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*NOTE*

# Flavonoids from *Psidium guaijava*

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The leaves of *Psidium guaijava* yielded a new flavonol glycoside: queretin 4′-glucuronoide, and its known derivatives: 3-sulphate, 3-glucoside, 3-rhamnoside, also kaempferol, 3-sulphate and 1,3,5-trihydroxybenzoic acid were found.

Earlier phytochemical investigation on the flavonoids in *Psidium guaijava* L. (Myrtacae) revealed the presence of only 3-arabinopyranoside and 3-arabinofuranoside of quercetin. The previous conclusion, that only two flavonoid compounds are present in *P. guaijava*[1], needs to be revised in the light of results of the present study, in which one new and four known flavonoid compounds have been isolated together with the phenolic compound, 1,3,5-trihydroxybenzoic acid.

Two-dimensional paper chromatography (PC) of the aqueous ethanol extract of the fresh leaves of *P. guijava* revealed glycosylated flavonoids, together with a phenolic compound. Paper chromatography followed by purification using Sephadex LH-20 afforded six pure compounds.

Acid hydrolysis of compound [1] gave quercetin and glucuronic acid identified by CoPC and authentic samples.

The UV spectral data of the new compound [1] in the presence of standard reagents for flavonoid analyses established free hydroxyl groups at the 3, 5, 7, and 3′ positions[2]. The sodium methoxide spectrum exhibited a bathochromic shift and a decrease in intensity for band 1 relative to methanol spectrum[2,3]; sodium acetate spectrum also gave a bathochromic shift +13 nm relative to band II and +5 nm relative to band I indicating the free 7 position. Colour was unchanged under UV light before and after hydrolysis (yellow) typical for a 3-O-free flavonol, which upon hydrolysis gave a flavonol aglycone (quercetin) and a sugar (glucuronic acid).

THe $^1$H NMR spectrum of [1] in DMSO-$d_6$ confirmed the suggested structure as the spectrum exhibted two protons as doublets at 6.2 ppm and 6.4 (J = 2.5 Hz), typical for H-6 and H-8, one proton as doublet at 6.81 ppm (J = 8.5 Hz) for H-5′, one proton as double doublet at 7.81 ppm (J = 8.5 Hz and 2.5 Hz) for H-6′ and one proton as doublet at 7.51 ppm (J = 2.5 Hz) for H-2′. Furthermore, there was only one anomeric proton signal of a sugar moiety attached to a flavonoid skeleton (doublet at 5.49 ppm, J = 8.0 Hz).

$^{13}$C NMR spectrum showed all signals for flavonoid part same as in quercetin except carbon no. 4′ which appeared slightly shifted upfield at 148.2 ppm which

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confirmed the substitution of the sugar to the position also the sugar carbon signals prove it to be glucuronic acid.

UV, $^1H$ NMR and $^{13}C$ NMR established the substitution of the sugar moiety at 4′ position, further confirmation using MS spectrum which gave the molecular weight of compound [1] at m/e 477 (negative FABMS for M-1). Together these data established [1] to be quercetin 4′-O-glucuronoide as a new natural flavonoid compound. The other known compounds were identified by direct TLC, PC comparison and from spectral data in the literature.[4,5]

For PC, Whatman (3 MM) with MeOH for elution.

Plant material: leaves were collected in August 1995 from Giza, identified by Bolous.[6] A voucher specimen is deposited in the Herbarium of the NRC. Air-dried leaves (2 kg) were extracted with $CHCl_3$ (then 50% EtOH (3 × 21) at room temp for 24 h each). Solvent was removed under vacuum to afford 80 g of conc. extract. The aqueous conc. extract was submitted to PPC using BAW (*n*-butanol-acetic acid-water) (4 : 1 : 5, upper layer); the developed chromatogram exhibited, under UV light, four brown, one yellow and one blue band. Further purification using Sephadex LH-20, $H_2O$ and MeOH as eluting solvents afforded five flavonoids and one phenolic compound.

3,5,7,3′-tetrahydroxyflavone 4′-O-glucuronoide; quercetin 4′-O-glucuroniode (1): Yellow amorphous powder; UV 260,355; + NaOMe: 269,394 (dec int) + $AlCl_3$ 270,420; + $AlCl_3$ + HCl: 260,355; NaOAc: 265,368; + NaOAc + $H_3BO_3$: 260,365

$^1H$ NMR (500 MHz, DMSO-$d_6$ TMS, δ ppm: 7.52 (1 H, d, J = 2.5 Hz, H-2′), 7.81 (1 H, dd, H-6), J = 8.5 Hz, 2.5 Hz), 6.81 (1H, d, j = 8.5 Hz), H-5′, 6.4 (1H, J = 2 Hz, H-8), 6.2 (1H, d, 1 = 2 Hz), 5.49 (1 H, d, J = 8.0 Hz, H-1″), 3.0–3.50 (4 H, m, sugar protons, H-2, H-3, H-4, H-5). $^{13}C$ NMR (125 MHz, DMSO-$d_6$, TMS, ppm) aglycone moiety: C-2 (156.2), C-3 (134.5), C-4 (177.7), C-5 (161), C-6 (98.4), C-7 (164.2), C-8 (93.9), C-9 (156), C-10 (104), C-1′ (120.4), C1-2′ (115.4), C-3′ (145), C-4′ (148.2), C-5′ (116.6), C-6′ (121.8), Sugar moiety, C-1″ (102), C-2″ (71.6), C-3″ (74), C-4″ (75.8), C-5″ (76.2), C-6″ (172).

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