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Research Article

Extraction, isolation and characterization of bioactive compounds derived from *Sanchezia oblonga* plant extract

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ABSTRACT

Medicinal plants, owing the richest source of drugs for the traditional medicine, food supplements, modern as well as folk medicines, fragrances, significant efforts have been paid for driving the quest for potential bioactive chemicals derived from them. Plant extracts have been used to cure a variety of illnesses for a very long time in many civilizations. In many cases, efforts are made to properly validate and comprehend the usefulness of these folk treatments without analyzing the bioactive chemicals in plants i.e. the mature leaves of Sanchezia oblonga Ruiz & Pav. is crushed into little pieces and applied to the body to treat cyanosis, tendonitis, and backaches. Herein leaf extracts of Sanchezia oblonga Ruiz & Pav. were used to test for the presence of phytochemicals and investigate the plant's pharmacological properties. The isolation of phytochemicals using TLC, GC-MS, analysis and UV visible spectroscopy reveals the existence of nine bioactive compounds. Additionally, in-silico and DFT analysis clearly indicates that Stearic Acid possesses highest activity affinity for binding and pharmacological potential against different target proteins among the isolated phytochemicals.

INTRODUCTION

A medicinal plant is any plant that contains compounds that can be utilized for therapeutic purposes or that serves as a precursor for the creation of important pharmaceuticals. Normally, scientific researchers are responsible of assessing the benefit of plant families. Local people, on the other hand, are best qualified to determine the usefulness of specific plant species for a given

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application because they can draw on empirical knowledge gathered over a period of time[1]. Over millions of years, they have changed and adapted to fend off bacteria, insects, fungi, and the environment to create distinctive secondary metabolites with a variety of structural characteristics. Their ethno pharmacological properties have been used as a primary source of medicines for early drug discovery [2]. According to the World Health Organization (WHO), 80% of people still rely on plant based traditional medicines for primary health care (Farnsworth et al., 1985) and 80% of the plant derived drugs were related to their original ethno pharmacological purpose [3]. People have looked for natural remedies for their illnesses since ancient times. As is the case with animals, the first uses of medicinal plants were instinctual. Natural products have been used since ancient times and in folklore for the treatment of many diseases and illnesses[4]. They have been the source of most of the active ingredients of medicines. This is widely accepted to be true when applied to drug discovery in 'olden times' before the advent of high through screening and the post genomicera [5]. In truth, everything depended on practice because there wasn't enough information available at the time about the causes of the ailments or the best plant to use as a preventive medicine. As specific medicinal plants for treating particular ailments came to light over antiquity, the empirical base for their use grew and they started to be used as explanatory evidence. Up until the invention of medical science in the 16th century, prevention and therapy were provided by plants (Sofowora 2013)[6]. Since 5000 BC, medicinal herbs have been used in India as part of the Ayurvedic medical system. For the purpose of preventing and treating disease, this approach comprises dietary guidelines and herbal medicines that are tailored to the body, mind, and spirit [7]. According to reports, herbal medicines and their active ingredients can effectively heal human diseases and disorders while also having positive impacts on long term fitness.[3]. Since the beginning of time, people have researched using herbal remedies to treat a variety of illnesses and relieve pain. In addition to the aforementioned, the usage of medicinal plants dates back 60,000 years, when a Sumerian clay slab, a sort of equipment, was unearthed and used to verify the use of medicinal plants in the production of medications. Today, more than 50% of medications are natural and have some connection to plants in their origin.[3] Currently, both developed and developing nations frequently employ herbal medications for healthcare. Herbal medications are regarded as mixes of chemical substances produced by plants, and their effectiveness is constrained due to poor oral absorption. In the current situation, it becomes vital to standardise herbal goods and evaluate medicine quality in order to determine the quantity of their active constituents. The first record of using medicinal plants to make medications dates back to roughly 5000 years ago and was discovered on a Sumerian slab of clay from Nagpur. It contains 12 drug synthesis formulas that allude to more than 250 different plants, some of which contain alkaloids including mandrake, poppy, and henbane [3] . Proof from the Old Testament and the most sacred Jewish scripture called the Talmud showed that aromatic herbs like myrtle and incense were used during numerous rites following a treatment.[3] Many of the drugs that are currently on the market have either been directly or indirectly produced from plants, which have historically been an excellent source of pharmaceuticals. According to ethnobotanical data, 800 plants may have anti-diabetic properties (Alarcon-Aguilara et al., 1998)[8]. When tested using currently available experimental procedures, a number of these herbs have demonstrated anti-diabetic action. According to Bailey and Day (1989), Ivorra et al. (1988), Marles and Farnsworth (1995), a variety of active

principles derived from plants that represent a variety of chemical compounds have shown activity commensurate with their potential application for the therapeutic use of Non-Insulin-Dependent-Diabetes. [9]. They play a key role in offering basic healthcare to people who live in rural areas. They are also used as essential components for the production of both conventional and modern medications as well as therapeutic agents. Tropical rainforests in central and south America are home to the perennial evergreen shrub Sanchezia nobilis (Acanthaceae)[10]. Plants in the Sanchezia genus can be utilised as anti-tuberculosis, anti-tumor, anticonvulsants, cough sedatives, and expectorants in traditional medicine [11].The world's greatest diversity of plant species can be found in tropical regions, some of which may have therapeutic benefits. During the course of this investigation, Sanchezia nobilis, a tropical plant, was examined for its leaves. The lowland regions of tropical Central and South America are home to members of this genus, which are shrubs, small trees, and occasionally plants. The three species S. nobilis, S. parvibracteata, and S. speciosa are examples of well-known species [12]. Some species have become recognised for their therapeutic properties and are frequently utilised, but it is unknown whether the majority of plants in tropical forests contain active ingredients [13]. As a result, comprehensive scientific screening is needed to assess these plants. Therefore, the goal of this research effort was to look for bioactive substances and assess the pharmacological effects of this plant's leaves. According to studies, these substances have anti-inflammatory, anti-bacterial, anti-fungal, anti-cancer, and antioxidant activities. There haven't been many investigations into Sanchezia speciosa's pharmacological properties and chemical composition. Therefore, there is no exhaustive identification of the basic chemical constituents and comprehensive quality control of this genus. S. speciosa contains cardiac and flavonoid glycosides and their extracts exhibit antioxidant and anti-inflammatory activities [14]. Extracts of the same species exerted cytotoxicity in human epithelial cervical cancer cell lines[14]. *Sanchezia oblonga* Ruiz & Pav. (syn. Sanchezia nobilis Hook. f.) is a perennial evergreen shrub from the rainforests of Central and South America[15]. An previous study discovered that *S. nobilis* extracts include syringin, flavone glycosides, cinnamyl and benzyl alcohol glycosides, and neolignan glucoside in addition to the matsutake alcohol glycosides. When necessary, the bioactive ingredient is then extracted, fractionated, and isolated. In addition, it comprises determination of quantity and quality of bioactive compounds. Efficacy and ease of administration are among the reasons that plants are becoming increasingly popular as source of medicine, especially since they are natural, are available in local communities, and are cheaper to buy. Furthermore, herbal medicine may be a substitute to conventional medicine in cases where a drug's side effects are severe and drug resistance exists. When extracting medicinal plants, active substances such alkaloids, flavonoids, terpenes, saponins, steroids, and glycosides are separated from inert or inactive material using a suitable solvent and accepted extraction techniques. Plant products with high levels of phenolic and flavonoid chemicals have been shown to have antioxidant characteristics and are therefore utilised to treat age-related illnesses like Alzheimer's disease, Parkinsonism, anxiety, and depression[16]. The process of obtaining medicinal plants was carried out in a variety of ways such as maceration, infusion, decoction, percolation, digestion and Soxhlet extraction, superficial extraction, ultrasound-assisted, and microwave-assisted extraction[17]. In addition, thin-layer chromatography (TLC), high-performance liquid chromatography (HPLC),

paper chromatography (PC), and gas chromatography (GC) were used in purification and separation of the secondary metabolites. When choosing an extraction technique, solvent to be employed, solvent pH, temperature, and solvent to sample ratio, it is crucial to take the nature of the plant material into account. It also relies on how the finished products are going to be used. The objective of this study was to evaluate various extraction solvents, procedures, fractionation, and purification techniques as well as phytochemical screening and identification of bioactive chemicals in *Sanchezia oblonga*medicinal plants.

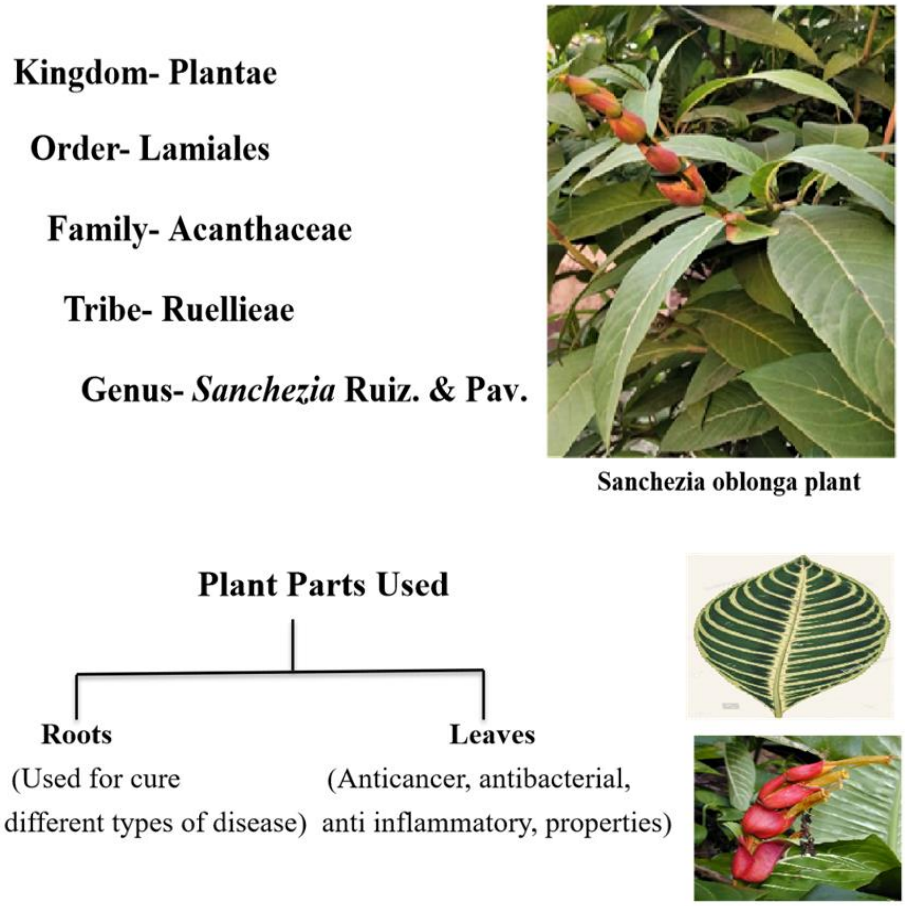


Figure 1: Plant taxonomy and different parts of *Sanchezia oblonga*medicinal plants

2. Taxonomy and nomenclature

Sanchezia is a genus of the family Acanthaceae and tribe is Ruellieae was first briefly described by Ruiz and Pavon in 1974 and named by Jose Sanchez. The Plant is cultivated in India and mostly found in Western Ghat & Eastern GhatRoots and Leaves are the most important parts of the plant as shown in **Table 1**.The taxonomic classification of plants at the family stage is crucial in figuring out which plant species are valuable to the local population. According to Phillips and Gentry [18], certain plant families are unquestionably more helpful than others in particular use categories.According to Scotland and Vollesen [19], the family Acanthaceae has roughly 221 genera and 4000 species that are found widely throughout the Old and New World Tropics. An exceptional variety of taxa, morphological and ecological features, and geographical distribution distinguish the Acanthaceae as a global group of flowering plants. More than 93% of the Acanthaceae species on

Madagascar are considered endemic, making it the island with the highest degree of endemism [20]**.** Furthermore, Acanthaceae boast a remarkably rich fossil record as well as marked taxonomic diversity [21]. Most species of Acanthaceae live in small populations, especially in tropical ecosystems that exhibit high alpha diversity. Tropical botanists have struggled with this for a long time as we attempt to understand the evolution of species in these regions. The genus Sanchezia is included in the subfamily Ruellieae. This genus is native to the New World and comprises 59 species which are diverse morphologically, ecologically, and geographically [22]. Sanchezia species are widely commercialized as ornamentals are often planted as street shrubs or living fences (Scotland and Vollesen, 2000).*Sanchezia oblonga* Ruiz & Pav. (Acanthaceae) belong to the family of neotropical herbs and shrubs. *Sanchezia oblonga* is a small, semi-woody erect evergreen shrub growing 1.3 to 2.4 meters. Stems are bright green to purple. Leaves are large, up to 26 centimeters in length, opposite, lanceolate. Green blade with clearly visible veins of white or yellow. Flowers are yellow, tubular, with red bracts, about 5 centimeters long, and borne in terminal spikes of 6 to 10 as shown in **Figure 1**. Fruits are oblong capsules with 6 to 8 circular, compressed seeds. Several species of *Sanchezia*, such as *S. parvibracteata*, *S. nobilis* and *S. speciosa*, are cultivated as ornamentals in tropical areas and botanical gardens due to their colorful leaves and conspicuous bright and colorful bracts and flowers. Recently, this genus was revised by Leonard and Smith (1964); among 58 species, over half were newly described [23].*Sanchezia* is named for José Sánchez, a nineteenth-century professor of botany at Cádiz, Spain (Clay *et al.,* 1987).They reported Species of ot this genus are *S. lampra, S. ovata Ruiz & Pav.***,** *S. parvibracteata* **,** *S. parviflora***,** *S. peruviana***,** *S. putumayensis* **,** *S. sericea***,** *S.* speciosa**,** *S.* nobilis Hook.f. (Wiersema and León, 2013)[24], *S. oblonga* (wikispecies: *Sanchezia oblonga*).

Table 1: Distribution of plants in different regions of Indian

Continent/Country/Region	Distribution	Origin	Reference	Notes
Andhra Pradesh	Present	Introduced	India Biodiversity (2014)	Cultivated
Karnataka	Present	Introduced	India Biodiversity (2014)	Cultivated
Tamil Nadu	Present	Introduced	India Biodiversity (2014)	Cultivated
West Bengal	Present	Introduced	India Biodiversity (2014)	Cultivated

3. MATERIALS AND METHODS

3.1. Reagents and chemicals : Analytical grade (HPLC) solvents, chemicals and reagents, Merck chemicals, Research-Lab Fine Chemical Industries, Mumbai, India, and Sigma Aldrich, Germany provided all of the chemicals.

3.2. Plant collection and identification and ethnomedicine survey: Plant will be collected from Balurghat College campus and identified by Professor Monoranjan Chowdhury, Plant taxonomy Laboratory, University of North Bengal. The plant material were properly washed with tap water and then rinsed with distilled water, dried in oven at 600°C until plant parts became well dried for grinding.

3.3. Plants parts used : Roots and Leaves are the most important parts of this plants. In the present study leaves had roots are used for the extraction purpose.

3.4. Preparation of powder sample

After drying, the plant materials were ground well into fine powder. The fresh leaves along with their petioles (1 kg) of the above plant were dried at 60 °C in a hot-air oven for 3–4 days. The dried leaves (300 g) were crushed into fine powder using mixer grinder.

3.5. Extraction of active compounds

The 100 g of powder drug was extracted in a Soxhlet extractor in 500 mL of 95% methanol and double distilled water separately at room temperature (30 °C) for 72–96 h. Then the extracts were filtered using Whatman No.1 filter paper. The pigments of the filtrate were removed by running in activated charcoal column. The pigment free samples were concentrated using rotary vacuum evaporator (Superfit Rotary Vacuum Evaporator, R-150, Mumbai, India) at 40 °C. From the final dry weight of 300 g of plant sample, 30 g of active methanol extract of Sanchezia oblonga was recovered. The active extracts of planti.e methanol extractswas kept aseptically at 4°C until use.

3.5.1. Preparation of powder sample: The fresh leaves along with their petioles (1 kg) of the above plant were dried at 60 °C in a hot-air oven for 3–4 days. The dried leaves (300 g) were crushed into fine powder using mixer grinder.

3.5.2. Moisture content: Moist sample was weighed immediately and recorded as ‘wet weight of sample’. The wet sample was dried at a temperature not exceeding 115°c using hot air oven.

Solvent extraction and pigment free : The 100 g of powder drug was extracted in a Soxhlet extractor in 500 mL of 95% analytical graded methanol at room temperature (30 °C) for 72–96 h. Then the extracts were filtered using Whatman No.1 filter paper. The pigments of the filtrate were removed by running in activated charcoal column.

3.6. Qualitative Analysis by thin Layer Chromatography:

Extract was to begin with, checked by TLC was performed after separation of major purified compound using MERCK TLC silica gel 60 F_{254} aluminium sheet. TLC with the separated purified compound used as stationery phase was carried out eluted by a standardized mixture of n-hexane and ethyl acetate in a ratio of 1:1 as mobile phase and visualized under 254 nm UV light. The R_f value was determined by calculating the ratio of the distance run by stationary phase to the distance run by mobile phase. The above prepared plant extracts were applied on precoated TLC plates by using capillary tubes and developed in a TLC chamber using suitable mobile phase. The developed TLC plates were air dried and observed under ultra violet light UV at both 254 nm and 366 nm. They were later sprayed with different spraying reagents and some were placed in hot air oven for 1 min for the development of color in separated bands. The movement of the analyze was expressed by its retention factor (R*f*). Values were calculated for different sample.

$$Rf = \frac{\text{Distance travel by solute}}{\text{Distance travel by solvent}}$$ (Where R*f*- Retention factor)

After drying the plates, they were exposed to Iodine vapours by placing in a chamber that was saturated with iodine vapours and also exposed to different spraying reagents. All plates were visualized directly after drying and with the help of UV at 254 nm and 366 nm in UV TLC viewer. The R*f* value of the different pots that were observed was calculated.

3.7. GC–MSanalysis :

To account the active photochemical in the fraction active fraction, gas chromatography-mass spectrometry (GC–MS) of the methanol fraction was carried out in a GC–MS instrument (Instrument No: GC-240 Ion Trap MS, Model:7890B, Agilent Technologies, USA) armored with a capillary column VF-5MS (ID-0.25MM, Film-0.25 µm, Length 31.98 min, Max temp. 325 °C).

3.8. Antibacterial activity by the Agar well Diffusion Method:

Assessment of antibacterial activity of crude sample against Gram negative bacteria (*E. coli*) was measured by the agar well diffusion method. 5 mm wells were cut in each fresh inoculated bacterial plates and 10 µl of different concentration of the test sample was loaded into the 5 mm diameter well seeded with test bacteria and incubated for 24 h. at 37 °C. The potency was measured by zone diameter of growth inhibition of crude extracts.

3.9. Computational Details:

In this study, all simulations were conducted using density functional theory (DFT) within the Gaussian 16 software package[25]. The ground-state geometries of all the phytochemicals were optimized at the B3LYP/6-31+G(d) level of theory[25]. To ensure that the optimized geometries correspond to true minima on the potential energy surfaces, a vibrational frequency analysis was performed at the same theoretical level, confirming the absence of imaginary frequencies. Optimized geometries are plotted using Gausview 6 program package[26].

3.10. Methodology for Molecular Docking Analysis:

Molecular Docking of the extracted compounds has been carried out by Autodock Vina programm package[27, 28]. The “sdf” files (3D-conformer) molecular structures of the nine extracted compounds are downloaded from PubChem (https://pubchem.ncbi.nlm.nih. gov/) and was converted to respective pdb files[29].

3.10.1. Ligand and protein preparation :

The crystal structure of two SARS-CoV-2 proteins (PDB ID:6LU7 and PDB ID:6w9c) and two Ebola virus proteins (PDB ID:1eS6 PDB ID: 4z9p), were retrieved from Protein Data bank (www.rcsb.org)[30]. All the structures of proteins were cleaned by removing hetero-atoms and water molecules using UCSF Chimera and site dependent run were carried outto evaluate the best binding sites of the extracted nine phytochemicals. To elucidate the binding site identification along with structural features of protein-drug com posite UCSF Chimera and Discovery Studio Visualizer have been used[31].

4. RESULTS AND DISCUSSION:

Phytochemical tests for bioactive constituents such as glycosides, saponins, anthraquinone derivatives, flavonoids, sterols, tannins, alkaloids, triterpenoids, phenols and leucoanthocyanidins were carried out on portion of residual material using standard phytochemical procedures as shown in the **Table 2**. The positive tests of these

observations clearly indicates that *Sanchezia oblonga* is a source of phytochemicals like Tannins, Alkaloids, steroids, Flavonoids natural products.

Table 2: Phytochemical testsof the active constituents in *Sanchezia oblonga* extract

Experiments	Observation	Bioactive Compounds Present
Plant material+ FeCl3+ distilled Water	Blue-black precipitation	Presence of Tannins
Plant material + Methanol + HCl + Dragendorff solution	Brownish-red precipitation	Presence of Alkaloids
Plant material + Water+ filtration	Shaken vigorously for 2 minutes and stable foam formed	Presence of Saponins
Plant material + Chloroform + Ac etic anhydride (1:1)	Formation of blue-green ring	Presence of Steroids
Plant material + dil. NH3 + Conc. H2SO4	Yellow colour formed	Presence of Flavonoids
Plant material + 10% NH3 + CHC l3	Rose-pink colour formed	Presence of Anthraquinone

4.1. Macro and Microscopic evaluation: The root and leaves extracts are examined macroscopically for parameters such as shape, size, colour, external features, and odour. Fresh samples of leaves, and roots were allowed to extract in diiferent solvents like methanol, ethnol, n-hexane, water, glycerol for microchemical tests as shown in **Figure 2**.

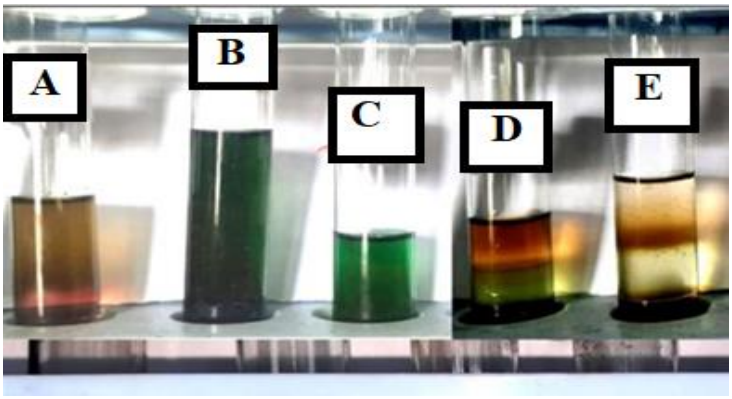


Figure 2. Microchemical colour reaction test of *Sanchezia oblonga* extractA: Ethanolic extract of the leaf powder; B- Methanolic extract of the leaf powder; C: n-Hexen extract of the leaf powder; D: Water extract of the leaf powder; E: Glycerol extract of the leaf powder.

4.2. Thin layer Chromatography analysis (TLC) Chromatographic separation of the constituent phytochemicals of the*Sanchezia oblonga* extract by TLC revealed three distinct spots

with Rf values of 0.29 (C2), 0.78 (C3) and 0.87 (C4), as shown in the **Figure 3** . These different sub-fractions of from TLC scraped is collected separately and allowed for bioassay. Among the sub-fraction of TLC plate 0.78 (C3) was the potentially active.

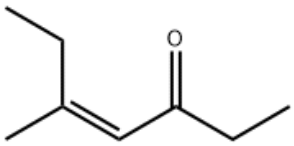
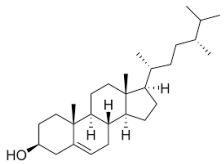
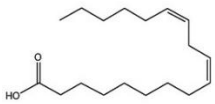
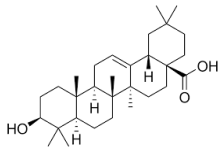
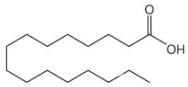
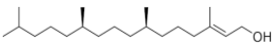


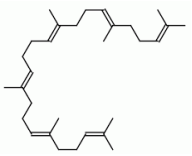
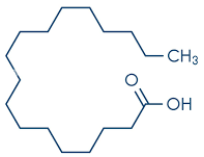
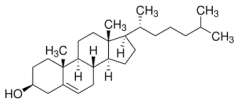
Figure 3 : Thin layer chromatography analysis of *Sanchezia oblonga* extract

4.3. Gas Chromatography Mass Spectrometry Analysis

In order to explore the presence of the phytochemicals derived from*Sanchezia oblonga* the plant extract we have used Gas Chromatography Mass Spectrometryanalysis. GC-MS analysis showed there are nine major compounds are present in the methanolic extract. Table 3 illustrated the names, molecular mormula, molecular weight along with molecular structure of these major nine compounds.

Table3: GC-MS profiling of the active phytochemicals of Sanchezia oblonga:

Sl. No.	Chemical name	Molecular formula	Molecular weight (g/mol)	Molecular structure
1	5methyl4hepten3one	C8H14O	126.20 g/mol	
2	Campesterol	C28H48O	400.7 g/mol	
3	Linoleic acid	C18H32O2	280.45 (g/mol)	
4	Oleanolic Acid	C30H48O3,	456.7 g/mol	
5	Palmitic Acid	C16H32O2,	256.43 (g/mol)	
6	Phytol	C20H40O	296.5 g/mol	

7	Squalene	C30H50	410.7 g/mol	
8	Stearic Acid	C18H36O2	284.5 g/mol	
9	Stigmasterol	C29H48O	412.7 g/mol	

4.4. Molecular docking The binding affinities of nine major compounds against two different proteins of two different targets viz. of two SARS-CoV-2 proteins (PDB ID:6LU7 and PDB ID:6w9c) and two Ebola virus proteins (PDB ID:1eS6 PDB ID: 4z9p), were analysed and tabulated in the tabulated in Table 4. From the Table 4 it is clear that among the phytochemicals stearic acid possessed highest docking affinity against the two different targets. 3D and 2D Docked structures of the two proteins against stearic acid are illustrated in the Figure 4 and 5.

Table 4 : Binding affinities of the the phytochemicals derived from *Sanchezia oblonga* againts Covid protein and Ebola Virus proteins

Drugs	6lu7 Covid protein	6w9c Covid protein	1eS6 Ebola Virus	4z9p Ebola Virus
5_methyl_4_hepten_3_one	-3.8	-4.3	-4.2	-4.0
Campesterol	-6.7	-6.4	-6.6	-6.2
Linoleic acid	-4.6	-4.4	-4.4	-3.9
Oleanolic Acid	-7.4	-6.8	-8.4	-6.8
Palmitic Acid	-4.1	-4.1	-4.3	-3.8
Phytol	-4.9	-4.9	-4.3	-4.1
Squalene	-4.8	-4.7	-4.5	-4.2
Stearic acid	-8.9	-8.4	-8.5	-8.1
Stigmasterol	-7.1	-6.4	-6.7	-6.7

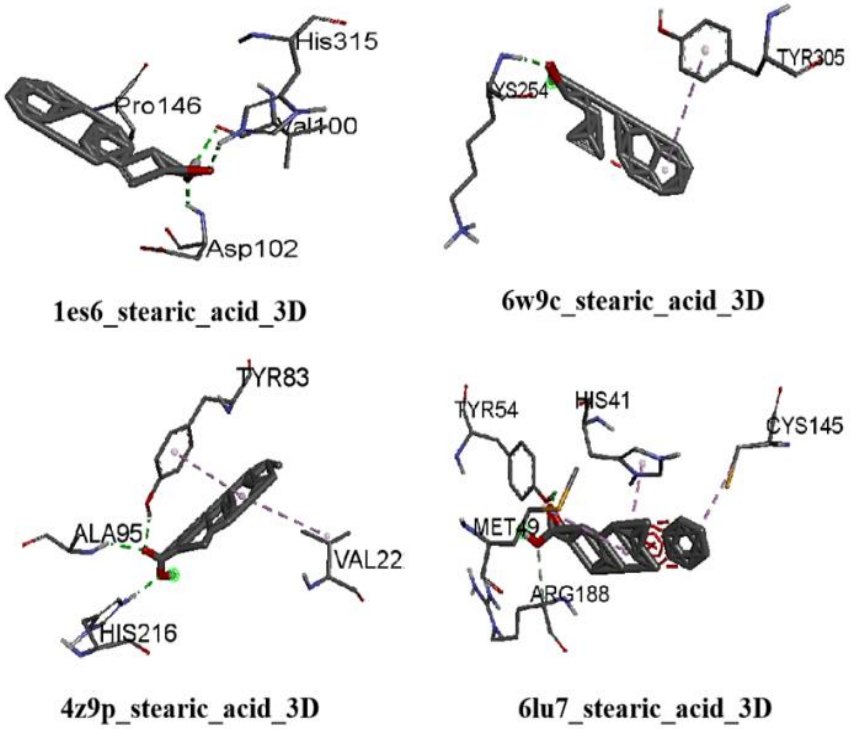


Figure 4: 3D structures of the dockedphytochemicals derived from *Sanchezia oblonga* againts Covid protein and Ebola Virus proteins

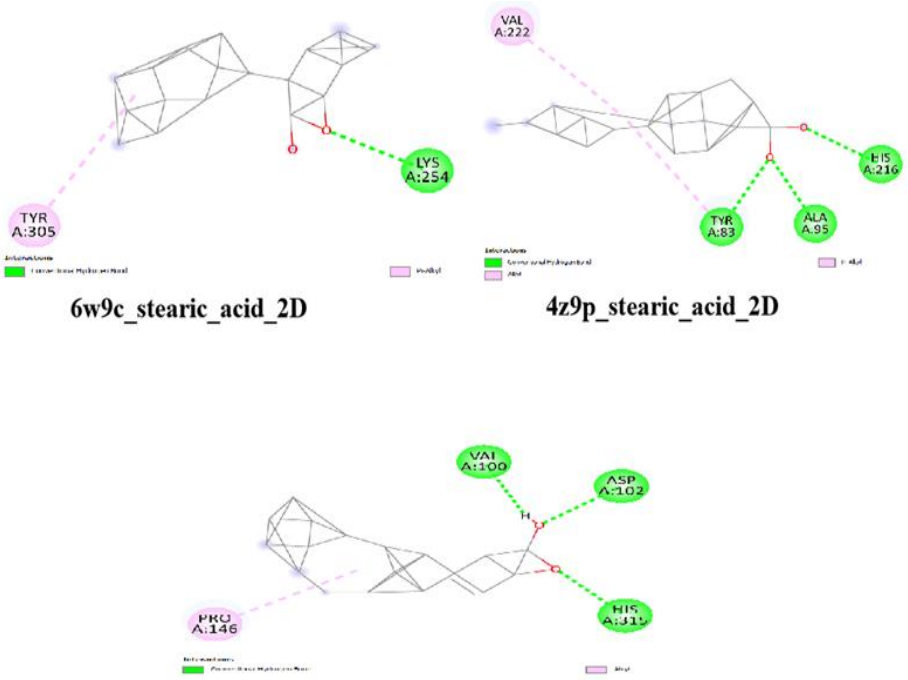


Figure 5: 2D structures of the docked phytochemicals derived from *Sanchezia oblonga* against Covid protein and Ebola Virus proteins

4.5. UV Visible Spectroscopy:

UV-Vis spectroscopy is an analytical technique that measures the amount of discrete wavelengths of UV or visible light that are absorbed by or transmitted through a sample in comparison to a reference or blank sample. This property is influenced by the sample composition, potentially providing information on what is in the sample and at what concentration. UV spectra ofthe methanol extract of*Sanchezia oblonga* at 50µg/ml concentration and its UV-VIS spectrum was determined in the wavelength range 200-800 nm a UV- VIS spectrophotometer (Shimadzu 1800) against methanol blank. Here we find a UV-vis peak of 210-280nm which is a characteristic peak of fatty acids as shown in the **Figure 6**. Our GC-MS analysis is concordant with this observations.

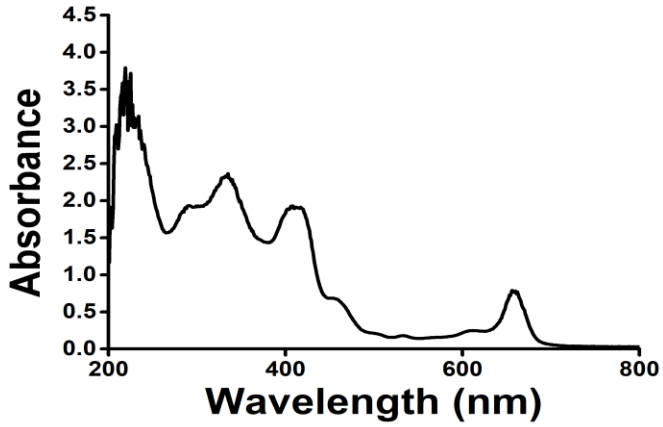


Figure 6. UV spectra of extract derived from *Sanchezia oblonga*

4.6. ADMET Analysis

ADMET (i.e. Absorption, Distribution, Metabolism, Excretion, and Toxicity) profiling of the phytochemicals were performed with the help of pkCSM online server. All the studied compounds have a skin permeability ranging from -2.86 to -1.78. Most of the phytochemicals do not inhibit P-glycoprotein I and II. Blood-brain barrier (BBB) permeability and CNS permeability values are laying between -0.11 to +0.86 and -2.19 to -0.96 respectively. Most of the phytochemicals also do not inhibit CYP2C19, CYP2C9, CYP2D6, CYP3A4, CYP1A2, inhibitors and they do not interact with renal OCT2 substrate. These data are tabulated in **Table 5**. Here it is very important to note that all the phytochemicals do not show AMES toxicity nor inhibit hERGI inhibitor.

Table 5 : ADMET analysis of UV spectra of extract derived from *Sanchezia oblonga*

Compound	Caco2 permeability	Skin Permeability	P-glycoprotein substrate	P-glycoprotein I inhi	P-glycoprotein II inhi	BBB Permeability	CNS permeability	CYP2D6 substr	CYP3A4 substrate	CYP1A2 inhibitor	CYP2C19	CYP2C9 inhi	CYP2D6 inhibitor	CYP3A4 inhibitor	Total Clearance	Renal OCT2 substrate	AMES toxicity

				bitor	bitor			ate			inhibitor	bitor					
5methyl4hepten3one	**1.407**	**-1.783**	No	No	No	**0.598**	**-2.192**	**No**	No	No	No	No	No	No	**0.456**	**No**	**No**
Campesterol	**1.223**	**-2.86**	No	Yes	Yes	**0.774**	**-1.758**	No	Yes	No	No	No	No	No	**0.572**	No	**No**
Linoleic acid	**1.57**	**-2.723**	No	No	No	**-0.142**	**-1.6**	No	Yes	Yes	No	No	No	No	**1.936**	No	No
Oleanolic Acid	**1.17**	**-2.735**	No	No	No	**-0.14**	**-1.157**	No	Yes	No	No	No	No	No	**-0.081**	No	No
Palmitic Acid	**1.558**	**-2.717**	No	No	No	**-0.111**	**-1.816**	No	Yes	No	No	No	No	No	**1.763**	No	No
Phytol	**1.515**	**-2.576**	No	No	Yes	**0.806**	**-1.563**	No	Yes	Yes	No	No	No	No	**1.686**	No	No
Squalene	**1.216**	**-2.768**	No	No	Yes	**0.981**	**-0.955**	No	Yes	No	No	No	No	No	**1.791**	No	No
Stearic Acid	**1.556**	**-2.726**	No	No	No	**-0.195**	**-1.707**	No	Yes	Yes	No	No	No	No	**1.832**	No	No
Stigmasterol	**1.213**	**-2.783**	No	Yes	Yes	**0.771**	**-1.652**	No	Yes	No	No	No	No	No	**0.618**	No	No

4.7. Antimicrobial activity:

The antimicrobial activity of crude extract used against *E. coli* bacteria as shown in **Figure 7**. Bio-assay analysis clearly indicates that the methanolic extract derived from *Sanchezia oblonga* is a source of phytochemicals which possessed antimicrobial activity.

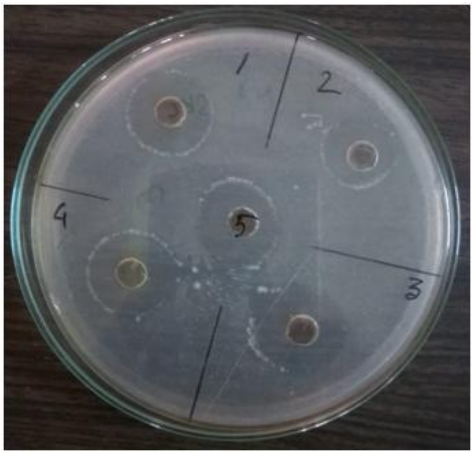


Figure 7: Bio-assay analysis of methanolic extract derived from *Sanchezia oblonga*

4.8. Computational analysis:

We have also carried out the computational analysis of the phytochemicals derived from the methanolic exact of *Sanchezia oblonga* plant. The ground state optimized geometries of the phytochemicals are shown in the **Figure 8**. To find the reactivity parameters we have calculated the HOMO, LUMO energy levels of the phytochemicals and tabulated in the Figure

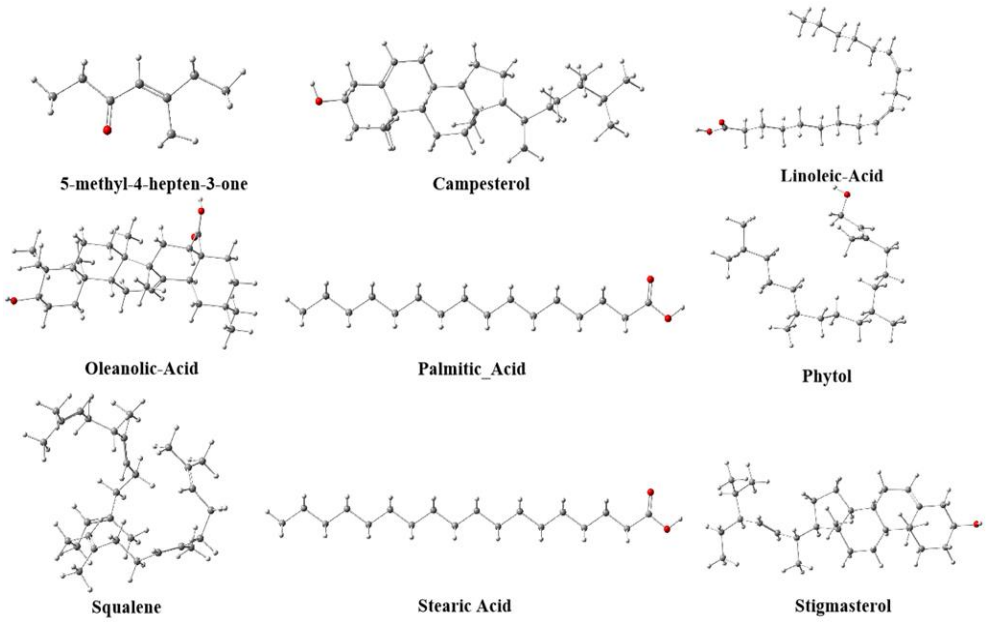


Figure 8: Ground state geometries of the phytochemicals derived from methanolic extract at B3LYP/6-31+g(d) level of theory

From the above analysis it is clear that stearic acid possesses highest band gap and highest LUMO energy levels which is responsible for showing highest activity against two different targets in the docking analysis as shown **Table 6**.

Table 6 : HOMO, LUMO energy levels and Bandgap of the phytochemicals derived from methanolic extract derived from *Sanchezia oblonga*

Name of Compounds	Homo (eV)	Lumo (eV)	Δ(Homo-Lumo) (eV)
5 methyl 4 hepten 3 one	-6.61	-1.50	5.11
Campesterol	-6.42	-0.14	6.28
Linoleic-Acid	-6.65	-0.19	6.46
Oleanolic-Acid	-6.22	-0.33	5.89
Palmitic Acid	-7.86	-0.17	7.69
Phytol	-6.59	-0.36	6.23

Squalene	-6.05	-0.22	5.83
Stearic Acid	-7.85	-0.17	7.68
Stigmasterol	-6.41	-0.18	6.23

5. CONCLUSION

In the present study we have made a systematic analysis of the methanolic leaf extracts of *Sanchezia oblonga* were used to identify the presence of phytochemicals and investigate the plant's pharmacological properties. TLC analysis indicates the presence of three major components present in the methanolic leaf extracts of *Sanchezia oblonga. GC-MS* analysis indicates the presence of nine phytochemicals whose antimicrobial activity of crude extract used against *E. coli. UV-vis* analysis clearly indicates the presence of fatty acids in the extrcat. Additionally, *in-silico* and DFT analysis clearly indicates that Stearic Acid possesses highest binding afinity against two different targets viz. of two SARS-CoV-2 proteins (PDB ID:6LU7 and PDB ID:6w9c) and two Ebola virus proteins (PDB ID:1eS6 PDB ID: 4z9p). This analysis open up new opportunity for the discovery of drugs from the leaf extracts of *Sanchezia oblonga.*

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Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Clinical trial : Not Applicable

Clinical trial No: Not Applicable

Author Contributions Statement

Tanmoy Mazumdar: Drafting of the manuscript, concept, original research

Mainak Banerjee: Supervision, Drafting of the manuscript, concept, original research

Tanmoy Dutta: Drafting of the manuscript, concept

Surajit Saha : Drafting of the manuscript, concept, original research

Swapan Kumar Chowdhury: Supervision, Drafting of the manuscript, concept, original research

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