Supporting Information

Rec. Nat. Prod. 16:5 (2022) 471-476

A New Benzophenone Derivative from the Endophyte *Shiraia* sp. BYJB-1

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Compounds	IC50 ° (µM)	
	SMMC7721	HepG2
1	N/A ^b	N/A
2	N/A	N/A
3	N/A	N/A
4	N/A	N/A
5	N/A	N/A
6	25.94 ± 2.07	50.48 ± 1.94
7	45.82 ± 1.32	N/A
8	N/A	N/A
Sorafenib ^a	2.19 ± 0.04	4.80 ± 0.08

 Table S1: Cytotoxicity activities of compounds 1-8.

^a positive control. ^b N/A: No active.

^c Results are the mean \pm SD (n = 3).

Table S2 : Antimicrobia	l activities of	compounds 1-8 .
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Compounds	MIC (µg/mL)	
	MRSA	E. coil
1	> 500	> 500
2	> 500	> 500
3	> 500	> 500
4	> 500	> 500
5	> 500	> 500
6	62.5	> 500
7	62.5	> 500
8	62.5	> 500
Vancomycin ^a	1.25	-
Kanamycin ^a	-	1.25

^a positive control.

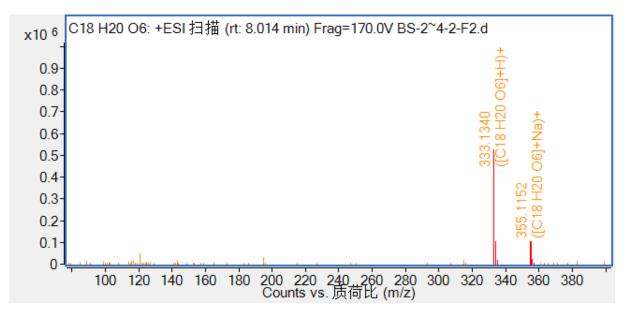


Figure S1: HR-ESI-MS spectrum of 1

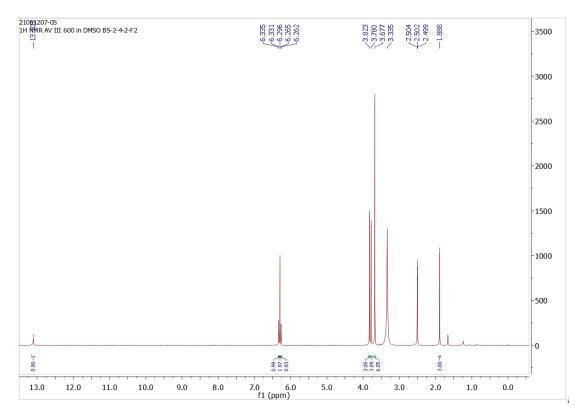


Figure S2: ¹H-NMR (600 MHz, DMSO-*d*₆) spectrum of **1**

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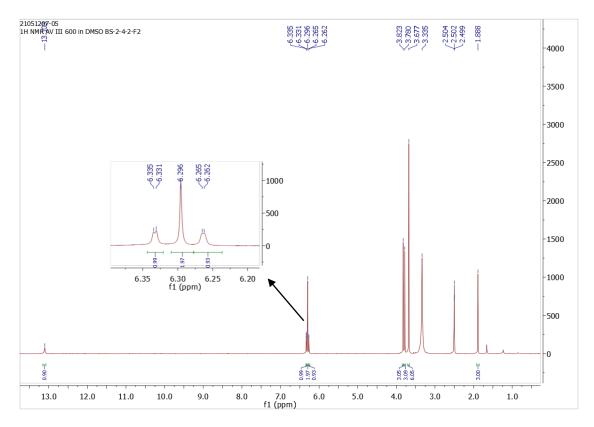


Figure S3: ¹³C-NMR (150 MHz, DMSO-*d*₆) spectrum of 1

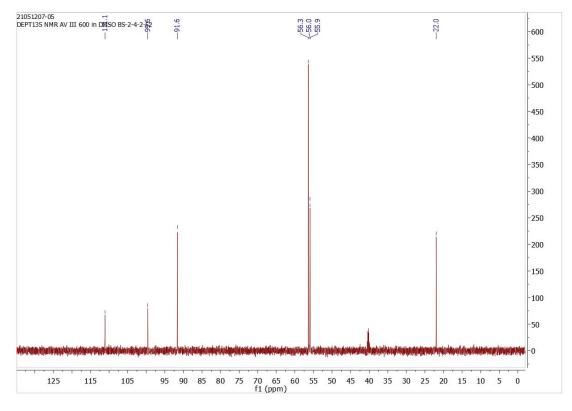


Figure S4: DEPT135 (150 MHz, DMSO-d₆) spectrum of 1

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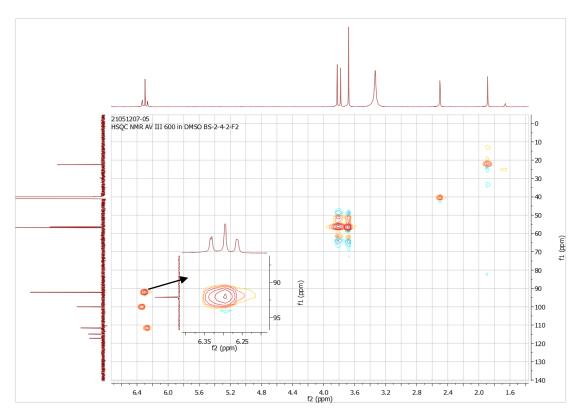


Figure S5: HSQC spectrum of 1

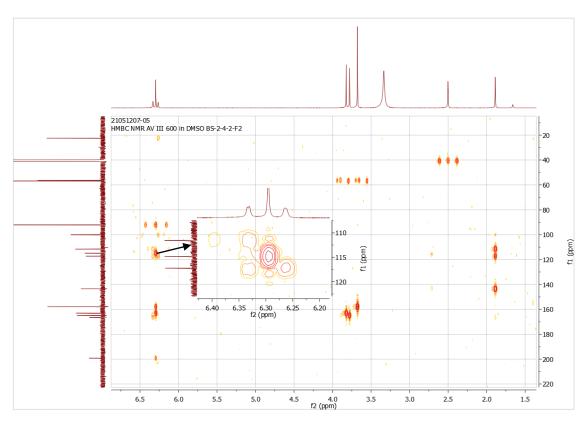
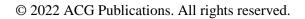


Figure S6: HMBC spectrum of 1



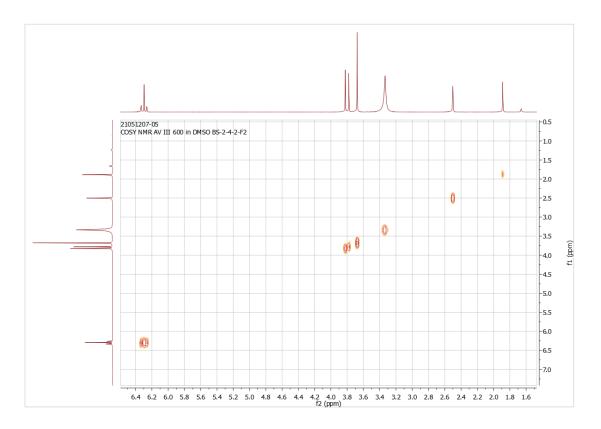


Figure S7: ¹H-¹H COSY spectrum of 1

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SciFinder® Page 1 Score: 99 Score: 96 Score: 96 2. 101744-11-0 52806-38-9 52806-43-6 ó C₁₉ H₂₀ D₂ O₆ Methanone, (4.5-dimethoxy-2-methylphenyl)(3.4,5-trimethoxyphenyl-2,6-d₂)-(9Cl) Related Info: C₁₈ H₂₀ O₆ Benzophenone, 2-hydroxy-4,4',5,5'-tetramethoxy-2'-methyl- (6CI) C₁₉ H₂₂ O₆ Methanone, (4,5-dimethoxy-2-methylphenyl)(3,4,5-trimethoxy oxyph Key Physical Properties: Key Physical Properties: Mol cular Weight ecular Weight 346.37 32.35 1 References
 2 Commercial Sources 332.35 Bolling Point (Predicted) Value: 481.4545.0 °C | Condition: Press: 760 Density (Predicted) Dansity (Predicted) Value: 1.1944.0.06 g/cm3 | Condition: Temp: °C Press: 760 Torr pfa (Predicted) Value: 7.5840.48 | Condition: Most Acidic Te 25 °C Boiling Point (Predicted) Value: 485.5±45.0 °C | Condition: Press: 760 Torr Density (Predicted) Value: 1.139±0.06 g/cm3 | Condition: Temp: 20 *C Press: 760 Torr : 20 Related Info: ~ 1 References ~ 2 Commercial Sources Related Info: ~ 1 References ~ 2 Commercial Sources Score: 96 Score: 96 Score: 96 5. 102162-90-3 6. 102162-91-4 56890-08-5 Y ŝ) ſĭ ٩. . 1 сń C₁₉ H₂₂ O₆ Methanone, (3,4-dimethoxyph trimethoxy-2-methylphenyl)-C₁₉ H₂₂ O₆ Benzonhor C 19 H22 O6 Benzophenone, 2-ethyl-2'-hydroxy-4,4',5,5'-tetramethoxy- (6CI) myl)(3,4,5-Benzophenone, 2'-hydroxy-3,4,4',5'-etramethoxy-2,6-dimethyl- (6CI) terramentoxy (6cr) Key Physical Properties: Molecular Weight 346.37 Bolling Point (Predicted) Value: 537.3±50.0 °C | Condition: Press: 760 Torr Key Physical Properties: Key Physical Properties: Molecular Weight Molecular Weight 346.37 Boiling Point (Predicted) Value: 480.7±45.0 °C | Cor Torr 346.37 Boiling Point (Predicted) Value: 471.2±45.0 °C | Cor Torr Torr Density (Predicted) Value: 1.175±0.06 g/cm3 | Condition: Temp: 20 "C Press: 760 Torr pKa (Predicted) Value: 7.59±0.48 | Condition: Most Acidic Temp: 25 °C Torr Torr Density (Predicted) Value: 1:174±0.06 g/cm3 | Condition: Tem *C Press: 760 Torr pKa (Predicted) Value: 7:55±0.48 | Condition: Most Acidic 25 *C Density (Predicted) Value: 1.139±0.06 g/c °C Press: 760 Torr 20 Related Info: ~ 1 References ~ 5 Commercial Sources Related Info: ~ 1 References ~ 2 Commercial Sources Related Info: Spectra ~ 1 References ~ 2 Commercial Sources SciFinder® Page 2 Score: 96 Score: 95 Score: 95 2253623-31-1 102162-92-5 129103-92-0 P U . M____ á C₁₉ H₂₂ O₆ Benzophenone, 2,4,4',5,5'-pentam methyl- (6CI) C₁₈ H₂₀ O₆ Methanone, (2-hydroxy-3-methoxy-6-methylphenyl)(2,4,5-trimethoxyphenyl Key Physical Properties: C18 H20 O6 INDEX NAME NOT YET ASSIGNED athoxy-2 Key Physical Properties: Key Physical Properties: Molecular Weight 332.35 Boiling Point (Predicted) Value: 496.3±45.0 °C | Condition: F Torr Molecular Weight 346.37 Boiling Point (Predicted) Value: 518.1±50.0 °C | Con Molecular Weight 332.35 Boiling Point (Predicted) Value: 493.4±45.0 °C | Con Torr n' Pre ss[.] 760
 Torr
 Density (Predicted)

 Density (Predicted)
 Value: 1.1942-0.06 (gr03)

 Constraints
 Constraints

 Cress: 700 Torr
 pKa (Predicted)

 Value: 7.21:0.45 | Condition: Most Acidic Temp: 26 °C
 Torr Torr Density (Predicted) Value: 1.1944.0.06 g(cm3 | Condition: Temp: 20 "C Press: 760 Torr PKa (Predicted) Value: 7.49±0.40 | Condition: Most Acidic Temp 25 "C Porries (Predicted) Value: 1.139±0.06 g/cm3 | Co °C Press: 760 Torr on: Temp: Related Info: ~ 1 References ~ 2 Commercial Sources Related Info: Related Info ~ 3 References Reactions ~ 2 References actions Score: 95 10. 1101903-04-1 Of Contraction C₁₉ H₂₂ O₆ Methanone, (6-hydroxy-3-methoxy-2-methylphenyl)(2,3,4-trimethoxy-6-methylphenyl)-Key Physical Properties Molecular Weight 346.37 Boiling Point (Predicted) Value: 486.6±45.0 °C | Condition: Press: 760 Torr Density (Predicted) Value: 1.175±0.06 g/cm3 | Condition: Temp: 20 "C Press: 760 Torr pKa (Predicted) Value: 7.99±0.48 | Condition: Most Acidic Temp: 25 "C Related Info: ~ 1 References

Figure S8: Scifinder search reports

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