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ORIGINAL ARTICLE

New phytoconstituents from the roots of *Aralia cachemirica* Decne

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Abstract *Aralia* species are used in traditional medicine to treat rheumatic arthritis, nephritis, lumbago, lameness, gastritis, inflammation and diabetes mellitus. Phytochemical investigation of the roots of *Aralia cachemirica* Decne (Araliaceae) collected from the Aharbal region of Kashmir afforded four new phytoconstituents identified as *n*-tetracont-19-enoic acid (**1**), 4α,4β,8β,10β,13β,17β-hexamethyl perhydrophenanthrenyl-3β-*n*-decanoate (**3**), tetrahydrocontinentalic acid (**4**) and 1β,4α,4β-trimethyl-6-(10,14,18-trimethyl-tridec-6-enyl)-cyclohexane-4β-ol (**5**) along with the known compounds continentalic acid (**2**), maltose (**6**) and sucrose (**7**). The structures of these phytoconstituents have been elucidated on the basis of spectral data analysis.

1. Introduction

Aralia cachemirica Decne (Araliaceae), known as Khoree and Banakhor, is a perennial aromatic lax shrub, up to 3 m tall, distributed in Afghanistan, Tibet, Kashmir, Himachal Pradesh, Uttarakhand and Sikkim (Pusalkar, 2009). *Aralia* species are used in traditional medicine to treat gastritis, rheumatic arthritis, inflammation, nephritis and diabetes mellitus (Oh et al., 2009; Liu et al., 2000). It is eaten by goats as a nutrient (Anon., 2003). *A. cachemirica* yielded aralosides (George et al., 1984), β-sitosterol (Anon., 2003), sugars (Bhat et al., 2010), essential oil (Shawl et al., 2009; Verma et al., 2010) and continentalic acid (Sharma et al., 2011). The plant showed hyperglycaemic (Bhat et al., 2005) and antibacterial (Sangwan et al., 2008) activities. This manuscript describes the isolation and characterization of new fatty acids, tetraterpinolide and diterpenic acid from the roots of *A. cachemirica*.

2. Materials and methods

2.1. General

The melting points were determined on a Perfit apparatus and are uncorrected. The IR spectra were recorded on KBr pellet using a jasco FT/IR-5000 instrument (FTS 135, Hongkong). The ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra were scanned on DRX-400 Avance 400 MHz spectrometer (Bruker-Biospin, Rheinstetten, Germany) using $CDCl_3$ as solvent and TMS as internal standard. FAB-MS were

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measured using JEOL-JMS-DX 303 spectrometer (Peabody, MA, USA). Column ($450 \times 4 \times 0.2$ cm) chromatography was performed on silica gel (60–120 mesh, Qualigens, Mumbai, India) and thin layer chromatography on silica gel G-coated TLC plates (Merck). Spots were visualized by exposure to iodine vapours, UV radiation and by spraying reagents.

2.2. Plant material

The dried roots of *A. cachemirica* were collected from the Aharbal region of Kashmir and was authenticated by Dr. A.R. Naqshi, the Department of Taxonomy, University of Kashmir, Srinagar with a voucher specimen No. PS/UKS/AR-1 and was deposited in herbarium for future reference in the Department of Pharmaceutical Sciences, University of Kashmir, Srinagar.

2.3. Extraction and isolation

The air dried roots (2.5 kg) were coarsely powdered and extracted exhaustively in a Soxhlet apparatus with methanol for 72 h. The methanolic extract was concentrated under reduced pressure to obtain a dark brown viscous mass (210 g). Small portion of extract was analyzed chemically to determine the presence of different chemical constituents. The concentrated extract (150 g) was dissolved in methanol (250 ml) and adsorbed on silica gel (60–120 mesh) for column chromatography. The slurry was air dried and chromatographed over silica gel column packed in petroleum ether. The column was eluted successively with petroleum ether, mixture of petroleum ether and chloroform (9:1, 3:1, 1:1, and 1:3), pure chloroform and finally the mixture of chloroform and methanol (99:1, 97:3, 19:1, 23:2, 9:1, 3:1, and 1:1, 1:3). Various fractions were collected separately and matched by TLC to check homogeneity. Similar fractions having same R_f values were combined and crystallized. The isolated compounds were recrystallized to get pure compounds. The following compounds were isolated:

2.4. n-Tetracont-19-enoic acid (*1*)

Elution of the column with petroleum ether gave colourless amorphous powder of **1**, recrystallized from acetone–methanol (1:1), yield 0.36%, m.p. 54–55 °C, R_f 0.3 (petroleum ether–chloroform, 9:1); IR ν_{max} (KBr): 3300, 2950, 2843, 1690, 1643, 1410, 1315, 1280, 1130, 721 cm^{-1}; ^1H NMR ($CDCl_3$): δ 5.03 (1H, m, $w_{1/2}$ = 9.8 Hz, H-19), 5.00 (1H, m, $w_{1/2}$ = 9.8 Hz, H-20), 2.14 (2H, t, J = 7.1 Hz, H_2-2), 2.01 (2H, m, H_2-18), 1.98 (2H, m, H_2-21), 1.52 (4H, m, 2×CH_2), 1.29 (62H, brs, 31×CH_2), 0.91 (3H, t, J = 6.5 Hz, Me-40); ^{13}C NMR ($CDCl_3$): δ 180.06 (C-1), 122.31 (C-19), 115.02 (C-20), 55.20 (C-2), 40.17 (CH_2), 39.52 (CH_2), 37.61 (CH_2), 35.42 (CH_2), 31.87 (CH_2), 28.12 (CH_2), 29.45 (28×CH_2), 22.56 (CH_2), 18.51 (Me-40); +ve FAB MS m/z (rel. int): 591 $[M+H]^+$ ($C_{40}H_{79}O_2$) (12.3), 283 (9.8), 307 (19.5).

2.5. Continentalic acid (*2*)

Elution of the column with petroleum ether–chloroform (9:1) afforded colourless crystals of **2**, recrystallized from methanol, yield 1.36%; m.p. 159–160 °C, IR ν_{max} (KBr): 3280, 1693, cm^{-1}; ^1H NMR ($CDCl_3$): δ 6.55 (1H, brs, H-14), 5.73 (1H, dd, J = 9.9 Hz, 7.2 Hz, H-15), 5.14 (1H, brs, H_2-16a), 4.92 (2H, d, J = 12.6 Hz, H_2-16b), 1.25 (3H, brs, Me-19), 1.01 (3H, brs, Me-20), 0.65 (3H, brs, Me-17); ^{13}C NMR ($CDCl_3$): δ 38.51 (C-1), 19.22 (C-2), 36.40 (C-3), 44.04 (C-4), 56.09 (C-5), 29.21 (C-6), 35.78 (C-7), 137.93 (C-8), 50.51 (C-9), 37.90 (C-10), 29.71 (C-11), 29.35 (C-12), 39.15 (C-13), 127.96 (C-14), 147.14 (C-15), 112.91 (C-16), 24.08 (C-17), 184.83 (C-18), 19.56 (C-19), 13.79 (C-20); +ve FAB MS m/z (rel. int): 303 $[M+H]^+$ ($C_{20}H_{31}O_2$) (11.2).

2.6. Cachemiridiol (*3*)

Elution of column with petroleum ether–chloroform (9:1) afforded colourless crystals of **3**, recrystallized from acetone–methanol (1:1), yield 0.36%, R_f 0.4 (petroleum ether–benzene, 17:3), m.p. 85–86 °C, IR ν_{max} (KBr): 3410, 2925, 2872, 1725, 1642, 1430, 1210, 1145, 1052 cm^{-1}; ^1H NMR ($CDCl_3$): δ 5.26 (1H, d, J = 5.6, H-6), 5.07 (1H, m, H-11), 4.25 (1H, dd, J = 5.5, 9.6 Hz, H-3α), 3.25 (2H, t, J = 9.5 Hz, H_2-19), 2.53 (2H, t, J = 7.2 Hz, H_2-2′), 2.27 (2H, m, H_2-7), 2.18 (2H, m, H_2-12), 1.58 (2H, m, H_2-2), 1.98 (1H, m, H-14), 1.85 (2H, m, H_2-1), 1.71 (1H, m, H-13), 1.68 (1H, m, H-17), 1.63 (2H, m, H_2-15), 1.58 (2H, m, CH_2), 1.54 (4H, m, 2×CH_2), 1.42 (16H, brs, 8×CH_2), 1.19 (3H, brs, Me-22), 1.02 (3H, d, J = 6.2 Hz, Me-24), 0.95 (3H, d, J = 6.5 Hz, Me-25), 0.88 (3H, brs, Me-20), 0.83 (3H, t, J = 6.1 Hz, Me-10′), 0.80 (3H, brs, Me-21), 0.68 (3H, brs, Me-23); ^{13}C NMR ($CDCl_3$): δ 45.07 (C-1), 34.18 (C-2), 69.94 (C-3), 42.01 (C-4), 140.92 (C-5), 120.22 (C-6), 39.22 (C-7), 56.28 (C-8), 137.82 (C-9), 38.36 (C-10), 127.46 (C-11), 38.96 (C-12), 49.52 (C-13), 55.28 (C-14), 35.28 (C-15), 33.48 (C-16), 50.52 (C-17), 33.28 (C-18), 61.52 (C-19), 25.35 (C-20), 20.46 (C-21), 18.95 (C-22), 18.65 (C-23), 20.48 (C-24), 21.19 (C-25), 172.12 (C-1′), 31.24 (C-2′), 28.96 (C-3′), 28.96 (C-4′), 28.96 (C-5′), 28.96 (C-6′), 28.52 (C-7′), 28.52 (C-8′), 22.34 (C-9′), 14.21 (C-10′); +ve FAB MS m/z (rel. int): 529 $[M+H]^+$ ($C_{35}H_{61}O_3$) (9.3), 373 (22.15), 155 (12.5).

2.7. Tetrahydrocontinentic acid (*4*)

Elution of column with chloroform–methanol (49:1) afforded colourless amorphous powder of **4**, recrystallized from acetone–methanol (1:1), yield 1.26%, R_f 0.5 (chloroform–ethyl acetate, 4:1), m.p. 115–116 °C, IR ν_{max} (KBr): 3410, 2926, 2850, 1697, 1539, 1470, 1370, 1250, 1120 cm^{-1}; ^1H NMR ($CDCl_3$): δ 2.16 (1H, m, H-5β), 1.98 (2H, m, H_2-1), 1.86 (2H, m, H_2-2), 1.79 (2H, m, H_2-3), 1.71 (2H, m, H_2-14), 1.68 (2H, m, H_2-7), 1.53 (1H, m, H-9), 1.47 (1H, m, H-8), 1.35 (2H, m, H_2-6), 1.32 (3H, brs, Me-19), 1.29 (2H, m, H_2-12), 1.23 (2H, m, H_2-11), 1.21 (2H, m, H_2-15), 1.16 (3H, brs, Me-20), 1.14 (3H, brs, Me-17), 0.85 (3H, t, J = 6.3 Hz, Me-16); ^{13}C NMR ($CDCl_3$): δ 41.20 (C-1), 23.60 (C-2), 39.35 (C-3), 47.51 (C-4), 56.81 (C-5), 28.73 (C-6), 37.25 (C-7), 55.05 (C-8), 55.86 (C-9), 38.73 (C-10), 25.96 (C-11), 36.60 (C-12), 42.50 (C-13), 44.31 (C-14), 21.37 (C-15), 14.77 (C-16), 28.16 (C-17), 179.05 (C-18), 18.25 (C-19), 17.39 (C-20); +ve FAB MS m/z (rel. int): 307 $[M+H]^+$ ($C_{20}H_{35}O_2$) (18.3).

2.8. Araliasesterterpenol (*5*)

Elution of column with chloroform–methanol (19:5) afforded colourless crystals of **5**, recrystallized from chloroform–methanol (1:1), yield 0.15%, R_f 0.25 (toluene–ethyl acetate, 4:1), m.p. 218–