Supporting Information

Bioassay-Guided Isolation of Iridoids and Phenylpropanoids from Aerial Parts of *Lamium album* and Their Anti-inflammatory Activity in Human Neutrophils

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Dedicated to Professor Dr. Max Wichtl in recognition of his outstanding contribution to pharmacognosy research.

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Fig. 1S The draft of isolation of compounds from the aqueous-methanolic extract from the aerial parts of *L. album*. Preparative HPLC conditions: Zorbax C18; mobile phase: 0.1%
HCOOH in water (A) and 0.1% HCOOH in acetonitrile (B); elution: 0% B – 40% B (0-60 min), 40% B – 50% B (60-65 min).
The structure of compound 3 identified as caryoptoside.

$^1$H NMR spectrum of compound 3 (300 MHz, CD$_3$OD) $\delta$ 7.37 (1H, s, H-3), 5.58 (1H, d, $J = 2.0$ Hz, H-1), 4.63 (2H, d, $J = 7.9$ Hz, H-1'), 3.89 (1H, dd, $J = 11.9, 1.7$ Hz, CH$_2$-6'), 3.66 (1H, m, CH$_2$-6'), 3.36 (1H, t, H-3'), 3.27 (1H, d, $J = 8.5$ Hz, H-5'), 3.25 (1H, m, H-4'), 3.18 (1H, d, $J = 8.0$ Hz, H-2'), 2.58 (1H, d, $J = 10.5$ Hz, H-9), 2.22 (1H, m, $J = 14.4, 9.4, 3.0$ Hz, CH$_2$-6), 1.65 (1H, dt, $J = 14.4, 5.7$ Hz, CH$_2$-6), 1.19 (3H, s, CH$_3$-10).

$^{13}$C NMR spectrum of compound 3 (75 MHz, CD$_3$OD) $\delta$ 169.17 (C-11), 151.51 (C-3), 114.22 (C-4), 99.80 (C-1'), 95.12 (C-1), 79.92 (C-8), 79.06 (C-7), 78.32 (C-5'), 77.99 (C-3'), 74.65 (C-2'), 71.64 (C-4'), 62.86 (CH$_2$-6'), 51.64 (C-9, -OCH$_3$), 38.77 (C-6), 27.61 (C-5), 21.88 (-OCH$_3$).

The structure of compound 11 identified as caffeic acid.

$^1$H NMR spectrum of compound 11 (300 MHz, CD$_3$OD) $\delta$ 7.53 (1H, d, $J = 15.9$ Hz, H-7), 7.03 (1H, d, $J = 2.0$ Hz, H-2), 6.93 (1H, dd, $J = 8.2, 2.0$ Hz, H-6), 6.78 (1H, d, $J = 8.2$ Hz, H-5), 6.22 (1H, d, $J = 15.9$ Hz, H-8). Compound 11 was identified by comparing the above spectral data with those in the literature [1].
The structure of compound 17 identified as lamiuside A (lamalboside, 2-(3,4-dihydroxyphenyl)ethyl-O-β-D-galactopyranosyl-(1→2)-α-L-rhamnopyranosyl-(1→3)-(4-O-trans-cafeoyl)-β-D-glucopyranoside).

\(^1\)H NMR spectrum of compound 17 (300 MHz, CD\(_3\)OD) \(\delta\) 7.60 (1H, d, \(J = 15.9\) Hz, H-7'), 7.06 (1H, d, \(J = 1.8\) Hz, H-2'), 6.96 (1H, dd, \(J = 8.2\) Hz, H-6'), 6.78 (1H, d, \(J = 8.2\) Hz, H-5'), 6.71 (1H, d, \(J = 1.8\) Hz, H-2), 6.68 (1H, d, \(J = 8.0\) Hz, H-5), 6.57 (1H, dd, H-6), 6.27 (1H, d, \(J = 15.9\) Hz, H-8'), 5.57 (1H, s, H-1''), 4.93 (1H, t, \(J = 9.2\) Hz, H-4''), 4.36 (2H, t, \(J = 7.6\) Hz, H-1''', H-1''), 4.04 (1H, m, Hb-8), 3.75 (1H, m, Ha-8), 2.79 (2H, t, \(J = 7.3\) Hz, H-7), 1.05 (3H, d, \(J = 6.1\) Hz, H-6''). Compound 17 was identified by comparing the above spectral data with those in the literature [2,3].

The structure of compound 21 identified as 6''-O-β-D-glucopyranosylmartynoside (trans-lamiuside E, 2-(3-hydroxy-4-methoxyphenyl)ethyl-O-α-L-rhamnopyranosyl-(1→3)-(4-O-trans-cafeoyl)-β-D-glucopyranosyl-(1→6)-(4-O-trans-feruloyl)-β-D-glucopyranoside).

\(^1\)H NMR spectrum of compound 21 (300 MHz, CD\(_3\)OD) \(\delta\) 7.89 (1H, s, H-2'), 7.67 (1H, d, \(J = 15.9\) Hz, H-7'), 7.20 (1H, s, H-6'), 7.09 (1H, d, \(J = 8.3\) Hz, H-5'), 6.82 (1H, dd, \(J = 8.1, 5.2\) Hz, H-5), 6.73 (1H, d, H-2), 6.69 (1H, s, H-6), 6.38 (1H, d, \(J = 15.9\) Hz, H-8'), 5.19 (1H, br s, H-1''), 4.40 (1H, d, \(J = 7.9\) Hz, H-1''), 4.30 (1H, d, \(J = 7.6\) Hz, H-1'''), 3.89 (3H, s, CH\(_3\)O-3'), 3.82 (3H, s, CH\(_3\)O-4'), 2.83 (1H, br t, \(J = 7.2\) Hz, H-7), 1.09 (3H, d, \(J = 6.1\) Hz, H-6''). Compound 21 was identified by comparing the above spectral data with those in the literature [2].
The structure of compound 23 identified as lamiuside B (2-(3,4-dihydroxyphenyl)ethyl-O-β-D-galactopyranosyl-(1→2)-α-L-rhamnopyranosyl-(1→3)-(4-O-trans-feruoyl)-β-D-glucopyranoside).

\[ \text{Fig. 6S} \]

\[ \text{Fig. 7S} \]

**1**H NMR spectrum of compound 23 (300 MHz, CD\textsubscript{3}OD) \( \delta \) 7.66 (1H, d, \( J = 15.9 \) Hz, H-7'), 7.20 (1H, s, H-2'), 7.09 (1H, d, \( J = 10.0 \) Hz, H-6'), 6.82 (1H, d, \( J = 8.2 \) Hz, H-5'), 6.71 (1H, d, \( J = 1.9 \) Hz, H-2), 6.68 (1H, d, \( J = 8.0 \) Hz, H-5), 6.57 (1H, dd, \( J = 8.1, 1.9 \) Hz, H-6), 6.38 (1H, d, \( J = 15.9 \) Hz, H-8'), 5.58 (1H, s, H-1''), 4.93 (1H, t, \( J = 9.3 \) Hz, H-4''), 4.37 (2H, t, \( J = 7.5 \) Hz, H-1'', H-1'''), 4.03 (1H, dd, \( J = 16.1, 8.5 \) Hz, H-8), 3.89 (3H, s, CH\textsubscript{3}O -3'), 3.75 (1H, m, Ha-8), 2.79 (1H, t, \( J = 7.2 \) Hz, H-7), 1.06 (3H, d, \( J = 6.1 \) Hz, H-6''). Compound 23 was identified by comparing the above spectral data with those in the literature [2].

**1**H NMR spectrum of compound 28 (300 MHz, DMSO) \( \delta \) 12.56 (1H, s, OH on C-5), 10.83 (1H, br s, OH on C-7), 10.14 (1H, s, br s, OH on C-4'), 10.00 (1H, s, br s, OH on C-4''), 7.98 (2H, d, \( J = 8.7 \) Hz, H-2', 6'), 7.37 (1H, d, \( J = 4.1 \) Hz, H-7''), 7.33 (2H, d, \( J = 11.6 \) Hz, H-2'', 6''), 6.85 (2H, d, \( J = 8.8 \) Hz, H-3',5'), 6.78 (2H, d, \( J = 8.5 \) Hz, H-3'',5''), 6.38 (1H, d, \( J = 1.6 \) Hz, H-8), 6.14 (1H, d, \( J = 1.7 \) Hz, H-6), 6.10 (1H, d, \( J = 16.0 \) Hz, H-8''), 5.44 (1H, d, \( J = 6.4 \) Hz, H-1''), 5.22 (1H, d, \( J = 5.4 \) Hz, sugar OH), 5.16 (1H, d, \( J = 4.1 \) Hz, H-1''), 4.26 (1H, d, \( J = 10.7 \) Hz, Ha-6''), 4.02 (1H, dd, \( J = 11.9, 6.3 \) Hz, Hb-6''), 3.38-3.20 (m, H-2'', 3'', 5''). Compound 28 was identified by comparing the above spectral data with those in the literature [3].
The structure of compound 29 identified as lamiumide C.

$^1$H NMR spectrum of compound 29 (300 MHz, CD$_3$OD) $\delta$ 7.56 (1H, d, $J = 15.9$ Hz, H-7'), 7.04 (1H, d, $J = 1.8$ Hz, H-2'), 6.89 (1H, dd, $J = 8.2$, 1.9 Hz, H-6'), 6.77 (1H, d, $J = 8.2$ Hz, H-5'), 6.68 (1H, d, $J = 1.9$ Hz, H-2), 6.64 (1H, d, $J = 8.1$ Hz, H-5), 6.54 (1H, dd, $J = 8.1$, 1.9 Hz, H-6), 6.29 (1H, d, $J = 15.9$ Hz, H-8'), 5.57 (1H, s, H-1''), 4.49 (1H, dd, $J = 11.9$, 1.9 Hz, Hb-6'), 4.39 (1H, d, $J = 7.6$ Hz, H-1'''), 4.34 (1H, d, $J = 8.0$ Hz, H-1''), 2.78 (1H, t, $J = 7.4$ Hz, H-7), 1.23 (3H, d, $J = 6.2$ Hz, H-6''). Compound 29 was identified by comparing the above spectral data with those in the literature [2].

References