; LEU 88; THR 74	Alkyl , VDW
2	CID 5364443	-3.5	ILE 90; LEU 88	Alkyl
3	CID 445639	-3.7	ILE 90; LEU 88, THR 74	Alkyl , VDW

4	CID 3037234	-4.3	ILE 90; LEU 88	CHB, Pi-Alkyl
6	CID 5282184	-4.1	ILE 90; LEU 88; PRO 92;THR 94; ARG 8	Alkyl, CHB
7	CID 5312308	-3.9	ILE 90; LEU 88	Alkyl
8	CID 5283306	-3.4	ILE 90; LEU 88	Alkyl
9	CID 75084	-3.9	ILE 90; LEU 88; PRO 92;THR 94; ARG 8	CHB, Alkyl
10	CID 31284	-3.4		
11	CID 71380066	-3.4	ILE 90; PHE 62; ALA 73;THR 74; LYS 46	CHB, Alkyl
12	CID 12366	-3.8	ILE 90; LEU 88	CHB, Alkyl
13	CID 102193811	-7.1	ILE 90; LEU 88; ALA 73;ASP 17;THR 74	Pi-sigma, Pi-Alkyl, CHB

VDW -Vander Waals force, CHB- Comprehensive Hydrogen bond

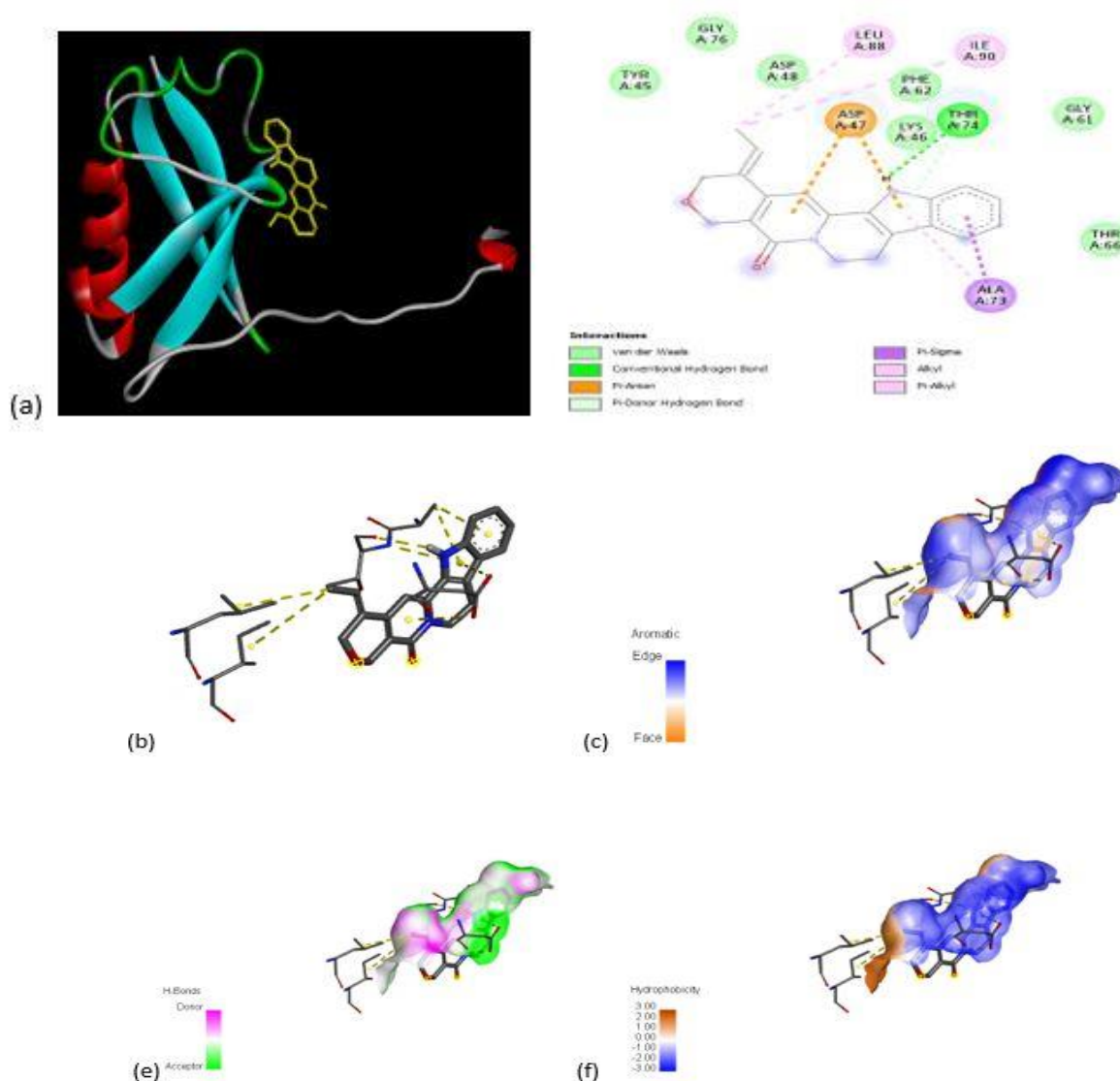


Figure 5: Ligand-receptor interaction of naucline (a) 3D-interaction (b) 2D-Interaction (c) ligand interaction (d) Aromatic interactions (e) Hydrogen bond interaction (f) Hydrophobic interaction.

Discussion

Previous reports on *Sarcocephalus latifolius* fruit have revealed a diverse array of phytochemicals, including alkaloids, flavonoids, tannins, and terpenoids. These compounds are primarily responsible for the plant's various bioactivities, such as anti-inflammatory, antimicrobial, and antioxidant effects [14,15,16]. Therefore, the antioxidant potential recorded on the fruit extract (figure 1.) may be due to the presence of flavonoids and tannins as reported by Hans et al. [17] that these phytochemicals contribute to their role in preventing oxidative stress-related diseases. Mfotie et al. [18] has also reported that flavonoids found in the fruit of *Sarcocephalus* may inhibit pro-inflammatory cytokines and reduce oxidative stress.

Several methodologies have been employed to isolate the phytochemicals from *S. latifolius* fruits. Common techniques include Solvent Extraction, which utilize various solvents to extract bioactive compounds efficiently. For instance, ethanol and methanol have been frequently used due to their polarity, aiding in the extraction of a broad spectrum of phytochemicals [19]. Also, chromatographic techniques such as High-Performance Liquid Chromatography (HPLC) and Thin Layer Chromatography (TLC) are essential in the purification and identification of individual compounds. These methods have been instrumental in characterizing the specific alkaloids and flavonoids present in the fruit [20]. Alongside isolation, structural elucidation of compounds often employs spectroscopic methods, including Nuclear Magnetic Resonance (NMR) and Mass Spectrometry (MS) [21]. These techniques provide detailed insights into the molecular structure of the phytochemicals, confirming their identities and elucidating their potential mechanisms of action [22].

Spectral elucidation of *S. latifolius* isolate revealed that the UV showed a maximum peak at λ_{max} 349 nm suggestive of a ketone moiety which is conjugated. The IR spectra of the pure compound carried out using Fourier infrared spectrophotometer showed vibrational frequencies for different organic molecules. 3291cm^{-1} indicates N-H stretching, 2922cm^{-1} Sp^2 and 2850cm^{-1} Sp^3 orbitals and this shows the presence of methylene and methyl groups. The unsymmetrical bending at the fingerprint region showed the presence of an amide at 1640cm^{-1} and 1738cm^{-1} bending frequency. Also, the band at 1640cm^{-1} of the IR spectra supports the presence of a secondary amide [23].

The Proposed structure of the compound was deduced from analysis ^1H and ^{13}C -NMR, DEPT Spectra of

Compound. The ^{13}C -NMR and DEPT Spectra data indicated that the molecule possesses one lactam carbonyl (169 ppm), eight aromatic carbons, one trisubstituted olefin, four methylene, six methines, and eight quaternary carbons. The signal at 62.7 and 66.6ppm was assigned as the resonances of two oxymethylene respectively [13]. The ^1H -NMR Spectrum showed the presence of four aromatic protons, a broad peak at -NH- (7.9ppm) and one $\text{CH}_2\text{-CH}_2\text{-N}$ -group were observed. Suggesting a β -carboline skeleton. Two of the four aromatic protons in ring A appeared as doublets at 7.49 ppm and the other as two doublets of doublets at 7.22 and 7.20 ppm were attributed to H- 9, H-12, H-10 and H-11. In addition, two up-field signals of H-19 (5.34ppm) and methyl protons at 0.99 ppm were characteristic of trisubstituted olefin with a methyl group at C-19 respectively [24].

The bioactive compounds derived from *S. latifolius* fruit have been reported to exhibit numerous therapeutic applications [5,25,26]. Mfotie et al. [27] reported that extracts from the fruit have shown efficacy against various pathogens, indicating potential applications in developing natural antimicrobial agents. Abbah et al. [3] evaluated the anti-nociceptive, anti-inflammatory and anti-pyretic activities of the aqueous extract of the root bark of *S. latifolia* in mice and rats. With significant reduction in egg-albumin induced oedema in rats in a dose-dependent manner, the study agreed with our findings which showed a significant reduction (in-vitro) for egg albumin and histamine inflammation by the *S. latifolius* fruit extracts (fig. 2). The anti-inflammatory effects of *S. latifolius* fruit extracts can be attributed to several mechanisms. Mfotie et al. [18] has reported that extracts from *S. pobeguinii* have been shown to inhibit cyclooxygenase (COX) and lipoxygenase (LOX) enzymes, which are critical in inflammatory responses. Inhibition of these enzymes can lead to decreased production of prostaglandins and leukotrienes, thereby reducing inflammation [28]. Mfotie et al. [18] observed that several studies have shown extracts from *S. latifolius*, can downregulate the production of key pro-inflammatory cytokines, such as TNF- α and IL-6, by inhibiting their transcription factors.

With Molecular docking becoming a corner stone in drug discovery, particularly for understanding how compounds can inhibit or activate specific biological pathways, an in-silico investigation of the GCMS and isolated compounds from *S. latifolius* fruit revealed moderate to low druggability with more violation of the drug-likeness. However, the isolated compound showed a good drug-likeness (Table 5). Most compounds

showed good Gastro-intestinal absorption (GI), while a few showed possibilities to cross the Blood brain barrier (BBB). The most potent ligands were obtained by examining molecular interaction of the ligands with the binding pocket of TNF- α 1. The results as shown (Table 6) unfold better interaction of the isolated compound (CID 102193811) than all other ligands. As the best ligand, CID 102193811 had lower $\Delta G_{\text{binding}}$ value and binds on the best position in the receptor binding site. While most of the compounds had between eight to nine interactions with the amino acid residues which were majorly alkyl, Vander-Waals and conventional hydrogen bonding, the isolated compound had twelve (12) interactions with the residues which were majorly Pi-sigma, Pi- alkyl, Pi- anion, Pi-donor hydrogen, Conventional hydrogen bonding and Vander-Waals. Most interactions occurred with amino acid residues such as ILE 90; LEU 88; PHE 62; ALA 73; THR 66; THR 74; LYS 46; THR 94. There is increasing evidence that specific amino acids can exert regulatory effects at various levels of cell activity, acting as mediators or signal molecules and, therefore, modulate numerous functions [29]. Newsholme [30] reported that the function of immune cells was reportedly improved by glutamine, arginine and cysteine. In addition, Amino acids were reported to modulate gene expression in several ways either as promoters of some genes or as activators of several transcription factors [31, 29]. For example, nuclear transcription factor kappa B (NF κ B) is often activated in intestinal inflammation [32,33,34]. Therefore, the mechanism of action of the compounds reported in this study may agree with the observation raised by Mfotie et al. [18]

Conclusion

The isolation and structural elucidation of phytochemicals from *S. latifolius* fruit revealed a complex tapestry of bioactive compounds with significant therapeutic potential. Through a combination of chromatographic and spectroscopic techniques, Naucleine has been characterized by providing a foundation for further research into its bioactivity and therapeutic applications. As the demand for natural compounds grows in the pharmaceutical industry, naucleine represents a promising candidate for future drug development efforts.

Also, the fruit extract of *S. latifolius* presents significant anti-inflammatory potential, supported by a rich phytochemical profile and various mechanisms of action. The ability to inhibit key inflammatory mediators, reduce oxidative stress, and modulate enzymatic activity underscores its therapeutic promise.

Therefore, continued research, particularly in clinical settings, will be crucial to validating these findings and exploring the application of *Sarcocephalus latifolius* extracts in managing inflammation-related diseases.

Author Contributions

HB: Conceptualization, Methodology, Investigation, Formal analysis, Writing-original draft, Visualization, Writing-review & editing. CA: Formal analysis, Resources, Writing-original draft, Visualization. HH: Formal analysis, Resources, Writing-original draft. ABB: Formal analysis, Resources, Writing-original draft.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Ethical Approval

Not applicable.

Data Availability

The raw data supporting the conclusions of this manuscript will be made available on genuine request.

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