SUPPLEMENTARY MATERIAL

A Novel Antimicrobial Flavonoid from the Stem Bark of *Commiphora Pedunculata* (Kotschy & Peyr.) Engl.

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Abstract: A new flavonoid, 2-(3,5-dihydroxy-4-methoxy-phenyl)-3,5-dihydroxy-8,8-dimethyl-2,3-dihydro-8H-pyrano[3,2]chromen-4-one together with previously reported epicatechin were isolated from the ethyl acetate soluble fraction of the methanol extract of the stem bark of *Commiphora pedunculata*. The structures of these compounds were elucidated based on extensive analysis of their spectral data, including 1 and 2D NMR. The compounds were active against nine out of twelve tested microorganisms including a resistant strain (VRE), *E. coli*, *S. aureus* and *C. albicans*. The zones of inhibition ranged between 22 and 34 mm against the microorganisms. The MIC was as low as 6.25 µg/mL against *S. dysenteriae*, *B. cereus* and *S. aureus*, while the MBC was as low as 50 µg/mL against *P. aeruginosa*, VRE and *C. albicans*. This is the first report of the isolation of this compound.

Keywords: 2D NMR; *Commiphora pedunculata*; Burseraceae; Flavonoids; VRE

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Table S1. NMR spectral data for compound **1** (CD₃OD, 400 MHz)

Figure S1. Selected HMBC correlations of compound **1**

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Figure S4. COSY spectrum of compound **1**

Figure S5. DEPT spectrum of compound **1**

Figure S6. HSQC spectrum of compound **1**

Figure S7. HMBC spectrum of compound **1**

Figure S8. IR spectrum of compound **1**

Table S1. NMR spectral data for compound **1** (CD₃OD, 400 MHz)

No.	δ_{H} [mult., <i>J</i> (Hz)]	δ_{C} (mult.)	HMBC
2	4.90 d (11.4)	85.04 (CH)	4, 1', 3
3	4.49 d (11.4)	73.71.01 (CH)	3, 4, 2
4	-	198.79 (C)	-
5	-	159.20 (C)	-
6	-	104.20 (C)	-
7	-	163.64 (C)	-
8	5.92 s	97.13 (CH)	8a, 4a, 6
8a	-	163.60 (C)	-
4a	-	102.33 (C)	-
1'	-	134.01 (C)	-
2'	6.55 s	108.27 (CH)	4', 3', 1', 2
3'	-	151.75 (C)	-
4'	-	137.29 (C)	-
5'	-	151.75 (C)	-
6'	6.55 s	108.27 (CH)	4', 3', 1', 2
2''	-	79.54 (C)	-
3''	5.61 d (10.0)	127.73 (CH)	6, 2'', 1'''
4''	6.61 d (10.0)	115.97 (CH)	7, 6, 5, 2''
1'''	1.44 brs	28.62 (CH ₃)	2'', 3''
2'''	1.43 brs	28.56 (CH ₃)	2'', 3''
4'-OCH ₃	3.83 s	60.78 (CH ₃)	4'

Figure S1. Selected HMBC correlations of compound 1

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Figure S2. Proton NMR spectrum of compound 1

Figure S3. ^{13}C NMR spectrum of compound 1

Figure S4. COSY spectrum of compound 1

Figure S5. DEPT spectrum of compound 1

Figure S6. HSQC spectrum of compound 1

Figure S7. HMBC spectrum of compound 1

Jun13-2013-ABU-James 36 1 /opt/topspin ABU

Jun13-2013-ABU-James 30 1 /opt/topepin ABU

W3 in cd3od

Jun13-2013-ABU-James 30 1 /opt/topspin ABU

N3 in cd3od

Operator: My Computer
Department: lab

TITLE: AYD_N3

Labels of AYD_N3:

Name	Value
Spectrometer model	MB3000
Accessory model	
Detector model	114690-131082
Detector Gain	27
Resolution	8
Scans	30
Filename	
Inst. Resolution	
Inst. OP Band Flag	
Inst. Laser Type	
Preamplifier ADC Channel	
Preamplifier Detector ID	
Preamplifier Sampling Factor	
Preamplifier 2nd Stage Gain	
Preamplifier 1st Stage Gain	

Figure S8. IR spectrum of compound 1