

**CHEMICAL CONSTITUENTS FROM THE SEEDS OF *BUTEA MONOSPERMA* (LAM.)  
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**ABSTRACT**

*Butea monosperma* (Lam.) Taub. (family Fabaceae) is a small-sized, deciduous tree. Its seeds are used as an anthelmintic, antiparasitic, diuretic, purgative and to treat abdominal troubles, eye diseases, inflammation, piles, scorpion sting, skin diseases and tumours. Our study was planned to isolate chemical constituents from a methanolic extract of the seeds of this plant and to characterize their structures on the basis spectral data analysis. Phytochemical investigation of the seeds of *B. monosperma* led to isolate a long chain aliphatic constituent characterized as *n*-triacontane (**1**), fatty acid esters identified as *n*-propyl *n*-docos-11-enoate (*n*-propyl cetoleate, **2**), *n*-pentyl *n*-docos-11-enoate (*n*-pentyl cetoleate, **4**), tetradecan-1-oyl *n*-docos-11-enoate (myristyl cetoleate, **5**) and eicosanyl octadecenoate (arachidyl stearate, **6**), a new lactone compound viz., hexadecan-3(Z)-en-1,5-olide (**3**), and a new steroidal glycosidic ester formulated as stigmast-5-en-3 $\beta$ -ol-3 $\alpha$ -D-glucuronopyranosyl - (9Z,12Z)-octadeca-9,12-dienoate ( $\beta$ -sitosterol 3 $\alpha$ -D- glucuranosyl linoleate, **7**).

**KEYWORDS:** *Butea monosperma*, seeds, phytoconstituents, isolation, spectral data analysis, structure characterization.

**INTRODUCTION**

*Butea monosperma* (Lam.) Taub. (family Fabaceae), known as dhak, Bengal kino, palash, and Flame of the forest, is a native to tropical and sub-tropical Indian subcontinent, Cambodia, Laos, Indonesia, Malaysia, Sri Lanka, Thailand and Vietnam. It is a small-sized, deciduous tree, trunk crooked, branches irregular; bark rough, ash coloured; leaves are pinnate, petiole 8 – 16 cm long, with three leaflets; flowers bright orange-red, racemose; fruit is a pod.<sup>[1]</sup> Its flowers are aphrodisiac, astringent, depurative, diuretic, emmenagogue, expectorant and tonic, used to treat biliousness, diarrhoea, eye diseases, gout, gonorrhoea, inflammation, leprosy, leucorrhoea, difficult micturition, skin diseases, strangury, sun stroke and thirst sensation.<sup>[2,4]</sup> The seeds are anthelmintic, antiparasitic, diuretic and purgative, utilized to subside eye diseases, inflammation, piles, scorpion sting and skin diseases.<sup>[5]</sup> The seed oil, known as Moodsga oil, is efficacious to cure abdominal troubles, skin diseases and tumours.<sup>[4]</sup> The roots are beneficial to relieve night blindness, defected eyes, elephantiasis, impotency and as an antidote for snake bite. *Butea* gum has anthelmintic, anti-conceptive, anticonvulsive, antidiabetic, antidiarrheal, antiestrogenic, antifertility, antimicrobial, antistress, aphrodisiac, astringent, haemagglutinating, hepatoprotective, liver tonic and wound healing activities. It is prescribed to

cure coughs, diarrhoea, dysentery, bladder and stomach haemorrhage, inflammation, excessive perspiration, phthisis, piles, ringworm, stomatitis, thoracic diseases and ulcers.<sup>[2,5]</sup> The leaves are considered as an anthelmintic, aphrodisiac, appetizer, astringent, carminative, diuretic and tonic, recommended to relieve colds, colic, boils, eye diseases, inflammation, lumbago, irregular menstruation, piles, pimples, sore throat and worm infestations. Petiole juice is sucked to overcome colds, cough, diabetes and stomach disorders.<sup>[2,4,6,7,10]</sup> The stem bark is anthelmintic, aphrodisiac, appetiser, astringent, bitter tonic, blood purifier, digestive, emollient and laxative, useful to prevent biliousness, body swelling, bone fractures, catarrh, colds, cough, dysmenorrhea, dysentery, gonorrhoea, hydrocele, injury, liver disorders, piles, scorpion sting, ulcers and tumours.<sup>[2,4,7,10]</sup> The root bark is considered as an aphrodisiac, analgesic and anthelmintic; efficacious against dropsy, piles, tumours and ulcers.<sup>[8]</sup>

The palash flowers contained butrin, butein, butin, isobutrin, coreopsin, isocoreopsin, sulphurein (glycoside), monospermoside (butein 3- $\beta$ -D-glucoside) and isomonospermoside, chalcones, aurones, flavonoids (palasitrin, prunetin), sugars, amino acids and steroids.<sup>[9,14]</sup>

The pods yielded an imide.<sup>[15]</sup> The seeds afforded a fixed oil,  $\beta$ -sitosterol, fatty acids and palasonin.<sup>[16,17]</sup> The seed coats possessed allophanic acid derivatives.<sup>[18]</sup> The stems furnished stigmasterol, its beta-D-glucoside, nonacosanoic acid, 3- $\alpha$ -hydroxyeuph-25-ene and 2,14-dihydroxy-11,12-dimethyl-8-oxo-octadec-11-enylcyclohexane.<sup>[19]</sup> The gum and stem bark produced leucocynidin, tannins, mucilaginous material, pyrocatechin, kino-tannic acid, gallic acid, (-)-3-hydroxy-9-methoxypterocarpan [(-)-medicarpin], lupenone, lupeol,  $\beta$ -sitosterol, 5-methoxygenistein and prunetin.<sup>[20]</sup> The leaves produced undecanyl oleate.<sup>[21]</sup> The presence of herbal chemical constituents vary due to many factors such as geographic regions, soils, seasonal changes, plant species and application of fertilizers. Keeping in views the various therapeutic values and variation aspects of chemical constituents of the plants and development of ecofriendly, biodegradable and safer herbal preparations, it has been aimed to establish chemical structures of phytoconstituents isolated from the seeds of *Butea monosperma*.

## MATERIALS AND METHODS

The protocols of all methodologies (procedures, experimental designs and spectral data analysis) were adopted from the earlier published work.<sup>[21, 25, 26]</sup>

### Collection and authentication of plant materials

The seeds of *Butea monosperma* were collected from a wild plant in Ghaziabad (U.P.) region. The plant material was identified and authenticated by Prof. M. P. Sharma, Taxonomist, Department of Botany, Jamia Hamdard, New Delhi. A voucher specimen of the plant material was preserved in the herbarium of the Department of Pharmacognosy and Phytochemistry, Jamia Hamdard, New Delhi.

### Extraction and isolation

The seeds of *Butea monosperma* (1 kg) were dried in air, coarsely powdered and extracted exhaustively with methanol in a Soxhlet apparatus. The extract was concentrated under reduced pressure to get a dark brown mass, 123.6 g. The dried residue (100 g) was dissolved in minimum amount of methanol and adsorbed on silica gel column grade (60-120 mesh) to obtain a slurry. It was air-dried and chromatographed over silica gel columns loaded in petroleum ether (b. p. 60 – 80 °C). The column was eluted with petroleum ether, petroleum ether - chloroform (9:1, 3:1, 1:1, 1:3, v/v), chloroform and chloroform - methanol (99:1, 49:1, 19:1, 9:1, v/v). Various fractions were collected separately and matched by TLC to check homogeneity. Similar fractions having the same  $R_f$  values were combined and crystallized with solvents. The isolated compounds were recrystallized to get pure compounds.

### *n*-Triacontane (1)

Elution of the column with petroleum ether – chloroform (3:1) produced colourless crystals of **1**, recrystallized from chloroform – methanol (1: 1) mixture, 114 mg

yield, m. p. 64 – 67 °C; UV  $\lambda_{max}$  (MeOH): 211 nm; IR  $\nu_{max}$  (KBr): 2919, 2849, 1466, 1377, 724  $cm^{-1}$ ; <sup>1</sup>H NMR (CDCl<sub>3</sub>):  $\delta$  1.54 (2H, m, H<sub>2</sub>-15), 1.25 (54H, brs, 27  $\times$  CH<sub>2</sub>), 0.90 (3H, t, J = 6.3 Hz, Me-1), 0.85 (3H, t, J = 6.9 Hz, Me-30); <sup>13</sup>C NMR (CDCl<sub>3</sub>):  $\delta$  35.71 (C-2), 31.92 (C-2), 30.15 (C-3), 29.68 (24  $\times$  CH<sub>2</sub>), 27.16 (C-28), 22.69 (C-29), 14.12 (Me-1, Me-35); +ve FAB MS  $m/z$  (rel. int.): 422 [M]<sup>+</sup> (C<sub>30</sub>H<sub>62</sub>) (5.1).

### *n*-Propyl cetoleate (2)

Elution of the column with petroleum ether – chloroform (1:1, v/v) afforded a colourless mass of **2**, recrystallized from acetone-methanol (1:1, v/v), yield 123 mg,  $R_f$ : 0.56 (chloroform – methanol, 9:1, v/v); m. p. 44 - 45 °C; UV  $\lambda_{max}$  (MeOH): 217 nm (log  $\epsilon$  4.3); IR  $\nu_{max}$  (KBr): 2924, 2854, 1740, 1645, 1462, 1377, 1169, 1114, 721  $cm^{-1}$ ; <sup>1</sup>H NMR (CDCl<sub>3</sub>):  $\delta$  5.34 (1H, m, H-11), 5.26 (1H, m, H-12), 4.30 (2H, t, J = 8.4 Hz, H<sub>2</sub>-1'), 2.34 (2H, t, J = 7.1 Hz, H<sub>2</sub>-2), 2.01 (2H, m, H<sub>2</sub>-10), 1.63 (2H, m, H<sub>2</sub>-13), 1.59 (2H, m, H<sub>2</sub>-3), 1.25 (30H, brs, 15  $\times$  CH<sub>2</sub>), 0.87 (3H, t, J = 6.8 Hz, Me-22), 0.84 (3H, t, J = 6.2 Hz, Me-3'); <sup>13</sup>C NMR (CDCl<sub>3</sub>):  $\delta$  173.38 (C-1), 39.04 (C-2), 33.96 (C-3), 31.90 (C-4), 29.30 (C-5), 29.30 (C-6), 29.30 (C-7), 29.44 (C-8), 30.02 (C-9), 36.63 (C-10), 129.99 (C-11), 129.65 (C-12), 34.38 (C-13), 29.93 (C-14), 29.59 (C-15), 29.44 (C-16), 29.24 (C-17), 29.08 (C-18), 28.62 (C-19), 24.96 (C-20), 22.66 (C-21), 14.20 (C-22), 62.09 (C-1'), 29.68 (C-2'), 14.08 (C-3'); +ve FAB MS  $m/z$  (rel. int.): 381 [M+H]<sup>+</sup> (C<sub>25</sub>H<sub>49</sub>O<sub>2</sub>) (31.8), 337 (32.5).

### Hexadecan-3(Z)-en-1,5-olide (3)

Further elution of the column with petroleum ether – chloroform (1:1, v/v) yielded a colourless mass of **3**, recrystallized from acetone - methanol (1:1, v/v), yield 102 mg, m. p. 71 - 73 °C; UV  $\lambda_{max}$  (MeOH): 282 nm (log  $\epsilon$  4.8); IR  $\nu_{max}$  (KBr): 2919, 2849, 1733, 1628, 1455, 1374, 1168, 1101, 1017, 725  $cm^{-1}$ ; <sup>1</sup>H NMR (CDCl<sub>3</sub>):  $\delta$  6.48 (1H, dd, J = 6.8, 7.4 Hz, H-3), 6.16 (1H, m,  $w_{1/2}$  = 8.3 Hz, H-4), 4.34 (1H, d, J = 6.9 Hz, H<sub>2</sub>-5 $\alpha$ ), 4.28 (1H, d, J = 5.6 Hz, H<sub>2</sub>-5 $\beta$ ), 3.24 (1H, brm,  $w_{1/2}$  = 18.6 Hz, H-2 $\alpha$ ), 2.09 (2H, m, H<sub>2</sub>-6), 1.58 (4H, m, H<sub>2</sub>-7, H<sub>2</sub>-8), 1.35 (24H, brs, 12  $\times$  CH<sub>2</sub>), 1.31 (12H, brs, 6  $\times$  CH<sub>2</sub>), 0.91 (3H, t, J = 6.3 Hz, Me-26); <sup>13</sup>C NMR (CDCl<sub>3</sub>):  $\delta$  171.63 (C-1), 41.45 (C-2), 126.36 (C-3), 124.19 (C-4), 64.36 (C-5), 30.54 (19  $\times$  CH<sub>2</sub>), 25.73 (C-25), 19.68 (C-26); +ve FAB MS  $m/z$  (rel. int.): 392 [M]<sup>+</sup> (C<sub>26</sub>H<sub>48</sub>O<sub>2</sub>) (32.6).

### *N*-Pentyl cetoleate (4)

Further elution of the column with petroleum ether – chloroform (1:1, v/v) produced a colourless mass of **4**, recrystallized from chloroform-methanol (1:1, v/v), yield 98 mg,  $R_f$ : 0.56 (chloroform – methanol, 9:1, v/v); m. p. 69 - 71 °C; UV  $\lambda_{max}$  (MeOH): 212 nm (log  $\epsilon$  5.1); IR  $\nu_{max}$  (KBr): 2927, 2852, 1738, 1632, 1463, 1379, 1166, 1031, 723  $cm^{-1}$ ; <sup>1</sup>H NMR (CDCl<sub>3</sub>):  $\delta$  5.37 (1H, m, H-11), 5.32 (1H, m, H-12), 4.12 (2H, t, J = 7.2 Hz, H<sub>2</sub>-1'), 2.31 (2H, t, J = 7.1 Hz, H<sub>2</sub>-2), 2.05 (2H, m, H<sub>2</sub>-10), 2.01 (2H, m, H<sub>2</sub>-13), 1.66 (2H, m, H<sub>2</sub>-3), 1.62 (2H, m, H<sub>2</sub>-4), 1.30 (6H, m, H<sub>2</sub>-9, H<sub>2</sub>-14, H<sub>2</sub>-15), 1.25 (26H, brs, 13  $\times$  CH<sub>2</sub>), 0.88 (3H, t, J = 6.4 Hz, Me-22), 0.85 (3H, t, J =

6.2 Hz, Me-5');  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ ):  $\delta$  175.51 (C-1), 51.81 (C-2), 41.10 (C-3), 39.54 (C-4), 38.34 (C-5), 34.83 (C-6), 33.13 (C-7), 30.91 (C-8), 30.86 (C-9), 44.15 (C-10), 130.82 (C-11), 128.91 (C-12), 42.09 (C-13), 30.77 (C-14), 30.68 (C-15), 30.66 (C-16), 30.52 (C-17), 30.38 (C-18), 27.26 (C-19), 26.48 (C-20), 23.68 (C-21), 14.55 (C-22), 61.39 (C-1'), 32.72 (C-2'), 30.55 (C-3'), 30.41 (C-4'), 14.74 (C-5'); +ve FAB MS  $m/z$  (rel. int.): 409  $[\text{M}+\text{H}]^+$  ( $\text{C}_{27}\text{H}_{53}\text{O}_2$ ) (21.9), 337 (42.7).

#### **N-Tetradecanyl cetoleate (5)**

Elution of the column with chloroform furnished a colourless mass of **5**, recrystallized from chloroform-methanol (1:1, v/v), yield 121 mg,  $R_f$ : 0.17 (chloroform); m. p. 83 - 85 °C; UV  $\lambda_{\text{max}}$  (MeOH): 214 nm ( $\log \epsilon$  4.3); IR  $\nu_{\text{max}}$  (KBr): 2919, 2850, 1744, 1645, 1466, 1368, 1164, 807, 724  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ ):  $\delta$  5.35 (1H, m, H-11), 5.29 (1H, m, H-12), 4.23 (2H, t,  $J$  = 7.2 Hz,  $\text{H}_2$ -1'), 2.32 (2H, t,  $J$  = 7.1 Hz,  $\text{H}_2$ -2), 2.07 (2H, m,  $\text{H}_2$ -10), 2.03 (2H, m,  $\text{H}_2$ -13), 1.65 (2H, m,  $\text{H}_2$ -3), 1.61 (4H, m,  $\text{H}_2$ -4,  $\text{H}_2$ -5), 1.32 (8H, m,  $\text{H}_2$ -9,  $\text{H}_2$ -14,  $\text{H}_2$ -15,  $\text{H}_2$ -16), 1.25 (40H, brs, 20 x  $\text{CH}_2$ ), 0.89 (3H, t,  $J$  = 6.5 Hz, Me-22), 0.84 (3H, t,  $J$  = 6.1 Hz, Me-14');  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ ):  $\delta$  173.10 (C-1), 42.83 (C-2), 30.74 (C-3 to C-9), 33.41 (C-10), 133.65 (C-11), 131.52 (C-12), 33.41 (C-13), 30.74 (C-14 to C-17), 29.86 (C-18), 28.82 (C-19), 28.77 (C-20), 22.58 (C-21), 14.53 (C-22), 63.85 (C-1'), 32.78 (C-2'), 30.74 (C-3' to C-11'), 28.77 (C-12'), 22.61 (C-13'), 14.42 (C-14'); +ve FAB MS  $m/z$  (rel. int.): 535  $[\text{M}+\text{H}]^+$  ( $\text{C}_{36}\text{H}_{71}\text{O}_2$ ) (25.6), 337 (56.1).

#### **Arachidyl stearate (6)**

Further elution of the column with chloroform yielded a colourless amorphous powder of **6**, yield 153 mg, recrystallized from chloroform-methanol (1:1), m. p. 88 - 91 °C; UV  $\lambda_{\text{max}}$  (MeOH): 211 nm ( $\log \epsilon$  3.3); IR  $\nu_{\text{max}}$  (KBr): 2919, 2849, 1734, 1466, 1261, 1173, 1105, 1024, 802, 724  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ ):  $\delta$  4.08 (2H, t,  $J$  = 6.6 Hz,  $\text{H}_2$ -1'), 2.21 (2H, t,  $J$  = 7.5 Hz,  $\text{H}_2$ -2), 1.58 (2H, m,  $\text{H}_2$ -3), 1.35 (2H, brs,  $\text{H}_2$ -2'), 1.27 (44H, brs, 22 x  $\text{CH}_2$ ), 1.25 (18H, brs, 9 x  $\text{CH}_2$ ), 0.93 (3H, t,  $J$  = 6.2 Hz, Me-18), 0.89 (3H, t,  $J$  = 6.5 Hz, Me-20');  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ ):  $\delta$  171.12 (C-1), 34.89 (C-2), 32.71 (C-3), 30.61 (C-4), 30.11 (C-5 to C-13), (C-14), 29.61 (C-15), 27.06 (C-16), 25.82 (C-17), 19.62 (C-18), 64.76 (C-1'), 30.11 (C-2' to C-16'), 28.09 (C-17'), 26.74 (C-18'), 23.48 (C-19'), 14.73 (C-20'); +ve FAB MS  $m/z$  (rel. int.): 564  $[\text{M}]^+$  ( $\text{C}_{38}\text{H}_{76}\text{O}_2$ ) (11.6), 281 (77.6), 267 (16.5).

#### **$\beta$ -Sitosterol glucuranosyl linoleate (7)**

Elution of the column with chloroform-methanol (9:1) yielded colourless powder of **7**, recrystallized from chloroform - methanol (1:1), 119 mg,  $R_f$  0.42 (chloroform - ethyl acetate, 9:1), m. p. 125 - 127 °C, UV  $\lambda_{\text{max}}$  (MeOH): 225 nm ( $\log \epsilon$  4.8); IR  $\nu_{\text{max}}$  (KBr): 3490, 3310, 31065, 2915, 2853, 1741, 1711, 1621, 1463, 1415, 1377, 1241, 1166, 1118, 1036, 943, 722  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR ( $\text{DMSO}-d_6$ ):  $\delta$  5.38 (1H, m, H-6), 3.85 (1H, brm,  $w_{1/2}$  = 18.5 Hz, H-3 $\alpha$ ), 2.33 (1H, m,  $\text{H}_2$ -2 $\alpha$ ), 2.30 (1H, m,  $\text{H}_2$ -2 $\alpha$ ), 2.28 (1H, m,  $\text{H}_2$ -4 $\alpha$ ), 2.25 (1H, m,  $\text{H}_2$ -7 $\alpha$ ), 2.08 (1H,

m,  $\text{H}_2$ -7 $\alpha$ ), 2.04 (1H, m,  $\text{H}_2$ -4 $\alpha$ ), 2.02 - 1.23 (23H, m, 8 x  $\text{CH}_2$ , 7 x CH), 1.02 (3H, brs, Me-19), 0.94 (3H, d,  $J$ =6.2 Hz, Me-21), 0.84 (3H, d,  $J$ =6.4 Hz, Me-26), 0.82 (3H, d,  $J$ =6.1 Hz, Me-27), 0.79 (3H, d,  $J$ =5.6 Hz, Me-29), 0.68 (3H, brs, Me-18), 5.25 (1H, d,  $J$ = 6.0 Hz, H-1' $\alpha$ ), 4.29 (1H, d,  $J$  = 4.2 Hz, H-5'), 4.15 (1H, dd,  $J$  = 6.0, 5.6 Hz, H-2'), 4.12 (1H, dd,  $J$  = 7.2, 4.2 Hz, H-4'), 3.66 (1H, m, H-3'), 5.35 (1H, m, H-9''), 5.32 (1H, m, H-10''), 5.30 (1H, m, H-12''), 5.28 (1H, m, H-13''), 2.82 (2H, m,  $\text{H}_2$ -11''), 2.76 (2H, m,  $\text{H}_2$ -2''), 2.35 (2H, m,  $\text{H}_2$ -8''), 2.31 (2H, m,  $\text{H}_2$ -14''), 1.62 (2H, m,  $\text{H}_2$ -3''), 1.25 (8H, brs,  $\text{H}_2$ -4'',  $\text{H}_2$ -5'',  $\text{H}_2$ -15'',  $\text{H}_2$ -16''), 1.20 (6H, m,  $\text{H}_2$ -6'',  $\text{H}_2$ -7'',  $\text{H}_2$ -17''), 0.84 (3H, t,  $J$  = 6.1 Hz, Me-18'');  $^{13}\text{C}$  NMR ( $\text{DMSO}-d_6$ ):  $\delta$  38.86 (C-1), 30.73 (C-2), 71.32 (C-3), 41.47 (C-4), 141.36 (C-5), 122.46 (C-6), 33.35 (C-7), 32.93 (C-8), 49.50 (C-9), 36.38 (C-10), 23.77 (C-11), 39.71 (C-12), 44.87 (C-13), 55.76 (C-14), 24.57 (C-15), 28.49 (C-16), 55.09 (C-17), 12.94 (C-18), 20.36 (C-19), 37.85 (C-20), 18.73 (C-21), 34.63 (C-22), 26.06 (C-23), 46.52 (C-24), 29.21 (C-25), 21.46 (C-26), 20.03 (C-27), 25.34 (C-28), 11.89 (C-29), 101.53 (C-1'), 69.83 (C-2'), 62.17 (C-3'), 67.99 (C-4'), 79.81 (C-5'), 177.53 (C-6'), 174.10 (C-1''), 48.61 (C-2''), 30.92 (C-3''), 39.95 (C-4''), 30.83 (C-5''), 36.76 (C-6''), 30.72 (C-7''), 30.68 (C-8''), 132.89 (C-9''), 131.08 (C-10''), 52.20 (C-11''), 129.38 (C-12''), 128.42 (C-13''), 30.63 (C-14''), 30.59 (C-15''), 30.51 (C-16''), 28.45 (C-17''), 14.93 (C-18''); +ve FAB ESI MS  $m/z$  (rel. Int.): 852  $[\text{M}]^+$  ( $\text{C}_{53}\text{H}_{88}\text{O}_8$ ) (1.3), 439 (8.3), 413 (41.7), 263 (11.6).

## **RESULTS AND DISCUSSION**

Compound **1** was a long chain aliphatic constituent characterized as *n*-triacontane.<sup>[22, 23]</sup>

Compound **2** showed IR absorption bands for an ester group (1740  $\text{cm}^{-1}$ ), unsaturation (1645  $\text{cm}^{-1}$ ) and long aliphatic chain (721  $\text{cm}^{-1}$ ). Its mass spectrum exhibited a molecular ion peak at  $m/z$  381  $[\text{M}+\text{H}]^+$  consistent with the molecular formula of a fatty acid ester,  $\text{C}_{25}\text{H}_{49}\text{O}_2$ . An important ion peak generated due to removal of propyl group at  $m/z$  337  $[\text{C}_1 - \text{O}$  fission,  $\text{CH}_3(\text{CH}_2)_9\text{-CH}=\text{CH}(\text{CH}_2)_9\text{-COO}]^+$  indicated that cetoleic acid was esterified with *n*-propyl alcohol. The  $^1\text{H}$  NMR spectrum of **2** displayed two one-proton deshielded multiplets at  $\delta$  5.34 and 5.26 assigned to vinylic H-11 and H-12 protons, respectively. Two two-proton triplets at  $\delta$  4.30 ( $J$  = 8.4 Hz) and 2.34 ( $J$  = 7.1 Hz) were ascribed correspondingly to oxymethylene  $\text{H}_2$ -1' and methylene  $\text{H}_2$ -2' protons adjacent to the ester function. The remaining methylene protons appeared as two-proton multiplets at  $\delta$  2.34, 2.01, 1.63 and 1.59 and as a broad singlet at  $\delta$  1.25 (30H). Two three-proton triplets at  $\delta$  0.87 ( $J$  = 6.8 Hz) and 0.84 ( $J$  = 6.2 Hz) were accounted to C-22 and C-3' primary methyl protons, respectively. The  $^{13}\text{C}$  NMR spectrum of **2** showed signals for the ester carbon at  $\delta$  173.38 (C-1), vinylic carbons at  $\delta$  129.99 (C-11) and 129.65 (C-12), oxymethylene carbon at  $\delta$  62.09 (C-1'), other methylene carbons between  $\delta$  39.04 - 22.66 and methyl carbons at  $\delta$  14.20 (C-22) and 14.08 (C-3'). On the basis of these spectral data analysis, the structure of **2**

has been elucidated as *n*-propyl *n*-docos-11-enoate (*n*-propyl cetoleate), a new fatty acid ester (Fig. 1).

Compound **3** had IR absorption bands for a lactone group ( $1733\text{ cm}^{-1}$ ), unsaturation ( $1628\text{ cm}^{-1}$ ) and long aliphatic chain ( $725\text{ cm}^{-1}$ ). Its mass spectrum exhibited a molecular ion peak at  $m/z$  392  $[M]^+$  relating to a molecular formula of a long chain containing lactone,  $C_{26}H_{48}O_2$ . The  $^1H$  NMR spectrum of **3** showed a one-proton deshielded double doublet at  $\delta$  6.48 ( $J = 6.8, 7.4$  Hz, H-3) and a one-proton multiplet at  $\delta$  6.16 with half-width of 8.3 Hz assigned to *cis* (Z)- oriented vinylic H-3 and H-4 protons, respectively. Two one-proton doublets at  $\delta$  4.34 ( $J = 6.9$  Hz) and 4.28 ( $J = 5.6$  Hz) were accounted to oxymethylene H<sub>2</sub>-5 protons. A one-proton multiplet at  $\delta$  3.24 ( $w_{1/2} = 18.6$  Hz) was ascribed to  $\alpha$ -oriented methine H-2 proton. Two multiplets at  $\delta$  2.09 (2H) and 1.58 (4H) and two broad singlets at  $\delta$  1.35 (24H) and 1.31 (12H) were associated with the methylene H<sub>2</sub>-6 to H<sub>2</sub>-25 protons. A three-proton triplet at  $\delta$  0.91 ( $J = 6.3$  Hz) was attributed to C-26 primary methyl protons. The  $^{13}C$  NMR spectrum of **3** showed signals for the lactone carbon at  $\delta$  171.63 (C-1), vinylic carbons at  $\delta$  126.36 (C-3) and 124.19 (C-4), oxymethylene carbon at  $\delta$  64.36 (C-5), methine carbon at  $\delta$  41.45 (C-2), methylene carbons at  $\delta$  30.54 (19 x CH<sub>2</sub>) and 25.73 (C-25) and methyl carbon at  $\delta$  19.68 (C-26). On the basis of these spectral data evidences, the structure of **3** has been established as hexadecan-3(Z)-en-1,5-olide, a new lactone compound (Fig. 1).

Compound **4** was a homologous compound of **2** and showed IR absorption bands for an ester group ( $1738\text{ cm}^{-1}$ ), unsaturation ( $1632\text{ cm}^{-1}$ ) and long aliphatic chain ( $723\text{ cm}^{-1}$ ). Its mass spectrum exhibited a molecular ion peak at  $m/z$  409  $[M+H]^+$  consistent with the molecular formula of a fatty acid ester,  $C_{27}H_{53}O_2$ . A prominent ion peak formed due to removal of pentyl group at  $m/z$  337  $[C_{1'} - O$  fission,  $CH_3(CH_2)_9-CH=CH-(CH_2)_9-COO]^+$  suggested that cetoleic acid was esterified with *n*-pentyl alcohol. The  $^1H$  NMR spectrum of **4** exhibited two one-proton downfield multiplets at  $\delta$  5.37 and 5.32 assigned to vinylic H-11 and H-12 protons, respectively. Two two-proton triplets at  $\delta$  4.12 ( $J = 7.2$  Hz) and 2.31 ( $J = 7.1$  Hz) were ascribed correspondingly to oxymethylene H<sub>2</sub>-1' and methylene H<sub>2</sub>-2 protons nearby to the ester function. The remaining methylene protons appeared as multiplets from  $\delta$  2.05 to 1.30 and as a broad singlet at  $\delta$  1.25 (26H). Two three-proton triplets at  $\delta$  0.88 ( $J = 6.4$  Hz) and 0.85 ( $J = 6.2$  Hz) were attributed to primary C-22 and C-5' methyl protons, respectively. The  $^{13}C$  NMR spectrum of **4** showed signals for the ester carbon at  $\delta$  175.51 (C-1), vinylic carbons at  $\delta$  130.82 (C-11) and 128.91 (C-12), oxymethylene carbon at  $\delta$  61.39 (C-1'), other methylene carbons between  $\delta$  51.81 – 23.68 and methyl carbons at  $\delta$  14.55 (C-22) and 14.74 (C-5'). On the basis of the afore-mentioned evidences, the structure of **4** has been elucidated as *n*-pentyl *n*-docos-11-enoate (*n*-pentyl cetoleate), a new fatty acid ester (Fig. 1).

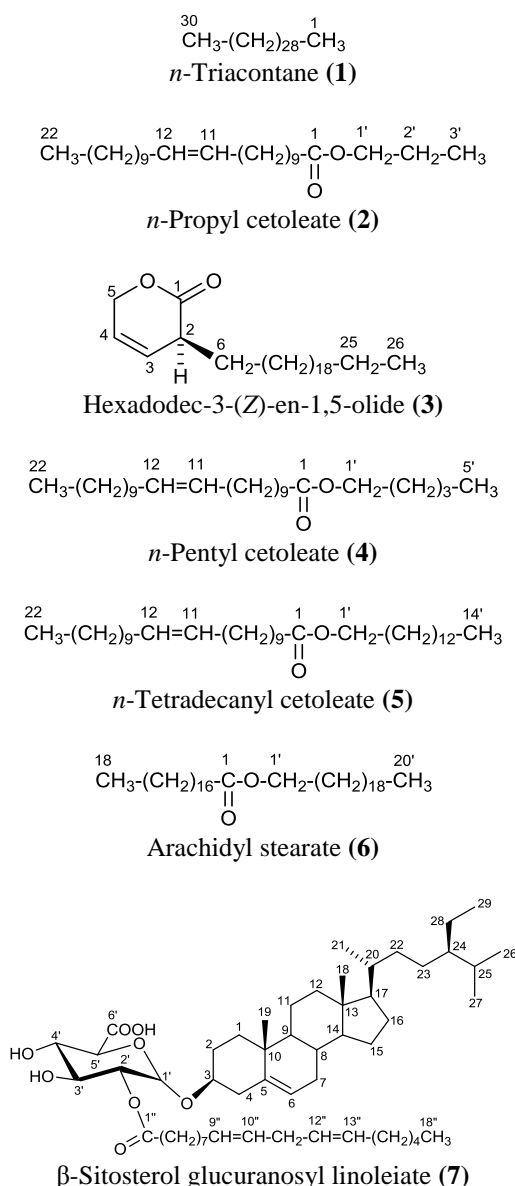
Compound **5** exhibited IR absorption bands for an ester group ( $1744\text{ cm}^{-1}$ ), unsaturation ( $1645\text{ cm}^{-1}$ ) and long aliphatic chain ( $724\text{ cm}^{-1}$ ). Its mass spectrum showed a molecular ion peak at  $m/z$  535  $[M+H]^+$  relating to a molecular formula of a fatty acid ester,  $C_{36}H_{71}O_2$ . A prominent ion peak formed due to removal of tetradecanyl group at  $m/z$  337  $[C_{1'} - O$  fission,  $CH_3(CH_2)_9-CH=CH-(CH_2)_9-COO]^+$  suggested that cetoleic acid was esterified with tetradecan-1-ol (myristyl alcohol). The  $^1H$  NMR spectrum of **5** exhibited two one-proton deshielded multiplets at  $\delta$  5.35 and 5.29 assigned to vinylic H-11 and H-12 protons, respectively. Two two-proton triplets at  $\delta$  4.23 ( $J = 7.2$  Hz) and 2.32 ( $J = 7.1$  Hz) were attributed correspondingly to oxymethylene H<sub>2</sub>-1' and methylene H<sub>2</sub>-2 protons adjacent to the ester function. The remaining methylene protons appeared as multiplets from  $\delta$  2.07 to 1.32 and as a broad singlet at  $\delta$  1.25 (40H). Two three-proton triplets at  $\delta$  0.89 ( $J = 6.5$  Hz) and 0.85 ( $J = 6.2$  Hz) were attributed to primary C-22 and C-14' methyl protons, respectively. The  $^{13}C$  NMR spectrum of **5** displayed signals for the ester carbon at  $\delta$  173.10 (C-1), vinylic carbons at  $\delta$  133.65 (C-11) and 131.52 (C-12), oxymethylene carbon at  $\delta$  63.85 (C-1'), other methylene carbons between  $\delta$  42.83 – 22.58 and methyl carbons at  $\delta$  14.53 (C-22) and 14.42 (C-14'). On the basis of above discussion the structure of **5** has been characterized as tetradecan-1-oyl *n*-docos-11-enoate (myristyl cetoleate), a new fatty acid ester (Fig. 1).

Compound **6** was a known fatty acid ester characterized as eicosanyl octadecenoate (eicosanyl stearate, arachidyl stearate, Fig. 1).<sup>[24]</sup>

Compound **7**, named  $\beta$ -sitosterol glucuranosyl linoleate, gave positive tests of glycosides and showed characteristics IR absorption bands for hydroxyl groups ( $3490, 3310\text{ cm}^{-1}$ ), ester function ( $1741\text{ cm}^{-1}$ ), carboxylic group ( $3106, 1711\text{ cm}^{-1}$ ), unsaturation ( $1621\text{ cm}^{-1}$ ) and a long aliphatic chain ( $722\text{ cm}^{-1}$ ). On the basis of mass and  $^{13}C$  NMR spectra, the molecular ion peak of **7** was determined at  $m/z$  852 corresponding to the molecular formula of a steroidal glycosidic ester,  $C_{53}H_{88}O_8$ . A prominent ion fragment produced at  $m/z$  413  $[C_{1'} - O$  fission,  $C_{29}H_{49}O]^+$  supported the presence of the steroidal unit attached to the sugar moiety. An ion fragment arising at  $m/z$  263  $[C_{1''} - O$  fission,  $CH_3-(CH_2)_4-CH=CH-CH_2-CH=CH-(CH_2)_7-CO]^+$  indicated that linoleic acid was esterified with the glycosidic unit linked with the steroidal unit. The  $^1H$  NMR spectrum of **7** showed five one-proton multiplets at  $\delta$  5.38, 5.35, 5.32, 5.30 and 5.28 assigned to vinylic H-6, H-9'', H-10'', H-12'' and H-13'' protons, respectively. A one-proton broad multiplet at  $\delta$  3.85 with half-width of 18.5 Hz was attributed to oxygenated  $\alpha$ -oriented H-3 methine proton. Two three-proton singlets at  $\delta$  1.02 and 0.68, and four three-proton doublets at 0.94 ( $J=6.2$  Hz), 0.84 ( $J=6.4$  Hz), 0.82 ( $J=6.1$  Hz) and 0.79 ( $J=5.6$  Hz) were associated with the tertiary C-19 and C-18, secondary C-21, C-26 and C-27 and primary C-29 methyl protons, respectively. A one-

proton doublet at  $\delta$  5.25 ( $J=6.0$  Hz) was ascribed to  $\beta$ -oriented anomeric H-1' proton. Four one-proton signals as a doublet at  $\delta$  4.29 ( $J = 4.2$  Hz), as double doublets at  $\delta$  4.15 ( $J = 6.0, 5.6$  Hz) and 4.12 ( $J = 7.2, 4.2$  Hz) and as a multiplet at  $\delta$  3.66 were ascribed correspondingly to sugar oxymethine H-5', H-2', H-4', and H-3' protons. A three-proton triplet at  $\delta$  0.84 ( $J = 6.1$  Hz) was accommodated to primary C-18'' methyl protons. The remaining methine and methylene protons resonated from  $\delta$  2.82 to 1.20. The appearance of the sugar C-2' proton in the deshielded region at  $\delta$  4.15 suggested the attachment of the ester group at C-2' carbon of the sugar unit. The  $^{13}\text{C}$  NMR spectrum of **7** showed important signals for steroidal vinylic carbons at  $\delta$  141.36 (C-5) and 122.46 (C-6), oxymethine carbon at  $\delta$  71.32 (C-3), methyl carbons at  $\delta$  12.94 (C-18), 20.36 (C-19), 18.73 (C-21), 21.46 (C-26) and 11.89 (C-29), sugar anomeric carbon at  $\delta$  101.53 (C-1'), carboxylic carbon at  $\delta$  177.53

(C-6') and other sugar carbons from  $\delta$  79.81 to 62.17, and acyl signals for the ester carbon at  $\delta$  174.10 (C-1''), vinylic carbons at  $\delta$  132.89 (C-9''), 131.08 (C-10''), 129.38 (C-12'') and 128.42 (C-13'') and methyl carbon at  $\delta$  14.93 (C-18''). The  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectral data of the steroidal nucleus were compared with other stigmastene-type molecules.<sup>[25,26]</sup> Acid hydrolysis of **7** yielded  $\beta$ -sitosterol, m. p. 136 – 138 °, D-glucuronic acid, m. p. 159 – 161 °C,  $[\alpha]_D^{25} 35 - 37^\circ$ , conc. 6 % w/v in water,  $R_f = 0.26$  (*n*-butanol – pyridine – water, 6: 4: 3, v/v) and linoleic acid,  $R_f = 0.48$  (glacial acetic acid, 85 %). On the basis of spectral data analysis and chemical reactions, the structure of **7** has been formulated as stigmast-5-en-3 $\beta$ -ol-3 $\alpha$ -D-glucuronopyranosyl - (9*Z*,12*Z*)-octadeca-9,12-dienoate ( $\beta$ -sitosterol 3 $\alpha$ -D-glucuronosyl linoleate), a new steroidal glycosidic ester (Fig. 1).



**Fig. 1: Chemical constituents 1 to 7 isolated from the leaves of *Butea monosperma* (Lam.) Taub.**

## CONCLUSION

Phytochemical investigation of the seeds of *B. monosperma* led to isolate a long chain aliphatic

constituent characterized as *n*-triacontane (**1**), fatty acid esters identified as *n*-propyl *n*-docos-11-enoate (*n*-propyl cetoleate, **2**), *n*-pentyl *n*-docos-11-enoate (*n*-pentyl cetoleate, **4**), tetradecan-1-oyl *n*-docos-11-enoate (myristyl cetoleate, **5**), eicosanyl octadecenoate (arachidyl stearate, **6**), a new lactone compound viz., hexadecan-3(Z)-en-1,5-olide (**3**), and a new steroidal glycosidic ester formulated as stigmast-5-en-3 $\beta$ -ol-3 $\alpha$ -D-glucuronopyranosyl - (9Z,12Z)-octadeca-9,12-dienoate ( $\beta$ -sitosterol 3 $\alpha$ -D-glucuronosyl linoleate, **7**). This work has enhanced understanding about the chemical constituents of the undertaken plants. Further research is recommended to screen bioactivities of the isolated phytoconstituents with a view for supplementing conventional drug development especially in developing countries.

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