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Phytochemical investigation of the roots of *Jatropha curcas*L.

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ORIGINAL RESEARCH ARTICLE

ABSTRACT

Background: *Jatropha curcas* L. (Euphorbiaceae), is grown in tropical and subtropical regions of the world mainly in Africa, Asia and Pacific region. The plant is used to treat allergies, burns, cuts, cough, diabetes, diarrhoea, gum diseases, herpes, leucoderma, skin diseases, paralysis, piles, splenomegaly, toothache, tumours, ulcers, whitlow, warts and syphilis. Our study was planned to isolate chemical constituents from the rhizomes of *C. rotundus* and to characterize their structures.

Material and methods: The air-dried root powder was exhaustively extracted with methanol and the concentrated extract was adsorbed on silica gel (60-120 mesh) for the preparation of slurry. The dried slurry was chromatographed over silica gel column packed in petroleum ether. The column was eluted with petroleum ether, chloroform and methanol, successively, in order of increasing polarity to isolate the compounds.

Results: Phytochemical investigation of the roots led to isolate 2-hydroxybenzyl *n*-octanoate (salicyl caprylate, 1), 2-hydroxybenzyl *n*-dodecanoate (salicyl laurate, 2), benzyl *n*-tetradecanoate (benzyl myristate, 3), *n*-butanoyl-β-D-glucopyranoside (4), 2β-D-galactopyranosyloxybenzyl *n*-hexanoate (2β-D-galactosyloxybenzyl caproate, 5), 2β-D-glucopyranosyloxybenzyl *n*-octanoate (2β-D-glucopyranosyloxybenzyl caprylate, 6) and *n*-caproyl O-β-D-glucopyranosyl-(2'→1'')-O-β-D-glucopyranoside (*n*-caproyl diglucoside, 7). The structures of these compounds have been established on the basis of spectral data analysis and chemical means.

Conclusion: The roots of *J. curcas* possessed three aromatic esters, their glycosides and acyl glucosides.

Keywords: *Jatropha curcas* L., Roots, Chemical constituents, Isolation, Characterization.

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INTRODUCTION

Jatropha curcas L., syn. *J. afrocurcas* Pax, *J. edulis* Sessé, *Curcas indica* A. Rich. (Euphorbiaceae), known as jamalgota, Barbados nut, chander-jyoti, physic nut and jatropa, is a native to Central America and Mexico and grown in tropical and subtropical regions of the world mainly in Africa, Asia and Pacific region. It occurs as a multipurpose and drought resistant, perennial, 2-5 m tall shrub, with watery latex; bark smooth; branches glaucous-gray, glabrous, sparsely lenticellate; capsules globose, yellow; seeds ellipsoidal and black (Jones and Miller,

1992; Uche and Aprioku, 2008). The entire plant is used as an abortifacient, analgesic, anti-inflammatory, laxative, styptic and to treat allergies, burns, cuts, cough, diabetes, diarrhea, dropsy, gum diseases, herpes, leucoderma, skin ailments like eczema, ringworm and scabies, paralysis, piles, rheumatism, sores, splenomegaly, toothache, tumors, ulcers, venereal diseases, whitlow, warts, wounds and syphilis. The young twigs are edible; the mature twigs are used to clean the teeth and to cure joint pain, toothache, gum inflammation and pyorrhoea. The leaves are anticonvulsant, antidiarrhoeal, febrifuge, hemostatic and lactagogue, utilized to alleviate anemia,

asthma, cough, edema, epilepsy, dysentery, fever, flu, headache, jaundice, toothache and urinary tract infection (Jones and Miller, 1992; Najda et al., 2013). The bark is beneficial to subside itches, eczema, leprosy and ulcers (Quattrocchi, 2012). The seed oil is applied externally to treat dropsy, cancer, paralysis, piles, rheumatism, sciatica, skin diseases and snakes bites (Okujagu et al., 2006). The oil burns with clear smoke free flame, tested successfully as a fuel for simple diesel engines (Islam et al., 2011). In Ayurveda, the seeds are considered as an antimalarial, anthelmintic, antiseptic, cathartic and highly toxic. The seed by-products are used as cakes in organic fertilizers; the oil possesses insecticidal properties (Gübitz et al., 1999; Openshaw, 2000). The stem bark is a fish poison and applied to heal wounds of animal bites; root bark is used to cure sores (Laxane et al., 2013). The latex is styptic and vulnerary, effective to relieve asthma, burns, cuts, dysentery, earache, rheumatism, scabies, mouth sores, sprains, ulcers and wounds (Quattrocchi, 2012). The roots are used as an abortifacient, anthelmintic, anticonvulsant, antihypertensive, anti-inflammatory, febrifuge and for treating chest and kidney diseases, dysentery, eczema, malaria, joint pain, rheumatism, jaundice and sore throat (Okujagu et al., 2006; Quattrocchi, 2012).

The seeds contained curcin, arabinose, 12-deoxy- 16-hydroxyphorbol derivatives, dulcitol, steroids, raffinose and stachyose (Oskoueian et al., 2011; Tongpoothorn et al., 2012; Yao et al., 2012; Nzikou et al., 2009). The latex possessed curcacyclines and a cyclic octapeptide curcain (Van den Berg et al., 1995). The roots yielded β -sitosterol and its D-glucoside, marmesin, propacin, the curculathyrans A and B and the curcusones A–D, jatrophol and jatropholone A and B, tomentin, Jatrophin and taraxerol (Kong et al., 1996). The leaves gave α -amyrin, isovitexin, N-1-triacontanol, steroids, complex of 5-hydroxyl- pyrrolidin-2-one and pyrimidine-2,4-dione, campesterol, stigmasterol, β -sitosterol, apigenin, vitexin and isovitexin. The plant yielded tetradecyl-(E)-ferulate, 3-O- (Z)-coumaroyl oleanolic acid, heudelotone, epiisojatro -grossidiones, 2-methoxyanthraquinone, curcusones, coumaric acids, p-hydroxybenzoic acid, protocatechuic acid, resorsilic acid, saponins and tannins (Najda et al, 2013; Ribeiro et al., 2012). The bark and plant parts possessed β -amyrin, tannins and taraxasterol (Igbinosa et al., 2011; Khafagy et al., 1977; Hufford and Oguntimein, 1987; Ravindranath et al., 2004; Adebawale and Adedire, 2006; Namuli, 2011; Sachdeva et al., 2011; Zhang et al., 2012; Saosoong and Ruangviriyachai, 2016). This manuscript describes isolation and characterization of aromatic esters, their glycosides and acyl glucoside from the roots of *J. curcas*.

MATERIAL AND METHODS

General procedures

Melting points were determined on a Perfit melting apparatus (Ambala, Haryana, India) and are uncorrected. UV spectra were measured with a Lambda Bio 20 spectrophotometer (Perkin Elmer-Rotkreuz, Switzerland) in methanol. Infrared spectra were recorded on Bio-Rad FTIR 5000 spectrophotometer (FTS 135, Kawloon, and Hong Hong) using KBr pellets; γ_{\max} values are given in cm^{-1} . The ^1H and ^{13}C NMR spectra were screened on Advance DRX Bruker spectrospro 400 and 100 MHz, respectively, instruments (Karlsruhe, Germany) using CDCl_3 or DMSO-d_6 as a solvent and TMS as an internal standard. Mass spectra were scanned by effecting ionization at 70 eV on a JEOL-JMS-DX 303 spectrometer (Japan) equipped with direct inlet probe system. Column chromatography was performed on silica gel (60-120 mesh; Qualigen, Mumbai, India). TLC was run on silica gel G (Qualigen). Spots were visualized by exposing to iodine vapours, UV radiation and spraying with ceric sulphate solution.

Plant material

The roots of *J. curcas* were collected from Sonapat, Haryana and identified by Dr. H. B. Singh, Head, Raw Materials Herbarium and Museum, NISCAIR, New Delhi under voucher specimen No. NISCAIR/RHMD/11-12/1887/187. A voucher specimen has been retained in the Department of Pharmaceutical Sciences, G J University of Science and Technology, Hissar, Haryana.

Preparation of extract

The dried roots (1.0 kg) were coarsely powdered and exhaustively extracted in a Soxhlet apparatus with methanol. The methanolic extract was concentrated under reduced pressure to yield a dark brown viscous mass (11.8 g). A small portion of the extract was analyzed chemically to determine the presence of different chemical constituents.

Isolation of phytoconstituents

The viscous dark brown extract (150 g) was dissolved in small quantity of methanol and adsorbed onto silica gel (60 - 120 mesh) for preparation of a slurry. The slurry was air dried and subjected to chromatography over silica gel column packed in petroleum ether. The column was eluted successively with petroleum ether, mixture of petroleum ether - chloroform (9:1, 3:1, 1:1, 1:3), chloroform and the mixture of chloroform - methanol (99:1, 97:3, 95:5, 92:8, 9:1, 3:1, 1:1, 1:3). Various fractions were collected separately and matched by TLC to check the homogeneity. Similar fractions having the same R_f values were combined and crystallized. The isolated

compounds were recrystallized to get the following compounds:

Salicyl caprylate (1)

Elution of the column with chloroform - methanol (9:1) gave yellow crystals of **1**, 181 mg (0.24 % yield), R_f : 0.46 (chloroform - methanol, 9 : 1), m. p. 125-126°C; IR ν_{max} (KBr): 3425, 2918, 2842, 1725, 1630, 1525, 1465, 1380, 1235, 1180, 1075, 985 cm^{-1} ; 1H NMR ($CDCl_3$): δ 7.33 (1H, m, H-3), 7.08 (1H, m, H-6), 6.82 (1H, m, H-5), 6.72 (1H, m, H-4), 4.08 (2H, brs, H_2 -7), 2.45 (2H, t, $J = 7.2$ Hz, H_2 -2'), 1.51 (2H, m, CH_2), 1.24 (8H, brs, $4 \times CH_2$), 0.88 (3H, t, $J = 6.3$ Hz, Me-8'); ^{13}C NMR ($CDCl_3$): δ 146.06 (C-1), 166.82 (C-2), 138.89 (C-3), 115.51 (C-4), 109.03 (C-5), 119.83 (C-6), 70.63 (C-7), 173.34 (C-1'), 56.10 (C-2'), 35.50 (C-3'), 34.13 (C-4'), 29.49 (C-5'), 29.53 (C-6'), 22.58 (C-7'), 14.41 (C-8'); TOF MS m/z (rel. int.): 250 $[M]^+$ ($C_{15}H_{22}O_3$) (2.2).

Salicyl laurate (2)

Elution of the column with chloroform - methanol (9:1) furnished brown crystals of **2**, 278 mg (0.37 % yield), R_f : 0.40 (chloroform - methanol, 9 : 1), m. p. 117-118°C; IR ν_{max} (KBr): 3410, 2928, 2841, 1722, 1525, 1455, 1403, 1358, 1325, 1266, 1215, 1170, 1022 cm^{-1} ; 1H NMR ($CDCl_3$): δ 6.99 (1H, m, H-3), 6.85 (1H, m, H-6), 6.78 (1H, m, H-5), 6.67 (1H, m, H-4), 4.09 (2H, brs, H_2 -7), 2.20 (2H, t, $J = 7.1$ Hz, H_2 -2'), 1.95 (2H, m, CH_2), 1.51 (2H, m, CH_2), 1.24 (14H, brs, $7 \times CH_2$), 0.86 (3H, t, $J = 6.3$ Hz, Me-12'); ^{13}C NMR ($CDCl_3$): δ 147.48 (C-1), 162.48 (C-2), 131.96 (C-3), 115.60 (C-4), 121.26 (C-5), 119.35 (C-6), 69.65 (C-7), 173.41 (C-1'), 56.38 (C-2'), 31.77 (C-3'), 29.55 (C-4'), 29.51 (C-5'), 29.47 (C-6'), 29.47 (C-7'), 29.37 (C-8'), 29.18 (C-9'), 24.83 (C-10'), 22.57 (C-11'), 14.41 (C-12'); TOF MS m/z (rel. int.): 306 $[M]^+$ ($C_{19}H_{30}O_3$) (2.5).

Benzyl myristate (3)

Elution of the column with chloroform - methanol (9:1) gave yellow crystals of **3**, 253 mg (0.33 % yield), R_f : 0.35 (chloroform - methanol, 9 : 1), m. p. 76 - 78°C; IR ν_{max} (KBr): 2919, 2841, 1722, 1635, 1455, 1365, 1260, 1015, 835 cm^{-1} ; 1H NMR ($CDCl_3$): δ 7.23 (1H, m, H-2), 7.01 (1H, m, H-6), 6.93 (2H, m, H-3, H-5), 6.65 (1H, m, H-4), 4.08 (2H, brs, H_2 -7), 2.28 (2H, t, $J = 7.2$ Hz, H_2 -2'), 2.01 (2H, m, H_2 -3'), 1.48 (2H, m, CH_2), 1.23 (20H, brs, $10 \times CH_2$), 0.85 (3H, t, $J = 6.5$ Hz, Me-14'); ^{13}C NMR ($CDCl_3$): δ 146.52 (C-1), 120.16 (C-2), 113.46 (C-3), 115.08 (C-4), 115.21 (C-5), 115.18 (C-6), 69.67 (C-7), 173.09 (C-1'), 56.46 (C-2'), 51.84 (C-3'), 37.15 (C-4'), 34.97 (C-5'), 31.77 (C-6'), 29.46 (C-7'), 29.37 (C-8'), 29.13 (C-9'), 28.99 (C-10'), 27.08 (C-11'), 24.94 (C-12'), 22.57 (C-13'), 14.39 (C-14'); TOF MS m/z (rel.int.): 318 $[M]^+$ ($C_{21}H_{34}O_2$) (1.3).

n-Butanoyl-O- β -D-glucufuranoside (4)

Elution of the column with chloroform - methanol (17:3) yielded pale yellow crystals of **4**, 319 mg (0.43 % yield), R_f : 0.23 (chloroform - methanol, 9 : 1), m. p. 86-87°C; IR ν_{max} (KBr): 3455, 3365, 2918, 2841, 1730, 1590, 1456, 1410, 1227, 1175, 1085, 965 cm^{-1} ; 1H NMR (DMSO- d_6): δ 6.68 (1H, d, $J = 7.6$ Hz, H-1'), 4.72 (1H, m, H-4'), 3.76 (1H, m, H-2'), 3.51 (1H, m, H-3'), 3.42 (1H, m, H-5'), 3.27 (2H, d, $J = 6.0$ Hz, H_2 -6'), 2.51 (1H, t, $J = 3.2$ Hz, H_2 -2), 1.24 (2H, m, H_2 -3), 0.89 (3H, t, $J = 6.1$ Hz, Me-4'); ^{13}C NMR (DMSO d_6): δ 173.27 (C-1), 37.19 (C-2), 29.61 (C-3), 14.28 (C-4), 107.84 (C-1'), 81.25 (C-2'), 77.37 (C-3'), 83.06 (C-4'), 72.96 (C-5'), 63.55 (C-6'); TOF MS m/z (rel. int.): 250 $[M]^+$ ($C_{10}H_{18}O_7$) (2.1).

2 β -D-Galactosyloxybenzyl caproate (5)

Further elution of the column with chloroform - methanol (17:3) gave yellow crystals of **5**, 337 mg (0.45 % yield), R_f : 0.35 (chloroform - methanol, 17 : 3), m. p. 104-105 °C; IR ν_{max} (KBr): 3425, 3365, 3280, 2928, 2843, 1735, 1645, 1525, 1445, 1336, 1260, 1185, 1022 cm^{-1} ; 1H NMR (DMSO d_6): δ 7.06 (1H, m, H-3), 6.93 (1H, m, H-6), 6.82 (1H, m, H-5), 6.71 (1H, m, H-4), 5.61 (1H, d, $J = 7.1$ Hz, H-1"), 4.36 (1H, m, H-5"), 3.86 (2H, brs, H_2 -7), 3.81 (1H, m, H_2 -2"), 3.75 (1H, m, H-3"), 3.62 (1H, m, H-4"), 3.16 (2H, d, $J = 5.6$ Hz, H_2 -6"), 2.51 (2H, m, H_2 -2'), 1.51 (2H, m, CH_2), 1.24 (4H, brs, $2 \times CH_2$), 0.86 (3H, t, $J = 6.5$ Hz, Me-6'); ^{13}C NMR (DMSO d_6): δ 145.88 (C-1), 167.75 (C-2), 138.48 (C-3), 120.95 (C-4), 127.59 (C-5), 133.26 (C-6), 72.95 (C-7), 168.76 (C-1'), 57.54 (C-2'), 31.47 (C-3'), 29.25 (C-4'), 22.71 (C-5'), 14.33 (C-6'), 109.22 (C-1"), 72.85 (C-2"), 71.65 (C-3"), 66.69 (C-4"), 76.21 (C-5"), 62.57 (C-6"); TOF MS m/z (rel. int.): 384 $[M]^+$ ($C_{17}H_{28}O_8$) (1.6).

2 β -D-Glucopyranosyloxybenzyl caprylate (6)

Elution of the column with chloroform - methanol (4:1) gave yellow crystals of **6**, 403 mg (0.53 % yield), R_f : 0.45 (chloroform - methanol, 17 : 3), m. p. 117-118 °C; IR ν_{max} (KBr): 3415, 3340, 3265, 2918, 2837, 1723, 1635, 1527, 1455, 1362, 1260, 1180, 1035, 910 cm^{-1} ; 1H NMR (DMSO d_6): δ 7.10 (1H, m, H-3), 6.92 (1H, m, H-6), 6.89 (1H, m, H-5), 6.71 (1H, m, H-4), 5.54 (1H, d, $J = 7.4$ Hz, H-1"), 4.25 (1H, m, H-5"), 4.01 (2H, brs, H_2 -7), 3.85 (1H, m, H_2 -2"), 3.74 (1H, m, H-3"), 3.43 (1H, m, H-4"), 3.21 (2H, d, $J = 7.2$ Hz, H_2 -6"), 2.41 (2H, t, $J = 7.3$ Hz, H_2 -2'), 1.51 (2H, m, CH_2), 1.23 (8H, brs, $4 \times CH_2$), 0.85 (3H, t, $J = 6.5$ Hz, Me-8'); ^{13}C NMR (DMSO d_6): δ 145.89 (C-1), 163.22 (C-2), 133.24 (C-3), 118.13 (C-4), 127.57 (C-5), 130.09 (C-6), 72.02 (C-7), 171.86 (C-1'), 53.04 (C-2'), 31.43 (C-3'), 29.46 (C-4'), 29.41 (C-5'), 29.32 (C-6'), 22.68 (C-7'), 14.12 (C-8'), 102.45 (C-1"), 73.06 (C-2"), 71.62 (C-3"), 66.67 (C-4"),

79.60 (C-5''), 63.16 (C-6''); TOF MS m/z (rel. int.): 412 $[M]^+$ ($C_{21}H_{32}O_8$) (12.7).

n-Caproyl diglucoside (7)

Elution of the column with chloroform - methanol (3:1) yielded colourless crystals of **7**, 431 mg (0.57 % yield), R_f : 0.53 (chloroform - methanol, 3 : 1), m.p. 81-82°C; IR ν_{max} (KBr): 3510, 3425, 3322, 1725, 1635, 1455, 1365, 1260, 1082 cm^{-1} ; 1H NMR (DMSO d_6): δ 5.31 (1H, d, $J = 7.3$ Hz, H-1'), 5.16 (1H, d, $J = 7.2$ Hz, H-1''), 4.73 (1H, m, H-2'), 4.56 (1H, m, H-5''), 4.32 (1H, m, H-5''), 4.21 (1H, m, H-2''), 3.84 (1H, m, H-3'), 3.81 (1H, m, H-3''), 3.65 (1H, m, H-4''), 3.48 (1H, m, H-4''), 3.17 (2H, d, $J = 8.2$ Hz, H₂-6'), 3.06 (2H, d, $J = 9.1$ Hz, H₂-6''), 2.39 (2H, t, $J = 7.2$ Hz, H₂-2), 1.26 (4H, brs, $2 \times CH_2$), 0.93 (3H, t, $J = 6.3$ Hz, Me-6); ^{13}C NMR (DMSO d_6): δ 169.83 (C-1), 33.43 (C-2), 29.56 (C-3), 29.37 (C-4), 22.68 (C-5), 14.21 (C-6), 102.61 (C-1'), 82.18 (C-2'), 71.01 (C-3'), 64.14 (C-4'), 75.93 (C-5'), 61.54 (C-6'), 98.04 (C-1''), 71.91 (C-2''), 70.62 (C-3''), 63.35 (C-4''), 76.11 (C-5''), 60.89 (C-6''); TOF MS m/z (rel.int.): 440 $[M]^+$ ($C_{18}H_{32}O_{12}$) (50.2).

RESULTS AND DISCUSSION

Compound **1**, named salicyl caprylate, showed IR spectrum absorption bands for hydroxyl group (3425 cm^{-1}), aromatic ring (1630, 1525, 1075 cm^{-1}) and ester group (1725 cm^{-1}). On the basis of mass and ^{13}C NMR spectra the molecular ion peak of **1** was established at m/z 250 corresponding to a benzyl ester, $C_{15}H_{22}O_3$. The 1H NMR spectrum of **1** displayed four one-proton multiplets between δ 7.33 - 6.72 assigned to aromatic H-3, H-6, H-5 and H-4 protons and a two-proton broad singlet at δ 4.08 ascribed to C-7 oxymethylene protons adjacent to the ester group. A two-proton triplet at δ 2.45 ($J = 7.2$ Hz) was associated with methylene H₂-2' nearby the ester group. A three-proton triplet at δ 0.88 ($J = 6.3$ Hz) was attributed to C-8' primary methyl protons. The remaining methylene protons resonated as a multiplet at δ 1.51 (2H) and as a singlet at δ 1.24 (8H). The ^{13}C NMR spectrum of **1** displayed signals for aromatic carbons between δ 166.82 - 109.03, ester carbon at δ 173.34 (C-1'), oxymethylene carbon at δ 70.63 (C-7), methyl carbon at 14.41 (Me-8') and other methylene carbons between δ 56.10 - 22.58. Acid hydrolysis of **1** yielded salicylic alcohol, m. p. 83 - 85 °C, R_f 0.70 (ethyl acetate - methanol - water, 77 : 13 : 10) and caprylic acid, m. p. 16 °C, R_f 0.74 (0.1 N ethyl amine). On the basis of spectral data analysis, the structure of **1** has been characterized as 2-hydroxybenzyl *n*-octanoate, a new aromatic ester (Fig. 1).

Compound **2**, named salicyl laurate, displayed characteristic IR absorption bands for hydroxyl group at 3410 cm^{-1} , aromatic ring (1525, 1022 cm^{-1}) and ester group at 1722 cm^{-1} . On the basis of mass and ^{13}C NMR

spectra the molecular ion peak of **2** was established at m/z 306 corresponding to a benzyl ester, $C_{19}H_{30}O_3$. The 1H NMR spectrum of **2** exhibited four one-proton multiplets between δ 6.99-6.67 attributed to aromatic protons and a two-proton broad singlet at δ 4.09 accounted to oxymethylene H₂-7 protons linked to the aromatic ring. A two-proton triplet at δ 2.20 ($J = 7.1$ Hz) was associated with the methylene H₂-2' protons located nearby to the ester carbon. A three-proton triplet at δ 0.86 ($J = 6.3$ Hz) was ascribed to C-12' primary methyl protons. The remaining methylene protons resonated between δ 1.95 - 1.24. The ^{13}C NMR spectrum of **2** displayed signals for ester carbon at δ 173.41 (C-1'), oxygenated methylene carbon at δ 69.65 (C-7), aromatic carbons from δ 162.48 to 115.60, methyl carbon at 14.41 (Me-12') and methylene carbons between δ 56.38 - 22.57. Acid hydrolysis of **2** yielded salicylic alcohol, m. p. 83 - 85 °C, R_f 0.70 (ethyl acetate - methanol - water, 77 : 13 : 10) and lauric acid, m. p. 43 °C, R_f 0.73 (0.1 N ethyl amine). On the basis of these evidences, the structure of compound **2** was elucidated as 2-hydroxybenzyl *n*-dodecanoate, a new aromatic ester (Fig. 1).

Compound **3**, designated as benzyl myristate, $[M]^+$ m/z 318 ($C_{21}H_{34}O_2$), showed IR absorption bands for ester group (1722 cm^{-1}). The 1H -NMR spectrum of **3** showed three one-proton multiplets at δ 7.23, 7.01 and 6.65 attributed to aromatic H-2, H-6 and H-4 protons, respectively, and a two-proton multiplet at δ 6.93 ascribed to aromatic H-3 and H-5 protons. A two-proton broad singlet at δ 4.08 was associated with oxymethylene H₂-7 protons. A three-proton triplet at δ 0.85 ($J=6.5$ Hz) was accounted to terminal primary C-14' methyl protons. The other methylene protons resonated as two-proton signals between δ 2.28 - 1.23. The ^{13}C NMR spectrum of **3** exhibited signals for phenyl carbons between δ 146.52 - 113.46, ester carbon at δ 173.09 (C-1'), oxymethylene carbon at δ 69.67 (C-7), methylene carbons from δ 56.46 to 22.57 and methyl carbon at δ 14.39 (C-14'). Acid hydrolysis of **3** yielded benzyl alcohol, and myristic acid, m. p. 54 °C. On the basis of spectral data analysis, the structure of compound **3** has been determined as benzyl *n*-tetradecanoate (benzyl myristate), a new aromatic ester (Fig. 1).

Compound **4**, $[M]^+$ at m/z 250 ($C_{10}H_{18}O_7$), displayed distinctive IR absorption bands for hydroxyl groups (3455, 3365 cm^{-1}) and ester function (1730 cm^{-1}). The 1H NMR spectrum of **4** showed a one-proton doublet at δ 6.68 ($J = 7.6$ Hz) ascribed to anomeric H-1' proton. The other sugar protons appeared from δ 4.72 to 3.27. The methylene protons appeared as a two-proton triplet at δ 2.51 ($J = 3.2$ Hz, H₂-2) and as a two-proton multiplet at δ 1.24 (H₂-3). A three-proton triplet at δ 0.89 ($J = 6.1$ Hz)

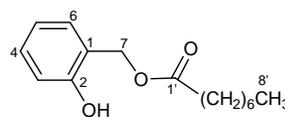
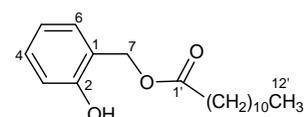
was ascribed to terminal C-4 primary methyl protons of the alkyl chain. The ^{13}C NMR spectrum of **4** displayed signals for ester carbon at δ 173.27 (C-1), anomeric carbon at δ 107.84 (C-1'), other sugar carbons from δ 83.06 to 63.55, methyl carbon at 14.28 (Me-4) and methylene carbons at δ 37.19 and 29.61. The presence of anomeric proton in the deshielded region at δ 6.68 in the ^1H NMR spectrum and anomeric carbon at δ 107.84 (C-1'), C-2' at δ 81.25 and C-4' at δ 83.06 suggested furanic form of the sugar unit. On the basis of these evidences the structure of compound **4** has been depicted as *n*-butanoyl- β -D-glucofuranoside, a new acyl glucoside (Fig. 1).

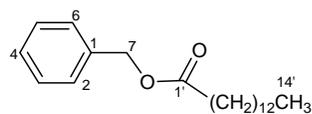
Compound **5**, named 2 β -D-galactosyloxybenzyl caproate, $[\text{M}]^+$ at m/z 384 ($\text{C}_{19}\text{H}_{28}\text{O}_8$), gave positive tests of glycosides and exhibited IR absorption bands for hydroxyl groups (3425, 3365 and 3280 cm^{-1}) and ester function (1735 cm^{-1}). The ^1H NMR spectrum of **5** demonstrated four one-proton multiplets between δ 7.06 - 6.71 attributed to aromatic protons, a one-proton doublet at δ 5.61 ($J = 7.1\text{ Hz}$) ascribed to anomeric H-1'' proton, other sugar protons between δ 4.36 - 3.16, a three-proton triplet at δ 0.86 ($J = 6.5\text{ Hz}$) accounted to C-6' primary methyl protons and the remaining methylene protons from δ 2.51 to 1.24. The ^{13}C NMR spectrum of **5** displayed signals for aromatic carbon from δ 167.75 to 120.95, anomeric carbon at δ 109.22 (C-1''), other sugar carbons between δ 76.21 - 62.57, ester carbon at δ 168.76 (C-1'), methylene group attached to ester carbon at δ 57.54, other methylene carbons at δ in the range of δ 57.54 - 22.71 and terminal methyl carbon at 14.33 (Me-6'). Acid hydrolysis of **5** yielded salicylic alcohol, m. p. $83 - 85^\circ\text{C}$, R_f 0.70 (ethyl acetate - methanol - water, 77 : 13 : 10), caproic acid, R_f 0.63 (0.1 N ethylamine) and D-galactose, R_f 0.23 (*n*-butanol- acetic acid - water, 4 : 1 : 5). On the basis of spectral data analysis and chemical reactions, the structure of **5** had been formulated as 2 β -D-galactopyranosyloxybenzyl *n*-hexanoate, a new aromatic ester (Fig. 1).

Compound **6**, $[\text{M}]^+$ m/z 412 ($\text{C}_{21}\text{H}_{32}\text{O}_8$), gave positive tests of glycosides and showed IR absorption bands for hydroxyl groups ($3415, 3340, 3265\text{ cm}^{-1}$), ester function (1723 cm^{-1}) and aromatic ring ($1635, 1527, 1035\text{ cm}^{-1}$). The ^1H -NMR spectrum of **6** showed four one-proton multiplets from δ 7.10 to 6.71 attributed to aromatic protons, a one-proton doublet at δ 5.54 ($J=7.4\text{ Hz}$) ascribed to anomeric H-1'', other sugar protons between δ 4.25 - 3.21, a two-proton triplet at δ 2.41 ($J=7.3\text{ Hz}$) accounted to methylene H₂-2' protons adjacent to the ester function, other methylene protons at δ 1.51 (2H) and 1.23 (8H) and a three - proton triplet at δ 0.85 ($J = 6.5\text{ Hz}$) assigned to C-8' primary methyl protons. The ^{13}C

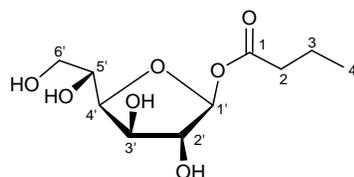
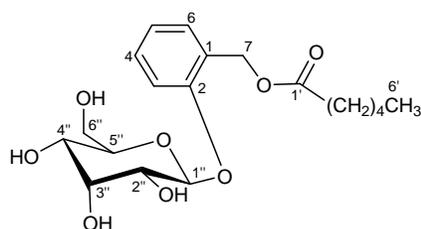
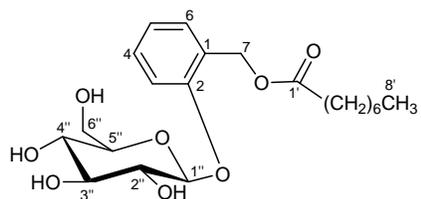
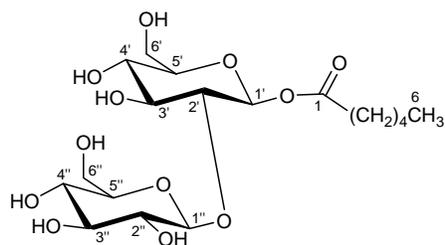
NMR spectrum of **6** demonstrated signals for ester carbon at δ 171.86 (C-1'), aromatic carbons from δ 163.22 to 118.13, methylene carbons in the range of δ 53.04 - 22.68, terminal methyl carbon at 14.12 (Me-8'), anomeric carbon at δ 102.45 (C-1'') and other sugar carbons between δ 79.60 - 63.16. Acid hydrolysis of **6** yielded salicylic alcohol, m. p. $83 - 85^\circ\text{C}$, R_f 0.70 (ethyl acetate - methanol - water, 77 : 13 : 10), caprylic acid, m. p. 16°C , R_f 0.74 (0.1 N ethyl amine) and D-glucose, R_f 0.26 (*n*-butanol- acetic acid - water, 4 : 1 : 5). On the basis of these evidences, the structure of **6** has been characterized as 2 β -D-glucopyranosyloxybenzyl *n*-octanoate (Fig. 1).

Compound **7**, designated as *n*-caproyl diglucoside, responded for glycoside tests positively and exhibited distinctive IR absorption bands for hydroxyl groups ($3510, 3425, 3322\text{ cm}^{-1}$) and ester function (1725 cm^{-1}). Its molecular ion peak was established at m/z 440 on the basis of mass and ^{13}C NMR spectra corresponding to the molecular formula of an acyl diglycoside, $\text{C}_{18}\text{H}_{32}\text{O}_{12}$. The ^1H NMR spectrum of **7** displayed two one - proton doublets at δ 5.31 ($J = 7.3\text{ Hz}$) and 5.16 ($J = 7.2\text{ Hz}$) assigned to anomeric H-1' and H-1'' protons, respectively. The other sugar protons appeared between δ 4.73 - 3.06. A two-proton triplet at δ 2.39 ($J=7.2\text{ Hz}$) and as a four-proton singlet at δ 1.26 were ascribed to methylene protons. A three - proton triplet at δ 0.93 ($J = 6.3\text{ Hz}$) was attributed to terminal C-6 primary methyl protons. The ^{13}C NMR spectrum of **7** displayed signals for ester carbon at δ 169.83 (C-1), anomeric carbons at δ 102.61 (C-1') and 98.04 (C-1''), other sugar carbons from δ 82.18 to 60.89, methyl carbon at δ 14.21 (C-6) and methylene carbons between δ 33.43 - 22.68. The presence of H-2' signal in the deshielded region at δ 4.73 in ^1H NMR spectrum and C-2' signal at δ 82.18 in the ^{13}C NMR spectrum suggested (2' \rightarrow 1'') linkages of the sugar units. Acid hydrolysis of **7** yielded caproic acid, R_f 0.63 (0.1 N ethylamine) and D-glucose, R_f 0.26 (*n*-butanol- acetic acid - water, 4 : 1 : 5). On the basis of foregoing discussion, the structure of compound **7** has been characterized as *n*-caproyl O- β -D-glucopyranosyl-(2' \rightarrow 1'')-O- β -D-glucopyranoside, a new fatty acid diglycoside (Fig. 1).

Salicyl caprylate (**1**)Salicyl laurate (**2**)



Benzyl myristate (3)

*n*-Butanoyl-O- β -D-glucopyranoside (4)2 β -D-Galactopyranosyloxybenzyl caproate (5)2 β -D-Glucopyranosyloxybenzyl caprate (6)

Caproyl diglucoside (7)

Figure 1. Structural formulae of the chemical constituents 1 – 7.

CONCLUSION

Phytochemical investigation of a methanolic extract of the roots of *Jatropha curcas* led to isolate three aromatic esters, their glycosides and acyl glucoside. This work has enhanced understanding about the phytoconstituents of the plant. These compounds may be used as chromatographic markers for standardization of the tubers of the plant.

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CONFLICTS OF INTERESTS

None declared.

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