**Disproof of the Structure Proposed for a Natural Phenylethanol
Isolated from a Mangrove *Avicennia marina***

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S 3

125 MHz, CDCl₃

(expansion)

S 5

400 MHz, CD₃OD

(expansion)

S 7

500 MHz, CDCl₃

6120 YYQ-1-55-2 PA-2 55 214 0.7

Sample Name:	YYQ-1-55-2 PA-2 55 214 0.7	Injection Volume:	3.0
Vial Number:	BC8	Channel:	UV_VIS_2
Sample Type:	unknown	Wavelength:	214.0
Control Program:	test-dad3	Bandwidth:	4
Quantif. Method:	WXL	Dilution Factor:	1.0000
Recording Time:	2015-7-13 14:58	Sample Weight:	1.0000
Run Time (min):	17.51	Sample Amount:	1.0000

No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	7.07	n.a.	3.269	0.622	4.94	n.a.	BMB*
2	8.17	n.a.	45.840	11.959	95.06	n.a.	BMB*
Total:			49.110	12.581	100.00	0.000	

Chiral HPLC analysis of (S)-1

6119 YYQ-1-69-2+- PA-2 55 214 0.7

Sample Name:	YYQ-1-69-2+- PA-2 55 214 0.7	Injection Volume:	6.0
Vial Number:	BD8	Channel:	UV_VIS_2
Sample Type:	unknown	Wavelength:	214.0
Control Program:	test-dad3	Bandwidth:	4
Quantif. Method:	WXL	Dilution Factor:	1.0000
Recording Time:	2015-7-13 13:45	Sample Weight:	1.0000
Run Time (min):	71.71	Sample Amount:	1.0000

No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	7.07	n.a.	610.617	115.217	49.56	n.a.	BM *
2	8.14	n.a.	447.814	117.280	50.44	n.a.	MB*
Total:			1058.432	232.497	100.00	0.000	

Chiral HPLC analysis of racemic 1

Table S-1. Comparison of ^1H NMR for the natural and synthetic **1**

Natural 1 (500 MHz, CD_3OD) ^a	Synthetic 1 (400 MHz, CD_3OD) ^b	Synthetic 1 (500 MHz, CDCl_3) ^c
7.14 (d, $J = 7.5$ Hz, 2H, H-2,6)	7.13 (d, $J = 8.8$ Hz, 2H)	7.15 (d, $J = 9.0$ Hz, 2H)
6.89 (d, $J = 7.5$ Hz, 2H, H-3,5)	6.88 (d, $J = 8.8$ Hz, 2H)	6.87 (d, $J = 9.0$ Hz, 2H)
4.23 (d, $J = 9.3$ Hz, 1H, H-1')	4.21 (dd, $J = 10, 2.8$ Hz, 1H)	4.13 (dd, $J = 9.5, 3.0$ Hz, 1H)
3.89 (d, $J = 9.3$, 1H, H-1')	3.88 (dd, $J = 10, 8.0$ Hz, 1H)	4.01 (dd, $J = 9.5, 7.5$ Hz, 1H)
3.75 (br s, 1H, H-2')	3.72-3.68 (m, 1H)	3.82 (t, $J = 6.5$ Hz, 2H)
3.69 (t, $J = 7.2$, 2H, H-8)	3.70 (t, $J = 7.2$ Hz, 2H)	3.78 (dd, $J = 7.5, 3.0$ Hz, 1H)
2.72 (t, $J = 7.2$ Hz, 2H, H-7)	2.75 (t, $J = 6.8$ Hz, 2H)	2.81 (t, $J = 6.5$ Hz, 2H)
1.27 (s, 3H, H-4')	1.26 (s, 3H)	1.32 (s, 3H)
1.23 (s, 3H, H-5')	1.23 (s, 3H)	1.27 (s, 3H)

^aTaken with assignments from (Zheng et al. 2014). ^bThis work.

Zheng, C.; Chen, Y.; Jiang, L. L.; Shi, X.M., 2014. Antiproliferative metabolites from the endophytic fungus *Penicillium* sp. FJ-1 isolated from a mangrove *Avicennia marina*. *Phytochem. Lett.* 10, 272-275.

(expansion)

(S)-1

H-2'
H-8

H-1'

H-1'

S 14

HMBC in CD₃OD

4

2013500-y2-53-1-inter	USER: -- DATE: Apr 30 2016			
F1: 499.910	F2: 125.714	SW1: 8013	OF1: 2995.7	PTS1d: 16384
EX: s2pul	PW: 3.8 usec	PD: 1.0 sec	NA: 8	Nuts - \$2013500-y2-53-1-inter_pslabel_01.fid
			LB: 0.0

4

H-1'

4

H-1'

(expansion)

S 18

HMBC in CDCl₃