Indian Journal of Chemistry
Vol. 48B, August 2009, pp. 1164-1169

Note

A new aliphatic acid from *Achyranthes aspera* Linn. Roots

Surendra Kr Sharma[a]*, Neeru Vasudeva[a] & M Ali[b]

[a]Department of Pharmaceutical Sciences, Guru Jambheshwar University of Science and Technology, Hisar 125 001 Haryana, India

[b]Faculty of Pharmaceutical Sciences, Jamia Hamdard, New Delhi.

E-mail: prof.sharmask@gmail.com

Received 10 October 2008; accepted (revised) 24 April 2009

A total of six compounds isolated from the ethanol extract of the roots of *Achyranthes aspera* Linn. (Amaranthaceae) are characterised as strigmasta-5, 22-dien-3-β-ol**,** *trans*-13-docasenoic acid, *n*-hexacosanyl *n*-decaniate, *n*-hexacos-17-enoic acid and *n*-hexacos-11-enoic acid on basis of spectral data and chemical means, including a new aliphatic acid, *n*-hexacos-14-enoic acid which is being reported for the first time from natural and synthetic source.

Keywords: *Achyranthes aspera,* Amaranthaceae, aliphatic acid.

The plant *Achyranthes aspera* Linn. (Amaranthaceae) is distributed throughout India as a weed in pastures, wastelands and roadside up to 1000 m altitude. The plant is traditionally valued as a potent medicinal agent. The decoction of the whole plant is diuretic and useful for treating renal dropsy and in large doses it acts as ecbolic. The juice of the plant is used to treat opthalmia and dysentery. The paste made from the roots is taken internally with buttermilk as an anti-fertility drug. To induce abortion a thin paste is obtained by grinding the inflorescence with water and applied to external genitalia. The decoction of the fresh roots is introduced into the vagina to terminate pregnancy. The paste of the roots is applied to external genitalia to induce labor pains[1]. The ethanol extract of the roots, *n*-butanol fraction of aerial parts, methanolic leaf extract and benzene extract of the dried stem bark of *A. aspera* are reported to have anti-implantation and abortifacient activity[2-5]. The ethanol extract of the root possesses spermicidal activity[6], and the aqueous extract of the entire plant of *A. aspera* is hepatoprotective[7]. The hydroalcohalic extract of *A. aspera* stimulates cell mediated immune system by increasing phagocytic function[8]. The aqueous and methanolic extracts of the whole plant of *A. aspera* has proven to be hypoglycemic[9]. The total methanol extract of the leaves of *A. aspera* has anti-tumor activity[10]. The roots of *A. aspera* are reported to contain ecdysterone[11-13]. Two nitrogenous bases, betaine[14] and achyranthine[15] have been isolated from whole plant of *A. aspera.* A number of oleanolic acid based saponins have been reported from the seeds, unripe fruits, inflorescence of *A. aspera*[16-18]. Numerous aliphatic compounds have been reported from the seeds and the shoots of *A. aspera*[19-23].

In the present paper six phytoconstituents isolated are being reported for the first time in the plant *A. aspera* of which *n*-hexacos-14-enoic acid, an aliphatic acid, is being reported for the first time from any natural and synthetic source.

Results and Discussion

Compound **NA-I** a phytosterol, was obtained as a colourless crystalline mass from petroleum ether:benzene 75:25 elute. It responded positively to Liebermann Burchard test for sterols. Its IR spectrum showed characteristic absorption bands for hydroxyl groups (3336 cm^{-1}) and unsaturation (1640 cm^{-1}). The mass spectrum of **NA-I** displayed a molecular ion peak at *m/z* 412 corresponding to the molecular formula of a sterol, $C_{29}H_{48}O$. It indicated six double bond equivalent; four of them were adjusted in the tetracyclic carbon framework of the sterol and the remaining two in the vinylic linkages. The ^1H NMR spectrum of **NA-I** exhibited three one proton deshielded multiplets at δ 5.35, 5.14 and 5.03 assigned to vinylic proton H-6, H-22 and H-23, respectively. A one-proton road multiplet at δ 3.55 with half-width of 18.5 Hz was accounted to C-3 α-carbinol proton. Two three-proton broad signals at δ 1.01 and 0.69 were ascribed to C-19 and C-18 tertiary methyl proton. Four doublets at δ 0.93 (J = 5.7 Hz), 0.84 (J = 6.0 Hz), 0.82 (J = 6.0 Hz) and 0.80 (J = 6.9 Hz) were attributed to secondary C-21, C-26, C-27 tertiary C-29 methyl protons, respectively. The ^{13}C NMR spectrum of **NA-I** showed the presence of 29 carbon signals. The important signals at δ 139.9, 122.0, 128.72, 128.11 and 72.09 were assigned to vinylic C-5, C-6, C-22 and C-23 and C-3 carbinol protons, respectively. The ^1H and ^{13}C NMR values were compared with the related compounds particularly β-sitosterol, stigmasterol, and lowsaritol[24,25]. On the basis of the

foregoing discussion and comparison of melting point and Co-TLC the structure of **NA-I** has been established as strigmasta-5, 22-dien-3-β-ol.

Compound **NA-II**, brassidic acid, was obtained as colourless crystals from petroleum ether:benzene 85:15 elute. It produced effervescences with sodium bicarbonate solution and decolourized bromine water indicating unsaturated fatty acid nature of the molecule. Its IR spectrum displayed characteristic absorption bands for carboxylic group (3490, 1705 cm^{-1}) unsaturation (1640 cm^{-1}) and long aliphatic chain (719 cm^{-1}). The mass spectrum of **NA-II** exhibited a molecular ion peak at *m/z* 338 corresponding to a molecular formula of unsaturated fatty acid, $C_{22}H_{42}O_2$. It indicated two double bond equivalents which were adjusted in the carboxylic group and vinylic linkage. The prominent ion fragments generated at *m/z* 199, 139 $[C_{12}\text{-}C_{13}$ fission$]^+$, 154 [199 - COOH]$^+$, 124 [139 - Me]$^+$, 180 $[C_{14}\text{-}C_{15}$ fission-COOH$]^+$ suggested the location of the vinylic linkage at C-13. The ^{1}H NMR spectrum of **NA-II** showed a two-proton multiplet at δ 5.34 assigned to vinylic H-13 and H-14. Two one-proton doublets at δ 2.37 (J = 7.5 Hz) and 2.31 (J = 7.5 Hz) were attributed to C-2 methylene protons adjacent to the carboxylic group. Two multiplets at δ 2.01 and 1.63, both integrated for two protons each accounted C-12 and C-15 methylene adjacent to the olefinic linkage, respectively. A three-proton triplet at δ 0.85 (J = 6.6 Hz) was ascribed to terminal primary methyl protons. The remaining methylene proton resonated as 30-proton broad signal. The ^{13}C NMR spectrum of **NA-II** exhibited signals for important signals for carboxylic carbon (δ 180.21) unsaturated carbons at δ 130.82 (C-11) and 130.01 and methyl carbon at δ 14.74 (C-22). The remaining methylene carbon resonated between δ 34.58 - 19.90. The absence of any signal between δ 5.34 - 2.37 in the ^{1}H NMR spectrum and between δ 130.01 - 34.58 in the ^{13}C NMR spectrum ruled out the presence of a hydroxyl group in the molecule. On the basis of spectral data analysis and chemical reactions the structure of **NA-II** has been characterized as *trans*-13-docasenoic acid.

Compound **NA-III**, was obtained as a colourless crystalline from benzene elute. It decolourized bromine water and gave effervescences with sodium bicarbonate suggesting unsaturated fatty acid nature of the molecule. Its IR spectrum displayed characteristic adsorption bands for carboxylic group (3450, 1707 cm^{-1}), unsaturation (1635 cm^{-1}) and long aliphatic chain (721 cm^{-1}). The mass spectrum of **NA-III** exhibited a molecular ion peak at *m/z* 394 corresponding to a molecular formula of unsaturated fatty acid $C_{26}H_{50}O_2$. It had two degrees of unsaturation which were adjusted one each in vinylic bond and carboxylic group. The prominent ion fragments generated at δ 213, 181 $[C_{13}\text{-}C_{14}$ fission$]^+$ and 155, 239 $[C_{15}\text{-}C_{16}$ fission$]^+$ supported the existence of the olefinic linkage at C-14. The ^{1}H NMR spectrum of **NA-III** showed two one-proton multiplets at δ 5.50 and 5.48 assigned to vinylic H-14 and H-15, respectively. Two one-proton doublets at δ 2.91 (J = 6.0 Hz) and 2.87 (J = 6.0 Hz) were ascribed to methylene H_2-2 adjacent to the carboxylic group. Two multiplets at δ 2.07 and 2.03, both integrated for two protons each, were attributed to methylene H_2-13 and H_2-16 nearby to the vinylic carbons. A three-proton triplet at δ 0.89 (J = 7.5 Hz) was associated with the terminal primary C-26 methyl protons. The remaining methylene protons resonated between δ 1.48-1.15. The ^{13}C NMR signal of **NA-III** presented signals for C-1 caroboxylic group at δ 179.31, vinylic carbons at δ 133.23 (C-14) and 130.31 (C-15), methyl carbon at δ 14.36 (C-26) and methylene carbon between 33.97-23.11. The absence of ^{1}H NMR signals between δ 5.48-2.91 and ^{13}C NMR signals between δ 130.31-33.97 supported the absence of carbinol proton in the molecule. On the basis of above mention discussion the structure of **NA-III** has been established as *n*-hexacos-14-enoic acid. This is a new phytoconstituent isolated from a plant for the first time.

Compound **NA-IV**, was obtained as a colourless crystalline mass from petroleum ether:benzene 95:5. Its IR spectrum showed characteristic adsorption bands for ester group (1736 cm^{-1}) and long aliphatic chain (799, 724 cm^{-1}). The mass spectrum of **NA-IV** displayed a molecular ion peak at *m/z* 536 corresponding to a molecular formula of a fatty acid ester, $C_{36}H_{72}O_2$. It indicated one double bond equivalent which was adjusted in the ester groups. The prominent ion fragments generated at *m/z* 155 [CO-O fission]$^+$ and 171 [O-C, fission]$^+$ suggested that C10 fatty was esterified with a C_{26} aliphatic alcohol. The ^{1}H NMR spectrum of **NA-IV** exhibited four one-proton doublets at δ 4.14 (J = 5.4 Hz), 4.09 (J = 5.4 Hz) and at 2.30 (J = 6.6 Hz) and 2.26 (J = 6.6 Hz) assigned correspondingly to oxygenated methylene H_2-1′ and methylene H_2-2 adjacent to the ester group. Two three-proton triplets at δ 0.87 (J = 6.3 Hz) and 0.85 (J = 6.1 Hz) were attributed to primary C-10 and C-26 methyl protons, respectively. The remaining methylene

protons resonated between 1.61-1.23. The ^{13}C NMR value of **NA-IV** exhibited important signals for ester carbons at δ 171.37, oxygenated methylene C-1′ carbon at δ 60.24, methyl carbons at δ 14.35 (C-10) and 14.21 (C-26′) and methylene carbon between δ 34.50-22.79. Acid hydrolysis of **NA-IV** yielded *n*-capric acid (TLC comparable). On the basis of spectral data analysis and chemical reaction the structure of NA-IV has been characterized as *n*-hexacosanyl-*n*-decaniate.

Compound **NA-V** was obtained as a colourless crystalline mass from petroleum ether:benzene 50:50 elute. Its decolourised bromine water and yielded effervescences with sodium bicarbonate solution indicating unsaturated fatty acid nature of the molecule. Its IR spectrum showed characteristics absorption bonds for carboxylic groups (3160, 1709 cm^{-1}) unsaturation (1635 cm^{-1}) and aliphatic long chain (723 cm^{-1}). The mass spectrum of NA-V exhibited a molecular ion peak at *m/z* 394 corresponding to a molecular formula $C_{26}H_{50}O_2$. It had two double bond equivalents which were adjusted in the carboxylic groups and vinylic linkage. The prominent ion peaks generated at *m/z* 281 [C_{18}-C_{19} fission]$^+$ and 139, 225 [C_{16}-C_{17} fission]$^+$ suggested the presence of the vinylic linkage at 17. The ^1H NMR signal of **NA-V** displayed two one-proton deshielded multiplates at δ 5.32 and 5.27 assigned to vinylic H-17 and H-18, respectively. Two one-proton doublets at δ 2.75 (J = 4.8 Hz) and 2.72 (J = 4.8 Hz) were accounted to C-2 methylene protons adjacent to the ester group. Two multiplets at δ 2.21 and 1.98, both integrated for two protons each, were ascribed to C-16 and C-19 methylene protons, respectively. A three-proton triplet at δ 0.55 (J = 6.3 Hz) was associated with C-26 primary methyl protons. The remaining methylene protons resonated between δ 1.54-1.25. The ^{13}C NMR spectrum of **NA-V** displayed important signals for ester carbons at δ 174.68 (C-1), vinylic carbon at δ 129.42 (C-17) and 127.57 (C-18), methyl carbon at δ 13.81 (C-26) and methylene carbons between δ 33.73-22.10. The absence of any signal between δ 5.27-2.75 in the ^1H NMR spectrum and between δ 127.57-33.73 in the ^{13}C NMR spectrum ruled out the existence of the carbinol carbon in the molecule. On the basis of spectral data analysis and chemical reactions the structure of NA-V has been identified as *n*-hexacos-17-enoic acid.

Compound **NA-VI,** was obtained as a colourless crystalline mass from benzene:chloroform, 85:15, 75:25, 50:50 elute. Its nature was inferred as unsaturated fatty acid on the basis of decolourization of bromine water and formation of effervescences with sodium bicarbonate solution. Its IR spectrum displayed characteristic absorption bonds for carboxylic group (3350, 1711 cm^{-1}), unsaturation (1640 cm^{-1}) and long aliphatic chain (722 cm^{-1}). The mass spectrum of **NA-VI** exhibited a molecular ion peat at *m/z* 394 corresponding to a molecular formula of unsaturated fatty acid $C_{26}H_{50}O_2$. It indicated two double bond equivalents which were adjusted in the vinylic linkage and carboxylic group. The Promination peaks arose at *m/z* 171, 223 [C_{10}-C_{11} fission]$^+$ and 197 [C_{12}-C_{13} fission]$^+$ suggested the existence of the vinylic linkage at D^{11}. The ^1H NMR spectrum of NA-VI showed two one-proton deshielded multiplates at δ 5.39 and 5.32 assigned to vinylic H-11 and H-12, respectively. Two one-proton doublets at δ 2.77 (J = 4.8 Hz) and 2.75 (J = 4.8 Hz) were accounted to C-2 methylene protons adjacent to the ester group. Two multiplets at δ 2.34 and 2.01, both integrated for two protons each, were ascribed to C-10 and C-13 methylene protons adjacent to the olefinic carbons. A three-proton triplet at δ 0.88 (J = 6.1 Hz) was ascribed with C-26 primary methyl proton. The remaining methylene protons resonated at δ 1.61 (2H), 1.30 (10H) and 1.25 (26 H). The ^{13}C NMR spectrum of **NA-VI** presented important signals for carboxylic carbon at δ 179.1 (C-1), vinylic carbons at δ 130.11 (C-11) and 127.99 (C-12), methyl carbon at δ 14.20 (C-26) and methylene carbons between δ 34.01-22.77. The absence of ^1H NMR signals between δ 5.32-2.77 and ^{13}C NMR signals between δ 127.99-34.01 ruled out the existence of any carbinol carbon in the molecule. On the basis of these evidences the structure of **NA-VI** has been established as *n*-hexacos-11-enoic acid.

Materials and Methods

All the melting points were determined in centigrade scale in one end open capillary. UV spectra were recorded in methanol on a Perkin-Elmer EZ301 spectrophotometer and λ max values are in nm. IR spectra were recorded on a Shimadzu FTIR 8201 spectrophotometer using KBr pellets and ν_{max} values are in cm^{-1}. ^1H NMR were recorded on a Bruker Avance 400 spectrometer using deuterated dimethylsulfoxide (DMSO-d_6), deuterated benzene (C_6D_6) and deuterated chloroform ($CDCl_3$) as solvents with TMS as internal standard. Chemical shifts are expressed in ppm with respect to internal trimethylsilane (TMS). ^{13}C NMR were recorded on a Bruker Avance 400 spectrometer in C_6D_6 and recorded in ppm with TMS as internal

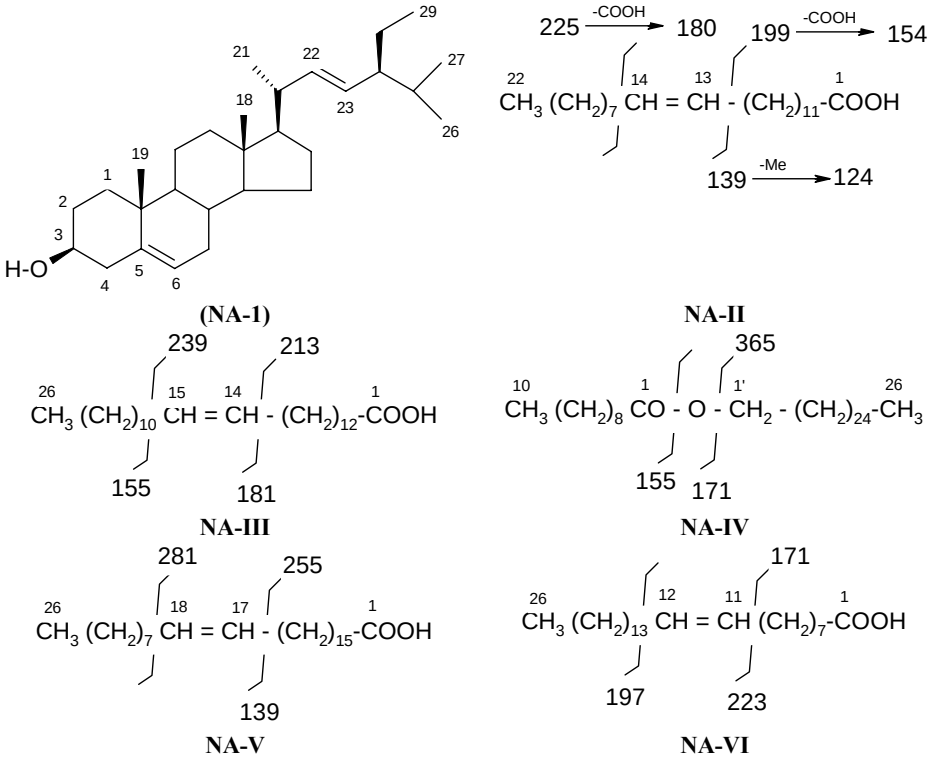

Figure 1 — Phytoconstituents isolated from the roots of *A. aspera* Linn.

standard. Fast atomic bombardment mass spectra (FABMS) data were recorded on a JEOL SX 102/DA-6000 mass spectrometer. *m/z* values of more intense peaks are mentioned.

Plant Material

The roots of *Achyranthes aspera* Linn. were collected from the campus of Guru Jambheshwar University of Science and Technology, Hisar, The plant was authenticated by Dr. M.P. Sharma, Taxonomist, Department of Botany, Faculty of Science, Jamia Hamdard, New Delhi. Herbaria were made and their voucher specimen retained in the department for future references.

Experimental Section

Extraction and Isolation

Shade dried (4.450 kg) of the roots of *A. aspera* Linn. were crushed to coarse powder and extracted exhaustively with 95% ethanol in a Soxhlet extractor. The extracts were concentrated to dryness under reduced pressure and controlled temperature (50-60°C) to yield a brown solid (250 g).

A portion (220 g) of the ethanol extract was dissolved in minimum amount of MeOH and adsorbed on silica gel (60-120 mesh), air dried and chromatographed over silica gel (540 g). The column was eluted with solvents in various proportions in increment of polarity. The fractions collected were subjected to thin layer chromatography to check the homogeneity of various fractions. The various compounds isolated from the extract are listed below along with their spectral data. Their structures are shown in **Figure 1**.

Strigmasta-5, 22-dien-3-β-ol (NA-I)

Elution of the column with pet. ether:benzene (75:25) furnished colourless amorphous powder of compound NA-I recrystallized from ethanol, 248 mg (0.056%), R_f 0.28 (pet. ether: benzene 3:1), m.p. 168-170°C, $[\alpha]_D^{30^\circ}$ –50 (c = 1.9, $CHCl_3$); IR (KBr): 3336, 2934, 2870, 1640, 1458, 1383, 1053, 970, 798 cm^{-1}; ^1H NMR ($CDCl_3$): δ 5.35 (1 H, m, H-6), 5.14 (1H, m, H-22), 5.03 (1H, m, H-23), 3.55 (1 H, br m, $w_{½}$ = 18.5 H_8, H-3α), 1.01 (3H, br s, Me-19), 0.93 (3H, d, *J* = 5.7 Hz, Me-21), 0.84 (3H, d, *J* = 6.0 Hz, Me-26), 0.82 (3H, d, *J* = 6.0- Hz, Me-27), 0.80 (3H, d, *J* = 6.9 Hz, Me-29), 0.69 (3H, br s, Me-18); ^{13}C NMR data is presented in **Table I**; +ve ion FABMS *m/z* 412 $[M]^+$ ($C_{29}H_{48}O$) (13.2).

Table I — ^{13}C NMR data of strigmasta-5, 22-dien-3-β-ol (NA-I, $CDCl_3$)

C	δ_C	C	δ_C
1	37.45	16	28.05
2	32.59	17	56.60
3	72.09	18	12.46
4	42.98	19	19.94
5	139.90	20	38.05
6	122.00	21	19.66
7	30.44	22	128.72
8	32.26	23	128.11
9	52.07	24	46.66
10	36.99	25	29.96
11	21.94	26	20.44
12	38.79	27	21.79
13	43.24	28	23.90
14	57.50	29	12.90
15	23.90		

Trans-13-docasenoic acid (NA-II)

Elution of the column with pet. ether:benzene (85:15) furnished colourless amorphous powder of compound NA-II recrystallized from methanol, 18 mg (0.004%), R_f 0.43 (pet. ether:benzene 3:1), m.p. 60-61°C, UV λ_{max} 238 nm (log ε 4.5); IR (KBr): 3490, 2816, 2848, 1705, 1640, 1463, 1409, 1164, 1099, 1018, 719 cm^{-1}; ^{1}H NMR (C_6D_6): δ 5.34 (2 H, m, H-13, H-14), 2.37 (2H, d, *J* = 7.5 Hz, H_2-2a), 2.37 (1H, d, *J* = 7.5 Hz, H_2-2a), 2.31 (1 H, d, *J* = 7.5 Hz, H_2-2b), 2.01 (2H, m, H_2-12), 1.63 (2H, m, H_2-15), 1.25 (30H, br s, 15×CH_2), 0.85 (3H, t, *J* = 6.6 Hz, Me-22); ^{13}C NMR (DMSO-d_6): δ 180.21 (C-1), 130.82 (C-11), 130.01 (C-12), 34.58 (C-2), 32.27 (C-10), 30.56 (C-13), 29.73 (10 × CH_2), 26.24 (CH_2), 25.38 (CH_2), 23.89 (CH_2), 22.26 (CH_2), 19.90 (CH_2), 14.74 (CH_3-22); +ve FABMS *m/z* (rel. int.) 338 $[M]^+$ ($C_{22}H_{42}O$) (46.8), 199 (13.6), 180 (913.5), 154 (71.2), 139 (23.6), 124 (31.8).

n-Hexacos-14-enoic acid (NA-III)

Elution of the column with benzene gave colourless amorphous powder of compound NA-III recrystallized from methanol, 14 mg (0.003%), R_f 0.62 (benzene: chloroform 9:1), m.p. 263-265°C, IR (KBr): 3450, 2918, 2850, 1707, 1635, 1463, 1296, 1205, 1016, 941, 721 cm^{-1}; ^{1}H NMR ($CDCl_3$): δ 5.50 (1 H, m, H-14), 5.48 (1H, m, H-15), 2.91 (1H, d, *J* = 6.0 Hz, H_2-2a), 2.87 (1 H, d, *J* = 6.0 Hz, H_2-2b), 2.07 (2H, m, H_2-13), 2.03 (2H, m, H_2-16), 1.48 (2 H, m, CH_2), 1.32 (32 H, br s, 16 × CH_2), 1.15 (4 H, m, 2 × CH_2), 0.89 (3H, t, *J* = 7.59 Hz, Me-26); ^{13}C NMR (C_6D_6): δ 179.31 (C-1), 133.23 (C-14), 130.31 (C-15), 33.97 (C-2), 32.33 (C-13), 30.17 (C-16), 29.83 (15 × CH_2), 29.46 (CH_2), 27.62 (CH_2), 26.41 (CH_2), 24.95 (CH_2), 23.11 (CH_2), 14.36 (CH_3-26); +ve FABMS *m/z* 394 $[M]^+$ ($C_{26}H_{50}O_2$) (43.8), 238 (41.7), 213 (27.2), 181 (12.7), 155 (22.1).

n-Hexacosanyl-*n*-decaniate (NA-IV)

Elution of the column with pet. ether:benzene 95:5 gave colourless crystals of compound NA-IV recrystallized from methanol, 61mg (0.014%), R_f 0.16 (pet. ether:benzene 95:5), m.p. 290-293°C; IR (KBr): 2934, 2854, 1736, 1459, 1375, 1245, 1175, 1019, 960, 799, 724 cm^{-1}; ^{1}H NMR ($CDCl_3$): δ 4.14 (1 H, d, *J* = 5.4 Hz, H_2-1′a), 4.09 (1H, d, *J* = 5.4 Hz, H_2-1′b), 2.30 (1H, d, *J* = 6.6 Hz, H_2-2a), 2.26 (1 H, d, *J* = 6.6 Hz, H_2-2b), 1.61 (2H, m, CH_2), 1.35 (2H, m, CH_2), 1.28 (10 H, br s, 5×CH_2), 1.25 (20 H, br s, 10 × CH_2), 1.23 (8 H, br s, 4× CH_2), 0.87 (3H, t, *J* = 6.1 Hz, Me-26′); ^{13}C NMR ($CDCl_3$): δ 171.37 (C-1), 60.24 (C-1′), 34.50 (CH_2), 32.02 (CH_2), 29.80 (15 × CH_2), 29.56 (5 × CH_2), 29.46 (4 × CH_2), 29.36 (4 × CH_2), 25.09 (CH_2), 22.79 (CH_2), 14.35 (Me-10), 14.21 (Me-26′); +ve ion FABMS *m/z* (rel. int.) 536 $[M]^+$ ($C_{26}H_{72}O_2$) (19.9), 171 (36.8), 155 (53.6).

n-Hexacos-17-enoic acid (NA-V)

Elution of the column with pet. ether:benzene 50:50 furnished colourless crystals of compound NA-V recrystallized from methanol, 52 mg (0.012%), R_f 0.1(pet. ether:benzene 1:3), m.p. 262-265°C; IR (KBr): 3160, 2922, 2853, 1709, 1635, 1462, 1412, 1378, 1290, 1080, 940, 723 cm^{-1}; ^{1}H NMR (DMSO-d_6) : δ 5.32 (1 H, m, H-17), 5.27 (1H, m, H-18), 2.75 (1H, d, *J* = 4.8 Hz, H_2-2a), 2.72 (1 H, d, *J* = 4.8 Hz, H_2-2b), 2.21 (2H, m, H_2-16), 1.98 (2H, m, H_2-19), 1.54 (2 H, m, H_2-3), 1.29 (16 H, br s, 8 × CH_2), 1.25 (20 H, br s, 10× CH_2), 0.85 (3H, t, *J* = 6.3 Hz, Me-26′); ^{13}C NMR ($CDCl_3$) : δ 174.68 (C-1), 129.42 (C-17), 127.57 (C-18), 33.73 (CH_2), 31.46 (CH_2), 31.03 (CH_2), 29.24 (18×CH_2), 29.09 (CH_2), 28.87 (CH_2), 28.80 (CH_2), 28.75 (CH_2), 28.71 (CH_2), 28.68 (CH_2), 26.71 (CH_2), 25.18 (CH_2), 24.54 (CH_2), 27.22 (CH_2), 22.10 (CH_2), 13.81 (CH_2-26); +ve ion FABMS *m/z* (ret. int.) 394 $[M]^+$ ($C_{26}H_{50}O_2$) (27.8), 281 (25.2), 25 (70.6), 139 (37.1).

n-Hexacos-11-enoic acid (NA-VI)

Elution of the column with benzene:chloroform 85:15, 75:25, 50:50 (fraction nos. 331-445) gave colourless crystals of compound NA-VI recrystallized from methanol, 21 mg (0.005%), R_f 0.91 (chloroform:methanol 5:1), m.p. 240-242°C; IR (KBr): 3350, 2924, 2854, 1711, 1640, 1463, 1378, 1210, 1172, 1016, 965, 722 cm^{-1} ; ^1H NMR ($CDCl_3$): δ 5.39 (1 H, m, H-11), 5.32 (1H, m, H-12), 2.77 (1H, d, J = 4.8 Hz, H_2-2a), 2.75 (1 H, d, J = 4.8 Hz, H_2-2b), 2.34 (2H, m, H_2-10), 2.01 (2H, m, H_2-13), 1.61 (2 H, m, CH_2), 1.30 (10 H, br s, 5 × CH_2), 1.25 (26 H, br s, 13 × CH_2), 0.88 (3H, t, J = 6.1 Hz, Me-26′); ^{13}C NMR ($CDCl_3$): δ 179.1 (C-1), 130.11 (C-11), 127.99 (C-12), 34.01 (CH_2), 32.01 (CH_2), 31.61 (CH_2), 29.78 (11×CH_2), 29.52 (CH_2), 29.44 (CH_2), 29.33 (CH_2), 29.16 (CH_2), 27.29 (CH_2), 25.71 (CH_2), 24.78 (CH_2), 22.77 (CH_2), 14.20 (Me-26); +ve ion FABMS *m/z* (ret. int.) 394 $[M]^+$ ($C_{26}H_{50}O_2$) (13.6), 223 (11.2), 197 (26.7), 171 (22.8).

References

1 Bhattacharjee S K & De L C, *Medicinal herbs and flowers* (Awishkar Publishers and Distributors, Jaipur, India) **1991**, 12.

2 Vasudeva N & Sharma S K, *J Ethanopharmacol,* 107, **2006**, 179.

3 Wadhwa V, Singh M M, Gupta D N, Singh C & Kamboj P, *Planta Medica*, 3, **1986**, 231.

4 Shibeshi W, Makonnen E, Zerihun L & Debella A, *Afr Health Science,* 6, **2006**, 108.

5 Pakrashi A & Bhattacharya N, *Indian J Experiment Biol*, 15, **1977**, 856.

6 Paul D, Bera S, Jana D, Maiti R & Ghosh D, *Contraception,* 73, **2006**, 284.

7 Katewa S S & Arora A, *Indian Drugs,* 38, **2001**, 332.

8 Mali R G, Hundiwale J C, Gatvi R S, Patil K S & Kulkarni M V, *J Natural Remedies*, 6/2, **2006**, 115.

9 Akhtar M S & Iqbal J, *J Ethnopharmacol,* 31, **1991**, 49.

10 Chakarborty A, Brantner A, Mukainaka T, Nobukuni Y, Kuchide M, Konoshima T, Tokuda H & Nishino H, *Cancer Lett,* 177, **2002**, 1.

11 Olaf K, Ernest H, Martin G S, Josef R, Franz B, Efrem M, Dawit A & Asfaw D, *Monatshefte fuer Chemie,* 131, **2000,** 195.

12 Banerji A, Chintalwar G I, Joshi N K & Chadha M S, *Phytochem,* 10, **1971,** 2225.

13 Banerji A & Chadha M S, *Phytochem,* 9, **1970**, 1671.

14 Kapoor V K & Singh H, *Indian J Chem*, 4, **1966,** 461.

15 Basu N, K, *J Proc Inst Chem,* 29, **1957**, 73.

16 Hariharan V & Rangaswami S, *Phytochem*, 9, **1970**, 409.

17 Seshadri V, Batla A K & Rangaswami S, *Indian J Chem*, 20B, **1981**, 773.

18 Srivastava S, Gupta M, Verma R K, Singh S C & Kumar S. *J Indian Chem Soc,* 79, **2002**, 286.

19 Misra T N, Singh R S, Pandey H S, Parsad C & Singh S, *Indian J Chem,* 35B, **1996**, 637.

20 Misra T N, Singh R S, Pandey H S, Parasad C & Singh B P, *Phytochem*, 33, **1993**, 221.

21 Misra T N, Singh R S, Pandey H S, Prasad C & Singh B P, *Phytochem,* 31, **1992**, 1811.

22 Misra T N, Singh, H S, Pandey H S & Prasad C, *Phytochem,* 1991; 30: 2076-2078.

23 Ali M, *Orient J Chem* 9, **1993**, 84.

24 Ali M, *Techniques in terpenoid isolation* (Birla Publisher, Delhi) **2001**.

25 Greca M D, Monaco P & Privitera L, *J Nat Prod,* 53(6), **1990,** 1430.