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Original Article

ISOLATION, CHARACTERIZATION AND PREDICTION OF BIOLOGICAL ACTIVITY OF TWO NEW FATTY ESTERS AND A PHENOL FROM THE HEARTWOOD OF *PTEROCARPUS MARSUPIUM* ROXB.

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ABSTRACT

Objective: The current investigation involves the isolation, characterization and prediction of biological activity spectra of the phytoconstituents from the ethanolic extract of the heartwood of *Pterocarpus marsupium* roxb. (Fabaceae).

Methods: The heartwood (3 kg) was extracted in alcohol by cold maceration for 21 d and the compounds were isolated by column chromatography. The compounds thus isolated were characterised and their structures were elucidated by using assorted spectral data analysis, i.e., infrared radiation spectroscopy (IR), proton nuclear magnetic resonance (^{1}HNMR), carbon thirteen nuclear magnetic resonance (^{13}C NMR) and direct analysis in real time mass spectrometry (DART-MS). PASS (prediction of activity spectra for substances) computer program was used to predict the biological activity spectra of the isolated compounds.

Results: Phytochemical investigation of ethanolic extract of the heartwood of *Pterocarpus marsupium* led to isolate two fatty esters and a phenolic compound characterised as *n*-octanyl *n*-octadeca-9,12-dienoate (*n*-octanyl linoleiate, 1), *n*-dodecanyl *n*-octadeca-9,12-dienoate (*n*-dodecanyl linoleiate, 2) and 2, 3-dioxymethylene phenol (3). These phytoconstituents are reported for first time in the heartwood of *Pterocarpus marsupium* Roxb. The *in silico* profiling of these phytoconstituents exhibited their broad spectra of biological activity. Compounds (1) and (2) showed their maximum activity as All-trans-retinyl-palmitate hydrolase inhibitor, anti eczematic, lipid metabolism regulator, etc. and compound (3) was found to be active as membrane integrity agonist, aspulvinone dimethylallyl transferases inhibitor, carminative, neurotransmitter uptake inhibitor, etc.

Conclusion: These isolated phytoconstituents can be used as the marker compounds to establish the identity, quality and purity of the drug. The results of PASS prediction shall be very useful for establishing these phytoconstituents as active pharmacological moieties.

Keywords: 2, 3-dioxymethylene phenol, Fabaceae, Fatty esters, Heartwood, *Pterocarpus marsupium,* PAAS

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INTRODUCTION

The wealthiest bio-resource of drugs includes the medicinal plants [1]. They have been extensively used by the traditional healers for treatment of various diseases [2]. One such traditional medicinal plant-*Pterocarpus marsupium* was selected for the current investigation.

Pterocarpus marsupium Roxb. (Fabaceae), also known as Malabar kino, Indian kino tree or Vijayasar, is a medium to large, deciduous tree that can grow up to 30 m tall with compound and imparipinnate leaves, terminal panicles of yellow flowers, flat, circular and winged pod, convex and bony seeds and dark brown to grey bark with surface fissures. It is native to India, Nepal and Sri Lanka, where it occurs in parts of the Western Ghats in the Karnataka-Kerala region and also in the forests of central India [3, 4].

Its heartwood is used as an astringent and to treat inflammation, diabetes, obesity, diarrhea, vitiligo, eczema, psoriasis and bleeding [5-8]. The heartwood and other parts of the plant contained pterostilbene, pterocarpol, flavonoids, 1-(2', 6'-dihydroxyphenyl)-β-D-glucopyranoside, lupeol, phytosterols, p-hydroxybenzaldehyde and pterocarposide [9-16].

Every phytoconstituent exhibits a broad spectrum of effects. Some may be beneficial and used for the treatment of various diseases while others may be toxic. Modern drug design and discovery utilise the various web-services for the prediction of physicochemical properties, biological activity and toxicity of chemical compounds. PASS is one such computer program which is able to evaluate any new compound in huge chemical-pharmacological space [17, 18].

The main objective of our study was to isolate, characterise and predict the biological activity spectra for the phytoconstituents from the heartwood of *Pterocarpus marsupium*.

MATERIALS AND METHODS

General experimental procedures

All melting points (mp) were determined in centigrade scale in one–end open capillary on a thermoelectrical melting point apparatus. The IR spectra were measured on IR affinity-1 Fourier transform infrared spectrometer model (Schimadzu). The mass spectra were recorded on a JEOL-Accu TOF (time of flight) JMS-T100LC mass spectrometer having a DART (direct analysis in real time) source. The m/z (mass to charge ratio) values of the more intense peaks are mentioned and the fig. in a bracket attached to each m/z values indicated relative intensities with respect to the base peak. The ^{1}H and ^{13}C NMR spectra were scanned on Bruker AvIII HD-300 and 75 MHz, respectively, an instrument in $CDCl_3$ and MeOD solvents using TMS as an internal standard. The coupling constants (J values) are expressed in Hertz (Hz). Column chromatography was performed on a silica gel (60-120 mesh; Qualigen, Mumbai, India) column. TLC (thin layer chromatography) was run on silica gel G 60 F 254 (Qualigen) coated aluminium sheets. Spots were visualised by exposing to iodine vapors, UV (ultraviolet) radiation and spraying with ceric sulfate solution.

Plant material

The plant material was procured from Khari Baoli, Delhi and it was authenticated as the heartwood of *Pterocarpus marsupium* Roxb. (Ref. No. NISCAIR/RHMD/Consult/2015/2911/104-3) by Dr. Sunita

Garg, chief scientist, Raw Material Herbarium and Museum, Delhi (RHMD), CSIR-NISCAIR. The voucher specimen is preserved in the herbarium section of Department of Pharmacognosy, KIET School of Pharmacy, Ghaziabad, Uttar Pradesh, India.

Extraction

The heartwood (3 kg) was air dried, crushed to smaller pieces, coarsely powdered and extracted with ethanol by cold maceration for 21 d. The ethanolic extract was filtered, concentrated under reduced pressure and dried on a water bath at a temperature below than 75 °C.

Preparation of slurry

The dried extract (55 g) was dissolved in minimum amount of methanol to attain the desired consistency. Silica gel for column chromatography (60-120 mesh) was added gradually with constant mixing to obtain a slurry. It was air dried and large lumps if any were broken into a smaller size. The uniform particle size of the slurry was obtained by passing it through sieve (# 8).

Isolation of phytoconstituents

The dried slurry was chromatographed over silica gel column (1.6 m x 16 mm x 2 mm) packed in petroleum ether. The column was eluted successively in increasing order of polarity in various combinations with petroleum ether (60-80 °C), chloroform in petroleum ether (0.5%, 1%, 2%, 5%, 10%, 15%, 20%, 25%, 30%, 35%, 40%, 45%, 50%, 55%, 60%, 65%, 70%, 75%, 80%, 85%, 90%, 95%) chloroform (100%), and methanol in chloroform(0.1%, 0.2%, 0.3%, 0.4%, 0.5%). The fractions were collected separately and matched by TLC to check homogeneity. Similar fractions having the same R_f (retention factor) values were combined and crystallized. The isolated compounds were recrystallized to get pure compounds.

Pass prediction

In this molecular modelling study, structures were generated with the aid of Chem3D Ultra-9.00 and HyperChem-v.6.02, Wolfram Research Mathematics 6.0 software. Lone pairs of electrons and hydrogen atoms were added where appropriated. The equilibrium geometries of compounds were located using MM+(for Hyper Chem) and MM2 (for Chem3D) functional set. In the next step, RHF calculation (semiempirical AM1 method, the self-consistent field of Hartree-Fock) were performed and bond length, angles, torsion angles and partial charges have been calculated. Calculations were performed on a Intel (R) Core2 (TM) CPU 6600 @ 2.4 GHz Pentium IV computer with 2 GB RAM.

RESULTS

Phytochemical investigation of the ethanolic extract (dark reddish brown mass, 210.58 g (7.02%)) of the heartwood of *Pterocarpus marsupium* led to isolate two fatty esters and a phenolic compound characterized as *n*-octanyl *n*-octadeca-9,12-dienoate (*n*-octanyl linoleiate, **1**), *n*-dodecanyl *n*-octadeca-9,12-dienoate (*n*-dodecanyl linoleiate, **2**) and 2, 3-dioxymethylene phenol (**3**). These phyto-constituents are reported for first time in the plant. The results of the isolation are compiled in table 1**.**

n-Octanyl linoleiate (1)

Elution of the column with petroleum ether afforded a dark reddish brown semi-solid mass of **1**, yield 73 mg (0.13%); R_f: 0.90 (chloroform: methanol, 9.5: 0.5), mp 74-75 °C; IR υ_{max} (KBr): 2927, 2851, 1731, 1635, 1463, 1378, 1268, 1248, 1186, 1081, 967, 719 cm^{-1}**.** ^{1}H NMR ($CDCl_3$): δ 5.34 (1H, m, H-12), 5.01 (1H, m, H-9), 4.94 (1H, m, H-9), 4.90 (1H, m, H-13), 4.09 (2H, d, J=6.6 Hz, H_2-1′), 2.78 (2H, m, H_2-11), 2.28 (2H, t, J=7.2 Hz, H_2-2), 2.04 (2H, m, H_2-8), 1.99 (2H, m, H_2-14), 1.56 (2H, m, CH_2), 1.32 (2H, m, CH_2), 1.28 (6H, brs, 3 x CH_2), 1.25 (16H, brs, 8 x CH_2), 0.89 (3H, t, J=6.5 Hz, Me-18), 0.85 (3H, t, J=6.3 Hz, Me-8′). ^{13}C NMR ($CDCl_3$): δ 170.63 (C-1), 45.33 (C-2), 30.39 (C-3), 32.26 (C-4), 29.92 (C-5), 29.55 (C-6), 29.85 (C-7), 32.48 (C-8), 124.20 (C-9), 130.56 (C-10), 37.32 (C-11), 147.30 (C-12), 129.95 (C-13), 31.64 (C-14), 29.73 (C-15), 29.67 (C-16), 29.61 (C-17), 14.16 (C-18), 63.89 (C-1′), 29.59 (C-2′), 29.38 (C-3′), 29.17 (C-4′), 28.19 (C-5′), 27.51 (C-6′), 22.91 (C-7′), 19.94 (C-8′). ESI MS m/z (rel. int.): 392 $[M]^+$($C_{26}H_{48}O_2$) (25.2), 279 (41.3), 113 (7.5).

n-Dodecanyl linoleiate (2)

Elution of the column with petroleum ether-chloroform (9:1) gave a grayish yellow solid mass of **2**, yield 67 mg (0.12%); R_f 0.725 (chloroform-methanol, 9.5: 0.5), mp 101-102 °C; IR υ_{max} (KBr): 2918, 2849, 1740, 1620, 1442, 1376, 1238, 1101, 1081, 947, 795, 729 cm^{-1}**.** ^{1}H NMR (MeOD): δ 5.33 (1H, m, H-12), 4.94 (1H, m, H-10), 4.88 (2H, m, H-9, H-13), 4.06 (2H, t, J=6.6 Hz, H_2-1′), 2.77 (2H, m, H_2-11), 2.04 (2H, t, J=7.2 Hz, H_2-2), 1.99 (2H, m, H_2-14), 1.83 (2H, m, H_2-8), 1.55 (2H, m, CH_2), 1.33 (2H, m, CH_2), 1.30 (2H, m, CH_2), 1.28 (30H, brs, 15 x CH_2), 0.90 (3H, t, J=6.6 Hz, Me-18), 0.87 (3H, t, J=6.4 Hz, Me-12′). ^{13}C NMR (MeOD): δ 172.31(C-1), 40.37 (C-2), 30.89 (C-3), 30.76 (C-4), 30.72 (C-5), 30.66 (C-6), 30.63 (C-7), 33.22 (C-8), 126.21 (C-9), 131.54 (C-10), 41.16 (C-11), 142.25 (C-12), 116.15 (C-13), 30.93 (C-14), 30.66 (C-15), 30.63 (C-16), 30.92 (C-17), 14.26 (C-18), 68.45 (C-1′), 30.58(C-2′), 30.55 (C-3′), 30.49 (C-4′), 30.46 (C-5′), 30.42 (C-6′), 30.39 (C-7′), 30.37 (C-8′), 30.94 (C-9′), 27.33 (C-10′), 23.89 (C-11′), 21.39 (C-12′). ESI MS m/z (rel. int.): 448 $[M]^+$($C_{30}H_{56}O_2$) (1.1), 279 (39.6).

2, 3-Dioxymethylene phenol (3)

Elution of column with chloroform-methanol (99.8: 0.2) yielded a reddish gray solid mass of **3**, 105 mg (0.19% yield); R_f 0.68 (chloroform), mp 90-91 °C; IR υ_{max} (KBr): 3365, 2917, 2885, 1604, 1529, 1485, 1382, 1297, 1168, 1144, 1084, 964, 844 cm^{-1}.^{1}H NMR (MeOD): δ 6.95(1H, m, H-6), 6.29 (1H, m, H-4), 6.27 (1H, m, H-5), 4.89 (2H, brs,-OCH_2-O). ^{13}C NMR ($CDCl_3$): δ 159.52 (C-1), 131.04 (C-2), 108.29 (C-3), 107.47 (C-4), 107.88 (C-5), 108.29 (C-6), 103.11 (-OCH_2-O-)**.** ESI MS m/z (rel. int.): 138 $[M]^+$($C_7H_6O_3$) (1.2).

Table 1: Chemical constituents isolated from *Pterocarpus marsupium* Roxb.

Comp-ound	Column eluant	R_f value mobile phase	Yield (%w/w)	Physical State	Colour	M. p. °C	Mol. wt. [Mol. for.]	Nomenclature
(1)	P	0.90 C: M (9.5:0.5)	73 mg (0.13%)	Semi solid	Dark reddish brown	74-75	392 $C_{26}H_{48}O_2$	*n*-octanyl *n*-octadeca-9,12-dienoate
(2)	10% C in P	0.725 C: M (9.5:0.5)	67 mg (0.12%)	solid	Grayish yellow	101-102	448 $C_{30}H_{56}O_2$	*n*-dodecanyl *n*-octadeca-9,12-dien-oate
(3)	0.2% M in C	0.68 C: M (8: 2)	105 mg (0.19%)	solid	Reddish gray	90-91	138 $C_7H_6O_3$	2, 3-dioxymethylene phenol

P–Petroleum ether (60-80 °C), C–Chloroform; M–Methanol

The results of PASS prediction which revealed the biological activity spectra of the isolated compound (1), (2) and (3) are depicted in table 2, 3 and 4 respectively.

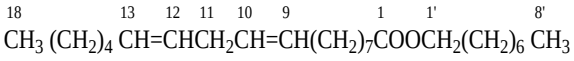
The first column in these tables show the percentage activity and the second show the percentage inactivity for the activity mentioned in column 3.

DISCUSSION

The compound 1 was obtained as a dark reddish brown semi-solid substance from petroleum ether eluants. Its IR spectrum exhibited characteristic absorption bands for ester group (1731 cm^{-1}), unsaturation (1635 cm^{-1}) and long aliphatic chain (719 cm^{-1}). The mass spectrum of 1 had a molecular ion peak at *m/z* 392 consistent

with the molecular formula an aliphatic ester, $C_{26}H_{48}O_2$. The prominent fragments generated at *m/z* 279 $[CH_3(CH_2)_3\text{-}(CH_2CH{=}CH)_2(CH_2)_7COO]^+$ and 113 $[(CH_2)_7CH_3]^+$ suggested that *n*-octanol was esterified with linoleic acid. The ^{1}H NMR spectrum of 1 showed four one-proton multiplets at δ 5.34, 5.01, 4.94 and 4.90 attributed to vinylic H-12, H-10, H-9 and H-13 protons, respectively. A two-proton doublet at δ 4.09 (J=6.6 Hz) and a two-proton triplet at δ 2.28 (J=7.2 Hz) were ascribed to oxygenated methylene H_2-1′ and methylene H_2-2 adjacent to the ester group, respectively. Five two-proton multiplets between δ 2.78-1.32 and two broad singlets at δ 1.28 (6H) and 1.25 (16H) were associated with the remaining methylene protons.

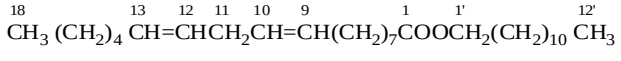
Two-three proton triplets at δ 0.89 (J=6.5 Hz) and δ 0.85 (J=6.3 Hz) were assigned to the terminal primary Me-18 and Me-8′ protons, respectively. The ^{13}C NMR spectrum of 1 exhibited the presence of ester carbon at δ 170.63 (C-1), vinylic carbons between δ 147.30-124.20 and methyl carbons at δ 14.16 (C-18) and 19.94 (C-8′). On the basis of the spectral data analysis, the structure of 1 has been established as *n*-octanyl *n*-octadeca-9, 12-dienoate. This phyto-constituent is first time reported in *P. marsupium*.



***n*-Octanyl *n*-octadeca-9,12-dienoate (1)**

The compound **2** was a greyish yellow solid mass isolated from petroleum ether-chloroform (9:1) eluants. Its IR spectrum showed distinctive absorption bands for ester group (1740 cm^{-1}), unsaturation (1620 cm^{-1}) and long aliphatic chain (729 cm^{-1}). The mass spectrum of **2** exhibited a molecular ion peak at *m/z* 448 corresponding to the molecular formula an aliphatic ester, $C_{30}H_{56}O_2$. The prominent fragment generated at *m/z* 279 $[CH_3(CH_2)_3\text{-}(CH_2CH{=}CH)_2(CH_2)_7COO]^+$indicated that linoleic acid was esterified with an aliphatic alcohol. The ^{1}H NMR spectrum of **2** displayed two one-proton multiplets at δ 5.33 and 4.94 and a two-proton multiplet 4.88 ascribed to vinylic H-12, H-10, H-9 and H-13 protons, respectively. Two two-proton triplets at δ 4.06 (J=6.6 Hz) and 2.04 (J=7.2 Hz) were ascribed to oxygenated methylene H_2-1′ and methylene H_2-2 adjacent to the ester group, respectively.

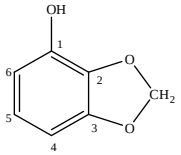
Six two-proton multiplets between δ 2.77-1.30 and a broad singlet at δ 1.28 (30 H) were associated with the remaining methylene protons. Two three-proton triplets at δ 0.90 (J=6.6 Hz) and δ 0.87 (J=6.4 Hz) were assigned correspondingly to the terminal primary Me-18 and Me-12′ protons. The ^{13}C NMR spectrum of **2** showed the presence of ester carbon at δ 172.31 (C-1), vinylic carbons between δ 142.25–116.15 and methyl carbons at δ 14.26 (C-18) and 21.39 (C-12′). On the basis of these evidence, the structure of **2** has been elucidated as *n*-dodecanyl *n*-octadeca-9, 12-dienoate. This phyto-constituent is first time reported in *P. marsupium*.



***n*-Dodecanyl *n*-octadeca-9,12-dienoate (2)**

The compound **3** was obtained as a reddish grey solid substance from chloroform: methanol (99.8: 0.2) eluants. It responded positive tests for phenol and had a molecular ion peak at *m/z* 138 in its mass spectrum corresponding to the molecular formula of a phenolic compound, $C_7H_6O_3$. Its IR spectrum exhibited distinct absorption bands for hydroxyl group (3365 cm^{-1}) and aromatic ring (1604, 1529, 1084 cm^{-1}). The ^{1}H NMR spectrum of **3** showed three one-proton multiplets at δ 6.95, 6.29 and 6.27 due to aromatic H-6, H-4 and H-5 protons, respectively.

A two-proton broad singlet at δ 4.89 was attributed to di-oxygenated methylene,–O-CH_2-O-, protons. Its ^{13}C NMR spectrum displayed signals for aromatic carbons from δ 159.52 to 107.47, and di-oxygenated methylene carbon at δ 103.11. These spectral data led to formulate the structure of **3** as 2, 3-dioxymethylene phenol. This phytoconstituent is first time reported in *P. marsupium.*



2, 3-Dioxymethylene phenol (3)

The PASS computer program, which is able to simultaneously predict more than one thousand biological and toxicological activities from only the structural formulas of the chemicals, was used to predict the biological activity profile of all the three new compounds isolated from *Pterocarpus marsupium.* Various novel pharmaceuticals have been discovered using PASS prediction. This application is a wonderful gift of technology to the mankind because it helps to discover new, potent and safe medicinal agents. It also provides an excellent opportunity for the multidisciplinary professionals (e. g. pharma and computational experts) to work together on a single platform and serve the society.

The PASS prediction profiles of the isolated compounds in the current research investigation have contributed towards the incredibility of this piece of work. n-octanyl linoleiate (1) showed the highest probability to be active as All-trans-retinyl-palmitate hydrolase inhibitor, anti eczematic, lipid metabolism regulator, CYP2J substrate, CYP2J2 substrate, phosphatidylcholine-retinol O-acyltransferase inhibitor, lipoprotein lipase inhibitor, phosphatidyl glycerophosphatase inhibitor, muco-membranous protector and alkenyl glycerophosphocholine hydrolase inhibitor. n-dodecanyl linoleiate (2) also exhibited a similar biological activity spectrum.

Table 2: Biological activity of n-octanyl linoleiate (1)

Percentage activity	Percentage inactivity	Name of activity
96.4	0.1	All-trans-retinyl-palmitate hydrolase inhibitor
95.6	0.2	Antieczematic
92.9	0.3	Lipid metabolism regulator
92.6	0.3	CYP2J substrate
92.0	0.3	CYP2J2 substrate
91.5	0.2	Phosphatidylcholine-retinol O-acyltransferase inhibitor
91.1	0.3	Lipoprotein lipase inhibitor
90.2	0.2	Phosphatidylglycerophosphatase inhibitor
90.4	0.5	Mucomembranous protector
89.9	0.5	Alkenylglycerophosphocholine hydrolase inhibitor
89.0	0.4	Alkylacetylglycerophosphatase inhibitor
88.6	0.3	Cutinase inhibitor
87.9	0.5	Acylcarnitine hydrolase inhibitor
86.9	0.4	Cholesterol antagonist
86.7	0.9	Polyporopepsin inhibitor
86.6	0.9	Saccharopepsin inhibitor
86.0	0.3	Macrophage colony stimulating factor agonist
85.3	0.4	Dextranase inhibitor

84.7	0.5	Fucosterol-epoxide lyase inhibitor
84.1	0.3	Preneoplastic conditions treatment
83.9	0.4	IgA-specific serine endopeptidase inhibitor
83.7	0.4	Antihypercholesterolemic
83.3	0.4	Antisecretoric
83.0	0.2	Angiogenesis stimulant
82.3	0.5	Linoleate diol synthase inhibitor
82.1	0.3	Phosphatidate phosphatase inhibitor
81.8	0.4	Poly(alpha-L-guluronate) lyase inhibitor
81.0	0.2	Protein-tyrosine sulfotransferase inhibitor
80.6	0.3	Poly(beta-D-mannuronate) lyase inhibitor
82.5	2.5	Ubiquinol-cytochrome-c reductase inhibitor
79.9	0.1	Thromboxane synthase stimulant
78.0	0.4	Leukopoiesis stimulant
77.9	0.5	IgA-specific metalloendopeptidase inhibitor
76.0	0.3	Ethanolamine-phosphate cytidylyltransferase inhibitor
75.8	0.3	Gastrin inhibitor
75.7	0.2	Pediculicide
76.2	0.9	Oxidoreductase inhibitor
75.3	0.4	Lactase inhibitor
74.5	0.1	Cyclooxygenase 1 substrate
73.5	1.1	Membrane integrity antagonist
72.5	0.4	Leukotriene-B4 20-monooxygenase inhibitor
72.0	0.7	Levanase inhibitor
71.5	0.8	CYP3A1 substrate
72.4	2.4	Pro-opiomelanocortin converting enzyme inhibitor
70.3	0.5	Cytoprotectant

Table 3: Biological activity of n-dodecanyl linoleiate (2)

Percentage activity	Percentage inactivity	Name of activity
96.4	0.1	All-trans-retinyl-palmitate hydrolase inhibitor
95.6	0.2	Antieczematic
92.9	0.3	Lipid metabolism regulator
92.0	0.3	CYP2J2 substrate
91.5	0.3	GST A substrate
90.2	0.2	Phosphatidylglycerophosphatase inhibitor
90.4	0.5	Mucomembranous protector
89.0	0.4	Alkylacetylglycerophosphatase inhibitor
88.4	0.1	Alcohol O-acetyltransferase inhibitor
87.2	0.1	Endocannabinoid uptake inhibitor
86.6	0.9	Saccharopepsin inhibitor
86.0	0.3	Macrophage colony stimulating factor agonist
85.4	0.5	Pullulanase inhibitor
84.7	0.5	Fucosterol-epoxide lyase inhibitor
84.1	0.3	Preneoplastic conditions treatment
83.7	0.5	Exoribonuclease II inhibitor
83.0	0.2	Angiogenesis stimulant
82.3	0.5	Linoleate diol synthase inhibitor
81.8	0.2	Phosphatidylinositol diacylglycerol-lyase inhibitor
81.0	0.2	Protein-tyrosine sulfotransferase inhibitor
80.7	0.4	CYP2E1 inhibitor
79.9	0.1	Thromboxane synthase stimulant
78.8	0.4	Ecdysone 20-monooxygenase inhibitor
78.0	0.4	Leukopoiesis stimulant
77.9	0.5	IgA-specific metalloendopeptidase inhibitor
76.2	0.2	Vanilloid 1 agonist
76.0	0.5	Sarcosine oxidase inhibitor
75.3	0.4	Lactase inhibitor
74.8	0.4	Anthranilate-CoA ligase inhibitor
73.2	0.4	Cyclomaltodextrinase inhibitor
73.3	0.5	Antimutagenic
73.5	1.1	Membrane integrity antagonist
72.5	0.4	Leukotriene-B4 20-monooxygenase inhibitor
73.4	1.5	Arginine 2-monooxygenase inhibitor
72.3	0.5	Alkenylglycerophosphoethanolamine hydrolase inhibitor
72.0	0.7	Levanase inhibitor
71.4	0.3	Sclerosant
71.5	0.8	CYP3A1 substrate
70.6	0.3	CYP4A substrate
70.3	0.5	Cytoprotectant
70.4	0.8	HMOX1 expression enhancer

This also proves the fact that the structure of the compound is related to its activity and also that compounds with similar chemical structure exhibit similarity in their activity profiles also. 2, 3-dioxymethylene phenol (3) was found to be active as membrane integrity agonist, aspulvinone dimethylallyl transferases inhibitor, carminative, neurotransmitter uptake inhibitor, a dehydro-L-gulonate decarboxylase inhibitor, MAP kinase stimulant, ubiquinol-cytochrome-c reductase inhibitor, JAK2 expression inhibitor, NADPH peroxidase inhibitor, glutathione thioesterase inhibitor, GABA aminotransferase inhibitor and antiseptic.

Table 4: Biological activity of 2, 3-Dioxymethylene phenol (3)

Percentage activity	Percentage inactivity	Name of activity
95.2	0.3	Membrane Integrity Agonist
90.6	0.7	Aspulvinone dimethylallyl transferases inhibitor
89.9	0.2	Carminative
87.8	0.2	Neurotransmitter uptake inhibitor
82.7	0.7	Dehydro-L-gulonate decarboxylase inhibitor
81.3	0.3	MAP kinase stimulant
81.8	0.27	Ubiquinol-cytochrome-c reductase inhibitor
79.8	0.8	JAK2 expression inhibitor
79.9	1.2	NADPH peroxidase inhibitor
79.3	0.8	Glutathione thiolesterase inhibitor
78.5	0.3	GABA aminotransferase inhibitor
77.9	0.4	Antiseptic
80.7	3.5	CYP2C12 substrate
79.3	2.1	Chlordecone reductase inhibitor
77.3	0.7	Antidyskinetic
77.8	1.4	Feruloyl esterase inhibitor
76.3	0.8	Caspase 3 stimulant
77.8	2.3	Antiseborrheic
75.6	0.4	MMP9 expression inhibitor
75.8	1.0	Alkane 1-monooxygenase inhibitor
76.3	2.2	Sugar-phosphatase inhibitor
76.1	2.3	Methylenetetrahydrofolate reductase (NADPH) inhibitor
77.1	3.3	Testosterone 17beta-dehydrogenase (NADP+) inhibitor
74.2	1.4	Glucan endo-1,6-beta-glucosidase inhibitor
74.6	2.2	Nicotinic alpha6beta3beta4alpha5 receptor antagonist
74.2	2.6	Alkenylglycerophosphocholine hydrolase inhibitor
73.4	2.0	Glucose oxidase inhibitor
72.3	1.4	NADPH-cytochrome-c2 reductase inhibitor
71.4	0.5	Ovulation inhibitor
71.5	0.6	Anesthetic general
74.0	3.4	Acrocylindropepsin inhibitor
74.0	3.4	Chymosin inhibitor
74.0	3.4	Saccharopepsin inhibitor
71.9	1.7	Ribulose-phosphate 3-epimerase inhibitor
70.9	0.8	Ecdysone 20-monooxygenase inhibitor
70.4	1.0	Thioredoxin inhibitor
70.4	1.8	Complement factor D inhibitor
70.7	2.6	Glutamyl endopeptidase II inhibitor
70.0	1.6	Arylacetonitrilase inhibitor
70.7	2.6	Glutamyl endopeptidase II inhibitor

CONCLUSION

Currently, PASS web-service is being utilised by more than 8700 registered users from more than 7o countries. Predictions for more than 250,000 organic compounds have been obtained from this computer program. More than 4,000 pharmacological effects, specific toxicities, mode of action, effect on gene expression, the interaction of metabolic enzymes, etc. have been predicted so far.

The isolated phytoconstituents in the current investigation are being reported for the first time so these can be utilised as fingerprinting markers for the various chromatographic techniques for establishing the identity, quality and purity of the drug. The *in silico* profiling of these phytoconstituents shall be more beneficial than the animal studies because of the significant variation in the genetic pattern of the humans and the rodents. The results of this study shall be very helpful for the upcoming research investigations to establish these new compounds as the pharmacologically active moieties.

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CONFLICTS OF INTERESTS

There are no conflicts of interest.

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