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CHEMICAL CONSTITUENTS FROM THE INFLORESCENCES OF *Ouratea hexasperma*

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In the course of our phytochemical investigation of Brazilian plants, we have studied some species of *Ouratea*, *Luxemburgia*, and *Salvagesia* (Ochnaceae). The studies of *Ouratea* allowed us to identify many classes of compounds besides the flavonoid dimers [1–4]. In the northeast of Brazil *Ouratea* species are used in folk medicine for several purposes with the trivial name "batiputa oil" [5]. The present work reports the first phytochemical study of *O. hexasperma* inflorescences and identifies three steroids, a saponin, and five known active glycopyranosyl flavonoids. The yellow inflorescences of *O. hexasperma* were collected in the Tabuleiro Region, Joao Pessoa-PB, Brazil, and a voucher sample was deposited at Herbarium Lauro Pires Xavier, Joao Pessoa-PB by the botanist Maria de Fatima Agra. The flowers (350.0 g) were dried, powdered, and extracted with methanol at room temperature. The solvent was removed under vacuum to yield a residue (50.0 g). The crude methanol residue was suspended in MeOH–H_2O (9:1) and successively partitioned with hexane and ethyl acetate. Each fraction was chromatographed on a silica gel column eluted with binary mixtures of hexane–ethyl acetate–methanol in increasing polarity gradients besides the pure solvents and Sephadex LH-20 to yield compounds **1–9**. The compounds were investigated by spectroscopic methods, including NMR and mass spectrometry. The compounds were identified as campesterol (**1**), sitosterol (**2**), stigmasterol (**3**) [6], sitosterol β-D-glucopyranoside (**4**) [7, 8], rutin (**5**) [9], orientin (**6**) [10, 11], vitexin (**7**) [10, 11], swertisin (**8**) [12], and swertiajaponin (**9**) [12].

Orientin (6). Yellow powder. IR (KBr, ν_{max}, cm^{-1}): 3384, 3246 (ν_{O-H}), 1655 ($\nu_{C=O}$), 1614, 1508, 1428 (δ_{C-H}), 1094–1041 (ν_{C-O}). ^{1}H NMR (200 MHz, DMSO-d_6, ppm, δ, J/Hz): 13.17 (s, 5-OH), 7.50 (1H, dd, J_1 = 8.0, J_2 = 2.1, H-6′), 7.44 (1H d, J = 2.1, H-2′), 6.90 (1H, d, J = 8.2, H-5′), 6.65 (1H, s, H-3), 6.25 (1H, s, H-6), 4.72 (1H, d, J = 9.4, H-1″), 3.82 (1H, t, J = 9.4, H-2″), 3.24 (1H, m, H-3″), 3.37 (1H, t, J = 9.4, H-4″), 3.21 (1H, m, H-5″), 3.75 (2H, m, H-6″). ^{13}C NMR (50.3 MHz, DMSO-d_6, δ, ppm): 164.2 (C-2), 102.4 (C-3), 182.0 (C-4), 160.5 (C-5), 98.3 (C-6), 162.8 (C-7), 104.6 (C-8), 156.0 (C-9), 103.9 (C-10), 121.9 (C-1′), 114.1 (C-2′), 145.9 (C-3′), 149.9 (C-4′), 115.8 (C-5′), 119.4 (C-6′), 73.5 (C-1″), 70.9 (C-2″), 78.9 (C-3″), 70.8 (C-4″), 82.0 (C-5″), 61.8 (C-6″) [10, 11].

Vitexin (7). Yellow powder. ^{1}H NMR (200 MHz, DMSO-d_6, δ, ppm, J/Hz): 13.2 (s, 5-HO), 8.26 (2H, J = 8.7, H-2′, 6′), 7.05 (2H, d, J = 8.7, H-3′, 5′), 6.94 (1H, s, H-3), 6.44 (1H, s, H-6), 4.94 (1H, d, J = 9.8, H-1″), 3.82 (1H, t, J = 9.6, H-2″), 3.37 (1H t, J = 9.4, H-4″), 3.24 (1H m, H-3″), 3.21 (1H, m, H-5″), 3.75 (1H, br.d, J = 11.6, 2H-6″). ^{13}C NMR (50.3 MHz, DMSO-d_6, δ, ppm): 164.9 (C-2), 102.5 (C-3), 182.7 (C-4), 160.3 (C-5), 98.4 (C-6), 162.3 (C-7), 104.6 (C-8), 155.6 (C-9), 104.1 (C-10), 122.1 (C-1′), 128.9 (C-2′), 115.0 (C-3′), 161.3 (C-4′), 115.0 (C-5′), 128.9 (C-6′), 73.9 (C-1″), 71.0 (C-2″), 79.0 (C-3″), 70.2 (C-4″), 81.2 (C-5″), 61.4 (C-6″) [10, 11].

Swertisin (8). Yellow amorphous solid. ^{1}H NMR (200 MHz, DMSO-d_6, δ, ppm, J/Hz): 13.17 (s, OH, H-5), 8.02 (2H, d, J = 8.0, H-2′, 6′), 6.89 (2H, d, J = 8.0, H-3′, 5′), 6.81 (1H, s, H-3), 6.51 (1H, s, H-8), 4.72 (1H, d, J = 10.0, H-1″), 3.82 (1H, m, H-2″), 3.25–3.75 (4H, m, H-3″, 4″, 5″, 6″) [12].

Swertiajaponin (9). Yellow amorphous solid. ^{1}H NMR (200 MHz, DMSO-d_6, δ, ppm, J/Hz): 13.15 (s, OH, H-5), 7.56 (1H, br.d, J = 8.5, H-6′), 7.55 (1H, br.s, H-2′), 6.92 (1H, d, J = 8.5, H-5′), 6.79 (1H, s, H-3), 6.59 (1H, s, H-8), 4.76 (1H, d, J = 10.0, H-1″), 3.2–3.8 (5H, m, H-2″-6″), 3.86 (3H, s, OCH_3). ^{13}C NMR (50.3 MHz, DMSO-d_6, δ, ppm): 164.5 (C-2),

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102.3 (C-3), 182.3 (C-4), 161.3 (C-5), 108.6 (C-6), 163.3 (C-7), 94.9 (C-8), 155.6 (C-9), 104.4 (C-10), 121.7 (C-1′), 113.9 (C-2′), 145.9 (C-3′), 150.1 (C-4′), 115.0 (C-5′), 119.5 (C-6′), 73.1 (C-1″), 70.7 (C-2″), 78.7 (C-3″), 70.7 (C-4″), 82.9 (C-5″), 61.6 (C-6″), 56.6 (OCH_3) [12].

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