

ALCOHOLS FROM WHOLE PLANT OF *LYCHNIS CORONARIA* L

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Article Received on: 04/11/10 Revised on: 20/11/10 Approved for publication: 01/12/10

ABSTRACT

Petroleum ether extract of whole plant of *Lychnis coronaria* L. (Caryophyllaceae) afforded new aliphatic alcohols characterized as *n*-Octacosanol (**1**), *n*-Nonacosanol (**2**), *n*-Tetracontanol (**3**) and Nonadecan-4,10-diene, 6-one, 1-ol (**4**). Their structures were established on the basis of spectral analysis.

KEYWORDS: *Lychnis coronaria* L, Octacosanol, *n*-Nonacosanol, *n*-Tetracontanol and Nonadecan-4,10-diene, 6-one, 1-ol.

INTRODUCTION

Lychnis coronaria L. (Caryophyllaceae) is a small herb and grows abundantly in Kashmir at Dachigam, below Gulmarg, Aharbal and wooded hill side at 8000 ft. It is also commonly known as “Rose champion” or “Mullein pink”^{1,2}. It is a white wooly herb, 30 to 75cm high, with spatulate to oblong-lanceolate leaves. Purplish, flowers on long stalk, calyx 2 to 2.5 cm long conical^{3,4}. The literature survey reveals that various parts of *L. coronaria* have been used as a folklore medicine for curing various ailments like disease of leprosy, diarrhoea, lungs and liver and also as a remedy for Beri-beri⁵. Decoction of the roots has been used in Spain for liver and lung complaints, and for infraction of the lymph glands and the mesentery¹. The plant extract was found to possess anti-inflammatory⁶, and antihepatotoxic⁷ properties. Hot aqueous extract from the aerial parts of the plant has been used for the treatment of hemorrhoids⁸.

Extensive studies have been carried out on *L. coronaria*. Three compounds have been isolated from the leaves of *L. coronaria* butanol extract. These compound were obtained after separation by thin-layer and 2-dimensional paper chromatography and were identified as pinitol, isoscoparin and feruloyl glucose by spectral data, hydrolysis, and acetylation. The presence of two glycosylflavones has been detected by spectral and chemical methods. The structure of glycosylflavones that have been detected are O- α -L-rhamnosylderivative and β -D-glucopranosyl flavone⁹. From the water-sol. part of the MeOH ext. from the leaves of *L. coronaria*, coumarins, saponins, and tannins were extracted. Coumarins and saponins were obtained in the CHCl₃ and Butanol extracts and tannins were seprated by polyamide sorbent¹⁰. The presence of 2-methyl butyl amine in *L. coronaria* was reported for the first time using chromatographic technique¹¹. Eleven compounds have also been isolated from ethanolic extract: triclin 7-O-glucopyranoside, (+)-isoscoparin, epoxyactinidionoside, 20 Rhydroxyecdysone, ecdysterone, polypodingB, ecdysterone 22-O- β -D-glucopyranoside, stigmast-5-ene-3-one, taraxerol, α -tocopherol and dehydrodiconiferyl alcohol-4-O- β -D-glucopyranoside¹¹. Qualitative analysis of alcoholic extract of *L. coronaria* leaves yielded coumarins, saponins and tannins¹². Glucose, galactose, mannose, xylose, arabinose and uronic acids were also found¹³. The present study gives an account of various aliphatic alcohols which were isolated from petroleum ether extract of *L. coronaria*.

MATERIALS AND METHODS

General experimental procedures

All the solvents are of Analytical grade Melting point was determined on Metler 9100 Electro thermal apparatus by open capillary method and are uncorrected. The IR spectra were recorded on KBr pellets on PYE UNICAM Spectrophotometer; Mass spectra on a Finnegan MAT 300 Mass Spectrophotometer; ^1H NMR on Bruker DRX 400 Spectrometer in CDCl_3 using TMS as internal standard reference, chemical shift in δ (ppm) and J values in Hz. Ultra Violet (UV) spectra were recorded on Beckman DU-64 Spectrophotometer in chloroform.

Plant material

The whole plant of *L. coronaria* was collected in the month of August from local areas of Aharbal, Srinagar (J&K) and authenticated by taxonomist. The voucher specimen (LC-FP-17) of the plant has been kept in the herbarium of Jamia Hamdard for further reference.

Extraction and isolation

The whole plant of *L. coronaria* (500 g) was crushed to coarse powder and then extracted successively by petroleum ether, chloroform and methanol using soxhlet apparatus till completely exhausted. The extracts thus obtained were dried under reduced pressure to yield 30, 45 and 75 gm of petroleum ether, chloroform and methanol extract respectively. Petroleum ether extract 20gm was dissolved in little solvent and adsorbed on the silica gel (60-120 mesh) for the preparation of slurry. It was then dried, packed on the top of silica gel column packed in petroleum ether. The column was then eluted with petroleum ether, chloroform and methanol successively in the order of increasing polarity. The fractions showing same TLC profile were combined together to isolate the following compounds as mentioned in Table No.1.

Compound characteristics

Compound – 1 occurs as white flakes, 20mg, m.p: 56-58°C; R_f : 0.67 (CHCl_3 -MeOH : 8:2); UV: λ_{max} 241, 265, 276 (sh) nm; IR (KBr): ν_{max} 3398 (OH), 2916 (CH_3), 2848 (CH_2), 1473, 1060 (C-O), 728, 719 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 0.82 (3 H, m, CH_3 -28), 1.18 (52 H, brs, 26 x CH_2 -), 3.56 (2 H, dd, $J = 6.0\text{Hz}$, $-\text{CH}_2$ -OH); EIMS (probe) 70 eV, m/z % (rel. int): 413(M^+ , $\text{C}_{28}\text{H}_{58}\text{O}$), 10%], 393.2 (100%), (71.9), 103.1 (100).

Compound – 2 occurs as white amorphous powder, 84mg, m.p: 70-72°C; R_f : 0.61 (Pet. Ether- CHCl_3 , 8:2); UV: λ_{max} 233, 236nm; IR (KBr): ν_{max} 3469 (OH), 2919 (CH_3), 2850 (CH_2), 1734 (C=O), 802 (C=C), 1022 (C-O), 861, 720 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 0.81 (3 H, m, $J = 6.0\text{Hz}$, CH_3 -19), 1.18 (24 H, brs, 7 x CH_2 -12-18, 3 x CH_2 - 7-9, 2 x CH_2 -2-3), 3.55 (2 H, m, $J = 6.0\text{Hz}$, $-\text{CH}_2$ -OH), 5.28 (1 H, ddd, $J = 6.0\text{Hz}$, =CH-4), 5.09 (1 H, ddd, $J = 6.0\text{Hz}$, =CH-5). 4.24 (1 H, ddd, $J = 6.0\text{Hz}$, =CH-10). 4.09 (1 H, ddd, $J = 6.0\text{Hz}$, =CH-11); EIMS (probe) 70 eV, m/z % (rel. int): 294 (M^+ , $\text{C}_{19}\text{H}_{34}\text{O}_2$) (10), 274 (26), 181 (16), 155 (27), 113 (11).

Compound – 3 occurs as yellow buff coloured amorphous solid, 38mg, m.p: 62-64°C; R_f : 0.60 (CHCl_3 -pet. Ether, 7:3); UV: λ_{max} 243, 275 (sh) nm; IR (KBr): ν_{max} 3398 (OH), 2916 (CH_3), 2848 (CH_2), 1470, 1462 (C-O), 1061, 729, 719 cm^{-1} ; ^1H NMR (CDCl_3): δ 0.80 (3 H, m, CH_3 -29), 1.25 (54 H, brs, 27 x CH_2 -2-28), 3.32 (2 H, dd, $J = 6.0\text{Hz}$, $-\text{CH}_2$ -OH); EIMS (probe) 70 eV, m/z % (rel. int): 423[M^+] ($\text{C}_{29}\text{H}_{60}\text{O}$), (36.6%).

Compound – 4 occurs as yellow buff coloured amorphous powder, 42mg, m.p: 67-69°C; R_f : 0.59 (CHCl_3 -Pet.ether, 8:2); UV: λ_{max} 275 (sh), 242 nm; IR (KBr): ν_{max} 3450 (OH), 2917 (CH_3), 2849 (CH_2), 1470, 956 (C-O), 729, 720 cm^{-1} ; ^1H NMR (CDCl_3): δ 1.10 (3 H, m, CH_3 -40), 1.16 (76 H, brs, 38 x CH_2 -2-39), 3.82 (2 H, dd, $J = 6.0\text{Hz}$, $-\text{CH}_2$ -OH); EIMS (probe) 70 eV, m/z % (rel. int): 579 [M^+] ($\text{C}_{40}\text{H}_{82}\text{O}$), (36.6%).

RESULT AND DISCUSSION

Compound 1 was obtained as white flakes from CHCl_3 eluants. It did not give color test for steroids and terpenes indicating it to be a fatty alcohol. Its IR showed absorption bands for hydroxyl group (3398 cm^{-1}), methyl group (2916 cm^{-1}) and long aliphatic chain (782, 719 cm^{-1}). It did not respond to bromine water test for unsaturation. Its Mass spectrum displayed a molecular ion peak at m/z 413 consistent with

molecular formula of an aliphatic alcohol $C_{28}H_{58}O$. The 1H NMR spectrum of compound **-1** showed two one-proton doublet at δ 3.56 ($J=6.0$ Hz) assigned to oxygenated methylene protons of C-1. The methylene protons appeared as 52-proton broad signal at δ 1.18. A three-proton multiplet at δ 0.82 was assigned to Me-28 terminal primary methyl protons. A single proton of hydroxyl group of C-1 appeared at δ 7.2. The ^{13}C NMR spectrum of compound **-1** exhibited important signals for oxygenated methylene carbons at C-1 at δ 63.11 and a primary methyl carbon C-28 at δ 14.12. All the methylene carbons resonate between δ 32.83-22.70. On the basis of above discussion the structure of compound **1** has been elucidated as *n*-octacosanol.

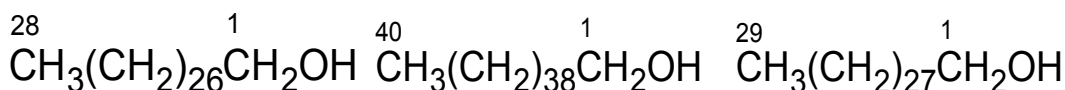
Compound 2 was obtained as white amorphous powder, had molecular formula $C_{19}H_{34}O_2$ as determined on the basis of Mass spectra (M^+ 294) and ^{13}C NMR spectrum. It did not give color test for steroids and terpenes indicating it to be a fatty alcohol. The IR spectrum exhibited absorption bands of hydroxyl group (3469 cm^{-1}), methyl group (2919 cm^{-1}), methylene groups (2850 cm^{-1}), carbonyl group (1743 cm^{-1}), olefinic linkage (820 cm^{-1}) and C-O alcoholic groups (1022 cm^{-1}). The 1H NMR spectrum exhibited peaks at δ 0.81 (3 H, *d*, $J = 6.0$ Hz, CH_3 -19) indicating one methyl group in the molecule. The 1H NMR spectrum also displayed a broad peak at δ 1.18 (24 H, brs, 7 x CH_2 -12-18, 3 x CH_2 -7-9, 2 x CH_2 -2-3) due to twelve methylene groups, which could be assigned at C-12 to C-18, C-7 to C-9, C-2 to 3. The peaks at δ 4.09 (1 H, ddd, $J = 6.0$ Hz, $>CH$ -11) and δ 4.24 (1 H, ddd, $J = 6.0$ Hz, $>CH$ -10) indicated the presence of an olefinic linkage between C-10 and C-11. The peaks at δ 5.09 (1 H, ddd, $J = 6.0$ Hz, $>CH$ -5) and δ 5.28 (1 H, ddd, $J = 6.0$ Hz, $>CH$ -4) indicated the presence of another olefinic linkage between C-5 and C-4. The peak at δ 3.55 (2 H, m, $J = 6.0$ Hz, $-CH_2-OH$ -1) was assigned to the alcoholic methylene group at positioned C-1.

The structure of the compound-**2** was also further confirmed on the basis of mass fragmentation pattern, which exhibited prominent peaks at m/z 294 due to molecular ion peak, m/z 279 due to elimination methyl group, m/z 181 due to further elimination of seven CH_2 groups, m/z 155 due to further elimination of olefinic linkage at C-10, m/z 113 due to further elimination of three CH_2 groups. Peaks at m/z 85 due to elimination of carbonyl group, m/z 59 due to further elimination of olefinic linkage, m/z 31 due to elimination of two methyl groups. The peak at m/z 31 due to elimination of terminal $-CH_2-OH$ was also obtained. The position of one hydroxyl group was assigned at C-1 on the basis of above mass spectrum fragmentation pattern. Thus on the basis of these findings the structure of compound **2** was established as nonadecan-4,10-diene, 6-one, 1-ol.

Compound 3 was obtained as buff yellow amorphous powder from $CHCl_3$ eluants. Its IR showed absorption bands at 3398 (OH), 2916 (CH_3), 2848 (CH_2) and long aliphatic chain at 729, 719 cm^{-1} . It did not respond to bromine water test for unsaturation. Its Mass spectrum displayed a molecular ion peak at m/z 423 consistent with molecular formula of an aliphatic alcohol $C_{29}H_{60}O$. The 1H NMR spectrum of compound **2** showed one-proton doublet at δ 3.32 ($J=6.0$ Hz) assigned to oxygenated methylene protons of C-1. The methylene protons appeared as 54-proton broad signal at δ 1.25. A three-proton multiplet at δ 0.82 was assigned to Me-29 terminal primary methyl protons. A single proton of hydroxyl group of C-1 appeared at δ 7.1. The ^{13}C NMR spectrum of compound **3** exhibited important signals for oxygenated methylene carbons at C-1 at δ 63.10 and a primary methyl carbon C-29 at δ 14.12. All the methylene carbons resonate between δ 32.81-22.69. On the basis of above discussion the structure of compound **3** has been elucidated as *n*-nonacosanol.

Compound 4 was obtained as buff yellow amorphous powder from $CHCl_3$ eluants. Its IR showed absorption bands at 3450 (OH), 2917 (CH_3), 2849 (CH_2) and long aliphatic chain at 729, 720 cm^{-1} . It did not respond to bromine water test for unsaturation. Its Mass spectrum displayed a molecular ion peak at m/z 579 consistent with molecular formula of an aliphatic alcohol $C_{40}H_{82}O$. The 1H NMR spectrum of compound **4** showed one-proton doublet at δ 3.82 ($J=6.0$ Hz) assigned to oxygenated methylene protons of C-1. The methylene protons appeared as 76-proton broad signal at δ 1.16. A three-proton multiplet at δ 1.1 was assigned to Me-40 terminal primary methyl protons. A single proton of hydroxyl group of C-1 appeared at δ 8.5. The ^{13}C NMR spectrum of compound **4** exhibited important signals for oxygenated methylene carbons at C-1 at δ 65.73 and a primary methyl carbon C-40 at δ 15.45. All the methylene

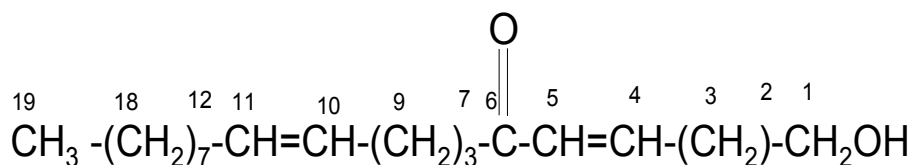
carbons resonate between δ 35.73-24.01. On the basis of above discussion the structure of compound 4 has been elucidated as *n*-tetracontanol.



n-Octacosanol

n-Tetracontanol

n-Nonacosanol



Nonadecan-4, 10-diene, 6-one, 1-ol.

ACKNOWLEDGEMENTS

The authors are thankful to the Head Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Jamia Hamdard University, New Delhi for providing necessary research facilities and to Prof. A. R. Naqshi (Dept. of Botany, University of Kashmir, Srinagar, India for identifying the plant material.

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Table No. 1: Alcohols isolated from whole plant of *Lychnis coronaria*

Name	Polarity	m.p (°C)	Mol. Formula/ Mol. Wt.	IUPAC Name
1	CHCl ₃ -MeOH (8:2)	56-58	C ₂₈ H ₅₈ O 413	<i>n</i> -Octacosanol
2	Pet. Ether-CHCl ₃ , (8:2)	70-72	C ₁₉ H ₃₄ O ₂ 294	Nonadecan-4, 10-diene, 6-one, 1-ol.
3	CHCl ₃ -pet. Ether, (7:3)	62-64	C ₂₉ H ₆₀ O 423	<i>n</i> -Nonacosanol
4	CHCl ₃ -Pet.ether, (8:2)	67-69	C ₄₀ H ₈₂ O 579	<i>n</i> -Tetracontanol

Source of support: Nil, Conflict of interest: None Declared