SUPPLEMENTARY MATERIAL

A new diketopiperazine derivative from a deep sea-derived *Streptomyces* sp. SCSIO 04496

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A new diketopiperazine (DKP) derivative, (6*R*,3*Z*)-3-benzylidene-6-isobutyl-1-methyl piperazine-2,5-dione (**1**), as well as five known DKPs **2-6** were isolated from a deep sea-derived *Streptomyces* sp. SCSIO 04496. The structure of **1** was elucidated using a combination of 1D and 2D NMR, HR-ESI-MS, chiral-phase HPLC techniques. Compounds **1-6** didn't show cytotoxic activity at concentration of 100 μ M in bioactivity assay.

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Figure S1. Chemical structures of the known compounds **2–6**.

Figure S2. Phylogenetic tree of *Streptomyces* sp. SCSIO 04496

Figure S3. Pure culture in dish (A) and scanning electron micrographs of spore chains and aerial mycelia (B) of *Streptomyces* sp SCSIO 04496 after incubation for 7 d on modified ISP-4 medium at 28 °C.

Figure S4 HR-ESI-MS spectrum of compound **1**

Figure S5 ^1H NMR (500 MHz) spectrum of compound **1** in CDCl_3

Figure S6 ^{13}C NMR (125 MHz) spectrum of compound **1** in CDCl_3

Figure S7 HMQC spectrum of compound **1** in CDCl₃

Figure S8 HMBC spectrum of compound **1** in CDCl₃

Figure S9 NOESY spectrum of compound **1** in CDCl₃

Figure S10 Chiral-phase HPLC analysis of the hydrolysate of compound **1**.

Figure S11 Key HMBC and NOESY correlations of compound **2**.

Table S1 ^1H -NMR (500 MHz) and ^{13}C -NMR (125 MHz) spectroscopic data of compound **2**.

position	Compound 2 ^a	
	δ_{H} (multi. J in Hz)	δ_{C}
1-NCH ₃	3.27 (s)	33.5 CH ₃
2		160.2 C
3		124.7 C
4-NH	7.85 (br s)	
5		160.4 C
6		129.8 C
7	5.59 (d, 10.0)	135.3 CH
8	3.72 (m)	27.9 CH
9	1.06 (d, 7.0)	23.6 CH ₃
10	1.06 (d, 7.0)	23.6 CH ₃
11	6.85 (s)	118.7 CH
12		125.7 C
13, 17	7.37 (d, 8.5)	131.7 CH
14, 16	6.85 (t, 8.5)	116.9 CH
15		159.2 C

^a Measured in CD₃OD/CDCl₃.