

Supplementary Materials: Inhibitory Activities of Blasticidin S Derivatives on Aflatoxin Production by *Aspergillus Flavus*

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Table S1. NMR spectroscopic data for blasticidin S derivatives.

position	MeBcS (3)		DahMeBcS (4)		PyBcS (5)		cytomycin (6)		7	
	$\delta_{\text{C}}^{\text{a}}$	$\delta_{\text{H}}^{\text{a}}$ (J in Hz)	$\delta_{\text{C}}^{\text{a}}$	$\delta_{\text{H}}^{\text{a}}$ (J in Hz)	$\delta_{\text{C}}^{\text{b}}$	$\delta_{\text{H}}^{\text{b}}$ (J in Hz)	$\delta_{\text{C}}^{\text{a}}$	$\delta_{\text{H}}^{\text{a}}$ (J in Hz)	$\delta_{\text{C}}^{\text{a}}$	$\delta_{\text{H}}^{\text{a}}$ (J in Hz)
1	148.8		151.8		148.6		148.7		148.6	
2	159.6		166.2		159.5		159.6		159.5	
3	95.6	6.24, d (7.8)	102.7	5.91, d (8.2)	95.6	6.22, d (7.8)	95.5	6.23, d (7.8)	95.5	6.24, d (7.9)
4	145.4	7.82, d (7.8)	142.7	7.64, d (8.2)	145.5	7.81, d (7.8)	145.5	7.84, d (7.8)	145.5	7.83, d (7.9)
5	79.4	6.57, s, br	78.8	6.54, s, br	79.3	6.55, s, br	79.4	6.54, s, br	79.2	6.57, s, br
6	124.6	6.26, dt (10.5, 2.5)	125.3	6.25, dt (10.4, 2.4)	124.6	6.24, dt (10.5, 2.3)	124.5	6.22, dt (10.5, 2.3)	124.2	6.25, dt (10.0, 2.4)
7	133.1	5.96, dt (10.5, 2.1)	132.4	5.99, dt (10.4, 2.0)	133.5	5.94, dt (10.5, 2.1)	134.0	5.90, dt (10.5, 2.1)	133.5	5.94, dt (10.0, 2.1)
8	44.5	4.83, ddd (8.2, 2.5, 2.1)	44.6	4.85, ddd (8.2, 2.4, 2.0)	44.5	4.83, ddd (8.2, 2.3, 2.1)	44.9	4.82, ddd (8.7, 2.3, 2.1)	44.5	4.82, ddd (8.2, 2.4, 2.1)
9	75.1	4.55, d (8.2)	75.0	4.55, d (8.2)	75.2	4.43, d (8.2)	76.3	4.28, d (8.7)	75.1	4.47, d (8.2)
10	171.3		171.2		172.1		173.3		172.7	
11	170.3		170.4		171.4		172.3		171.9	
12	36.5	2.74, m	36.5	2.77, m	36.7	2.77, m	36.5	2.52, m	41.2	2.52, m
13	46.4	3.68, m	46.4	3.70, m	46.3	3.62, m	45.7	3.84, m	45.2	4.05, m
14	29.3	2.06, m	29.2	2.09, m	29.4	2.10, m	25.4	2.12, m	31.0	1.96, m
								1.86, m		1.85, m
15	46.7	3.49, m	46.6	3.52, m	46.7	3.94, m	46.0	3.43, m	46.1	3.10, m
16	35.9	3.05, s	35.8	3.08, s	35.4	3.26, s	40.9	3.02, s	32.8	2.73, s
17	156.7		156.6		153.9		153.5		160.8	
18	-		-		157.7	8.58, s, br	-		-	
19	-		-		109.4	7.04, t (5.5)	-		-	
20	-		-		157.7	8.58, s, br	-		-	
COOCH ₃	53.5	3.76, s	53.4	3.78, s	-		-		-	

^a 125 MHz (δ_{C}) and 500 MHz (δ_{H}) in D₂O. ^b 125 MHz (δ_{C}) and 500 MHz (δ_{H}) in DMSO-d₆.

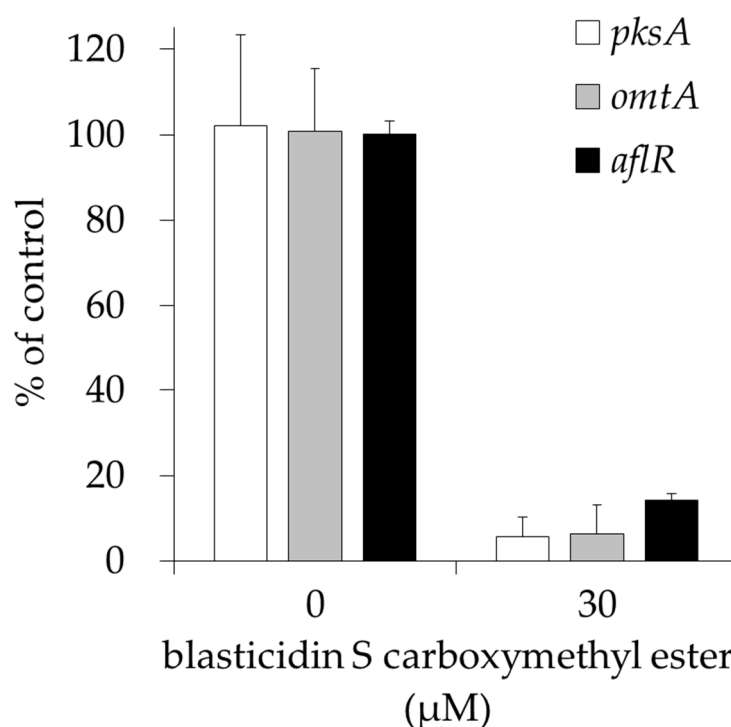


Figure S1. Effect of blasticidin S carboxymethyl ester on the transcription of genes encoding proteins involved in aflatoxin biosynthesis. The mRNA levels of the three genes were analyzed by quantitative PCR according to the method in our previous work [1]. Data are presented as the mean $\pm$ SD ($n = 6$).

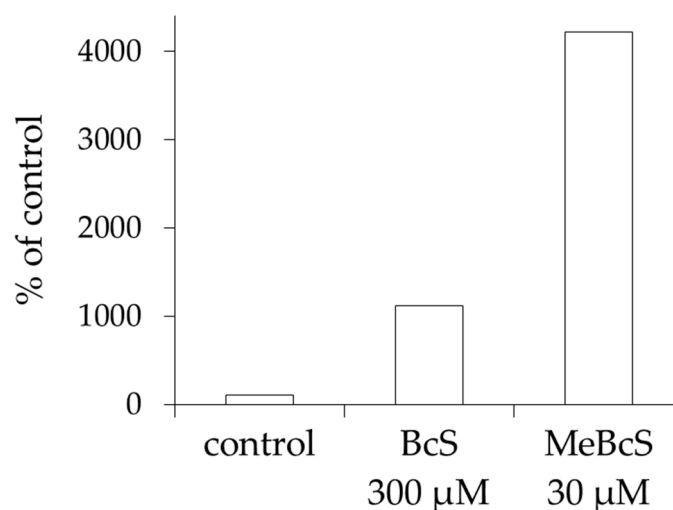


Figure S2. Effect of blasticidin S (BcS) and its carboxymethyl ester (MeBcS) on the transcription of blasticidin S deaminase. The mRNA level was analyzed by quantitative PCR according to the method in our previous work [1]. The primers used were 5'-GGCAGGTTTTGTGGGATTG-3' and 5'-CCCCTCCTCCCTAAAACAAT-3'. Data are presented as the mean ($n = 2$).

References

1. Yoshinari, T.; Sakuda, S.; Watanabe, M.; Kamata, Y.; Ohnishi, T.; Sugita-Konishi, Y. New metabolic pathway for converting blasticidin S in *Aspergillus flavus* and inhibitory activity of aflatoxin production by blasticidin S metabolites. *J. Agric. Food Chem.* **2013**, *61*, 7925–7931.