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B R I E F C O M M U N I C A T I O N S

CONSTITUENTS OF *Ipomoea cairica* ETHANOLIC EXTRACT

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Aerial parts of *Ipomoea cairica* L. Sweet (*Convolvulaceae*), a folk medicinal plant found in Brazil and elsewhere, were collected at Governador Valadares, Minas Gerais, Brazil, in May, 2000, and a voucher specimen (No. BHCB 16525) was deposited at Herbarium of Natural History Museum of Universidade Federal de Minas Gerais. The plant material was dried, reduced to powder (3.297 g), and macerated with ethanol for seven days. The crude extract yielded 250 g after evaporation to dryness. The ethanolic extract (100 g) was partitioned in a triphasic mixture of hexane–acetonitrile–$CHCl_3$–H_2O (2:3.4:1:1). The aqueous layer yielded 57 g and part (37 g) was fractionated by silica gel CC using a gradient starting with CH_2Cl_2–MeOH–H_2O (80:20:1) with increasing polarity up to (10:90:12). The fraction eluted with CH_2Cl_2–MeOH–H_2O (45:55:8) was chromatographed on modified silica gel 60A (phosphate buffer (NaH_2PO_4/H_3PO_4)) [1] eluted with hexane:EtOAc (up to 100% EtOAc) and EtOAc:MeOH (up to 40% MeOH) to obtain **1** (9 mg) and **2** (36 mg) in fractions eluted with EtOAc–MeOH (95:5). Compounds **1** and **2** have been isolated from *I. cairica* for the first time.

3,5-Di-O-caffeoylquinic Acid (1). White powder; UV spectrum (MeOH, λ_{max}, nm): 218, 241, 300, 326 (log ε 2.27, 2.14, 2.29, 2.41). IR spectrum (KBr, ν, cm^{-1}): 1692, 1630 (C=O), 1515, 1445 (Ar). PMR (400 MHz, CD_3OD, δ, ppm, J/Hz): 2.14–2.24 (2H, m, H-2), 2.25–2.34 (2H, m, H-6), 3.97 (1H, dd, J_{trans} = 7.44, J_{cis} = 3.28, H-4), 5.36–5.45 (2H, m, H-3, H-5), 6.28 (1H, d, $J_{8''7''}$ = 16.00, H-8″, 6.36 (1H, d, $J_{8'7'}$ = 16.00, H-8′), 6.79 (2H, d, $J_{5'6'}$, $_{5''6''}$ = 8.16, H-5′, H-5″), 6.95–6.99 (2H, m, H-6′, H-6″), 7.08 (2H, s, H-2′, H-2″), 7.58 (1H, d, $J_{7''8''}$ = 16.32, H-7″), 7.61 (1H, d, $J_{7'8'}$ = 16.32, H-7′). ^{13}C NMR (100 MHz, CD_3OD): 36.0 (CH_2, C-6), 37.7 (CH_2, C-2), 70.7 (CH, C-4), 72.1 (CH, C-5), 72.6 (CH, C-3), 74.8 (C, C-1), 115.1 (CH, C-8″), 115.2 (CH, C-2″), 115.3 (CH, C-2′), 115.6 (CH, C-8′), 116.5 (2CH, C-5′, C-5″), 123.0, 123.1 (CH, C-6′, C-6″), 127.8, 127.9 (C, C-1′, C-1″), 146.7 (2C, C-7′, C-7″), 147.1, 147.3 (CH, C-3′, C-3″), 149.5, 149.6 (C, C-4′, C-4″), 168.6, 168.9 (C=O, C-9′, C-9″), 177.4 (C=O, C-7), according to previously published spectral data [2].

4,5-Di-O-caffeoylquinic Acid (2). White powder; (MeOH, λ_{max}, nm): 218, 242, 300, 326 (log ε 2.69, 2.56, 2.72, 2.81). IR spectrum (KBr, ν, cm^{-1}): 1700, 1630 (C=O), 1515, 1445 (Ar). PMR (400 MHz, CD_3OD, δ, ppm, J/Hz): 2.09–2.20 (2H, m, H-2), 2.22–2.32 (2H, m, H-6), 5.12 (1H, dd, J_{trans} = 10.00, J_{cis} = 2.96, H-4), 5.58–5.67 (1H, m, H-5), 4.36–4.39 (1H, m, H-3), 6.19 (1H, d, $J_{8''7''}$ = 15.88, H-8″), 6.27 (1H, d, $J_{8'7'}$ = 15.88, H-8′), 6.75 (1H, d, $J_{5'6'}$ = 8.16, H-5″), 6.76 (1H, d, $J_{5'6'}$ = 8.16, H-5′), 6.89–6.93 (2H, m, H-6′, H-6″), 7.01 (1H, d, $J_{2''6''}$ = 1.92, H-2″), 7.03 (1H, d, $J_{2'6'}$ = 1.92, H-2′), 7.51 (1H, d, $J_{7''8''}$ = 15.88, H-7″), 7.59 (1H, d, $J_{7'8'}$ = 15.88, H-7′). ^{13}C NMR (100 MHz, CD_3OD): 38.5 (CH_2, C-2), 39.5 (CH_2, C-6), 69.1 (CH, C-3), 69.5 (CH, C-5), 75.9 (CH, C-4), 76.2 (C, C-1), 114.8 (CH, C-8″), 114.9 (CH, C-8′), 115.4 (2CH, C-2′, C-2″), 116.7 (2CH, C-5′, C-5″), 123.3 (2CH, C-6′, C-6″), 127.8 (2C, C-1′, C-1″), 146.9 (2C, C-3′, C-3″), 147.8, 147.9 (CH, C-7′, C-7″), 149.8 (2C, C-4′, C-4″), 168.4, 168.8 (C=O, C-9′, C-9″), 177.0 (C=O, C-7). These data are consistent with previously published results [3]. Assignments were confirmed by COSY, HSQC, and HMBC.

REFERENCES

1. C. Balis and M. G. Payne, *Phytopathology*, **61**, 1477 (1971).
2. M. Lavault and P. Richomme, *Chem. of Nat. Comp.*, **40**, 118 (2004).
3. B. H. Um, M. Polat, A. Lobstein, B. Weniger, R. Aragon, L. Declercq, and R. Anton, *Fitoterapia*, **73**, 550 (2002).

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