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 (1H NMR), carbon thirteen nuclear magnetic resonance (13C 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-octanoyl n-octadeca-9,12-dienoate (n-octanoyl linoleate, 1), n-dodecanoyl n-octadeca-9,12-dienoate (n-dodecanoyl linoleate, 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 dimethyl allyl 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

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 pterocarpol [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 thermo electrical melting point apparatus. The IR spectra were measured on IR Affinity-1 Fourier transform infrared spectrometer model (Shimadzu). The mass spectra were recorded on a JEOL-Acou TOF (time of flight) JMS-T100LQ 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 indicated relative intensities with respect to the base peak. The 1H and 13C NMR spectra were scanned on Bruker AvIII HD-300 and 75 MHz, respectively, an instrument in CDC13, 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...
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 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 Mathematica 6.0 software. Lone pairs of electrons and hydrogen atoms were added where appropriate. The equilibrium geometries of compounds were located using MM+ (for Hyper Chem) and MM2 (for Chem3D) functional set. In the next step, RBH 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-octanal n-octadeca-9,12-dienoate (n-octanolineate, 1), n-dodecanol n-octadeca-9,12-dienoate (n-dodecanol n-octadeca-9,12-dienoate, 2) and 2,3-dioxymethylene phenol (3). These phytoconstituents are reported for first time in the plant. The results of the isolation are compiled in table 1.

Table 1: Chemical constituents isolated from Pterocarpus marsupium Roxb.

| Compound | Column eluant | Rf value mobile phase | Yield (g/w) | Physical State | Colour | M. p. °C | Mol. wt. (Mol. for.) | Nomenclature |
|----------|---------------|-----------------------|-------------|----------------|--------|----------|---------------------|--------------|
| (1)      | P             | C (9.0:0.5)           | 0.90        | Semi           | Dark reddish | 75-76     | 392                 | n-octanoyl n-octadeca-9,12-dienoate |
| (2)      | 10%           | C in P (9.0:0.5)      | 0.725       | Solid          | Yellow     | 101-102  | 448                 | n-dodecanoyl n-octadeca-9,12-dienoate |
| (3)      | 0.2%          | M in C (0.2)         | 0.68        | Solid          | Reddish    | 90-91    | 138                 | 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_{30}H_{56}O_{2}. The prominent fragments generated at m/z 279 \{CH_3(CH_2)_2-\}, \{CH_2CH=CH(CH_2)_7COO\}^- and 113 \{CH_3(CH_2)_2\} suggested that n-octanoic acid was esterified with linoleic acid. The \textit{H} NMR spectrum of 1 showed four one-proton multiplets at δ 5.34, 5.01, 4.94 and 4.90 attributed to vinyl H-2, 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_2-2 and methylene H-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 (I=6.5 Hz) and δ 0.85 (I=6.3 Hz) were assigned to the terminal primary Me-1-8 and Me-9' protons, respectively. The \textit{13}C NMR spectrum of 1 exhibited the presence of ester carbon at δ 170.63 (C-1), vinylcarbon 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-octanoyl n-octadeca-9,12-dienoate. This phytoconstituent is first time reported in \textit{P. marsupium}.

\begin{table}[h]
\centering
\begin{tabular}{cccc}
\textbf{Percentage activity} & \textbf{Percentage inactivity} & \textbf{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 & CYP2J substrate \\
91.5 & 0.2 & Phosphatidylcholine-retinol O-acyltransferase inhibitor \\
91.1 & 0.3 & Lipid protein lipase inhibitor \\
90.2 & 0.2 & Phosphatidylglycerophosphatase inhibitor \\
90.4 & 0.5 & Mucomembranous protector \\
89.9 & 0.5 & Allkenyglycerophosphocholine hydrolase inhibitor \\
89.0 & 0.4 & Allkenyglycerophosphatase 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 \\
\end{tabular}
\caption{Table 2: Biological activity of n-octanoyl linoleate (1)}
\end{table}

The compound 2 was obtained as a reddish yellow solid mass isolated from petroleum ether-chloroform (9:1) eluants. Its IR spectrum showed distinct absorption bands for hydroxyl group (3365 cm^{-1}) and aromatic ring (1604, 1529, 1084 cm^{-1}). The \textit{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=O-, protons. Its \textit{13}C NMR spectrum displayed signals for aromatic carbons from δ 159.52 to 107.47, and dioxygenated 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 \textit{P. marsupium}.
### 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                   | Alkylacylglycerophosphatase 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 |
| 83.9                | 0.4                   | IgA-specific serine endopeptidase inhibitor |
| 83.7                | 0.4                   | Anti hypercholesteremic |
| 83.3                | 0.4                   | Anti-secretory     |
| 83.0                | 0.2                   | Angiogenesis stimulant |
| 82.3                | 0.5                   | Linoate diol synthase inhibitor |
| 82.1                | 0.3                   | Phoshatidate phosphatase inhibitor |
| 81.8                | 0.4                   | Poly(alpha-L-gulurate)-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 |
| 75.0                | 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     |
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 aminotransfere 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 thioesterase inhibitor            |
| 78.5                | 0.3                   | GABA aminotransfere 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                   | Furaloyl esterase inhibitor                   |
| 76.3                | 0.8                   | Caspase 3 stimulant                           |
| 77.3                | 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                   | Methyleneeterahydroolate reductase (NADPH) inhibitor |
| 77.1                | 3.3                   | Testosterone 17beta-dehydrogenase (NADP+) inhibitor |
| 74.2                | 1.4                   | Glican endo-1,6-beta-glucosidase inhibitor     |
| 74.6                | 2.2                   | Nicotinic alpha6beta4alpha5 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                   | Acrocyndropepsin 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                   | Ecrysone 20-monooxygenase inhibitor            |
| 70.4                | 1.0                   | Thioexocrine inhibitor                        |
| 70.4                | 1.8                   | Complement factor D inhibitor                 |
| 70.7                | 2.6                   | Glicamylendopeptidase II inhibitor             |
| 70.0                | 1.6                   | Arylacetoniitrilase inhibitor                 |
| 70.7                | 2.6                   | Glicamylendopeptidase II inhibitor             |

CONCLUSION

Currently, PASS web-service is being utilised by more than 9700 registered users from more than 70 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.

REFERENCES

1. Sharma V, Chaudhary U. Pharmacognostical and phytochemical screening of Helicteres isora roots. Asian J Pharm Clin Res 2016;9:96-101.
2. Kripa KG, Sangeetha R, Chamundeeswari D. Pharmacognostical and physicochemical evaluation of the plant Leucas Apetala. Asian J Pharm Clin Res 2016;9:263-8.
3. Saldanha CJ. Flora of Karnataka. Vol. I. Oxford: IBH Publishing; 1984. p. 21.
4. Matthew KM. The Flora of Tamil Nadu Carnatic. St. Josephs College: Tiruchirapalli, India; 1983.
5. Warrier PK. Indian medicinal plants: a compendium of 500 species. Vol. 3. Universities Press; 1995. p. 280.
6. Pullaiah T. Medicinal plants of Andhra Pradesh. New Delhi, India: Regency Publications; 1999. p. 63.
7. Devgun M, Nanda A, Ansari SH. *Pterocarpus marsupium* Roxb.-A comprehensive review. Pharmacogn Rev 2009;3:359-63.
8. Katiyar D, Singh V, Ali M. Phytochemical and pharmacological profile of *Pterocarpus marsupium*: a review. Pharma Innovation J 2016;5:31-9.
9. Maurya R, Ray AB. Constituents of *Pterocarpus marsupium*. J Nat Prod 1984;47:179-81.
10. Chakravarthy BK, Gode KD. Isolation of (-) Epicatechin from *Pterocarpus marsupium* and its pharmacological actions. Planta Med 1985;51:56-9.
11. Tripathi J, Joshi T. Flavonoids from *Pterocarpus marsupium*. Planta Med 1988;54:371-2.
12. Tripathi J, Joshi T. Phytochemical investigation of roots of *Pterocarpus marsupium*: isolation and structural studies of two new flavanone glycosides. Z Naturforsch C 1988;43:184-6.
13. Jahromi MAF, Ray AB. Antihyperlipidemic effect of flavonoids from *Pterocarpus marsupium*. J Nat Prod 1993;56:989-94.
14. Handa SS, Singh R, Maurya R, Satti NK, Suri KA, Suri OP. Pterocaroside, an isaurone C-glucoside from *Pterocarpus marsupium*. Tetrahedron Lett 2000;41:1579-81.
15. Suri KA, Satti NK, Gupta BD, Suri OP. 1-[(2’, 6’ dihydroxyphenyl)-(D-glucopyranoside, a novel C-glycoside from *Pterocarpus marsupium*. Indian J Chem 2003;42B:432-3.
16. Maurya R, Singh R, Deepak M, Handa SS, Yadav PP, Mishra PK. Constituents of *Pterocarpus marsupium*: a crude ayurvedic drug. Phytochemicals 2004;65:915-20.
17. Lagunin A, Stepanchikova A, Filimonov D, Poroikov, PASS: prediction of activity spectra for biologically active substances. Bioinformatics Applications Note 2000;16:747-8.
18. Porovikov V, Filimonov D, Borodina Yu, Langunin A, Kos A. Robustness of biological activity spectra predicting by computer program PASS for non-Congeneric sets of chemical compounds. J Chem Inf Comput Sci 2000;40:1349-55.

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