Profile of Phytochemicals and GCMS Analysis of Bioactive Compounds in Natural Dried-Seed Removed Ripened Pods Methanolic Extracts of Moringa oleifera

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Abstract

*Moringa oleifera* has been reported to be the store-house of wide range of bioactive compounds. Most commonly used plant part has been the leaves which are reported to be rich in Vitamins, Carotenoids, Polyphenols, Phenolic Acids, Flavonoids Alkaloids, Glucosinolates, Isoyanides, Tannins and Saponins. *Moringa* leaves are used as Keerai while, green pods are commonly used as vegetable in the traditional preparation of Sambar in south India. MO is gaining popularity because of its nutrient-rich root, leaves, flowers and fruits, having immense traditional medicinal uses and proved pharmacological properties. Not much of work has been carried out on analysis of bioactive compounds present in the pods. In the present study an attempt has been made to screen and analyze the range of bioactive compounds present in *Moringa oleifera* seed removed ripened natural dried pods. Phytochemical screening and GCMS analysis revealed the presence of 12 compounds namely - 7-Octadecene, 2-methyl- (C_{15}H_{31}O); 3,7,11,15-Tetramethyl-2-hexadecene-1-ol (C_{22}H_{45}O); 3,7,11,15-Tetramethyl-2-hexadecene-1-ol (C_{22}H_{45}O); 6,9,12,15-Docosaetaëric acid, me (C_{23}H_{46}O); Cyclohexanol, 5-methyl-2-{1-methylthethyl}- (C_{10}H_{19}O); 3,7,11,15-Tetramethyl-2-hexadecene-1-ol (C_{22}H_{45}O); Palmitic acid vinyl ester (C_{15}H_{26}O_{3}); gamma-Tocopherol (C_{29}H_{48}O_{2}); Vitamin E (C_{30}H_{48}O_{2}); Cholest-7a-(11)-dien-3-ol, 4,4-dim (C_{26}H_{46}O); gamma-Sitosterol (C_{28}H_{46}O); Stigmast-5,24(28)-dien-3-ol, (3.beta,24Z) - (C_{28}H_{46}O). Further, in-silico ADMET analysis is expected to provide in-depth physiochemical and biomolecular details of these molecules in order to exploit them for production of novel drugs for the pharma market with wide array of bio medical applications.

Keywords: Bioactive Compounds; GCMS; Phytochemical Screening; MOPME; Plant Based Natural Products;

INTRODUCTION

*Moringa oleifera* Lam. (Fam: Moringaceae) is a potential medicinal plant native to India, however, distributed in tropical and sub-tropical regions of the world. Furthermore, this plant has now been cultivated in other countries of the world.1 *M. oleifera* is considered to be ware-house of plant based natural products (PNPNs). The tree is endowed with far-fetched richness of bioactive compounds that serve as nutraceuticals and bio-pharmaceuticals. This tree is used as a natural source of nutrient supplement for women, infants and children.2 MO has a wide range of culinary applications besides bioremediation and medicinal properties.3 Edible part(s) of MO (leaves and green pods) contain - proteins, essential and non-essential amino acids, vitamins, minerals, antioxidants and phenolic compounds, Palmitic acid, Oleic acid, Linoleic acid, Gallic acid, p-Coumaric acid, Ferulic acid, Catechin, Quercetin, Kaempferol, Niazimicin, Vitamins (B, A, C, D and K). Quercetin, myricetin glycosides, caffeoylquinic acid, coumaroylquinic acid, hydroxybenzoic acid, kaempferol, glucorapaeolin, glucosinolain, glucoraphanin, glucoromargin, glucoiberin, glucosinolates, apigenin, luteolin, lutein,
luteoxanthin, zeaxanthin, b-carotene and isothiocyanates were identified as the main compounds in the extracts from moringa. Phenolic compounds from M. oleifera seed, such as gallic acid, ellagic acid and kaempferol are endowed with significant antioxidant activity.

There are 13 species with in the genus Moringa, of all, M. oleifera is best known, widely distributed, and popular species due to its manifold uses5. Leaves, bark, flowers and green pods of MO has reported antioxidant, antidiabetic, antibacterial, antifungal, anti-tumor, anti-inflammatory, antilulcer, antispasmodic, diuretic, antihypertensive, hepatoprotective, antipyretic, antiepileptic, cardioprotective and cholesterol-lowering activities4.

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. 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 levels5. Though, significant variation in composition of different species exists13-14 versatile nature of phytochemicals remains the key aspect of nutrition for people suffering from malnutrition5. Due to overwhelming nutritive and medicinal value of the pods, it is indicated that Moringa can be widely exploited for its nutritionally important phytoconstituents in the development of functional foods, nutraceuticals and therapeutic agent on a commercial by fortification to eradicate malnutrition20,21. Several bioactive compounds have been isolated and identified from different parts of Moringa (leaves, seeds, bark, flowers, pods, and root). Prospecting BANPs in pods of MO using in-silico ADMET predictions is expected to chart-out a new road map for drug discovery is the basic aspect sustainable exploitation of bioactive natural products22,27. The aim of this study is to identify phytochemicals in the natural dried-seed removed ripened pods by phytochemical screening followed by GC-MS so as to exploit them for the development of novel leads considering it’s nutritional and bio-pharmaceutical applications.

MATERIAL AND METHODS

COLLECTION OF THE PLANT MATERIAL

The plant specimen (dried pods) was collected from the fields (Organic Farms) near the Foothills of Alagarkovil Reserve Forest, Madurai, Tamil Nadu, India. The plant type specimen was identified and authenticated by Prof. Dr. S. Sutha at The Department of Medicinal Botany, Govt. Siddha Medical College, Palayamkottai, Tirunelveli District, Tamil Nadu, India.

PHYTOCHEMICAL SCREENING OF THE POD

The methanolic extracts were subjected to chemical tests for the detection of phytoconstituents using standard procedures15-25.

TEST FOR ALKALOIDS

Mayer’s test: Few drops of Mayer’s reagent was added to 1 mL of plant extract, appearance of a deep yellow or white precipitate indicated the presence of alkaloids in the solution. (Mayer’s reagent was freshly prepared by dissolving mercuric acetate in glacial acetic acid and potassium iodide in 100 ml water).

Dragendorff’s test: To 2 mL of the extract added 1 mL of Dragendorff’s reagent along the side of the test tube. Formation of orange or orange reddish brown precipitate indicated the presence of alkaloids. Dragendorff’s reagent was prepared by Sol A: 0.85g bismuth subnitrate, 40mL water, and 10mL glacial acetic acid and Sol B: 8g potassium iodide and 20mL water. 5mL each of Sol A & B with 20mL of glacial acetic acid and 70-100 mL of water is mixed to prepare Dragendorff’s reagent.

Hager’s test: Hager’s test was done by adding a few drops of Hager’s reagent to plant extracts and appearance of a yellow-color precipitate indicated the presence of alkaloids in the solution. Hager’s reagent is saturated solution of picric acid.

Wagner’s 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. Wagner’s Reagent was prepared by mixing 2.5 gm iodine in 12.5 gm of potassium iodide (KI 2); add 250 ml of water to produce solution.

TEST FOR GLYCOSIDES

Test For Anthraquinones Glycosides

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 CHCl3 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.

Bailjet test: Part of plant containing cardiac glycoside is dipped in sodium pircate solution; formation of a yellow to orange colour indicates the presence of aglycones or glycosides in the plant tissues.

Legal’s Test: To the concentrated ethanolic extract few drops of 10% NaOH were added, to make it alkaline. Then freshly prepared sodium nitroprusside was added to the solution. Presence of blue coloration indicated the presence of glycosides in the extract.

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 CARBOHYDRATES

Molisch’s test: Small portion of the plant extract was put in a test tube; 10 ml of distilled water was added and shaken vigorously and gently. The mixture was then filters and divided into two portions. To the first portion, two drops of Molish’s reagent was added followed by few drops of concentrated sulphuric acid by the wall of the test tube. Formation of brown or purple ring at the interphase indicated the presence of carbohydrates.

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 PHYTOSTEROLS**

Libermann Burchard's Test: Dissolve one or two crystals of cholesterol in dry chloroform in a dry test tube. Add few drops of acetic anhydride and then 2 drops of concentrated H2SO4 and mix well. The formation of a green or green-blue colour after a few minutes indicates the presence of phytosterols. After the reaction, concentration of cholesterol can be measured spectrophotometry.

Salkowski's Test: On adding a few drops of conc. Sulphuric acid to the plant extract and allow the solution to stand for some time, formation of brown ring indicated the presence of phytosterols in the plant extract.

**TEST FOR FLAVONOIDS**

FeCl₃ 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 flavonoids. Shinoda Test: To 2 ml of the extract, 1 ml of 1% ammonium solution was added. Appearance of yellow colour indicates the presence of flavonoids.

Shinoda's Test: In this test, four pieces of magnesium fillings (ribbon) are added to the ethanolic extract followed by a few drops of concentrated hydrochloric acid. A reddish colour indicates the presence of flavonoid.

**TEST FOR FIXED OILS AND FATS**

Spot test: Take the sample to be tested, press a little in the folds of the filter paper. On folding, if there is the appearance of greasy spot indicates the presence of oils or fats. The spot grows larger on heating and drying the filter paper.

Saponification: Take approximately 100 mg of oil or fat in a test tube. Add 3 mL of alcoholic-KOH and mix well. Place the tube in a boiling water bath for 15-20 min. Saponification value represents mg of potassium hydroxide required to saponify one gram of fat under the conditions specified. It is a measure of the average molecular weight of all the fatty acids present in the sample as triglycerides.

**TEST FOR FREE AMINO ACIDS**

Millon's reagent test: Millon's reagent is specific to phenol containing structures (tyrosine is the only common phenolic amino acid). Millon's reagent is concentrated HNO₃, in which mercury is dissolved. As a result of the reaction a red precipitate or a red solution is considered as positive test.

Ninhydrin reagent test: A 2% solution of ninhydrin is prepared by dissolving 0.2 grams of ninhydrin in 10ml of either ethanol or acetone. 1% solution of the amino acid (analyte) in distilled water is prepared, few drops of 2% ninhydrin solution is added to this solution. Test tube is kept in a warm water bath for 5 min, development of a deep blue/violet colour indicates presence of amino acids.

**TESTS FOR FIXED OILS AND FATS**

Spot test: Take the sample and place it between the folds of filter paper and rub it lightly. Presence of translucent spots on the filter paper confirms the presence of fats in the plant material.

Saponification: Take a sample a test tube, add strong alkali NaOH, boil the solution in a water bath for 5 min, add ethanol. Observe for the appearance of froth, formation of surfact in the test tube indicates the presence of fat in the sample.

**TEST FOR TANNINS**

5% Ferric chloride test: 5 mg of extract was taken and 0.5 ml of 5% ferric chloride was added. The development of dark bluish black color indicates the presence of tannins.

10% Lead acetate test: 10 mg of extract was taken and 0.5 ml of 1% lead acetate solution was added and the formation of precipitate indicates the presence of tannins and phenolic compounds.

**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.

**GUMS & MUCILAGE**

Ruthenium red test: 50 mg of dried mucilage powder was dissolved in 2 mL of distilled water, mixed with a few drops of Ruthenium red solution. Observed for pink color indicates the presence of gums and mucilage.

**GC-MS-MS Analysis**

Pod samples of were collected from the fields (Organic Farms) near the Foothills of Alagarkovil Reserve Forest, Madurai, Tamilnadu, India. The samples were processed and the methanolic extractions were carried out as described previously for GCMS analysis. GC-MS-MS analysis was carried out using Varian 4000 Ion trap GC/MS/MS with Fused silica 15m x 0.2 mm ID x 1μm of capillary column. The instrument was set to an initial temperature of 110 °C, and maintained at this temperature for 2 min. At the end of this period the oven temperature was rose up to 280 °C, at the rate of an increase of 5 °C/min, and maintained for 9 min. Injection port temperature was ensured as 250 °C and Helium flow rate as 1 ml/min. The ionization voltage was 70eV. The samples were injected in split mode as 10:1. Mass spectral scan range was set at 45-450 (m/z). Using computer searches on a NIST Ver.2.1 MS data library and comparing the spectrum obtained through GC-MS-MS compounds present in the plants sample were identified.

**Identification of Phytochemicals**

Interpretation on mass-spectrum GC-MS-MS was conducted using the database of National institute Standard and Technology (NIST) having more 62,000 patterns. The spectrum of the unknown compounds was compared with the spectrum of known components stored in the NIST library. The name, molecular weight and structure of the components of the test materials were ascertained.

**RESULTS**

Phytochemical analysis of MOMPE revealed the presence of alkaloids, carbohydrates, coumarins, flavonoids, glycosides, phenol, proteins, quinones, saponins, steroids, tannins and terpenoids. However, gums were not detected in the samples analyzed (Table 1). GCMS analysis revealed the presence of the following 12 phyto-compounds 7-Octadecyne, 2-methyl-
(C20H30); 3.7,11,15-Tetramethyl-2-hexadecen-1-ol (C20H30O); 3.7,11,15-Tetramethyl-2-hexadecen-1-ol (C20H30O); 3.7,11,15-Docosatetraenoic acid, me (C22H30O2); Cyclohexanol, 5-methyl-2-(1-methylthyl) (C7H12O); 3.7,11,15-Tetramethyl-2-hexadecen-1-ol (C20H30O); Palmmitic acid vinyl ester (C19H30O2); .gamma.-Tocopherol (C29H48O); Vitamin E (C22H30); Cholesta-7,9(11)-dien-3-ol, 4,4-dim (C20H30O); gamma.-Sitosterol (C29H46O); Stigmasta-5,24(28)-dien-3-ol, (3.beta,24Z)- (C20H30O) Table 1, 2; Fig. 1, 2.


Table 1 Phytochemical profile of *M. oleifera* Methanolic Pod Extracts (MOMPE)

<table>
<thead>
<tr>
<th>S. No</th>
<th>Plant constituents tested &amp; Reagent used</th>
<th>Observation/Results of the Test</th>
<th>M. oleifera Pod (Dried)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>TEST FOR ALKALOIDS</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.1</td>
<td><em>Mayer’s test</em></td>
<td>Absence of Creamy White ppt</td>
<td>++</td>
</tr>
<tr>
<td>1.2</td>
<td><em>Dragendorff’s test</em></td>
<td>Absence of Reddish Orange ppt</td>
<td>++</td>
</tr>
<tr>
<td>1.3</td>
<td><em>Hager’s test</em></td>
<td>Absence of Yellow precipitate</td>
<td>++</td>
</tr>
<tr>
<td>1.4</td>
<td><em>Wagner’s test</em></td>
<td>Absence of Reddish-Brown ppt</td>
<td>++</td>
</tr>
<tr>
<td>2.1</td>
<td>TEST FOR GLYCOSIDES - Anthroquinone</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.1.1</td>
<td><em>Borntrager’s test</em></td>
<td>Formation of Rose – Pink color</td>
<td>++</td>
</tr>
<tr>
<td>2.1.2</td>
<td><em>Baljet test</em></td>
<td>Formation of Yellow Orange color</td>
<td>+++</td>
</tr>
<tr>
<td>2.1.3</td>
<td><em>Legal’s test</em></td>
<td>Formation of pink to red colour</td>
<td>++</td>
</tr>
<tr>
<td>2.2</td>
<td>TEST FOR GLYCOSIDES - Cardiac</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.2.1</td>
<td><em>Keller-Killani test</em></td>
<td>Violet ring appears below brown</td>
<td>++</td>
</tr>
<tr>
<td>3</td>
<td>TEST FOR CARBOHYDRATES</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.1</td>
<td><em>Molish’s test</em></td>
<td>Formation of ring at junction</td>
<td>++</td>
</tr>
<tr>
<td>3.2</td>
<td><em>Fehling’s solution test</em></td>
<td>Formation of red precipitate</td>
<td>+++</td>
</tr>
<tr>
<td>3.3</td>
<td><em>Benedict’s reagent test</em></td>
<td>Formation of reddish-brown ppt</td>
<td>++</td>
</tr>
<tr>
<td>4</td>
<td>TEST FOR PHYTOSTEROLS</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.1</td>
<td><em>Libermann Burchard’s</em></td>
<td>Formation of a green-blue colour</td>
<td>+</td>
</tr>
<tr>
<td>4.2</td>
<td><em>Salkowski’s test</em></td>
<td>Formation of clear Brown Ring</td>
<td>+</td>
</tr>
<tr>
<td>5</td>
<td>TEST FOR FLAVONIODS</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5.1</td>
<td><em>Ferric chloride test</em></td>
<td>Appearance of Yellow Colour</td>
<td>++</td>
</tr>
<tr>
<td>5.2</td>
<td><em>Shinod’s test</em></td>
<td>Formation of a Reddish Colour</td>
<td>++</td>
</tr>
<tr>
<td>6</td>
<td>TEST FOR FIXED OILS AND FATS</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6.1</td>
<td><em>Spot test</em></td>
<td>Appearance of Greasy Spot</td>
<td>-</td>
</tr>
<tr>
<td>6.2</td>
<td><em>Saponification</em></td>
<td>mg of KOH to saponify 1g of fat</td>
<td>-</td>
</tr>
<tr>
<td>7</td>
<td>TEST FOR FREE AMINO ACIDS</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7.1</td>
<td><em>Millon’s reagent test</em></td>
<td>Red precipitate or a Red solution</td>
<td>+</td>
</tr>
<tr>
<td>7.2</td>
<td><em>Ninhydrin reagent test</em></td>
<td>Formation of a Blue/Violet color</td>
<td>+</td>
</tr>
<tr>
<td>8</td>
<td>TEST FOR TANNINS</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8.1</td>
<td><em>5% Ferric chloride</em></td>
<td>Development of bluish-black color</td>
<td>++</td>
</tr>
<tr>
<td>8.2</td>
<td><em>10% Lead acetate</em></td>
<td>Formation of a clear precipitate</td>
<td>++</td>
</tr>
<tr>
<td>9</td>
<td>TEST FOR SAPONINS</td>
<td></td>
<td></td>
</tr>
<tr>
<td>9.1</td>
<td><em>Foam test</em></td>
<td>Formation of stable foam</td>
<td>++</td>
</tr>
<tr>
<td>10</td>
<td>GUMS &amp; MUCILAGE</td>
<td>Formation of a Pink color</td>
<td>-</td>
</tr>
</tbody>
</table>

*Note: (++) - Indicate active constituents in high amount; (+) - Indicate active constituents in low amount; (−) - Indicate the absence of active constituents.*
Table 2: List of Bioactive Compounds in the GCMS profile of MOMPE

<table>
<thead>
<tr>
<th>RT</th>
<th>COMPOUND NAME</th>
<th>MF</th>
<th>MW</th>
<th>PA%</th>
</tr>
</thead>
<tbody>
<tr>
<td>13.189</td>
<td>7-Octadecyne, 2-methyl-</td>
<td>C19H36</td>
<td>264.5</td>
<td>5.803</td>
</tr>
<tr>
<td>13.486</td>
<td>3,7,11,15-Tetramethyl-2-hexadecen-1-ol</td>
<td>C20H40O</td>
<td>296.5</td>
<td>1.045</td>
</tr>
<tr>
<td>13.718</td>
<td>3,7,11,15-Tetramethyl-2-hexadecen-1-ol</td>
<td>C20H40O</td>
<td>296.5</td>
<td>2.073</td>
</tr>
<tr>
<td>16.670</td>
<td>6,9,12,15-Docosatetraenoic acid, me</td>
<td>C23H38O2</td>
<td>322.5</td>
<td>1.420</td>
</tr>
<tr>
<td>16.800</td>
<td>Cyclohexanol, 5-methyl-2-(1-methylethyl)-</td>
<td>C10H20O</td>
<td>198.3</td>
<td>2.969</td>
</tr>
<tr>
<td>17.874</td>
<td>3,7,11,15-Tetramethyl-2-hexadecen-1-ol</td>
<td>C20H40O</td>
<td>296.5</td>
<td>1.045</td>
</tr>
<tr>
<td>24.751</td>
<td>Palmitic acid vinyl ester</td>
<td>C18H34O2</td>
<td>282.5</td>
<td>1.051</td>
</tr>
<tr>
<td>30.188</td>
<td>Vitamin E</td>
<td>C29H50O2</td>
<td>416.7</td>
<td>3.184</td>
</tr>
<tr>
<td>31.580</td>
<td>Cholest-7,9(11)-dien-3-ol, 4,4-dim</td>
<td>C29H44O</td>
<td>412.7</td>
<td>1.933</td>
</tr>
<tr>
<td>34.341</td>
<td>gamma-Sitosterol</td>
<td>C29H52O2</td>
<td>432.7</td>
<td>8.456</td>
</tr>
<tr>
<td>36.344</td>
<td>Stigmasta-5,24(28)-dien-3-ol, (3.beta.,24Z)-</td>
<td>C29H46O</td>
<td>412.7</td>
<td>8.810</td>
</tr>
</tbody>
</table>

Table 3: IUPAC Name, CID, and SMILES of Bioactive Compounds in MOMPE

<table>
<thead>
<tr>
<th>IUPAC NAME</th>
<th>CID</th>
<th>SMILES</th>
</tr>
</thead>
<tbody>
<tr>
<td>2-methyloctadec-7-yn-</td>
<td>118810</td>
<td>CCCCCCCCCC<a href="CC%5BC@H%5D(C)C">C@H</a></td>
</tr>
<tr>
<td>(E)-3,7,11,15-tetramethylhexadec-2-en-1-ol</td>
<td>5366244</td>
<td>CC(CCCCCC)CCCC<a href="C">C@H</a>C(C)C(C)C(C)C(C)C</td>
</tr>
<tr>
<td>(E)-3,7,11,15-tetramethylhexadec-2-en-1-ol</td>
<td>5366244</td>
<td>CC(CCCCCC)CCCC<a href="C">C@H</a>C(C)C(C)C(C)C(C)C</td>
</tr>
<tr>
<td>[(1R,2R,5R)-5-methyl-2-propan-2-ylocyclohexyl acetate]</td>
<td>88692</td>
<td>C[C@H]1CC[C@H]1<a href="C">(C@H)</a>C(C)C</td>
</tr>
<tr>
<td>(E)-3,7,11,15-tetramethylhexadec-2-en-1-ol ethenyl hexadecanoate</td>
<td>5366244</td>
<td>CC(CCCCCC)CCCC<a href="C">C@H</a>C(C)C(C)C(C)C</td>
</tr>
<tr>
<td>2,7,8-trimethyl-2-(4,8,12-trimethyltridecyl)-3,4-(2R)-5,7,8-tetramethyl-2-[(4R,8R)-4,8,12-trimethyltridecyl]-3,4-dihydroinden-6-ol</td>
<td>14986</td>
<td>C(C=C(C=C(C))O=C=C(C=O)C(C)(C)(C)=C(C)C)</td>
</tr>
<tr>
<td>(3S,5R,10S,13R,14R,17R)-4,4,10,13-tetramethyl-17-[(2R)-6-methylheptan-2-yl]-1,2,3,5,6,12,14,15,16,17-</td>
<td>14985</td>
<td>C(C=C(C=C(C))O=C=C(C=O)C(C)(C)(C)=C(C)C)</td>
</tr>
<tr>
<td>(3S,5S,9S,10R,13S,14S,17R)-17-[(2R,5S)-5-ethyl-6-methylheptan-2-yl]-10,13-dimethyl-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthen-3-ol</td>
<td>22296805</td>
<td>C(C=C(C=C(C))O=C=C(C=O)C(C)(C)(C)=C(C)C)</td>
</tr>
<tr>
<td>(3S,5S,9S,10R,13R,14S,17R)-17-[(2R,5S)-5-propyl-5-ylhept-5-en-2-yl]-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthen-3-ol</td>
<td>133082557</td>
<td>C(C=C(C=C(C))O=C=C(C=O)C(C)(C)(C)=C(C)C)</td>
</tr>
<tr>
<td>(3S,5S,9S,10R,13R,14S,17R)-10,13-dimethyl-17-[(2S,5R)-5-propyl-5-ylhept-5-en-2-yl]-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthen-3-ol</td>
<td>5281326</td>
<td>C=C(C=C(C=C(C))O=C=C(C=O)C(C)(C)(C)=C(C)C)</td>
</tr>
</tbody>
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Figure 2: MS profile and 2D structure of Bioactive Compounds in MOMPE