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Research Article

Phytochemical Screening, GCMS Profile, and *In-silico* properties of Bioactive Compounds in Methanolic Leaf Extracts of *Moringa oleifera*

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Abstract

Plant Based Natural Products (PBNPs) have been subject of interest since ancient time due to their use in food, industrial and biomedical applications. Research attention has further augmented to explore their phytochemical composition, properties, and potential application in the post-COVID era. In the present study phytochemical screening has been carried out with Methanolic Leaf Extracts of *Moringa oleifera* (MLEMO) followed by Gas Chromatography-Mass Spectrometry (GCMS) analysis. Phytochemical analysis of MLEMO revealed the presence of Alkaloids, Carbohydrates, Coumarins, Flavonoids, Glycosides, Phenol, Proteins, Quinones, Saponins, Steroids, Tannins and Terpenoids. Further, GCMS analysis revealed the presence of 41 compounds of which Dihydroxyacetone; Monomethyl malonate; 4H-Pyran-4-one,2,3-dihydro-3,5-dihydroxy-6-methyl; 1,3-Propanediol, 2-ethyl-2-(hydroxymethyl); Propanoic acid, 2-methyl-, octyl ester; 3-Deoxy-d-mannoic lactone; Sorbitol; Inositol; Cyclohexanemethanol, alpha-methyl-4-(1-methylethyl), Hexadecanoic acid, Methyl palmitate; n-Hexadecanoic acid (Palmitic acid); 9-Octadecenoic acid, methyl ester; Phytol; 9,12,15-Octadecatrienoic acid; Octadecanoic acid; 9-Octadecenamide were prominent. Most of the compounds in the list are bioactive and possess medicinal properties that are expected to serve as a baseline lead for the development of therapeutic agents.

Keywords: Phytochemical screening; GCMS; Bioactive Natural Products; *Moringa oleifera*; MLEMO; Biomedical application

INTRODUCTION

Moringa oleifera Lam. (Family: Moringaceae) is a medicinal plant native to India, geographically distributed in tropical and sub-tropical climatic regions. However, has now been cultivated in other regions of the world[1]. *M. oleifera* is considered to be ware-house of plant based natural products (PBNPs) further it has been recognized as economically and nutritionally important crop owing to its health benefits. The tree is endowed with splendid diversity and incredible richness of bioactive compounds that serve as main source of nutraceuticals in maintaining health and wellbeing and overcome the malnutrition problem. The use of this tree is encouraged as a nutritional supplement for infants and children[2].

It has a wide range of culinary applications besides bioremediation, nutritional and medicinal properties[3]. Edible parts of this plant contain nutrients viz., proteins, essential and non-essential amino acids, vitamins, minerals, antioxidants and phenolic compounds. *M. oleifera* allele-chemicals [Amino Acids (Threonine, Methionine, Phenylalanine), Fatty Acids (Palmitic acid, Oleic acid, Linoleic acid), Phenols (Gallic acid, p-Coumaric acid, Ferulic acid) Flavonoids (Catechin, Quercetin, Kaempferol, Niazimicin) and other Bioactive Compounds, Vitamins (B, A, C, D and K)], Zeatin and Essential Macro (Potassium, Magnesium, Phosphorus) and Microelements (Iron, Zinc). Leaves, roots, seed, bark, fruit, flowers and immature pods of *Moringa* has been endowed with antioxidant, antidiabetic, antibacterial, antifungal, anti-tumor, anti-inflammatory, antiulcer, antispasmodic, diuretic, antihypertensive, hepatoprotective, antipyretic, antiepileptic, cardioprotective and cholesterol-lowering activities[4].

The plant is perennial tree; the fruit is known as DRUM-STICK and hence the plant is known as 'drumstick tree'[4]. Though there are 13 species in the genus *Moringa*, *M. oleifera* is best

known and probably the most widely distributed, and popular species due to its manifold uses[5]. In the meantime, it must be pointed out that the remaining 12 species in the genus have not yet been fully explored for their potential and medicinal properties[5]. This boils down to the fact that *M. oleifera* is the most extensively cultivated and undoubtedly exploited plant in the genus so far[6,7].

Factually, *M. oleifera* is native to India, commonly found in the southern region of the India-Subcontinent and the South East Asian Region. It is cultivated in Sub-Himalayan North-Eastern Pakistan to West Bengal in India; Southern part of Deccan Plains, North-Western Gangetic Plains; Central India to Dry Regions of Peninsular India. It is also cultivated in other regions of the world including Asia, Africa, and Europe[4]. It is a deciduous tree with brittle stem, whitish-gray corky bark with branches; leaves pale green, bipinnate/ tri-pinnate with opposite, ovate leaflets[8]. This crop can be cultivated on marginal lands under water-scarcity and elevated temperatures[9]. Optimum growth is observed in soil with alkaline pH; temperature range of 25-35°C however, it can withstand elevated temperatures, and frost[8].

M. oleifera recognized as "**The Miracle Tree**" due to its versatile nutraceutical uses[10]. National Institute of Health (NIH) has declared this plant as "**Botanical of the Year – 2007**"[3]. The tree is a rich source of essential nutrients such as proteins, vitamins, minerals, carbohydrates, with a potential to overcome malnutrition. Apart from the nutritional aspect *M. oleifera* is a rich source of other phytochemicals. Nearly, all parts of the plant including leaves, roots, pods, seeds, and flowers have been explored for their nutraceutical properties and biomedical applications[2,8].

Of all parts, the leaves are inexpensive and abundantly available but largely underutilized, ignored and often discarded. Different pharmaceutical products from this plant have been manufactured and marketed in both the Indian and worldwide markets due to these medicinal advantages. Recently, attempts have been made to evaluate the effect of processing methods on leaves to formulate Ready-to-Eat functional value-added foods. Furthermore, leaves are the most explored part of the tree due to the presence of nutrients, essential amino acids and minerals like Iron, Calcium, and Potassium[11]. In addition, low calorific value of leaves makes them a suitable candidate for obese diet[12]. Seeds have high lipid content (42%); however superior to soybean in composition[8].

M. oleifera has been traditionally utilized in folk remedies to cure conjunctivitis, and given to lactating mothers for enhancing milk production. The juice obtained from leaves is used to normalize blood pressure and blood glucose levels[5]. The accepted and safe dose of *M. oleifera* powder is 14 g daily[13]. Pharmacological studies have indicated that the extracts obtained from the plant have antioxidants[14], anti-diabetic[12], anti-bacterial, anti-fungal[15], and anti-carcinogenic[16]properties.

No adverse effects have been reported on rabbits[17] rats[18] during toxicity study with aqueous leaf extract *Moringa*. Though, significant variation in composition of different species exists[19] versatile nature of phytochemicals remains the key aspect of nutrition for people suffering from malnutrition and food security[3]. Due to overwhelming nutritive and medicinal use of the plant, it is indicated that *Moringa* can be widely exploited for its nutritionally important phytoconstituents in the development of functional foods, nutraceutical products and therapeutic agent on a commercial by fortification to eradicate malnutrition[20,21]. *Moringa* possesses immense potential for betterment of nutrition, enhanced food security and promotes sustainable rural development. Prospecting BASM using in-silico ADMET predictions to chart a new road map for drug discovery is the basic aspect sustainable exploitation of bioactive natural products[22-27]. The aim of this study is to identify phytochemicals by GC-MS analysis followed by. Compounds with maximum peak area in GCMS profile have been prospected for the molecular and biological properties so as to exploit them for the development of novel leads considering its nutritional, pharmaceutical and ethnopharmacological applications.

MATERIALS AND METHODS

Plant material:

Fresh leaves of *M. oleifera* were collected from farmlands near Alagarkovil Reserve Forest (longitude/ latitude geographical coordinates 10.0748° N, 78.2131° E, Eastern Ghats) Dindigul District, Tamilnadu during Jun-Jul 2021, taken to laboratory, cleaned and preserved as Herbarium, part of the collected sample was shade dried, powdered and subjected to extraction**.** Botanical identity of the plant was established using flora and confirmed by Department of Botany, Government Arts College, Melur, Madurai, India.

Botanical Description of the Plant

Habit: Trees to 12 m tall; **Stem**: Cylindrical; **Bark**: pale smooth to rugose but not fissured; **Leaves**: petiolate, 3-pinnate, 25-60 cm, stalked, glands often exuding clear or amber liquid at base of petiole and leaflets; **Leaflets**: 4-6 pairs, ovate, elliptic, or oblong, 1-2 × 0.5-1.2 cm, puberulous - young but glabrous - maturity, base rounded to cuneate, apex round to emarginate; petiolules slender, 1-2 mm; **Inflorescence**: widely spreading panicle; **Bracteate**: 10-30 cm; **Bracts**: linear, ca. 1 mm; **Flowers**: white to cream, fragrant, resembling an inverted Fabaceae flower with 2 dorsal sepals and 1 dorsal petal usually remaining un-reflexed and forming a projecting "keel" while perianth reflexes down to form a "banner" at right angles to the "keel", each flower borne on a false pedicel 7-15 mm; **Pedicel**: 1-2 mm; **Sepals**: lanceolate to linear-lanceolate, 0.7-1.4 mm, usually puberulent; **Petals**: spatulate, 1-2 cm, glabrous or puberulent at base; **Stamens**: hairy at base; **Ovary**: hairy. Fruits: Pod, Capsule 3-valved, 20-50 × 1-3 cm, dehiscent; **Seeds**: sub-globose, 3-angled, 8-15 mm in diam. excluding wings; wings 0.5-1 cm wide, rarely absent; **Fl**. - year round, **Fr**. - Jun-Dec[28] (Fig. 1).

Sample preparation

Using direct method of extraction, approximately 10 g of powder was extracted with 100 ml of methanol. The extract was transferred in to glass vials. The process was repeated 3 times with fresh solvent. The solvent was removed by Rota-vapor. The extracted residue was re-dissolved in the solvent to yield a final volume of 10mg/ml and the content was stored in cold (at 4°C) until further use.

Phytochemical Screening

The methanolic extracts were subjected to chemical tests for the detection of phytoconstituents using standard procedures[29-33].

Test for Phenols ($FeCl_3$ Test)

To 1 ml of the extract, 3 ml of distilled water followed by few drops of 10% aqueous Ferric chloride solution was added. Formation of blue or green colour indicates the presence of phenols.

Test for Flavonoids (Shinoda Test)

To 2 ml of the extract, 1 ml of 1% ammonia solution was added. Appearance of yellow colour indicates the presence of flavonoids.

Test for Tannins ($FeCl_3$ Test)

To 1 ml of the extract, 1 ml of 0.008 M Potassium ferricyanide was added and then add 1ml of 0.02 M Ferric chloride containing 0.1 N HCl. Appearance of blue-black colour indicates the presence of Tannins.

Test for Alkaloids (Wagner's Reagent Test)

Approximately, 1 ml of crude extract was mixed with 2 ml of Wagner's reagent. Reddish brown colour precipitate indicates the presence of alkaloids.

Test for Carbohydrates (Fehling's test, Benedict's test)

Fehling's test

Equal volume of Fehling A and Fehling B reagents were mixed together and then add 2ml of crude extract in it and gently boiled. A brick red precipitate appeared at the bottom of the test-tube indicates the presence of reducing sugars.

Benedict's test

1 ml of crude extract was mixed with 2ml of Benedict's reagent and boiled. A reddish brown precipitate was formed which indicates the presence of the carbohydrates.

Test for Proteins (Millon's Test, Ninhydrin Test)

Millon's test

1 ml of crude extract was mixed with 2ml of Millon's reagent; white precipitate appeared which turned red upon gentle heating that confirmed the presence of protein.

Ninhydrin test

1 ml of crude extract was mixed with 2ml of 0.2% solution of Ninhydrin and boiled. A violet colour precipitate was appeared suggesting the presence of amino acids and proteins.

Test for Cardiac glycosides (Keller-Kiliani test)

5 ml of extract was treated with 2 ml of glacial acetic acid containing one drop of ferric chloride solution. This was underlayed with 1 ml of concentrated sulphuric acid. A browning of the interface indicates a deoxy-sugar characteristic of carotenoids. A violet ring may appear below the brown ring, while in the acetic acid layer, a greenish ring may form just gradually throughout thin layer.

Test for Saponins (Foam Test)

2 ml of crude extract was mixed with 5 ml of distilled water in a test tube and it was shaken vigorously. Add some drops of olive oil. The formation of stable foam was taken as an indication for the presence of saponins.

Test for Coumarin (Sodium hydroxide Test)

10 % Sodium hydroxide was added to the extract and chloroform was added. Formation of yellow color shows the presence of Coumarin.

Test for Terpenoids (Salkowski test)

5 ml of extract was mixed with 2 ml of chloroform and 3 ml of concentrated sulphuric acid was carefully added to form a layer. A reddish brown coloration of the inter face was formed which indicates the presence of terpenoids.

Test for Steroids (Salkowski Test)

2 ml of acetic anhydride was added to 0.5 ml of crude extract containing 2 ml of sulphuric acid. The colour changed from violet to blue or green in samples indicates the presence of steroids.

Test for Quinones (Sodium hydroxide Test)

Diluted sodium hydroxide was added to the 1 ml of crude extract. Blue green or red coloration indicates the presence of quinones.

Test for Anthraquinones (Borntragers test)

0.5 g of extract was boiled with 10% hydrochloric acid for few minutes in water bath. It was filtered and allowed to cool. Equal volume of $CHCl_3$ was added to the filtrate. Few drops of 10% ammonia was added to the mixture and heated. Formation of rose – pink color indicates of n-hexane, chloroform, ethyl acetate and methanol of the presence of the anthroquinones.

GC-MS Analysis

Leaf samples of were collected from farmlands near Alagarkovil Reserve Forest (longitude/ latitude geographical coordinates 10.0748° N, 78.2131° E, Eastern Ghats) Dindigul District, Tamil Nadu, India. Phyto-components were identified using GC–MS detection system as described previously[26], however with modification, whereby portion of the extract was analysed directly by headspace sampling. GC–MS analysis was accomplished using an Agilent 7890A GC system set up with 5975C VL MSD (Agilent Technologies, CA, and USA). Capillary column used was DB-5MS (30 m × 0.25 mm, film thickness of 0.25 µm; J&W Scientific, CA, USA). Temperature program was set as: initial temperature 50°C held for 1 min, 5°C per min to 100°C, 9°C per min to 200°C held for 7.89 min, and the total run time was 30 min. The flow rate of helium as a carrier gas was 0.811851 mL/ min. MS system was performed in electron ionization (EI) mode with Selected Ion Monitoring (SIM). The ion source temperature and quadruple temperature were set at 230°C and 150°C, respectively. Identification of phyto-components was performed by comparison of their retention times and mass with those of authentic standards spectra using computer searches in NIST 08.L and Wiley 7n.l libraries[27].

RESULTS

Phytochemical analysis of MLEMO revealed the presence of alkaloids, carbohydrates, coumarins, flavonoids, glycosides, phenol, proteins, quinones, saponins, steroids, tannins and terpenoids. However, anthraquinones were not detected in the samples analyzed (Table 1). GCMS analysis revealed the presence of the following 41 phyto-compounds (listed in the decreasing order of abundancy) 1,3-Propanediol, 2-ethyl-2-(hydroxymethyl)- ($C_6H_{14}O_3$) 21.190; Propanoic acid, 2-methyl-, octyl ester ($C_{12}H_{24}O$) 15.027; 9,12,15-Octadecatrienoic acid, (Z,Z,Z)- ($C_{19}H_{30}O_2$) 10.006; Ethanamine, N-ethyl-N-nitroso- ($C_4H_{10}N_2O$) 5.216; 4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl- ($C_6H_8O_4$) 4.180; Benzeneacetonitrile, 4-hydroxy- (C_8H_7NO) 3.476; 3-Deoxy-d-mannoic lactone ($C_6H_{10}O_5$) 3.294; n-Hexadecanoic acid (Palmitic acid) ($C_{16}H_{32}O_2$) 2.570; Monomethyl malonate ($C_4H_6O_4$) 2.568; Dihydroxyacetone ($C_3H_6O_3$) 2.465; Inositol ($C_6H_{12}O_6$) 2.054; 1,7-Diaminoheptane ($C_7H_{18}N_2$) 1.799; 9-Octadecenamide, (Z)- ($C_{18}H_{35}NO$) 1.469; 1,2,3-Propanetriol, 1-acetate ($C_5H_{10}O_4$) 1.437; Octadecanoic acid ($C_{18}H_{36}O_2$) 1.205; 9-Octadecenoic acid (Z)-, methyl ester ($C_{19}H_{36}O_2$) 1.030; (1S)-Propanol, (2S)-[(tert.butyloxycarbonyl)amino]-1-phenyl- ($C_{17}H_{26}N_2O$) 0.967; Phytol ($C_{20}H_{40}O$) 0.966; Oxazolidine, 2-ethyl-2-methyl-

($C_6H_{13}NO$) 0.900; Hexadecanoic acid, Methyl palmitate ($C_{17}H_{34}O_2$) 0.851; 4,5-Diamino-6-hydroxypyrimidine ($C_4H_6N_4O$) 0.643; Benzyl .β.-d-glucoside ($C_{13}H_{18}O_6$) 0.605; 3-Piperidinol ($C_5H_{11}NO$) 0.597; Formamide, N,N-dimethyl- (C_3H_7NO) 0.584; d-Talonic acid lactone ($C_6H_{10}O_6$) 0.565; 2-Oxoglutaric acid ($C_5H_6O_5$) 0.546; 1,3-Benzenediol, 2-methyl- (C_7H_8O) 0.545; N-Methoxy-1-ribofuranosyl-4-imidazolecarboxylic amide ($C_{10}H_{15}N_3O_6$) 0.534; 1-Nitro-.β.-d-arabinofuranose, tetraacetate ($C_{13}H_{17}NO_{11}$) 0.511; Sorbitol ($C_6H_{14}O_6$) 0.482; Cyclohexanemethanol, alpha-methyl-4-(1-methylethyl)- ($C_{11}H_{22}O$) 0.482; N,N-Dimethylacetamide (C_4H_9NO) 0.454; 2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl- ($C_{11}H_{16}O_3$) 0.449; 6-methoxy-3-Pyridinecarboximidamide ($C_7H_9N_3O$) 0.429; 4-Allyl-3-(dimethylhydrazono)-2-methylhexane-2,5-diol ($C_{12}H_{24}N_2O_2$) 0.425; Benzenebutanal, .gamma.,4-dimethyl- ($C_{12}H_{16}O$) 0.395; D-erythro-Pentose, 2-deoxy- ($C_5H_{10}O$) 0.331; Furan, 2,3-dihydro-4-methyl- (C_5H_8O) 0.210; 3,4-Furandiol, tetrahydro-, trans- ($C_4H_8O_3$) 0.174; 4,6-dimethyl-2-propyl-1,3,5-dithiazinane ($C_8H_{17}NS_2$) 0.169; 1,8-Diamino-3,6-dioxaoctane ($C_6H_{16}N_2O_2$) 0.117 (Table 2). Calculated values pertaining to the molecular properties and predicted bioactivity scores relating functions of dihydroxyacetone phosphate; methylmalonic acid; 1,3-Propanediol, 2-ethyl-2-(hydroxymethyl)-; Benzeneacetonitrile, 4-hydroxy-; Ethanamine, N-ethyl-N-nitroso-; Propanoic acid, 2-methyl-, octyl ester; 3-Deoxy-d-mannoic lactone; Inositol; n-Hexadecanoic acid (Palmitic acid); 9,12,15-Octadecatrienoic acid, (Z,Z,Z)- is provided in Fig. **2 A-K** with their 3D structure. Data indicate that 9,12,15-Octadecatrienoic acid in the MLEMO holds significant GPCR ligand (0.33); Ion channel modulator (0.23); Kinase inhibitor (0.19); Nuclear receptor ligand (0.35); Protease inhibitor (0.13); Enzyme inhibitor (0.42) activity respectively (Table 3K).

DISCUSSION

Medicinal and biological activities of plant extract have been upheld by *in-vitro* assays[26,33-42]. In the leaf extracts of *M. oleifera* contains significantly high phenolic compounds primarily responsible for antioxidant effects[14,33,36]. Most of the compounds identified in methanolic leaf extract of *M. oleifera* - are endowed with medicinal properties and some of them are commonly present in many other medicinal plants used by local tribal people[33-42]. Dihydroxyacetone (DHA), rarely been detected in plant extracts have various applications; DHA is primarily used as an ingredient in sunless tanning products, synthesis of polymeric biomaterials[43]. 4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl- (DDMP) is a strong anti-oxidant in glucose–histidine Maillard reaction products[44]. Li et al.[45] indicated that the control of DDMP formation in the Maillard reaction is important to improve the thermally treated food quality as a result of its intense bitterness and potential toxicity.

M. oleifera leaves were reported to have anti-cancerous activity against HeLa cells by activating the apoptotic pathway[46]. Further, it has been reported that *Moringa* leaves extract induce apoptosis by up-regulating BAX and down-regulating BCL-2 expression, enhancing caspase-3-activity. Palmitic acid present in leaves inhibit cancer cell growth[47]. In G1 phase of cell cycle, D-allose present in MLEMO induces specific thioredoxin interacting protein (TXNIP) and stabilizes p27kip1 protein that inhibits cancer cells growth without affecting the normal cells in the system. As of now, there are evidences in the literature that support the fact that chronic inflammation may lead to malignancies of different organs including stomach, colon, breast, skin, prostate, pancreas[48]. Inhibition of NF-κB (nuclear factor kappa-light-chain-enhancer of activated B cells) signaling has potential therapeutic application in cancer therapy and management of metabolic inflammations.

Likewise, 4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl has been reported to suppresses the NF-κB target antiapoptotic genes Bcl-2 (B-cell lymphoma 2) while it induces expression of apoptotic genes Bax (Bcl-2-associated X protein), cleaved caspase-3 and cleaved PARP (Poly ADP-ribose polymerase). Methyl palmitate possesses a strong anti-fibrotic effect[48]. It inhibits NF-κB and consequent pro-inflammatory and oxidative stress response. Conjugated linoleic acids in methanolic leaf extracts of *Moringa* significantly decrease prostate cancer cell proliferation by down-regulating phorbol ester induced NFκB activation and subsequent COX-2(Cyclooxygenase2) expression[48,49]. Likewise, 9-Octadecenamide, an amide of oleic acid suppresses lipopolysaccharide induced expression of iNOS (inducible NO synthase) and COX-2 through inhibition of NF-kappa-B activation. A rationale for design and evaluation of novel antioxidant drug for atherosclerosis[50] wherein it has been pointed out that Hexadecanoic acid, Methyl palmitate displays antioxidant properties that reduce atherosclerosis significantly.

CONCLUSION

Therapeutic mechanism of a plant can be better understood with a proper investigation of its bioactive secondary metabolites. *M. oleifera* leaves remain an ideal sources of micro-nutrients and phytochemicals that can be used for the development of nutraceuticals and functional foods. *Moringa* leaves contain phytochemicals, which makes this plant ideal source of BASM. Therefore, food products based on the leaves contain more protein, dietary fibers, other nutrients, and antioxidants. The compounds identified by the GC-MS analysis of methanolic leaf extracts of *M. oleifera* in the present study relate their applications in folklore medicine. BASMs in *Moringa* prompt inspiration for further investigation to identify novel lead molecules in the drug discovery and design of novel herbal drugs of GRAS standard.

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Figure 1: *M. oleifera* a – Tree; b – leaf; c – flower; d – pod; e – seeds; f – gum; g – oil

Table 1: Phytochemical analysis of methanolic leaf extract of *M. oleifera*

Phytoconstituents	Test	Present/ Absent
Alkaloids	Wagner's reagent Test	**+**
Anthraquinones	Borntragers Test	**-**
Carbohydrates	Fehling's test, Benedict's test	**++**
Coumarins	Sodium hydroxide Test	**+**
Flavonoids	Shinoda Test	**++**
Glycosides	Keller-Kiliani Test	**+**
Phenol	$FeCl_3$ Test	**+++**
Proteins	Millon's Test, Ninhydrin Test	**++**
Quinones	Sodium hydroxide Test	**+**
Saponins	Foam Test	**+**
Steroids	Salkowski Test	**+**
Tannins	$FeCl_3$ Test	**++**
Terpenoids	Salkowski Test	**++**

+++ = Abundantly present; ++ = moderately present; + = slightly present; - = absent

Table 2 List of phytochemicals identified in GCMS analysis of methanolic leaf extract of *M. oleifera* (MLEMO) their retention time, with molecular formula, molecular weight and percentage peak area

RT	Name of the Compound	MF	MW(g/mol)	PA %
7.660	**Dihydroxyacetone**	**$C_3H_6O_3$**	**90.07**	**2.465**
14.061	**Monomethyl malonate**	**$C_4H_6O_4$**	**118.08**	**2.568**
15.562	4,5-Diamino-6-hydroxypyrimidine	$C_4H_6N_4O$	126.12	0.643
17.891	**4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-**	**$C_6H_8O_4$**	**144.12**	**4.180**
18.934	Furan, 2,3-dihydro-4-methyl-	C_5H_8O	84.11	0.210
21.010	1,2,3-Propanetriol, 1-acetate	$C_5H_{10}O_4$	134.13	1.437
21.227	3,4-Furandiol, tetrahydro-, trans-	$C_4H_8O_3$	104.10	0.174
21.410	1-Nitro-.β.-d-arabinofuranose, tetraacetate	$C_{13}H_{17}NO_{11}$	363.27	0.511
21.542	1,8-Diamino-3,6-dioxaoctane	$C_6H_{16}N_2O_2$	148.20	0.117
22.033	1,7-Diaminoheptane	$C_7H_{18}N_2$	130.23	1.799
22.660	N,N-Dimethylacetamide	C_4H_9NO	87.12	0.454
22.893	2-Oxoglutaric acid	$C_5H_6O_5$	146.10	0.546
23.149	Oxazolidine, 2-ethyl-2-methyl-	$C_6H_{13}NO$	115.17	0.900
25.455	6-methoxy-3-Pyridinecarboximidamide	$C_7H_9N_3O$	151.17	0.429
25.667	3-Piperidinol	$C_5H_{11}NO$	101.15	0.597
26.419	**1,3-Propanediol, 2-ethyl-2-(hydroxymethyl)-**	**$C_6H_{14}O_3$**	**134.17**	**21.190**
27.403	**Benzeneacetonitrile, 4-hydroxy-**	**C_8H_7NO**	**133.15**	**3.476**
27.681	Benzenebutanal, .gamma.,4-dimethyl-	$C_{12}H_{16}O$	176.25	0.395
28.820	2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-	$C_{11}H_{16}O_3$	180.24	0.449
30.002	**Ethanamine, N-ethyl-N-nitroso-**	**$C_4H_{10}N_2O$**	**102.13**	**5.216**
30.393	**Propanoic acid, 2-methyl-, octyl ester**	**$C_{12}H_{24}O$**	**200.31**	**15.027**
30.710	**3-Deoxy-d-mannoic lactone**	**$C_6H_{10}O_5$**	**162.14**	**3.294**

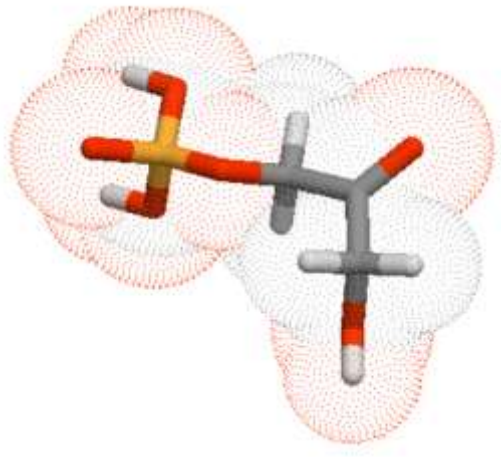
31.120	D-erythro-Pentose, 2-deoxy-	$C_5H_{10}O$	134.13	0.331
32.435	N-Methoxy-1-ribofuranosyl-4-imidazolecarboxylic amide	$C_{10}H_{15}N_3O_6$	273.24	0.534
33.228	Formamide, N,N-dimethyl-	C_3H_7NO	73.09	0.584
33.471	d-Talonic acid lactone	$C_6H_{10}O_6$	178.12	0.565
33.736	Sorbitol	$C_6H_{14}O_6$	182.17	0.482
34.899	**Inositol**	**$C_6H_{12}O_6$**	**180.16**	**2.054**
35.636	Cyclohexanemethanol, alpha-methyl-4-(1-methylethyl)-	$C_{11}H_{22}O$	170.29	0.482
37.376	Hexadecanoic acid, Methyl palmitate	$C_{17}H_{34}O_2$	270.50	0.851
37.982	**n-Hexadecanoic acid (Palmitic acid)**	**$C_{16}H_{32}O_2$**	**256.42**	**2.570**
39.293	(1S)-Propanol, (2S)-[(tert.butyloxycarbonyl)amino]-1-phenyl-	$C_{17}H_{26}N_2O$	251.71	0.967
39.722	9-Octadecenoic acid (Z)-, methyl ester	$C_{19}H_{36}O_2$	296.50	1.030
39.832	Phytol	$C_{20}H_{40}O$	296.57	0.966
40.041	**9,12,15-Octadecatrienoic acid, (Z,Z,Z)-**	**$C_{19}H_{30}O_2$**	**278.40**	**10.006**
40.218	Octadecanoic acid	$C_{18}H_{36}O_2$	284.50	1.205
40.383	4-Allyl-3-(dimethylhydrazono)-2-methylhexane-2,5-diol	$C_{12}H_{24}N_2O_2$	228.33	0.425
40.888	Benzyl .β.-d-glucoside	$C_{13}H_{18}O_6$	270.28	0.605
41.081	4,6-dimethyl-2-propyl-1,3,5-dithiazinane	$C_8H_{17}NS_2$	191.20	0.169
41.887	1,3-Benzenediol, 2-methyl-	C_7H_8O	124.13	0.545
42.062	9-Octadecenamide, (Z)-	$C_{18}H_{35}NO$	281.47	1.469

A

originalSMILES C(C(=O)COP(=O)(O)O)O

miSMILES: C(C(=O)COP(=O)(O)O)O

Dihydroxyacetone phosphate



Molecular Properties	Calculated Values
miLogP	-2.45
TPSA	104.06
Natoms	10
MW	170.06
nON	6
nOHNH	3
Nviolations	0
Nrotb	4
volume	126.61
Biological Properties	**Bioactivity Scores**
GPCR ligand	0.09
Ion channel modulator	0.84
Kinase inhibitor	-0.41
Nuclear receptor ligand	-0.28
Protease inhibitor	0.07
Enzyme inhibitor	1.29

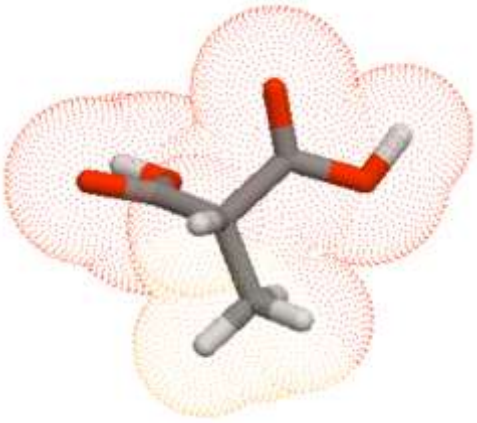
Figure 2(A): Structure (2D, 3D), molecular and biological properties of selected compounds in *M. oleifera*

B

originalSMILES CC(C(=O)O)C(=O)O

miSMILES: CC(C(=O)O)C(=O)O

Methylmalonic acid



Molecular Properties	Calculated Values
miLogP	-0.45
TPSA	74.60
Natoms	8
MW	118.09
nON	4
nOHNH	2
Nviolations	0
Nrotb	2
volume	100.03
Biological Properties	**Bioactivity Scores**
GPCR ligand	-2.94
Ion channel modulator	-2.53
Kinase inhibitor	-3.55
Nuclear receptor ligand	-2.70
Protease inhibitor	-2.75
Enzyme inhibitor	-2.60

Figure 2(B): Structure (2D, 3D), molecular and biological properties of selected compounds in *M. oleifera*

C

originalSMILES CC1=C(C(=O)C(CO1)O)O

miSMILES: CC1=C(C(=O)C(CO1)O)O

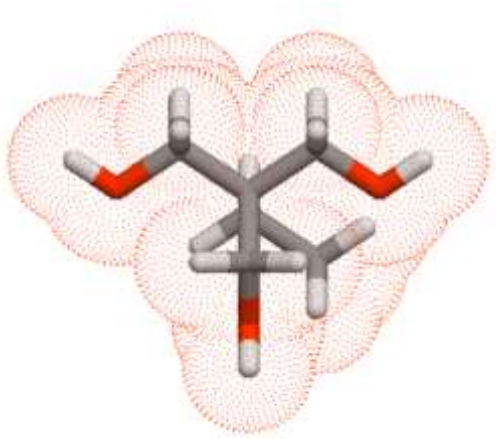
4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-

Molecular Properties	Calculated Values
miLogP	-0.46
TPSA	66.76
Natoms	10
MW	144.13
nON	4
nOHNH	2
Nviolations	0
Nrotb	0
volume	123.40
Biological Properties	**Bioactivity Scores**
GPCR ligand	-1.59
Ion channel modulator	-0.96
Kinase inhibitor	-2.25
Nuclear receptor ligand	-1.60
Protease inhibitor	-1.53
Enzyme inhibitor	-0.65

Figure 2(C): Structure (2D, 3D), molecular and biological properties of selected compounds in *M. oleifera*

D

originalSMILES CCC(CO)(CO)CO
miSMILES: CCC(CO)(CO)CO
Trimethylolpropane



Molecular Properties	Calculated Values
miLogP	-0.64
TPSA	60.68
Natoms	9
MW	134.18
nON	3
nOHNH	3
Nviolations	0
Nrotb	4
volume	136.96
Biological Properties	**Bioactivity Scores**
GPCR ligand	**--2.07**
Ion channel modulator	**--1.68**
Kinase inhibitor	**--2.66**
Nuclear receptor ligand	**-1.92**
Protease inhibitor	**-2.13**
Enzyme inhibitor	**-1.43**

Figure 2(D): Structure (2D, 3D), molecular and biological properties of selected compounds in *M. oleifera*

E

originalSMILES C1=CC(=CC=C1CC#N)O
miSMILES: C1=CC(=CC=C1CC#N)O
4-Hydroxybenzyl cyanide

Molecular Properties	Calculated Values
miLogP	1.42
TPSA	44.02
Natoms	10
MW	133.15
nON	2
nOHNH	1
Nviolations	0
Nrotb	1
volume	125.72
Biological Properties	**Bioactivity Scores**
GPCR ligand	**-0.92**
Ion channel modulator	**-0.82**
Kinase inhibitor	**-1.12**
Nuclear receptor ligand	**-0.91**
Protease inhibitor	**-1.05**
Enzyme inhibitor	**-0.73**

Figure 2(E): Structure (2D, 3D), molecular and biological properties of selected compounds in *M. oleifera*

F

originalSMILES CCN(CC)N=O
miSMILES: CCN(CC)N=O
N-nitrosodiethylamine

Molecular Properties	Calculated Values
miLogP	0.89
TPSA	32.67
Natoms	7
MW	102.14
nON	3
nOHNH	0
Nviolations	0
Nrotb	3
volume	106.97
Biological Properties	**Bioactivity Scores**
GPCR ligand	**-3.63**
Ion channel modulator	**-3.64**
Kinase inhibitor	**-3.76**
Nuclear receptor ligand	**-3.76**
Protease inhibitor	**-3.73**
Enzyme inhibitor	**-3.44**

Figure 2(F): Structure (2D, 3D), molecular and biological properties of selected compounds in *M. oleifera*

G

originalSMILES CCCCCCCCOC(=O)C(C)C

miSMILES: CCCCCCCCOC(=O)C(C)C

Octyl isobutyrate

Molecular Properties	Calculated Values
miLogP	4.76
TPSA	26.30
Natoms	14
MW	200.32
nON	2
nOHNH	0
Nviolations	0
Nrotb	9
volume	224.73
Biological Properties	**Bioactivity Scores**
GPCR ligand	**-0.57**
Ion channel modulator	**-0.21**
Kinase inhibitor	**-0.96**
Nuclear receptor ligand	**-0.51**
Protease inhibitor	**-0.53**
Enzyme inhibitor	**-0.27**

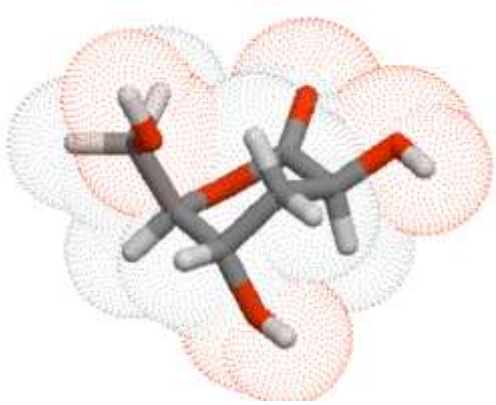
Figure 2(G): Structure (2D, 3D), molecular and biological properties of selected compounds in *M. oleifera*

H

originalSMILES C1C(C(OC(=O)C1O)CO)O

miSMILES: C1C(C(OC(=O)C1O)CO)O

3,5-Dihydroxy-6-(hydroxymethyl)oxan-2-one



Molecular Properties	Calculated Values
miLogP	-1.63
TPSA	86.99
Natoms	11
MW	162.14
nON	5
nOHNH	3
Nviolations	0
Nrotb	1
volume	137.90
Biological Properties	**Bioactivity Scores**
GPCR ligand	**-0.53**
Ion channel modulator	**-0.19**
Kinase inhibitor	**-1.12**
Nuclear receptor ligand	**-0.34**
Protease inhibitor	**-0.35**
Enzyme inhibitor	**0.35**

Figure 2(H): Structure (2D, 3D), molecular and biological properties of selected compounds in *M. oleifera*

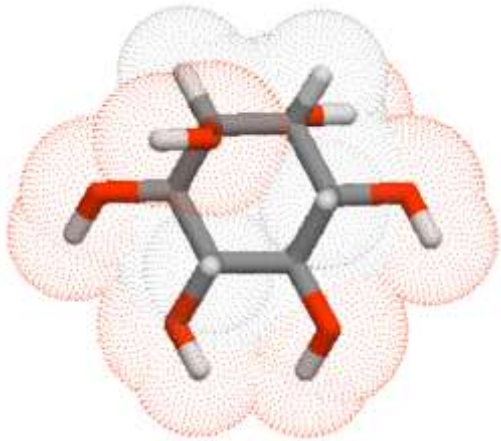
I

originalSMILES

C1(C(C(C(C(C1O)O)O)O)O)O

miSMILES: C1(C(C(C(C(C1O)O)O)O)O)O

Inositol



Molecular Properties	Calculated Values
miLogP	-2.39
TPSA	121.37
Natoms	12
MW	180.16
nON	6
nOHNH	6
Nviolations	1
Nrotb	0
volume	150.877
Biological Properties	**Bioactivity Scores**
GPCR ligand	**-0.67**
Ion channel modulator	**-0.11**
Kinase inhibitor	**-0.82**
Nuclear receptor ligand	**-0.73**
Protease inhibitor	**-0.67**
Enzyme inhibitor	**-0.17**

Figure 2(I): Structure (2D, 3D), molecular and biological properties of selected compounds in *M. oleifera*

J

originalSMILES CCCCCCCCCCCCCCCC(=O)O

miSMILES: CCCCCCCCCCCCCCCC(=O)O

Palmitic acid

Molecular Properties	Calculated Values
miLogP	7.06
TPSA	37.30
Natoms	18
MW	256.43
nON	2
nOHNH	1
Nviolations	1
Nrotb	14
volume	291.42
Biological Properties	**Bioactivity Scores**
GPCR ligand	**0.02**
Ion channel modulator	**0.06**
Kinase inhibitor	**-0.33**
Nuclear receptor ligand	**0.08**
Protease inhibitor	**-0.04**
Enzyme inhibitor	**0.18**

Figure 2(J): Structure (2D, 3D), molecular and biological properties of selected compounds in *M. oleifera*

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originalSMILES CCC=CCC=CCC=CCCCCCCCC(=O)O

miSMILES: CCC=CCC=CCC=CCCCCCCCC(=O)O

9,12,15-Octadecatrienoic acid

Molecular Properties	Calculated Values
miLogP	5.84
TPSA	37.30
Natoms	20
MW	278.44
nON	2
nOHNH	1
Nviolations	1
Nrotb	13
volume	306.47
Biological Properties	**Bioactivity Scores**
GPCR ligand	**0.33**
Ion channel modulator	**0.23**
Kinase inhibitor	**0.19**
Nuclear receptor ligand	**0.35**
Protease inhibitor	**0.13**
Enzyme inhibitor	**0.42**

Figure 2(K): Structure (2D, 3D), molecular and biological properties of selected compounds in *M. oleifera*