SUPPLEMENTARY MATERIAL

Isolation of a New Carboline Alkaloid from *Trigonostemon lii*

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Isolation of a New Carboline Alkaloid from *Trigonostemon lii*

A new carboline alkaloid, 1-(7-methoxy-quinoliny-4'-yl)-3,4-dihydro- β -carboline (**1**), was isolated from the leaves and twigs of *Trigonostemon lii* Y.T. Chang, together with three known ones, trigonostemonines C and D (**2-3**), and trigonoliimine A (**4**). Their structures were elucidated by spectroscopic analyses, including 2D-NMR techniques.

Keywords: *Trigonostemon lii*; Euphorbiaceae; carboline alkaloid

Supporting information

Spectroscopic data of the known compounds **2-4**.

Figure S1. Selective HMBC (H→C) correlations for compound **1**.

Original spectra of compound **1**.

^1H NMR Spectrum (500 MHz, CDCl_3)

^{13}C NMR Spectrum (125 MHz, CDCl_3)

COSY Spectrum

HSQC Spectrum

HMBC Spectrum

The enlarged spectrum of HMBC

HREIMS

EIMS

IR

Spectroscopic data of the known compounds **2-4**.

Trigonostemonine C (2)

Yellow amorphous solid, C₂₁H₁₅N₃O, MW: 325; ¹H NMR (CDCl₃, 500 MHz): δ 11.68 (1H, s, NH-9), 8.60 (1H, d, *J* = 5.2 Hz, H-3), 8.34 (1H, d, *J* = 4.1 Hz, H-2'), 8.15 (1H, d, *J* = 8.7 Hz, H-5), 8.06 (1H, d, *J* = 5.2 Hz, H-4), 7.77 (1H, d, *J* = 8.3 Hz, H-8'), 7.72 (1H, d, *J* = 8.2 Hz, H-5'), 7.45 (1H, m, H-7'), 7.43 (1H, d, *J* = 4.1 Hz, H-3'), 7.39 (1H, d, *J* = 7.8 Hz, H-6'), 7.13 (1H, d, *J* = 1.5 Hz, H-8), 7.01 (1H, dd, *J* = 8.7 and 1.9 Hz, H-6), 3.92 (3H, s, OCH₃-7); ¹³C-NMR (CDCl₃, 125 MHz): δ 161.4 (s, C-7), 148.6 (d, C-2'), 147.3 (s, C-8a'), 145.0 (s, C-4'), 143.3 (s, C-8a), 139.1 (s, C-1), 139.0 (d, C-3), 135.4 (s, C-9a), 130.2 (s, C-4a), 129.5 (d, C-7'), 128.5 (d, C-8'), 127.3 (d, C-6'), 126.4 (s, C-4a'), 125.9 (d, C-5'), 122.8 (d, C-5), 121.9 (d, C-3'), 115.2 (s, C-4b), 114.1 (d, C-4), 110.1 (d, C-6), 94.9 (d, C-8), 55.7 (q, OCH₃-7).

Trigonostemonine D (3)

Yellow amorphous solid, C₂₁H₁₅N₃O, MW: 325; ¹H NMR (CDCl₃, 500 MHz): δ 11.60 (1H, s, NH-9), 8.66 (1H, d, *J* = 5.2 Hz, H-2'), 8.47 (1H, d, *J* = 4.4 Hz, H-3), 8.30 (1H, d, *J* = 7.9 Hz, H-5), 8.16 (1H, d, *J* = 5.2 Hz, H-4), 7.73 (1H, d, *J* = 8.1 Hz, H-5'), 7.64 (1H, m, H-8'), 7.62 (1H, m, H-7), 7.40 (1H, m, H-8), 7.39 (1H, m, H-9'), 7.04 (1H, m, H-6), 7.02 (1H, m, H-6'), 3.73 (3H, s, OCH₃-7); ¹³C-NMR (CDCl₃, 125 MHz): δ 160.5 (s, C-7'), 149.5 (s, C-8a'), 149.0 (d, C-2'), 144.6 (s, C-4'), 141.6 (s, C-8a), 140.2 (s, C-1), 138.9 (d, C-3), 135.3 (s, C-9a), 129.9 (s, C-4a), 128.8 (d, C-7), 126.8 (d, C-5'), 121.9 (d, C-5), 121.5 (s, C-4a'), 121.5 (s, C-4b), 120.3 (d, C-6'), 120.1 (d, C-6), 119.8 (d, C-3'), 114.9 (d, C-4), 112.1 (d, C-8), 106.6 (d, C-8'), 55.3 (q, OCH₃-7).

Trigonoliimine A (4)

Light yellow gum, $C_{22}H_{20}N_4O$, MW: 357; 1H NMR ($CDCl_3$, 500 MHz): δ 9.32 (1H, s, H-1), 7.50 (1H, s, H-25), 7.49 (1H, m, H-4), 7.37 (1H, d, $J = 8.3$ Hz, H-7), 7.28 (1H, m, H-6), 7.11 (1H, t, $J = 7.5$ Hz, H-5), 6.82 (1H, s, H-15), 6.60 (1H, m, H-17), 6.59 (1H, m, H-18), 4.21 (1H, dd, $J = 16.1$ and 8.1 Hz, H-22 β), 4.00 (1H, m, H-11 α), 3.95 (1H, m, H-11 β), 3.75 (3H, s, OCH_3), 3.69 (1H, m, H-22 α), 3.23 (1H, m, H-10 α), 3.17 (1H, m, H-10 β), 2.36 (1H, m, H-21 β), 2.20 (1H, m, H-21 α); ^{13}C -NMR ($CDCl_3$, 125 MHz): δ 167.1 (s, C-24), 160.4 (s, C-16), 149.9 (d, C-25), 142.2 (s, C-14), 136.7 (s, C-8), 127.8 (s, C-2), 127.6 (s, C-9), 124.7 (d, C-6), 123.3 (d, C-18), 120.1 (d, C-5), 119.5 (d, C-4), 117.9 (s, C-3), 114.3 (s, C-19), 111.8 (d, C-7), 111.5 (d, C-17), 109.4 (d, C-15), 77.0 (d, C-20), 56.6 (t, C-22), 55.4 (q, OCH_3), 48.4 (t, C-11), 41.1 (t, C-21), 29.9 (t, C-10).

Figure S1. Selective HMBC (H→C) correlations for compound **1**.

Original spectra of compound **1**.

^1H NMR:

Original spectra of compound 1.

^{13}C NMR:

Original spectra of compound **1**.

^1H - ^1H COSY:

Original spectra of compound **1**.

HSQC:

Original spectra of compound **1**.

HMBC:

Original spectra of compound **1**.

The enlarged spectrum of HMBC:

Original spectra of compound **1**.

HREIMS:

Original spectra of compound **1**.

EIMS:

Original spectra of compound **1**.

IR:

Sample : NS-1	Frequency Range : 399.246 - 3996.32	Measured on : 21/10/2014
Technique : KBr	Resolution : 4	Instrument : Tensor27
Customer : 141021IR6	ZeroFilling : 2	Acquisition : Double Sided, For
		Sample Scans : 16