Supplementary Material

Title: Anti-Zika virus activity and chemical characterization by Ultra-High-Performance Liquid Chromatography (UPLC-DAD-UV-MS) of ethanol extracts in Tecoma species

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Mass spectrum of *Tecoma* species

**Figure 1S** – Mass spectrum in negative mode of *Tecoma castaneifolia* trunk
Figure 2S – Mass spectrum in negative mode of *Tecoma castaneifolia* leaves
Figure 3S – Mass spectrum in negative mode of *Tecoma garrocha* trunk
Figure 4S – Mass spectrum in negative mode of *Tecoma garrocha* leaves
Figure 5S – Mass spectrum in negative mode of *Tecoma stans* var. *angustata* trunk
Figure 6S – Mass spectrum in negative mode of *Tecoma stans* var. *angustata* leaves
Figure 7S – Mass spectrum in negative mode of *Tecoma stans* var. *stans* trunk
Figure 8S – Mass spectrum in negative mode of *Tecoma stans* var. *stans* leaves
NMR Data for Isolated Compound – Crenatoside

Spectroscopic Data for Crenatoside

Crenatoside: White solid (MeOH); m.p. Lit. 201-202 °C [21]; UV (MeOH) \( \lambda_{\text{max}} \) 330.5 nm; \(^1\)H NMR (DMSO-\textit{d6} and MeOD, 400 MHz): \( \delta \) 6.82 (1H, d, \( J = 1.8 \) Hz, H-2), 6.73 (1H, d, \( J = 8.1 \) Hz, H-5), 6.69 (1H, dd, \( J = 1.8/8.2 \) Hz, H-6), 4.60 (1H, dd, \( J = 2.6/10.5 \), H-\( \beta \)), 3.99 (2H, dd, \( J = 2.9/12.0 \) Hz, H-\( \alpha \) eq), 3.63 (2H, m, H-\( \alpha \) ax), 4.55 (1H, d, \( J = 7.8 \) Hz, H-1’), 3.47 (1H, m, H-2’), 4.13 (1H, t, \( J = 9.4 \) Hz, H-3’), 5.08 (1H, t, \( J = 9.6 \) Hz, H-4’), 3.75 (1H, sl, H-5’), 3.65 e 3.55 (1H, m, H-6’), 5.15 (1H, d, \( J = 1.4 \) Hz, H-1’’), 3.77 (1H, sl, H-2’’), 3.49 (1H, m, H-3’’), 3.25 (1H, t, \( J = 9.5 \) Hz, H-4’’), 3.57 (1H, m, H-5’’), 1.11 (1H, d, \( J = 6.2 \) Hz, H-6’’), 7.06 (1H, d, \( J = 2.0 \) Hz, H-2’’’), 6.78 (1H, d, \( J = 8.2 \) Hz, H-5’’’), 6.97 (1H, dd, \( J = 2.0/8.2 \) Hz, H-4’’’’), 7.60 (1H, d, \( J = 16.0 \) Hz, H-\( \beta \)’’), 6.28 (1H, d, \( J = 15.6 \) Hz, H-\( \alpha \)’’); \(^{13}\)C NMR (DMSO-\textit{d6} and MeOD, 100 MHz): \( \delta \) 129.8 (C-1), 114.5 (C-2), 146.3 (C-3), 146.3 (C-4), 116.2 (C-5), 118.8 (C-6), 72.7 (C-\( \alpha \)), 78.2 (C-\( \beta \)), 98.9 (C-1’), 81.9 (C-2’), 77.0 (C-3’), 70.0 (C-4’), 77.7 (C-5’), 61.9 (C-6’), 114.4 (C-\( \alpha \)’), 147.9 (C-\( \beta \)’), 101.9 (C-1’’), 71.9 (C-2’’), 71.8 (C-3’’), 73.3 (C-4’’), 70.2 (C-5’’), 18.3 (C-6’’), 127.3 (C-1’’’), 115.2 (C-2’’’), 146.8 (C-3’’’), 149.9 (C-4’’’), 116.5 (C-5’’’), 123.2 (C-6’’’), 167.6 (C=O); ESI-MS \( m/\ell \) 621.63 [M-H]\(^-\) and \( m/\ell \) 623.67 [M+H]\(^+\), (calcd. from C\(_{29}\)H\(_{34}\)O\(_{15}\), 622.12).

**Discussion of the Spectroscopic Data for Crenatoside**

The \(^1\)H-NMR spectrum displayed signals at \( \delta \) 4.55 (1H, d, \( J = 7.8 \) Hz) and \( \delta \) 5.15 (1H, d, \( J = 1.4 \) Hz) assignable to anomic protons of two sugar moieties and at the \(^{13}\)C-NMR spectrum the corresponding signals at \( \delta \) 98.9 and 101.9 ppm were assignable to the anomic carbons of two different sugar moieties. These chemical shifts are characteristics of the glucose and rhamnose, respectively [21, 31]. Furthermore, the value
of the coupling constant in the anomeric proton of the D-glucose \( (J = 7.8 \text{ Hz}) \) indicated a \( \beta \)-configuration, while that of the L-rhamnose \( (J = 1.8 \text{ Hz}) \) is consistent with an \( \alpha \)-configuration [21].

The \( ^1\)H-NMR displayed the aromatic signals at \( \delta \) 6.78; 6.97 and 7.06 ppm assigned to an ABX system that correspond to a caffeic acid. The two doublets at \( \delta \) 6.28 and 7.60 ppm are assigned to \( \alpha' \) and \( \beta' \) protons of the olefinic part of the caffeoyl unit, the coupling constant \( (J = 16.0 \text{ Hz}) \) indicating their trans configuration [21, 31].

A second aromatic ABX system was observed with chemical shifts at \( \delta \) 6.69; 6.73 and 6.82 ppm, by the protons of the 3,4-dihydroxyphenylethanol moiety. The chemical shift of the double doublet at \( \delta \) 4.60 ppm assignable to the proton at the \( \beta \) carbon indicated that this carbon is oxygenated, which was further confirmed from the upfield shift of its \( ^{13}\)C-NMR signal at \( \delta \) 78.2 ppm [21, 31].

The exact position of the sugar attachment (\( \beta \)-D-glucose and \( \alpha \)-L-rhamnose), caffeic acid and 3,4-dihydroxyphenylethanol were determined by signal comparison of the \( ^1\)H-NMR and \( ^{13}\)C-NMR with the previously reported data described [21]. Thus, the isolated compound was established as the phenylethanoid glycoside crenatoside \{1',2'-[\( \beta \)(3,4-dihydroxyphenyl)]-\( \alpha \), \( \beta \)-dioxoethanol]-4'-O-caffeoyl-O-\( \alpha \)-L-rhamnopyranosyl-(1\( \rightarrow \)3)-O-\( \beta \)-D-glucopyranoside\}. 
Figure 9S – $^1$H-NMR spectrum of crenatoside (400 MHz, DMSO-d6 e MeOD).
Figure 10S – $^1$H-NMR spectrum expansion 7.7 to 6.3 ppm of crenatoside (400 MHz, DMSO-d$_6$ e MeOD, δ)
Figure 11S – $^1$H-NMR spectrum expansion 5.2 to 4.5 ppm of crenatoside (400 MHz, DMSO-d$_6$ e MeOD, δ)

Figure 12S – $^1$H-NMR spectrum expansion 4.2 to 3.2 ppm of crenatoside (400 MHz, DMSO-d$_6$ e MeOD, δ)
Figure 13S – $^1$H-NMR spectrum expansion 1.3 to 0 ppm of crenatoside (400 MHz, DMSO-d6 e MeOD, δ)
Figure 14S – $^{13}$C-NMR spectrum of crenatoside (100 MHz, DMSO-d6 e MeOD, $\delta$)
$^{13}$C-NMR spectrum of crenatoside (DEPT-135, 100 MHz, DMSO-d$_6$ e MeOD, δ)