SUPPLEMENTARY MATERIAL

A New Sesquiterpene from the Entomogenous Fungus *Phomopsis amygdali*

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Abstract

A new sesquiterpene, (+)-*S*-1-methyl-abscisic-6-acid (**1**), together with five known compounds, (+)-*S*-abscisic acid (**2**), fusicoccin J (**3**), 3 α -hydroxyfusicoccin J (**4**), (*R*)-5-hydroxymethylmellein (**5**) and 4-hydroxyphenethyl acetate (**6**) were isolated from the fermentation extract of *Phomopsis amygdali*, an entomogenous fungus isolated from *Call midge*. Their structures were determined mainly by analysis of MS and NMR spectroscopic data. Compounds **1–6** were tested for antimicrobial activity against three plant pathogenic fungi: *Gibberella zeae*, *Verticillium albo-atrum*, and *Fusarium nivale*, and two bacteria: *Escherichia coli* and *Pseudomonas aeruginosa* 2033E. As a result, compounds **1–4** displayed antibacterial activity against Gram-negative *Pseudomonas aeruginosa* 2033E, the minimum

inhibition concentration (MIC value) of **1–4** are 30 $\mu\text{g/mL}$, 58 $\mu\text{g/mL}$, 26 $\mu\text{g/mL}$ and 26 $\mu\text{g/mL}$ respectively.

Keywords: Entomogenous fungus; *Phomopsis amygdali*; (+)-*S*-1-methyl-abscisic-6-acid; Antimicrobial activity; *Pseudomonas aeruginosa* 2033

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Table S1. ^1H NMR (500 MHz, in Acetone- d_6) and ^{13}C NMR (125 MHz, in Acetone- d_6) data for compounds **1** and **2**.

Position	1			2	
	$\delta_{\text{(H)}}$	$\delta_{\text{(C)}}$	HMBC	$\delta_{\text{(H)}}$	$\delta_{\text{(C)}}$
1	2.31(bris)	14.0	2, 3, 4, 6		167.2
2	5.88(s)	120.5	1, 4, 6	5.76(s)	118.6
3		152.4			151.1
4	6.58(d, $J = 15.7$ Hz)	134.4	1, 2, 3, 5, 1'	7.93(d, $J = 16.0$ Hz)	128.6
5	6.42(d, $J = 15.7$ Hz)	137.2	3, 4, 1'	6.39(d, $J = 16.0$ Hz)	138.4
6		168.0		2.06(d, $J = 2.1$ Hz)	19.2
1'		79.8			80.0
2'		162.8			163.2
3'	5.83(s)	127.4	1', 5', 7',	5.83(s)	127.3
4'		197.3			197.4
5'	2.18(d, $J = 16.8$ Hz)	50.3	1', 3', 4', 6', 8',	2.16(d, $J = 16.8$ Hz)	50.3
	2.57(d, $J = 16.8$ Hz)		4', 6', 8'	2.56(d, $J = 16.8$ Hz)	
6'		42.2			42.2
7'	1.89(bris)	19.1	1', 2', 3'	1.91(d, $J = 1.3$ Hz)	21.2
8'	1.07(s)	23.5	1', 5', 6'	1.07(s)	23.5
9'	1.03(s)	24.7	1', 5', 6'	1.04(s)	24.7

Table S2. ^1H NMR data for compound **1**.

Position	Acetone- d_6	CD_3OD
1	2.31(bris)	2.27(d, $J = 0.8$ Hz)
2	5.88(s)	5.93 – 5.90(m)
3		
4	6.58(d, $J = 15.7$ Hz)	6.48(d, $J = 15.7$ Hz)
5	6.42(d, $J = 15.7$ Hz)	6.27(d, $J = 15.7$ Hz)
6		
1'		
2'		
3'	5.83(s)	5.84(s)
4'		
5'	2.18(d, $J = 16.8$ Hz)	2.23(d, $J = 17.0$ Hz)
	2.57(d, $J = 16.8$ Hz)	2.55(d, $J = 17.0$ Hz)
6'		
7'	1.89(bris)	1.91(d, $J = 1.3$ Hz)
8'	1.07(s)	1.06(s)
9'	1.03(s)	1.02(s)