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NOTE

A New Flavonoidal Constituent from *Taraxacum officinale* (L.) Weber

RAJ NATH YADAVA* and SHIRIN KHAN

Natural Products Laboratory, Department of Chemistry, Dr. H.S. Gour Central University, Sagar-470 003, India

*Corresponding author: E-mail: rnyadava@rediffmail.com

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A new flavone glycoside (A) m.p. 265-268 ºC, m.f. $C_{33}H_{40}O_{21}$, $[M]^+$ 742 (FABMS), has been isolated from stem of *Taraxacum oficinale* (L.) Weber. It was characterized as 3,5,7,3',4'-pentahydroxy 8-C methyl flavone 7-O-β-D-xylopyranosyl (1→4)O-β-D glucopyranosyl 3'-O-α-L-rhamnopyranoside alongwith known compound ladanein B by various chemical degradations and spectral analysis.

Key Words: *Taraxacum officinale* (L.) Weber, Compositae, Stem, Flavone glycoside.

Taraxacum oficinale (L.) Weber[1-3] belongs to family Compositae. It is commonly known as 'Kanphool or Kukraundha' in Hindi. It is found in Himalayas and the Khasi Hills of Meghalaya, Mishmi Hills of Arunachal Pradesh and hills of South India at 3000-5000 m and Gujarat. It used in the treatment of kidney and liver problems. It is also useful in chromic diseases of the digestive organs especially hepatic affections and jaundice. It is used to make dandelion wine and the greens are used in salad. Earlier workers[4,5] have reported various constituents from this plant. In the present paper, we report the isolation and structural elucidation of a new flavone glycoside 3,5,7,3',4'-pentahydroxy 8-C methyl flavone 7-O-β-D-xylopyranosyl (1→4) O-β-D glucopyranosyl 3'-O-α-L-rhamnopyranoside (A) along with one known compound ladanein (B) from methanolic extract of the stems of this plant.

All the m.p. were determined on a thermoelectrical melting point apparatus and are uncorrected. The IR spectra were recorded in KBr disc. ^{1}H NMR spectra were recorded at 300 MHz in $CDCl_3$ using TMS as internal standard. ^{13}C NMR spectra were recorded at 90 MHz using $CDCl_3$ as solvent and mass spectra on a Jeol D 300 mass spectrometer.

The stem of *Taraxacum oficinale* (L.) Weber were collected from Patharia hills of Sagar district and authenticated by Department of Botany, Dr. H.S. Gour University, Sagar, India.

Isolation of compounds: Air dried and powdered stems (3 kg) of the plant were extracted with methanol. The methanol soluble fraction was concentrated under reduced pressure to give brown viscous mass (1.95 g). It gave two spots on TLC examination indicating it to be mixture of two compounds A and B. These compounds were separated by TLC and purified by column chromatography over silica gel and studied separately.

Study of compound A: It has m.p. 265-268 ºC, m.f. $C_{33}H_{40}O_{21}$, $[M^+]$ *m/z* 742. Found: C, 51.70; H, 5.17 calcd. for $C_{33}H_{40}O_{21}$ C, 51.75; H, 5.12 %. UV-VIS (MeOH): λ_{max} nm 262, 268, 276, 284, 364; IR (KBR, ν_{max}, cm^{-1}): 3438, 2891, 2855, 1731, 1657, 1620, 1568, 1446, 1388, 1347, 2865, 1083, 1024; ^{1}H NMR (300 MHz $CDCl_3$): δ 12.13 (1H, s, 5-OH), 3.87 (3H, s, 8-Me), 6.73 (1H, d, *J* 2.4 Hz, H-6), 8. 64 (1H, s, 3'-OH), 8.72 (1H, s, 4'-OH), 7.18 (1H, d, *J* 2.1 Hz, H-2'), 6.80 (1H, d, J 8.4 Hz, H-5'), 7.14 (1H, d, *J* 8.2, Hz, H-6'), 5.20 (1H, d, *J* 1.7 Hz, H-1"), 3.21-3.80 (4H, m, H-2", 3", 4", 5"), 3.82 (1H, dd, *J*, 12.0, 2.2 Hz, H-6"), 4.96 (1H, d, *J* 7.4 Hz, H-1'"), 3.33 (1H, m, H-2'"), 3.35 (1H, m, H-3'"), 3.35 (1H, m, H-4'"), 3.24 (2H, m, H-5'"), 5.28 (1H, d, *J* 7.8 Hz, H-1""), 4.12 (1H, dd, *J* 1.6, 3.6, Hz H-2""), 3.85 (1H, dd, *J*, 3.6,9.0 Hz, H-3""), 3.72 (1H, d, *J* 9.0 Hz, H-4""), 3.56 (1H, m, 5"") 1.88 (3H, d, *J* 5.8 Hz, H-6""); ^{13}C NMR (300 MHz, $CDCl_3$): δ 162.0 (C-2), 102.6 (C-3), 184.8 (C-4), 162.5 (C-5), 101.5 (C-6), 163.9 (C-7), 96.4 (C-8), 158.1 (C-9), 105.6 (C-10), 130.3 (C-1'), 117.3 (C-2'), 129.2 (C-3'), 132.7 (C-4'), 116.6 (C-5'), 123.9 (C-6'), 104.9 (C-1"), 78.6 (C-3"), 76.5 (C-5"), 76.0 (C-2"), 74.7 (C-4"), 68.0 (C-6"), 103.8 (C-1'"), 73.5 (C-2'"), 75.8 (C-3'"), 72.0 (C-4'"), 78.2 (C-5'"), 105 (C-1""), 78.4 (C-3""), 77.6 (C-5""), 75.6 (C-2""), 73.1 (C-4""), 62.9 (C-6"").

Acid hydrolysis of compound A: Compound A (100 mg) was dissolved in ethanol (20 mL) and refluxed with 10 mL of 10 % H_2SO_4 on water bath for 4 h. The reaction mixture was concentrated and allowed to cool and give compound **A-1** as aglycone which was identified as 3,5,7,3',4'-pentahydroxy 8

C-methyl flavone by comparison of its spectral data with reported literature values. The aqueous hydrolysate was neutralized with $BaCO_3$ and the $BaSO_4$ was filtered off. The filtrate was concentrated and subjected to paper chromatography examination using nBAW (4:1:5) solvent system and sugar were identified as L-rhamnose (R_f 0.37), D-xylose (R_f 0.25) and D-glucose (R_f 0.19), (Co-PC and Co-TLC).

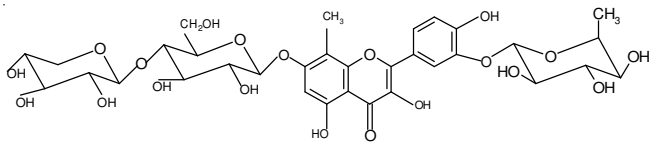
Study of Compound Aglycone (A-1): It has m.f. $C_{15}H_{12}O_7$, m.p 245-247 ºC, $[M]^+$ 304, found (%) C 59.28, H 3.88, calcd. for m.f. $C_{15}H_{12}O_7$, C 59.20, H 3.94; UV λ_{max} (nm) 275, 288, 340; IR (KBr, ν_{max}, cm^{-1}); 3297, 1646, 1600, 1520, 1461; ^{1}H NMR (300 MHz,$CDCl_3$): δ 11.7 (1H, s, C-5-OH), 5.00 (1H, d, *J* 11.5 Hz, H-2), 4.60 (1H, d, *J* 11.5 Hz, H-3), 5.98 (1H, d, *J* 2.0 Hz, H-6), 5.93 (1H, d, *J* 2.0 Hz, H-8), 7.05 (1H, d, *J* 1.9 Hz, H-2'), 6.85 (1H, d, *J* 8.1 Hz, H-5') 6.90 (1H, dd, *J* 8.1, 1.9 Hz, H-6'); ^{13}C NMR (300 MHz, $CDCl_3$) δ 85.09 (C-2); 73.64 (C-3); 198.37 (C-4); 164.27 (C-5); 97.29 (C-6); 168.72 (C-7); 96.27 (C-8); 164.47 (C-9); 101.79 (C-10); 129.82 (C-1'); 115.85 (C-2'); 146.28 (C-3'); 147.11 (C-4'); 116.05 (C-5'); 120.88 (C-6');

Permethylation of compound A: Compound A (40 mg) was refluxed with CH_3I (5 mL) and Ag_2O (20 mg) in DMF (25 mL) for 2 h and then filtered. The filtrate was hydrolyzed with 10 % ethanolic H_2SO_4 for 5 h. to give methylated aglycone identified 3,5,4'-trimethoxy 8C-methyl flavone and methylated sugars which were identified as 2,3,4-*tri*-O-methyl-L-rhamnose (R_f 0.37), 2,3,6-*tri*-O-methyl-D-glucose (R_f 1.0) and 2,3,4-*tri*-O-methyl-D-xylose (R_f 0.94).

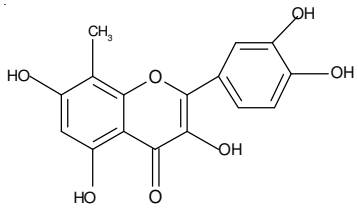
Enzymatic hydrolysis of compound A: Compound A (25 mg) was dissolved in MeOH (10 mL) and hydrolyzed with equal volume of takadiastase enzyme. The reaction mixture was allowed to stay at room temperature for 2 days and filtered off. The proaglycone and hydrolysate were studied separately.

The hydrolyzate was concentrated and subjected to paper chromatography examination using nBAW (4:1:5) as solvent system and aniline hydrogen phthalate as a spraying reagent which showed the presence of L-rhamnose (R_f 0.37). The proaglycone was dissolved in MeOH (20 mL) further hydrolyzed with equal volume of almond emulsin at room temperature as usual procedure yielded aglycone identified 3,5,7,3',4'-pentahydroxy 8C-methyl flavone and sugars were identified as D-xylose (R_f 0.26) and D-glucose (R_f 0.19) (Co-PC and Co-TLC).

Study of compound B: It has m.p. 214-216 ºC, m.f. $C_{17}H_{14}O_6$, $[M^+]$ *m/z* 314. Found: C 64.96; H 4.45 calcd. for $C_{17}H_{14}O_6$ C, 65.75; H, 4.55 %; UV:(MeOH) λ_{max} (nm) 274, 327; (+NaOH) 276, 365; (+$AlCl_3$) 260, 293, 350; (+HCl) 261, 302, 350; (+NaOAc) 275, 364; (+H_3BO_3) 279, 335. ^{1}H NMR (300 MHz $CDCl_3$): δ 12.78 (1H, s, 5-OH), 10.45 (1H, s, 6-OH), 6.90 (1H, s, H-3), 6.70 (1H, s, H-8), 8.05 (1H, d, *J* 8.9 Hz, H-2'), 7.12 (2H, d, *J* 8.9 Hz, H-3'), 7.10 (2H, d, *J* 8.7 Hz, H-5'), 8 (1H, d, *J* 8.8 Hz, H-6'), 3.91 (3H, s, OMe), ^{13}C NMR (300 MHz $CDCl_3$) δ (ppm): 162.90 (C-2), 103.45 (C-3), 183.02 (C-4), 152.09 (C-5), 130.92 (C-6), 61.27 (6-OMe), 157.70 (C-7), 93.04 (C-8), 151.89 (C-9), 103.99 (C-10), 123.64 (C-1'), 128.65 (C-2'), 11.20 (C-3'), 161.82 (C-4'), 11.10 (C-5'), 128.60 (C-6'), 54.78 (4'- OMe).



(A)



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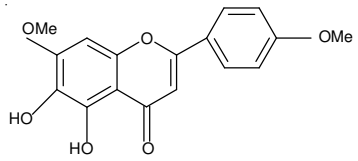

(B)

Structures of A, A-1, B

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