NEW LONG CHAIN ALIPHATIC COMPOUNDS FROM BUTEA MONOSPERMA (LAMK.)

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ABSTRACT:

*Butea monosperma, known as Palas, Khakhra in Hindi, is an Ayurvedic plant, and its various parts have been studied for their medicinal properties. It belongs to family leguminoceae, this research describes the isolation and structure elucidation of three new long chain and two known compounds from the acetone extract of the stem bark of this plant. The acetone extract of B. monosperma bark yields new aliphatic compounds-triacont-3, 17-diene **1**, 25-methyl-dotriacont-6, 20-diene-17-one **2**, undecylhexadecanoate **3** and two known compounds- stigmasterol **4**, and β-sitosterol **5**.these long chain aliphatic compounds showed antimicrobial activity.*

KEYWORDS: *Acetone extract, 25-methyl-dotriacont-6, triacont-3, 17-diene, 20-diene-17-one, undecylhexadecanoate, antimicrobial activity.*

1. INTRODUCTION

Butea monosperma in the traditional system of medicine is a medicinal plant. As reported by the Indian Ayurvedic texts, its leaves, stem, flowers, seeds, gum (stem) and roots have been widely used as traditional medicine [1]. It is commonly Forest due to its gorgeous canopy of scarlet flowers which looks like a flame [2]. Different species of Butea found in India are *Butea parviflora*, *Butea purpurea*, *Butea monosperma* and *Butea superb* [3]. It has various healing effects which are seen in treatment of many Diseases. The bark is an appetiser, lessens inflammation, used in liver disorders, fractures, topically in piles and purifies the blood. The leaf is an appetiser, astringent, anthelmintic, aphrodisiac, cures boils and piles. The flowers are astringent, diuretic and aphrodisiac and they are used to disperse swellings. The fruit and the seeds are bitter and oily and useful in piles, eye diseases and inflammation In the present work, the morphological, microscopical and phytochemical studies of different parts of *Butea monosperma*(Lamk.) Taub. Have been carried out which will be useful for proper identification and authentication of crude drug [4]. A beautiful tree has been reported to possess anti-inflammatory, antifungal activity, anthelmintic, antifertility, anti-diabetic and abortifacient activity [5].

2. MATERIALS AND METHODS

2.1 COLLECTION: The Bark of *B. monosperma* (15kg) were collected from the nearby area of Ujjain city and identified by School of studies in Botany, Vikram University; Ujjain 456010 (M.P.) India.

2.2 EXTRACTION AND ISOLATION: The bark of *B. monosperma* (15 Kg) were, dried, cleaned and powdered coarsely. It was extracted by acetone and excess of solvent was removed by rotatory film evaporator to afford dark brown solid extract (80 mg). The extracted showed positive test for the presence of steroids and terpenoids. This extract was fractionated on alumina grade III column. The column was eluted with various solvent and their mixture starting with n-hexane, benzene, ether, chloroform, ethanol and methanol. The fractions were collected in bulk and monitored by TLC. Repeated chromatography afforded 5 compounds in pure form.

2.3 EXPERIMENTAL SECTION : The IR spectra were recorded in KBr on Perkin Elmer-377, ^{1}H NMR spectra were recorded on 300 MHz varian XL spectrometer and 400 MHz Brucker WM spectrometer with TMS as internal standard, ^{13}C NMR spectra on varian XL 75 MHz spectrometer in $CDCl_3$ and EIMS on Jeol-JMS D 300 Mass spectrometer at 70 eV. The column chromatography was carried out on alumina Gr.III and TLC on silica gel G. Sports were visualized by exposure to iodine vapour or by spraying with $H_2SO_4^-$ vanillin solution followed by heating at 105^0C for 5 minutes.

2.3.1 TRIACONT-3, 17-DIENE: M^+ 418, $C_{30}H_{58}$, (chloroform: methanol, 20gm), m.p. 180 ^0C, isolated from hexane fraction of hexane elute of the column. TLC (hexane: ether 9.8: 0.2 v/v). IR (KBr): 2922, 2852, 1636, 1460, 1020, 760 and 720 cm^{-1}, ^{1}H NMR (200 MHz, $CDCl_3$): δ 0.91 (6H, t, 2x-CH_3), 1.31 (40H, s, 20x-CH_2), 1.6 (8H, brs, 4x-CH_2, α to unsaturation), 5.02 (4H, t, 2x- CH=CH), EIMS, m/z (rel. int., %): 418 [M^+] (1.2), 404 (1.1), 390 (1.3), 376 (2.0), 362 (2.0), 349 (2.1), 335 (3.6), 307 (3.6), 293 (2.0), 265 (1.9), 251(3.3), 237 (2.2), 233 (2.4), 210 (2.1), 196 (1.8), 182 (3.2), 168 (4.1), 154 (4.8), 136 (3.1), 136 (7.7), 124 (10.8), 122 (4.4), 110 (21.0), 96 (29.0), 71 (70.2), 57 (100).Anal. Found: C, 86.2, H, 13.8. Calcd for $C_{30}H_{58}$: C, 86.1, H, 13.9 %.

2.3.2 25-METHYL-DOTRIACONT-6, 20-DIENE-17-ONE: M^+ 474, $C_{33}H_{62}O$, (chloroform: methanol, 25gm), m.p. 240 ^0C, isolated from hexane: benzene fraction of hexane: benzene eluate of the column. TLC (hexane: ether: acetic acid 9:1:1 v/v). IR (KBr): 3020, 2928, 2855, 2709, 1627, 1466, 1410, 1215, 1019, 829 and 728 cm^{-1}, ^{1}H NMR (200 MHz, $CDCl_3$): δ 0.88(6H, t, 2x-CH_3), 5.34 (4H, m, 2x-

CH=CH), 2.29 (4H, t, 2x-CH_2, α to carbonyl group), 0.94 (3H, d, 2x- CH_3), 1.62 (1H, m,-CH_2-CH(CH_3)-CH_2-), 1.25 (44H, br s, 22CH_2)), EIMS, m/z (rel. int., %): 474 [M^+] (4.2), 460 (4.0), 446 (9.1), 432 (9.0), 418 (9.0), 405 (4.1), 404 (4.6), 390 (4.8), 389 (4.0), 375 (4.1), 359 (3.9), 319 (4.1), 291 (4.6), 265 (3.6), 258 (21.3), 216 (5.9), 183 (6.2), 182 (5.4), 172 (4.5), 165 (6.7), 153 (7.1), 141 (4.8), 139 (11.4), 137 (10.9), 125 (8.81), 123 (19.4), 109 (34.6), 95 (54.2), 70 (69.2), 56 (100).Anal. Found: C, 83.5, H, 13.1, O, 3.37. Calcd for $C_{33}H_{62}O$: C, 83.5, H, 13.0, O, 3.38 %.

2.3.3 UNDECYL HEXADECANOATE: M^+ 410, $C_{27}H_{54}O_2$, (chloroform: methanol, 25gm), m.p. 110 ^{0}C, isolated from benzene: ether fraction of hexane: benzene eluate of the column. TLC (benzene: methanol: acetic acid 8:2:1 v/v). IR (KBr): 2935, 2866, 1737, 1464, 1383, 1179, 1215, 1018, 835 and 720 cm-1, 1H NMR (200 MHz, CDCl3): δ 0.86 (6H, t, 2x-CH_3), 4.05 (2H, t, -CH_2-O-CO_2^-, J=8.0 Hz), 2.29 (2H, t, -CH_2-CO-O-, J=7.0 Hz), 1.50 (4H, br m, 2x-CH_2, β protons), 1.25 (40H, s, 20x-CH_2), EIMS, m/z (rel. int., %): 410 [M^+] (6.6), 397 (6.0), 383(6.2), 372 (4.6), 352 (5.6), 337 (4.5), 310 (4.4), 259 (37.9), 254 (73.2), 184 (11.6), 183 (6.8), 167 (6.6), 140 (15.4), 138 (9.8), 82 (40.2), 69 (100), 57 (77.9).Anal. Found: C, 79.1, H, 13.1, O, 7.8.Calcd for $C_{27}H_{54}O_2$: C, 79.0, H, 13.7, O, 7.8 %.

Alkaline hydrolysis[6] of 3 (3a) compound 3 (5mg) was refluxed with ethanolic KOH (2.5 ml, 5%) for 1 hr. at the end of reaction; the mixture was diluted with water (3.0 ml) and extracted with chloroform. The chloroform layer was dried over a hydro magnesium sulphate and concentrated. To separate both compounds it was put in deep freezer. After 4 days, some solid was separated out. After usual work –up it afforded an alcohol, identified as undecanol and an acid 3a respectively (IR: 1702 cm^{-1}).

2.3.4 STIGMASTEROL 4: M^+ 412, $C_{29}H_{48}O$, (chloroform: methanol, 24gm), m.p. 166-167 ^{0}C.[7]

2.3.5 B-SITOSTEROL 5: M^+ 414, $C_{29}H_{50}O$, (chloroform: methanol, 28gm), 138 ^{0}C.[8]

3. RESULTS AND DISCUSSION

3.1 COMPOUND 1: Triacont-3, 17-diene, m.p. 180 ^{0}C, M^+ 418, $C_{30}H_{58}$. IR showed absorption band at 760-720 cm^{-1} diagnostic[9-11]of $(CH_2)_n$ (where n is more then four) and at 1636cm^{-1} assignable to unsaturation in the molecule. The signal at δ 0.91 (t, 6H) in the ^{1}H NMR is assignable to the presence of 2 terminal –CH_3 groups while the triplet at δ 5.02 was assigned to olefinic protons. The methylene protons α to unsatuation appeared at δ 1.6 as broad peak. Rest of the methylene protons were resonated at δ 1.31 as a singlet. Mass spectrum showed [M^+] at m/z 418. In the mass spectrum separation of most of the peaks by 14 mass units and appearance of C_nH2_{n-1} ion series confirmed its long chain aliphatic nature. Abundant fragments at m/z 223, 363 formed by allylic cleavage indicated the position of double bond at

C-3 and C-17. On the basis of above evidences, compound 1 was assigned as triacont-3, 17-diene and being reported first time.

3.2 COMPOUND 2: 25-methyl-dotriacont-6, 20-diene-17-one, m.p. 240 ^{0}C, M^+ 474, $C_{33}H_{62}O$. The IR sprctrum showed the presence of unsaturation 1627cm^{-1} and long chain aliphatic nature of the molecule 758cm^{-1}. ^{1}H NMR spectrum showed a six proton triplet at δ 0.88 for the terminal methyl groups. A multiplet at δ 1.62 accounts for the methine proton .The olefinic proton resonated at δ 5.34 as multiplet. Rest of the methylene merged into a single peak at δ 1.24. The triplet at δ 2.29 was assigned to the methylenes attached to carbonyl group. Doublet at δ 0.94 was assigned to branched methyl protons. Mass spectrum showed the characteristic fragmentation pattern of long chain aliphatic compound. The fragment at m/z 319 was due to McLafferty rearrangement showed the presence of carbonyl group of the molecule. Major fragments were obtained at m/z 265, 319, 375, 446 indicated the position of carbonyl group and unsaturation. Thus compound 2 was characterized 25-methyl-dotriacont-6, 20-diene-17-one being first time reported.

3.3 COMPOUND 3: Undecyl hexadecanoate, m.p. 110 ^{0}C, M^+ 410, $C_{27}H_{54}O_2$. The IR sprctrum showed bands at 1179 and 720 cm^{-1} for aliphatic nature and at 1737 cm^{-1} for ester group. ^{1}H NMR spectrum showed a triplet at δ 0.86 (J=7.5Hz) for terminal methyl groups. Methylene protons of -CH_2-O-CO- and -CH_2-CO-O- moieties were resonated as triplets at δ 4.05 and δ 2.29 (J=7.0Hz) respectively. Methylene protons β to ester group were resonated at δ 1.50 as broad multiplet. Rest of the methylenes was resonated at δ 1.25 as singlet. Mass spectrum showed the characteristic fragmentation pattern of long chain aliphatic compound. The abundant peak at m/z 254 was due to the α-cleavage and loss of one hydrogen atom. The fragment at m/z 319 was due to McLafferty rearrangement showed the presence of ester group in the center of the molecule. Thus on the basis of above evidences, compound 3 was characterized as undecyl hexadecanoate and being first time reported by us.

3.4 COMPOUND 4: Stigmasterol, m.p. 166-167 ^{0}C, M^+ 412, $C_{29}H_{48}O$. Comparison of m.p., IR, ^{1}H NMR, ^{13}C NMR and Mass spectra of compound **4** with those reported in the literature, identified it as Stigmasterol.

3.5 COMPOUND 5: β-sitosterol, 138 ^{0}C, M^+ 414, $C_{29}H_{50}O$.Comparison of m.p., IR, ^{1}H NMR, ^{13}C NMR and Mass spectra of compound **5** with those reported in the literature, identified it as β-sitosterol.

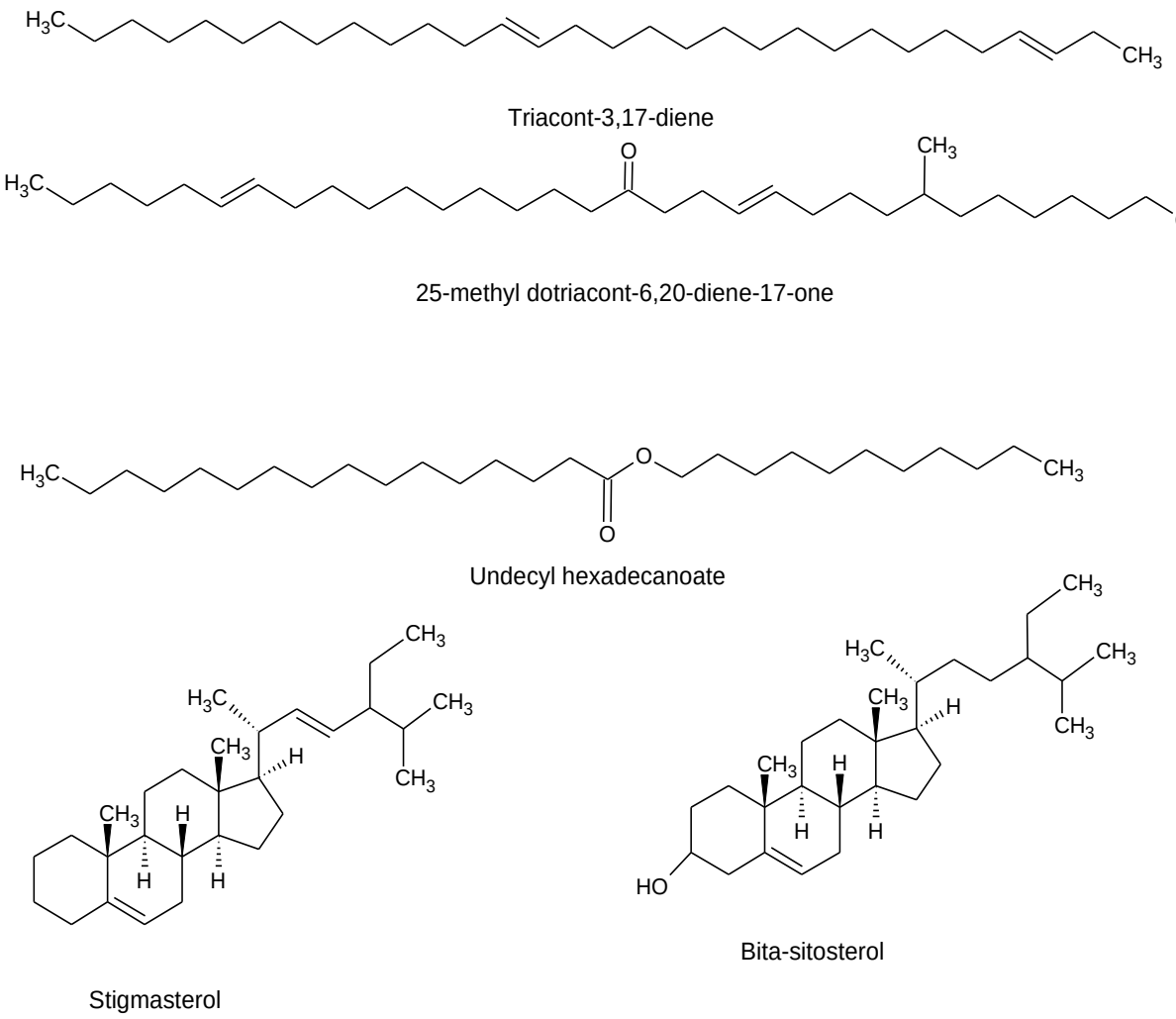

Fig. 1 Various New Aliphatic Compounds Compound

4. CONCLUSION

The phytochemical screening of acetone extract of *B. Monosperma* bark reveals the presence of new long chain aliphatic compounds and known stigma sterol and bita-sitosterol compounds. In the current work the acetone extract was subjected to column chromatography for isolation and 5 compounds were isolated. The chemical test reveals the presence of ester, further the structure of the compound was confirmed by spectral methods.

5. ACKNOWLEDGEMENT

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