Supporting Information

New Type of Trimeric and Pentameric Indole Alkaloids from *Psychotria rostrata*

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General experimental procedure, isolation and purification of alkaloids; S1—S2

¹H and ¹³C NMR spectra for compounds **1**; S3—S4

¹H—¹H COSY, HMQC, ¹H—¹³C HMBC, and ¹H—¹⁵N HMBC spectra for **1**; S5—S9

¹H and ¹³C NMR spectra for compounds **2**; S10—S11

¹H—¹H COSY, HMQC, and HMBC spectra for **2**; S12—S14

General UV: recorded in MeOH on a JASCO V-560 instrument. IR: recorded on a JASCO FT/IR-230 spectrophotometer. ¹H and ¹³C NMR spectra: recorded on JEOL JNM A-400, JNM A-500, JNM ECP-400, or JNM ECP-600 spectrometers, *J* values are given in Hz. EI-MS: direct probe insertion at 70 eV recorded on a JEOL JMS GC-mate spectrometer. FAB-MS: recorded on a JEOL JMS-HX110 mass spectrometer. Optical Rotation: measured using a JASCO P-1020 polarimeter. CD: recorded on a JASCO J-720WI spectrometer. TLC: precoated Kieselgel 60 F₂₅₄ plates (Merck, 0.25 mm thick). Column Chromatography: Kieselgel 60 [Merck, 70-230 (for open chromatography) and 230-400 mesh (for flash chromatography)], amino silica gel [Fuji Silysia Chemical, NH-DM1020], medium pressure liquid column chromatography: silica gel prepacked column Kusano CPS-HS-221-05.

Plant Material The plant sample was collected from Air Hitam Forest Reserve in central Peninsular Malaysia, and was identified by Dr. Ruth Kiew (Department of Biology, UPM). A voucher specimen is deposited at the herbarium of the Department of Biology, Universiti Putra Malaysia.

Extraction and Isolation of Alkaloids The air-dried powdered leaves (2.0 kg) of *P. rostrata* were initially extracted with petroleum ether, followed by exhaustive extraction with MeOH six times and filtered. The combined filtrates were concentrated under reduced pressure to give a crude extract (160 g), a part of which (10.0 g) was then dissolved in 2% aqueous sulfuric acid. The solution was washed with ethyl acetate, alkalized with Na₂CO₃ (pH 10), and then exhaustively extracted with 5% MeOH-CHCl₃ three times. The organic layer was washed with water, dried over MgSO₄, and evaporated to give a crude alkaloidal fraction (1.61 g), which was roughly separated by Sephadex LH-20 column chromatography using a H₂O—MeOH gradient to give 13 fractions. The MeOH eluate was purified by SiO₂ flash column chromatography (CHCl₃:MeOH:NH₄OH=90:10:1.5) followed by medium pressure liquid chromatography (CHCl₃:MeOH:NH₄OH=80:20:0.5) to give 21 mg of psychotrimine (**1**) and 5.4 mg of psychopentamine (**2**).

Psychotrimine (1): amorphous powder; $[\alpha]_D^{18} +179$ (*c* 0.2, CHCl₃); UV (MeOH) $\lambda_{\max}$ (log ϵ) 296 (3.99), 222.5 (4.57), 206.5 (4.55) nm; ¹H NMR (CDCl₃, 600 MHz) see Table 1 in the text; ¹³C NMR (CDCl₃, 150 MHz) see Table 1 in the text; ¹⁵N NMR (CDCl₃, 60 MHz) δ -235 (N-1''), -242 (N-1), -310 (N-8'), -327 (N-1'), -351 (N-10 and N-10''); FABMS (NBA) *m/z*:: 519 [M+H]⁺; HRFABMS (NBA/PEG) *m/z*:: 519.3206 (calcd for C₃₃H₃₉N₆, 519.3236). CD (*c* 0.22 mmol/L, MeOH, 24°C) λ_{nm} ($\Delta\epsilon$): 356 (−0.2), 305 (+7.0), 266 (+0.3), 236 (+13.0), 231 (0), 225 (−11.2), 212 (0), 203 (+12.1).

Psychopentamine (2): amorphous powder; $[\alpha]_D^{18} +42$ (*c* 0.2, CHCl₃); UV (MeOH) $\lambda_{\max}$ (log ϵ) 304 (4.10), 250.5 (4.37), 210 (4.81) nm; ¹H NMR (CDCl₃, 600 MHz) see Table 1 in the text; ¹³C NMR (CDCl₃, 150 MHz) see Table 1 in the text; EIMS *m/z*: (%): 862 (M⁺, 17), 590 (60), 516 (20), 344 (48), 250 (100), 149 (60); HRFABMS (NBA/PEG) *m/z*:: 863.5244 (calcd for C₅₅H₆₃N₁₀, 863.5237). CD (*c* 0.22 mmol/L, MeOH, 24°C) λ_{nm} ($\Delta\epsilon$): 349 (−0.3), 313 (+9.3), 275 (+1.8), 259 (+7.7), 247 (+2.7), 226 (+13.7), 219 (0), 211 (−31.6), 204 (0).

Figure S1: ^1H -NMR spectrum of psychotrimine (**1**) in CDCl_3 .

Figure S2: ^{13}C -NMR spectrum of psychotrimine (**1**) in CDCl_3 .

Figure S3: ^1H — ^1H COSY spectrum of psychotrimine (**1**) in CDCl_3 .

Figure S4: HMQC spectrum of psychotrimine (**1**) in CDCl_3 .

Figure S5: ^1H — ^{13}C HMBC spectrum of psychotrimine (**1**) in CDCl_3 .

Figure S6: ^1H - ^{15}N HMBC spectrum of psychotrimine (**1**) in CDCl_3 .

Figure S7: ^1H — ^{15}N HMBC spectrum of psychotrimine (**1**) in CDCl_3 .

Figure S8: ^1H -NMR spectrum of psychopentamine (**2**) in CDCl_3 .

Figure S9: ^{13}C -NMR spectrum of psychopentamine (**2**) in CDCl_3 .

Figure S10: ^1H - ^1H COSY spectrum of psychopentamine (**2**) in CDCl_3 .

Figure S11: HMQC spectrum of psychopentamine (**2**) in CDCl_3 .

Figure S12: HMBC spectrum of psychopentamine (**2**) in CDCl_3 .