SUPPLEMENTARY MATERIAL

Paenibacillin A, a new 2(1*H*)-pyrazinone ring-containing natural product from the endophytic bacterium *Paenibacillus* sp. Xy-2

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Abstract

A new 2(1*H*)-pyrazinone ring-containing natural product, paenibacillin A (**1**), together with five known diketopiperazine derivatives **2–6** and two known isoflavones **7–8**, was isolated from the culture of an endophytic bacterium *Paenibacillus* sp. Xy-2. The structure of compound **1** was elucidated by extensive spectral methods, including UV, IR, HR-ESI-MS, 1D and 2D NMR and ECD experiments. Compound **1** exhibited moderate cytotoxicity against HL-60 cell line with IC₅₀ value of 50.48 μM.

Keywords: *Paenibacillus* sp., endophytic bacterium, secondary metabolites, cytotoxicity

Table S1. ^1H (400MHz) and ^{13}C NMR (100MHz) spectroscopic data and HMBC correlations of paenibacillin A (**1**) in CDCl_3

Position	δ_{C}	δ_{H} (mult.; J in Hz)	HMBC
1		13.20 (1H, br s, -CONH)	
2	158.2		
3	161.0		
4			
5	120.5	7.25 (1H, s, H-5)	C-2, 3, 6, 1''
6	143.5		
1'	36.9	3.24 (1H, sext, $J = 6.8$ Hz, H-1')	C-2, 3, 2', 3', 4'
2'	27.7	1.55 (1H, dq, $J = 13.6$ Hz, 6.8 Hz, H _a -2') 1.82 (1H, dq, $J = 13.6$ Hz, 6.8 Hz, H _b -2')	C-3, 1', 3', 4'
3'	12.2	0.90 (3H, t, $J = 6.8$ Hz, H-3')	C-1', 2'
4'	17.8	1.22 (3H, d, $J = 6.8$ Hz, H-4')	C-3, 1', 2'
1''	30.2	2.85 (1H, sept, $J = 6.8$ Hz, H-1'')	C-5, 6, 2'', 3''
2'', 3''	21.2	1.35 (6H, d, $J = 6.8$ Hz, H-2'', 3'')	C-6, 1''

Figure S1. Key HMBC correlations of **1**

Figure S2. The HR-ESI-MS spectrum of compound **1**

Figure S3. The UV spectrum of compound **1**

Figure S4. The IR spectrum of compound **1**

Figure S5. The ¹H-NMR spectrum of compound **1** (400 MHz) in CDCl₃

Figure S6. The ¹³C-NMR spectrum of compound **1** (100 MHz) in CDCl₃

Figure S7. The HSQC spectrum of compound **1** (600 MHz) in CDCl₃

Figure S8. The HMBC spectrum of compound **1** (600 MHz) in CDCl₃