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Phytochemical investigation of flowers of *Rosa damascena* Mill

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Abstract

Rosa damascena Mill. (Rosaceae) has been appreciated for decorative, fragrance, cosmetics, food and folklore medicines to treat abdominal and chest pains, menstrual bleeding, digestive problems, constipation and to strengthen the heart. It is regarded as a symbol of affection, belief and magnificence. Phytochemical investigation of a methanolic extract of *R. damascena* flowers led to the isolation of four new compounds identified as *n*-cosan-5 β -ol (1), (*cis*)- 6, 10, 14-trimethylpentadec-3-en-7 β ,11 β -diol (damascene, 2), 7-hydroxy-4-(3'-methyl butanol)- coumarin- 3- en-one (rosacoumarin, 3) and cedr-6-en-12-ol-14-oic acid (rosacedrenic acid, 4). The structures of these compounds have been established on the basis of spectral data analysis and chemical means.

Keywords: *Rosa damascene*, flowers, phytoconstituents, Isolation, characterization

1. Introduction

Rosa damascena Mill. (Rosaceae), commonly known as Gole Mohammadi, Gul-e-Surkh (in Persian), Ward-e-Ahmar (in Arabic), Damascus rose or Otto rose (in English) and Gulab (in Hindi) [1-2], is a well-known ornamental plant, referred as the king of flowers having more than 200 species throughout the world [3]. The name of *R. damascena* is derived from the city name Damascus, Syria, where it exists as a wild plant. It is distributed in China, India, Middle East, North America and Europe and cultivated in different countries around the world. The Bulgarian and Taif rose flowers are known for the production of high quality rose essential oils [4]. Rose is the symbol of love, purity, faith and beauty since ancient times [5]. Traditionally it is used to treat abdominal and chest pains, menstrual bleeding, digestive problems, depression, nervous stress, skin problems, headache and as an anti-inflammatory and cardiotoxic [6]. Rose water is useful as an antiseptic agent for eye washing, mouth disinfecting and as antispasmodic to relieve the abdominal pains and bronchial and chest congestions [7-8]. A flower decoction is taken as a diuretic and to relieve fever, breast pain and menstrual problems. The rose petals are cooked with sugar or honey and ingested as a refrigerant [5]. Its rose petals are acrid, aromatic, aphrodisiac, appetizer, bitter, cardiotoxic, expectorant, febrifuge, laxative, refrigerant and tonic; used to alleviate leprosy, eye infections and excessive perspiration [9]. It is added as a chief ingredient in various polyherbal Unani formulation used as an antiobesity, cardio-protective, hepatoprotective, blood diseases and skin disorders [2, 10].

Potential bioactive compounds *viz.*, roxyloside A, isoquercitrin, afzelin, cyanidin-3-O- β -glucoside, quercetin gentiobioside, damaurones, rugaurone, maritimein, tetrahydroxyaurone, tetrahydroxy-dimethoxyaurone, siamaurone, damaurone B and flavonol glycosides have been reported from the plants [11-13]. The rose essential oil was consisted mainly of phenyl ethyl alcohol, citronellol, nonadecane, geraniol, nerol, heneicosane, nonadecane, tricosane, citronellal, citral, carvone, citronellyl acetate, eugenol, ethanol, farnesol, nonanol, nonanal, phenyl acetaldehyde, phenylmenthyl acetate and phenyl geraniol [14-18]. In this communication isolation and characterization of new phytoconstituents have been targeted from flowers of *R. damascena* procured from Delhi.

2. Materials and Methods

2.1. Materials

All chemicals were procured from Sigma-Aldrich unless otherwise stated. Melting points were determined on a thermoelectrically heated Perfit apparatus without correction. The IR spectra were measured in KBr pellet on a Bio-Red FT-IR spectrophotometer. UV spectra were obtained in methanol with a Lambda Bio 20 spectrophotometer. The ¹H (300 MHz) and ¹³C (75 MHz) NMR spectra were recorded on Bruker DRX 300 MHz instrument with TMS as an internal standard. Mass spectra were performed on a Jeol D-300 (EI/CI) system. Column chromatographic separations were carried out on silica gel (Merck, 60-120 mesh).

Pre-coated silica gel plates (Merck, Silica gel 60 F₂₅₄) were used for analytical thin layer chromatography and the spots were visualized by exposure to iodine vapors and UV radiations and spraying with ceric sulphate solution.

2.2 Methods

2.2.1 Plant Material

The flowers of *R. damascena* were procured from a local market, Khari Baoli, New Delhi and identified by Prof. M. P. Sharma, Department of Botany, Jamia Hamdard. A specimen voucher of the drug was deposited in the herbarium of the Phytochemistry Research Laboratory, Faculty of Pharmacy, Jamia Hamdard.

2.2.2 Preparation of Extract and Isolation

The pulverized flowers (1kg) were extracted exhausted with methanol using a Soxhlet extractor. The combined extracts were dried under reduced pressure to obtain a dark brown residue (190 g). The residue (100 g) was dissolved in minimum amount of methanol and adsorbed on silica gel column grade (60-120 mesh) to obtain a slurry. The slurry was dried in air and chromatographed over silica gel column loaded in chloroform. The column was eluted with chloroform and chloroform-methanol (99:1, 49:1, 93:7, 19:1, 3:1, 1:1, 1:3 v/v) in order of increasing polarity to isolate the following compounds 1-4.

2.3 *n*-Cosan-5 β -ol (1)

Elution of the column with chloroform gave a colorless amorphous powder of 1, recrystallized from chloroform-methanol (1:1), 92 mg, m. p. 73-74 °C; IR ν_{\max} (KBr): 3435, 2920, 2840, 1402, 1098, 794, 725 cm⁻¹. ¹H NMR (CDCl₃): δ 3.54 (1H, brm, $w_{1/2}$ = 16.3 Hz, H-5 α), 1.55 (2H, m CH₂), 1.34 (2H, m CH₂), 1.29 (6H, brs, 3 x CH₂), 1.25 (24H, m, 12 x CH₂), 0.83 (3H, t, J = 6.2 Hz, Me-1), 0.79 (3H, t, J = 6.8 Hz, Me-20); ¹³C NMR (CDCl₃): δ 66.11 (C-5), 38.30 (CH₂), 34.1 (CH₂), 30.83 (CH₂), 29.62 (8 x CH₂), 29.55 (CH₂), 29.42 (CH₂), 29.33 (CH₂), 27.72 (CH₂), 25.26 (CH₂), 22.59 (CH₂), 14.70 (C-20), 14.67 (C-1). EIMS m/z (rel. int.): 298 [M]⁺ (C₂₀H₄₂O) (6.9), 283 (7.5), 255 (10.3), 241 (15.3), 213 (7.8), 211 (16.6), 199 (6.7), 185 (11.2), 155 (12.6), 149 (19.6), 129 (16.7), 111 (15.8), 99 (16.1), 97 (27.2), 87 (13.6), 85 (73.2), 83 (27.1), 71 (74.3), 57 (100), 43 (93.8).

2.4 Damescanol (2)

Further elution of the column with chloroform afforded a colorless amorphous powder of 2, 181 mg, m. p. 69 - 71 °C; UV λ_{\max} (MeOH): 215 nm (log ϵ 3.1); IR ν_{\max} (KBr): 3430, 2952, 2853, 1635, 1462, 1378, 1253, 1168, 1097 cm⁻¹; ¹H NMR (CDCl₃): δ 5.31 (1H, m, $w_{1/2}$ = 8.9 Hz, H-3), 5.28 (1H, m, $w_{1/2}$ = 8.7 Hz, H-4), 3.73 (1H, brs, $w_{1/2}$ = 18.8 Hz, H-11), 3.47 (1H, brs, $w_{1/2}$ = 17.1 Hz, H-7 α), 2.53 (2H, m, H₂-5), 2.06 (1H, m, H₂-2), 1.99 (1H, m, H-6), 1.49 (1H, m, H-14), 1.44 (1H, m, H-10), 1.23 (6H, brs, H₂-8, H₂-9, H₂-12), 1.08 (2H, m, H₂-13), 0.88 (3H, d, J = 6.4 Hz, Me-16), 0.86 (3H, d, J = 6.2 Hz, Me-15), 0.83 (3H, d, J = 6.5 Hz, Me-18), 0.74 (3H, d, J = 6.1 Hz, Me-17), 0.65 (3H, t, J = 6.1 Hz, Me-1); ¹³C NMR (CDCl₃): δ 13.96 (C-1), 30.29 (C-2), 115.11 (C-3), 129.66 (C-4), 32.76 (C-5), 54.84 (C-6), 76.87 (C-7), 29.05 (C-8), 28.75 (C-9), 52.47 (C-10), 76.90 (C-11), 25.59 (C-12), 24.46 (C-13), 47.10 (C-14), 19.07 (C-15), 18.62 (C-16), 17.03 (C-17), 16.08 (C-18); EIMS m/z (rel. int.): 284 [M]⁺ (C₁₈H₃₆O₂) (3.6), 255 (5.1), 227 (43.8), 213 (98), 199 (7.1), 185 (6.2), 157 (9.8), 151 (12.3), 143 (8.3), 137 (19.8), 129 (13.1), 127 (8.9), 125 (11.8), 121 (40.3), 111 (15.3), 109 (19.3), 101 (20.1), 97

(36.2), 95 (37.8), 83 (42.3), 81 (44.1), 71 (30.6), 69 (70.1), 57 (58.1), 55 (100), 43 (80.2).

2.5 Rosacoumarin (3)

Elution of the column with chloroform-methanol (49:1) yielded pale yellow crystals of 3, recrystallized from chloroform-methanol (1:1), 394 mg, m. p. 157-159 °C; UV λ_{\max} (MeOH): 278, 320 nm (log ϵ 5.2, 2.1); IR ν_{\max} (MeOH): 3434, 2924, 2854, 1710, 1615, 1530, 1451, 1377, 1231, 1044 cm⁻¹; ¹H NMR (DMSO-d₆): δ 6.95 (1H, d, J = 7.6 Hz, H-5), 6.89 (1H, dd, J = 7.6, 3.0 Hz, H-6), 6.83 (1H, d, J = 3.0 Hz, H-8), 6.80 (1H, s, H-3), 3.65 (1H, d, J = 9.3 Hz, H₂-1'a), 3.55 (1H, d, J = 9.3 Hz, H₂-1'b), 2.48 (1H, m, H-3'), 1.28 (2H, m, H₂-2'), 0.89 (3H, d, J = 6.5 Hz, Me-4'), 0.86 (3H, d, J = 6.3 Hz, Me-5'); ¹³C NMR (DMSO-d₆): δ 167.60 (C-2), 128 (C-3), 165.45 (C-4), 115.47 (C-4a), 138.51 (C-5), 119.42 (C-6), 165.46 (C-7), 108.83 (C-8), 145.53 (C-8a), 62.74 (C-1'), 29.03 (C-2'), 47.04 (C-3'), 15.16 (C-4'), 14.03 (C-5'); EIMS m/z (rel. int.): 248 [M]⁺ (C₁₄H₁₆O₄) (46.7), 206 (10.1), 203 (29.3), 184 (32.6), 177 (5.3), 153 (100), 126 (36.1), 107 (32.3), 87 (53.4), 71 (5.5), 55 (65.5), 43 (78.9).

2.6 Rosacedrenoic acid (4)

Elution of the column with chloroform-methanol (19:1) furnished colorless crystals of 4, recrystallized from acetone - methanol (1:1) 118 mg, m. p. 56-57 °C; UV λ_{\max} (MeOH): 221 nm (log ϵ 4.2); IR ν_{\max} (KBr): 3455, 3426, 2926, 2854, 1709, 1636, 1463, 1376, 1245, 1175, 1096, 1032 cm⁻¹; ¹H NMR (DMSO-d₆): δ 5.28 (1H, s, H-7), 3.55 (2H, d, J = 10.2 Hz, H₂-12), 2.48 (1H, brm, $w_{1/2}$ = 12.8 Hz, H-11 α), 2.26 (1H, brm, $w_{1/2}$ = 11.9 Hz, H-4 α), 1.98 (1H, brm, $w_{1/2}$ = 11.6 Hz, H-1 α), 1.48 (2H, brm, H₂-9), 1.26 (6H, brs, CH₂-2, CH₂-3, CH₂-10), 1.21 (3H, s, Me-13), 0.87 (3H, d, J = 6.2 Hz, Me-15); ¹³C NMR (DMSO-d₆): δ 29.01 (C-1), 28.67 (C-2), 22.07 (C-3), 33.26 (C-4), 33.49 (C-5), 131.71 (C-6), 129.57 (C-7), 51.10 (C-8), 27.21 (C-9), 26.56 (C-10), 31.28 (C-11), 60.07 (C-12), 24.41 (C-13), 176.38 (C-14), 13.88 (C-15); EIMS m/z (rel. int.): 250 [M]⁺ (C₁₅H₂₂O₃) (3.5), 204 (7.6), 189 (7.7), 183 (5.9), 165 (7.2), 153 (13.3), 150 (29.6), 143 (9.6), 139 (10.1), 138 (14.3), 121 (23.6), 113 (10.5), 111 (19.3), 110 (20.6), 109 (15.9), 107 (17.2), 97 (36.5), 85 (20.2), 81 (38.1), 67 (33.2), 56 (100).

3. Results and Discussion

The compound 1 showed IR absorption bands for hydroxyl group (3435 cm⁻¹) and long aliphatic chain (794, 721 cm⁻¹). Its mass spectrum displayed a molecular ion peak at m/z 298 corresponding to a molecular formula of saturated aliphatic alcohol, C₂₀H₄₂O. Generation of prominent ion peaks at m/z 241, 57 [C₄-C₅ fission]⁺ and 211, 87 [C₅-C₆ fission]⁺ indicated the location of hydroxyl group at C-5. The ¹H NMR spectrum of 1 showed a one-proton broad multiplet at δ 3.54 with half width of 16.3 Hz ascribed to α -oriented carbinol H-5 proton. Two three-proton triplets at δ 0.83 (J = 6.2 Hz) and 0.79 (J = 6.8 Hz) were accounted to terminal C-1 and C-20 primary methyl protons, respectively. Two multiplets at δ 1.55 (2H), and 1.34 (2H), and two broad singlets at δ 1.29 (6H), and 1.25 (24H) were associated with the methylene protons.

The ¹³C NMR spectrum of 1 displayed signals for carbinol carbon at δ 66.11 (C-5), methylene carbons between δ 38.30 - 22.59 and methyl carbons at δ 14.70 (C-20) and 14.67 (C-1). The absence of any signal beyond δ 3.54 in ¹H NMR and 66.11 in ¹³C NMR spectra supported the saturated nature of the molecule. On the basis of these evidences the structure of 1 was elucidated as *n*-cosan-5 β -ol.

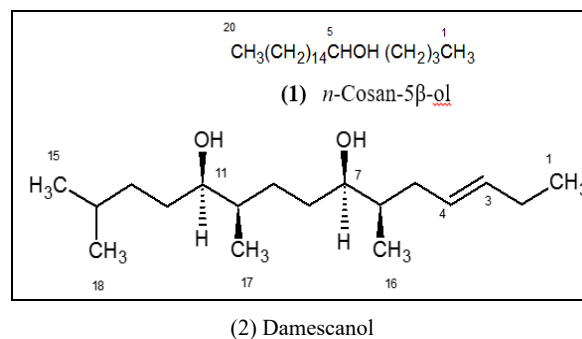
The compound 2, named Damescanol, had IR absorption

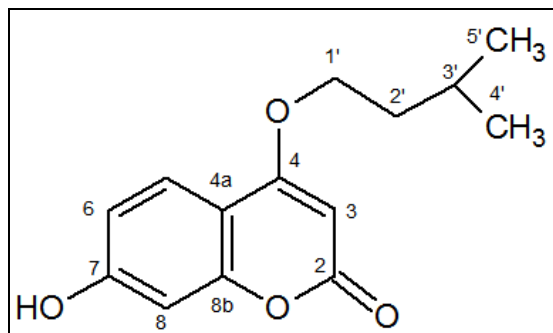
bands for hydroxyl groups (3430 cm^{-1}) and unsaturation (1635 cm^{-1}). Its mass spectrum showed a molecular ion peak at m/z 284 corresponding to a molecular formula to an acyclic norditerpenic diol, $\text{C}_{18}\text{H}_{36}\text{O}_2$. The generation of prominent ion peaks at m/z 255 [$\text{M} - \text{C}_2\text{H}_5$, $\text{C}_2\text{-C}_3$ fission] $^+$, 55 [$\text{C}_4\text{-C}_5$ fission, C_4H_7] $^+$ and 69 [$\text{C}_5\text{-C}_6$ fission, C_5H_9] $^+$ suggested the presence of the vinylic linkage at C-3. The ion peaks arising at m/z 97 [$\text{C}_6\text{-C}_7$ fission, C_7H_{13}] $^+$, 151 [$\text{M} - 97 - 2\text{H}_2\text{O}$ fission] $^+$, 157, 127 [$\text{C}_7\text{-C}_8$ fission] $^+$, 109 [$127\text{-H}_2\text{O}$] $^+$, 143 [$\text{C}_8\text{-C}_9$ fission, $\text{C}_9\text{H}_{19}\text{O}$] $^+$, 125 [$143\text{-H}_2\text{O}$] $^+$, 129 [$\text{C}_9\text{-C}_{10}$ fission, $\text{C}_8\text{H}_{17}\text{O}$] $^+$, 111 [$129\text{-H}_2\text{O}$] $^+$, and 137 [$\text{M} - 129 - \text{H}_2\text{O}$] $^+$ supported the location of hydroxyl group at C-7^[19]. The ion fragments formed at m/z 101 [$\text{C}_{10}\text{-C}_{11}$ fission, $\text{C}_6\text{H}_{13}\text{O}$] $^+$, 43 [$\text{C}_{13}\text{-C}_{14}$ fission, C_3H_7] $^+$, and 83 [$101\text{-H}_2\text{O}$] $^+$ indicated the existence of another hydroxyl group at C-11 and isopropyl group at terminal position of the carbon chain. The ^1H NMR spectrum of 2 showed two one-proton multiplet at δ 5.31 ($w_{1/2} = 8.9\text{ Hz}$) and 5.28 ($w_{1/2} = 8.7\text{ Hz}$) assigned to *cis*- oriented vinylic H-3 and H-4 protons, respectively. Two one-proton multiplets at δ 3.73 and 3.47 with half widths of 18.8 Hz and 17.1 Hz, respectively, were attributed correspondingly to α -oriented carbinol H-11 α and H-7 α protons. A two-proton broad singlet at δ 2.53 and two one-proton multiplets at δ 2.06 and 1.99 were ascribed to methylene H₂-5 and H₂-2 protons, adjacent to the vinylic linkage. Four three-proton doublets at δ 0.88 ($J = 6.4\text{ Hz}$, Me-16), 0.86 ($J = 6.2\text{ Hz}$, Me-15), 0.83 ($J = 6.5\text{ Hz}$, Me-18) and 0.74 ($J = 6.1\text{ Hz}$, Me-17) and a three-proton triplet at δ 0.65 ($J = 6.1\text{ Hz}$, Me-1) were associated with correspondingly secondary C-16, C-15, C-18 and C-17 and primary C-1 methyl protons, all located on saturated carbons. The remaining methylene and methine protons resonated between δ 2.04-1.08. The ^{13}C NMR spectrum of 2 displayed signals for vinylic carbons at δ 115.11 (C-3) and 129.66 (C-4), carbinol carbons at δ 76.87 (C-7) and 76.90 (C-11) and methyl carbons at δ 13.96 (C-1), 19.07 (C-15), 18.62 (C-16), 17.03 (C-17) and 16.08 (C-18). On the basis of these evidences the structure of 2 has been established as (*cis*)-6, 10, 14-trimethylpentadec-3-en-7 β , 11 β -diol, a new norditerpenic diol.

Compound 3, designated as rosacoumarin, exhibited UV absorption maxima for a coumarin at 232 and 335 nm^[20-21] and IR absorption bands for hydroxyl group (3434 cm^{-1}), carbonyl group (1710 cm^{-1}) and unsaturation (1615 , 1530 cm^{-1}). Its molecular ion peak was established at m/z 248 on the basis of mass and ^{13}C NMR spectra consistent to a molecular formula of a coumarin derivative, $\text{C}_{14}\text{H}_{16}\text{O}_4$. The ion fragments arising at m/z 71 [$\text{C}_{1'} - \text{O}$ fission] $^+$ and 177 [$\text{M} - 71$] $^+$ indicated attachment of an isopentyl chain to the coumarin unit. The ^1H NMR spectrum of 3 showed a one-proton doublet at δ 6.95 ($J = 7.6\text{ Hz}$), assigned to *ortho*-coupled aromatic H-5 proton. A one-proton doublet at δ 6.89 ($J = 7.6$, 3.0 Hz), a one-proton doublet at δ 6.83 ($J = 3.0\text{ Hz}$) and a one-proton singlet at δ 6.80 were ascribed to aromatic *ortho*, *meta*-coupled H-6, *meta*-coupled H-8 and H-3 protons, respectively. Two one-proton doublets at δ 3.65 ($J = 9.3\text{ Hz}$) and 3.55 ($J = 9.3\text{ Hz}$) were associated with H₂-1' oxy-methylene protons. Two three-proton doublets at δ 0.89 ($J = 6.5\text{ Hz}$) and 0.86 ($J = 6.3\text{ Hz}$) were accounted to secondary C-4' and C-5' methyl protons, respectively. A two-proton multiplet at δ 2.48 was attributed to methine H-3' proton. The ^{13}C NMR spectrum of 3 exhibited signals for carbonyl carbon at δ 167.60 (C-2), aromatic carbons in the range of δ 165.45 -

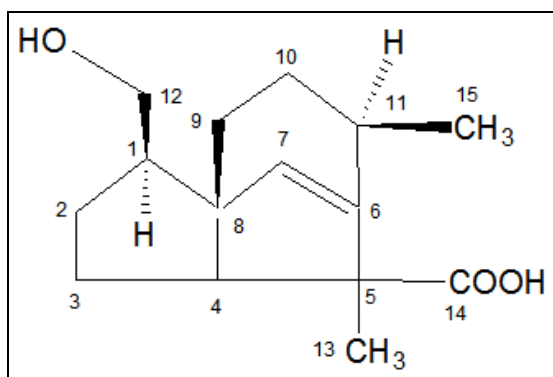
108.83, oxymethylene carbon at δ 62.74 (C-1') and methyl carbons at δ 15.16 (C-4') and 14.03 (C-5'). The ^1H and ^{13}C NMR values of the coumarin were compared with the reported data of other coumarins^[22-24]. On the basis of this discussion the structure of 3 has been established as 7-hydroxy-4-(3'-methyl butanol)-coumarin-3-en-one, a new coumarin derivative.

Compound 4, designated as rosacedrenoic acid, produced effervescence with sodium bicarbonate solution and decolorized bromine water indicating the presence of carboxylic acid group and unsaturation in the molecule. Its IR spectrum exhibited characteristic absorption bands for hydroxyl group (3455 cm^{-1}), carboxylic group (3426 , 1709 cm^{-1}) and unsaturation (1636 cm^{-1}). Its molecular ion peak was determined on the basis of mass and ^{13}C NMR spectra at m/z 250 consistent to a molecular formula of the cedrene-type sesquiterpenes, $\text{C}_{15}\text{H}_{22}\text{O}_3$. The important ion fragments appearing at the m/z 72 [$\text{C}_{3,4}\text{-C}_{1,8}$ fission] $^+$, 165, 85 [$\text{C}_{4,5}\text{-C}_{1,8}\text{-C}_{4,8}$ fission] $^+$, 121 [165-CO_2] $^+$, 153, 97 [$\text{C}_{4,5}\text{-C}_{8,9}$ fission] $^+$, 67 [$97\text{-CH}_2\text{OH}$] $^+$, 109 [153-CO_2] $^+$, 138 [$153\text{-Me-C}_{8,7}$] $^+$, 111, 139 [$\text{C}_{4,5}\text{-C}_{10,11}$ fission] $^+$, 110 [125-Me] $^+$, 81 [125-CO_2] $^+$, and 143, 107 [$\text{C}_{4,5}\text{-C}_{6,11}$ fission] $^+$ supported the existence of the hydroxyl methylene group at the C-1 and methyl and carboxylic groups at C-5. The ion peaks generating at m/z 56 [$\text{C}_{8,9}\text{-C}_{6,11}$ fission] $^+$, 81, 169 [$\text{C}_{8,9}\text{-C}_{5,6}\text{-C}_{8,7}$ fission] $^+$, 67, 183 [$\text{C}_{9,10}\text{-C}_{7,8}\text{-C}_{5,6}$ fission] $^+$, 204 [M-HCOOH] $^+$, 189 [204-Me] $^+$, 150 [$183\text{-Me-H}_2\text{O}$] $^+$ suggested the location of the vinylic linkage at C-6 and another methyl group at C-11^[25]. The ^1H NMR spectrum of 4 showed a deshielded one-proton singlet at δ 5.28 assigned to vinylic H-7. A two-proton doublet at δ 3.55 ($J = 10.2\text{ Hz}$) was ascribed to hydroxymethylene H₂-12 protons. Three one-proton multiplets at δ 2.48 ($w_{1/2} = 12.8\text{ Hz}$), 2.26 ($w_{1/2} = 11.9\text{ Hz}$) and 1.98 ($w_{1/2} = 11.6\text{ Hz}$) were accounted α -oriented methine H-11, H-4 and H-1 protons, respectively. A three-proton doublets at δ 0.87 ($J = 6.2\text{ Hz}$) was associated with C-15 secondary methyl protons. A six-proton broad singlet at δ 1.26 was ascribed to three methylene protons. A three-proton singlet at δ 1.21 was due to tertiary C-13 methyl protons. A two-proton multiplet δ 1.48 was due to methylene H₂-9 protons. The ^{13}C NMR spectrum of 4 exhibited important signals for vinylic carbons at δ 131.71 (C-6) and 129.59 (C-7), hydroxymethyl carbon at δ 60.07 (C-12), carboxylic carbons at δ 176.38 (C-14) and methyl carbons at δ 24.41 (C-13) and 13.88 (C-15). The ^1H and ^{13}C NMR spectra of the compound were compared with the reported values of cedrenes^[26-28]. On the basis of this discussion the structure of 4 has been established as cedr-6-en-12-ol-14-oic acid, a new sesquiterpene.





(3) Rosacoumarin



(4) Rosacedrenoic acid

4. Conclusion

The isolated secondary metabolites are valuable as they will provide necessary information for the further researchers as an effective analytical marker, identity, purity and quality control of this plant in future.

5. Acknowledgement

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