SUPPLEMENTARY MATERIALS

A possible glycosidic benzophenone with full substitution on B-ring from *Psidium guajava* leaves.

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Abstract.

Bidimensional NMR analysis may be a useful tool to resolve the structure of chemical compounds also in mixture. This letter would demonstrate how these techniques could be applied e.g. to the reported case on identification of benzophenone glycoside from *Psidium guajava*. A tentative structure for the secondary component, not yet described, was possibly proposed on the basis of observation and critic review of available 1D- and 2D-NMR spectra.

Keywords: Bidimensional NMR; Structure elucidation; Benzophenone glycosides.

Mono- and bidimensional NMR spectra and MS spectra were obtained from the supplementary materials (available on-line alongside the original paper) by Ukwueze and co-workers (Ukwueze et al. 2015).

¹H NMR 500 MHz MeOH δ = 7.57 (m, 2H), 7.48 (t, *J*=7.4, 2H), 7.39 (t, *J*=7.7, 3H), 6.20 (s, 1H), 4.72 (d, *J*=7.7, 1H), 3.87 (dd, *J*=2.1, 12.0, 1H), 3.65 (dd, *J*=5.9, 12.0, 1H), 3.25 (d, *J*=9.1, 2H), 3.14 (t, *J*=9.4, 1H), 2.51 (dd, *J*=7.7, 9.1, 1H), 2.02 (s, 3H).

Figure S1: The reported ¹H NMR spectrum of Guajaphenone A (2)

Figure S2: The reported ¹³C NMR spectrum of Guajaphenone A (2)

Figure S3: The reported H-H COSY spectrum of Guajaphenone A (2)

Figure S4: The reported HMQC spectrum of Guajaphenone A (2)

Figure S5: The reported HMBC spectrum of Guajaphenone A (2)

Andreas791 #757 RT: 21.38 AV: 1 NL: 1.75E8
F: + c ESI Full ms [100.00-1000.00]

Andreas791 #759 RT: 21.42 AV: 1 NL: 8.15E7
F: - c ESI Full ms [100.00-1000.00]

Figure S6: ESI-MS spectrum of Guajaphenone A (2)

References.

Ukwueze S.E., Osadebe P.O., Okoye F.B.C., 2015. A new antibacterial benzophenone glycoside from *Psidium guajava* (Linn.) leaves. Nat Prod Res, 29(18): 1728-1734. DOI: 10.1080/14786419.2014.1003188