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A BETULINIC ACID GLYCOSIDE FROM *SCHEFFLERA VENULOSA*

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Key Word Index—*Schefflera venulosa*; Araliaceae; triterpenic glycoside; betulinic acid.

Abstract—A new betulinic acid glycoside, lup-20(29)-en-28-oic-3-*O*-*β*-D-glucopyranosyl (2→1)-*O*-*β*-D-glucopyranoside has been characterized from the leaves of *Schefflera venulosa*.

INTRODUCTION

Extracts of different *Schefflera* species are used in the treatment of liver and rheumatic heart diseases [1] and in asthma [2]. We report the analysis and characterization of some known compounds together with the identification of a new betulinic acid glycoside from the leaves of *S. venulosa*.

RESULTS AND DISCUSSION

The ethanolic extract of the leaves of *S. venulosa* gave compound **1**, $C_{42}H_{68}O_{13}$, found to have a M_r of 780 from the appearance of a protonated $[M]^+$ at *m/z* 781 in its FAB mass spectrum. Peaks were observable at *m/z* 619 $[M+H-\text{hexose}]^+$ and at 457 $[M+H-2\text{ hexose}]^+$. It was hydrolysed with 10% HCl and the precipitated sapogenin filtered and purified by the usual K-salt method. This was identified as betulinic acid by IR, preparation of its acetyl and methyl derivatives and comparison with literature values [3, 4]. The hydrolysate revealed the presence of D-glucose only. The permethyl-ether of saponin **1a**, prepared by Kuhn's method, on methanolysis and subsequent hydrolysis yielded 2,3,4,6-tetra-*O*-methyl-D-glucose and Wallenfel's positive [5] 3,4,6-tri-*O*-methyl-D-glucose, indicating C-2 of the inner glucose as the point of linkage. Enzymatic hydrolysis of the saponin with *β*-glucosidase released glucose conforming *β*-linkage in the glucose. Therefore, the new saponin was characterized as lup-20(29)-en-28-oic-3-*O*-*β*-D-glucopyranosyl (2→1)-*O*-*β*-D-glucopyranoside.

EXPERIMENTAL

Defatted powdered leaves (6 kg) were exhaustively extracted with EtOH and the extract concd *in vacuo*. The residue (200 g) was fractionated by CC over silica gel (BDH, 100–120 mesh) with C_6H_6–EtOAc (4:1) first to isolate oleanolic acid and oleanonic acid; and then with $CHCl_3$–MeOH (4:1) to isolate *β*-sitosterol-*β*-D-glucoside and saponin (200 mg). Compound **1** was recrystallized from MeOH, mp 262–264° (dec). (Found: C, 64.93; H, 8.83; $C_{42}H_{68}O_{13}$ requires C, 64.61; H, 8.72%).

Acidic hydrolysis of **1**. Compound **1** (100 mg) was hydrolysed by refluxing with 10% HCl–MeOH (1:1, 20 ml) for 4 hr at 100°. The product were poured into H_2O, the ppt. sepd and purified by the K-salt method. It recrystallized from $CHCl_3$ as crystals, mp 314–317°, $[\alpha]_D^{25}+15°$ (pyridine). (Found: C, 78.83; H, 10.63; $C_{30}H_{48}O_3$ requires: C, 78.94; H, 10.52%). IR ν_{max}^{KBr} cm^{-1}: 3400, 1690, 1640, 1460, 1392, 1372, 890. UV λ_{max}^{EtOH} nm, 250. Acetate $C_{30}H_{48}O_2OCOMe$, mp 290–292°; Me ester $C_{31}H_{50}O_3$, mp 221–222°. ^1H NMR ($CDCl_3$): 0.74 (3H), 0.76 (3H), 0.90 (3H), 1.10, (3H), 1.15 (3H), 1.76 (3H), 2.1 (1H), 3.62 (3H), 4.69 (2H). MS *m/z* 470 $[M]^+$ (6). The hydrolysate was neutralised with Ag_2CO_3; the filtrate showed the presence of D-glucose only (PC, EtOAc–pyridine–H_2O (10:4:3), aniline hydrogen phthalate spray reagent, authentic sample run in parallel).

Permethylation of compound **1** *and hydrolysis of* **1a**. Compound **1** (50 mg) was treated with MeI (2 ml) and Ag_2O in DMF (3 ml) for 48 hr at room temp. The mixt. was filtered and the residue washed with a little DMF. The filtrate was evapd to dryness and the residue refluxed with 2 M HCl–MeOH (10 ml) for 3 hr and the concd aq. hydrolysate subjected to PC (*n*-BuOH–EtOH–H_2O, (5:1:4), to identify 2,3,4,6-tetra-*O*-methyl-D-glucose and 3,4,6-tri-*O*-methyl-D-glucose (R_G 1.0 and 0.84, respectively).

Enzymatic hydrolysis of compound **1**. Compound **1** (10 mg) in NaOAc buffer (pH 4.8–5.0) was treated with *β*-glucosidase (20 mg) at 37° for 24 hr. The soln was filtered and the filtrate checked by PC to show the presence of D-glucose only.

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