

Supplementary Materials: Biotransformation of Ergostane Triterpenoid Antcin K from *Antrodia cinnamomea* by Soil-Isolated *Psychrobacillus* sp. AK 1817

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Table S1. NMR spectroscopic data for compound (1)/(2) (in pyridine-d₅; 700MHz).

Position	δ_C	type	δ_H (J in Hz)	HMBC
1	36.7,	CH ₂	3.30, m ; 1.60, m;	H-2, H-19
2	34.4,	CH ₂	3.06, m ; 2.52, m;	H-1
3	214.2,	C		H-1, H-2, H-29
4	76.3,	C		H-6, H-29
5	50.6,	CH	1.79, dd (13.3, 2.4)	H-1, H-6, H-19, H-29
6	30.5,	CH ₂	2.52, m ; 2.67, m	H-5
7	70.3,	CH	4.66, t (8.4)	H-5, H-6
8	155.5,	C		H-6, H-14
9	141.8,	C		H-12, H-14, H-19
10	37.7,	C		H-1, H-5, H-6
11	201.2,	C		H-12
12	58.5	CH ₂	3.00, d (14.0); 2.48, d (14.0);	H-18
13	47.7	C		H-12, H-14, H-15, H-18
14	53.6	CH	2.79, dd (12.9, 7.0)	H-12, H-15, H-18
15	25.6	CH ₂	2.57, m ; 2.16, m	H-14
16	28.3	CH ₂	1.92, m ; 1.35, m	H-17
17	54.8	CH	1.41, m	H-16, H-21
18	12.5	CH ₃	0.87, s	H-12, H-14
19	20.7	CH ₃	1.91, s	H-1, H-5
20	36.2	CH	1.40, m	H-17, H-21
21	18.7	CH ₃	0.89, d (5.6)	
22	34.5	CH ₂	1.78, m ; 1.29, m	H-21
23	31.7	CH ₂	2.42, m ; 2.23, m	H-25, H-28
24	150.2	C		H-25, H-27
25	47.2	CH	3.48, dd (14.1, 7.1)	H-27, H-28
26	177.4,	C		H-25, H-27
27	17.3	CH ₃	1.51, d (7.1)	H-25
28	110.1	CH ₂	5.24, s ; 5.07, s	H-25
29	24.3	CH ₃	1.54, s	H-5

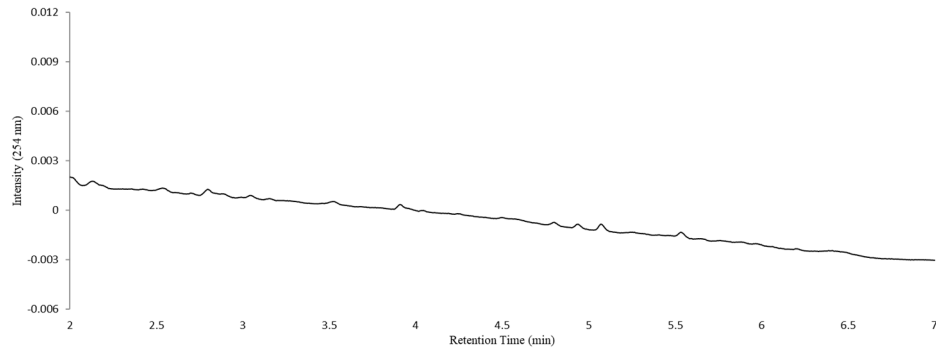


Figure S1. UPLC analysis of fermentation broth of the AK 1817 strain. The strain was cultivated in LB media without antcin K. The fermentation broth with cultivation of 72-h was analyzed by UPLC. The UPLC operation conditions were described in Materials and Methods.

TGAGGGAGGTGCTATACATGCAGTCGAGCGAATGATGAAGAAGCTTGCTTCTTC
TGATTTAGCGGCGGACGGGTGAGTAACACGTGGGCAACCTGCCCTGTAGATTGG
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AGCATGTGGTTTAATTCGAAGCAACGCGAAGAACCTTACCAGGTCTTGACATCCC
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CGCAACCCTTGATCTTAGTTGCCAGCATTAGTTGGGCACTCTAAGGTGACTGCC
GGTGATAAACCGGAGGAAGGTGGGGATGACGTCAAATCATCATGCCCTTATGA
CCTGGGCTACACACGTGCTACAATGGACGGTACAGAGGGTCGCAACCCCGCGAG
GGTGAGCTAATCCCATAAAACCGTTCTCAGTTCCGATTGTAGGCTGCAACTCGCC
TACATGAAGCCGGAATCGCTAGTAATCGTGATCAGCATGCCACGTATTAACCA

Figure S2. The partial 16S rRNA gene sequence of the AK 1817 strain. The partial 16S rRNA gene was amplified and sequenced by PCR with the bacteria specific 27F (5'-AGAGTTTGATCCTGGCTCAG-3') and 1391R (5'-GACGGGCRGTGWGTRCA-3') primer set. The PCR operation conditions were described in Materials and Methods.

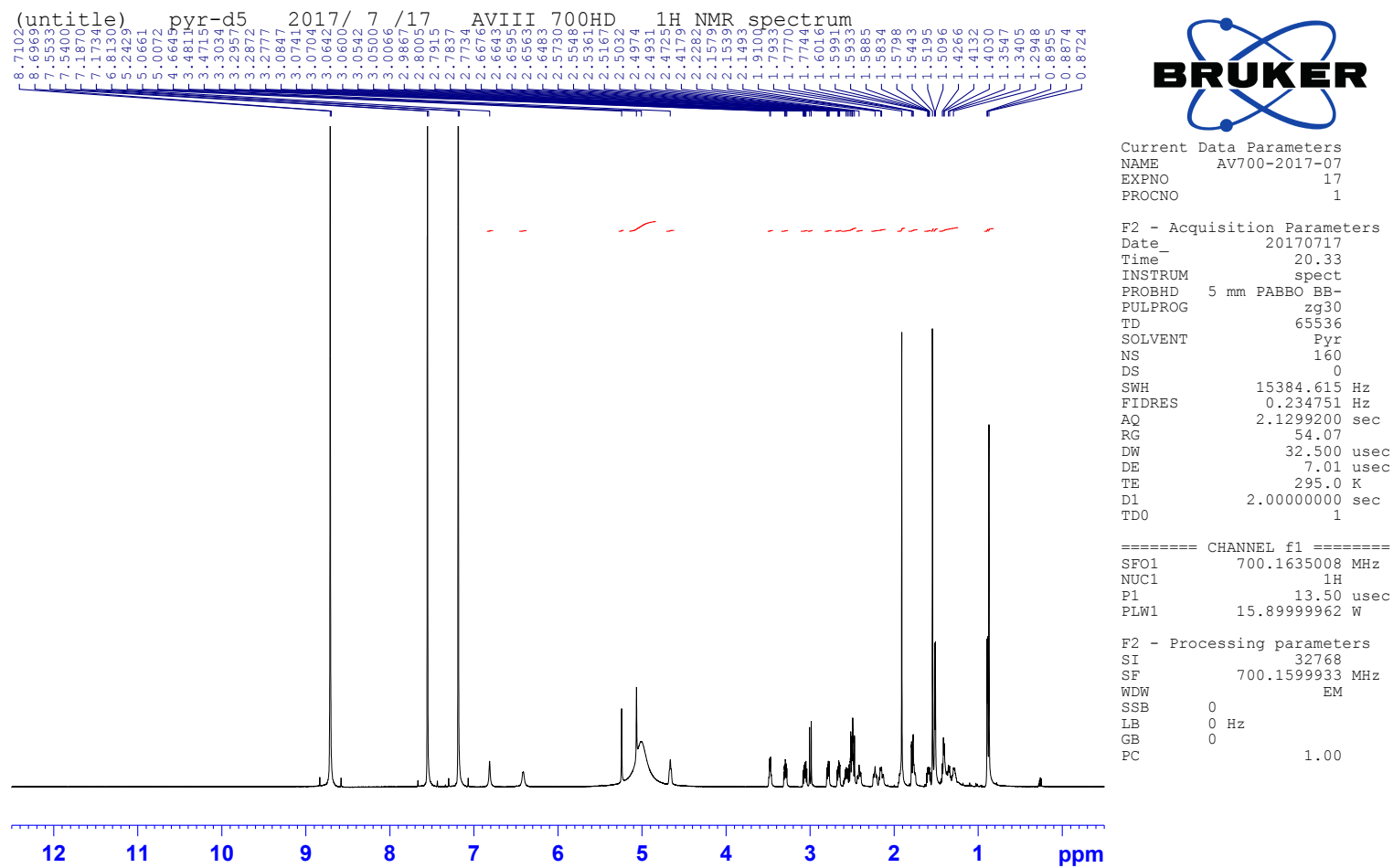


Figure S3. The ^1H -NMR (700 MHz, Pyridine- d_5) spectrum of compound (2).

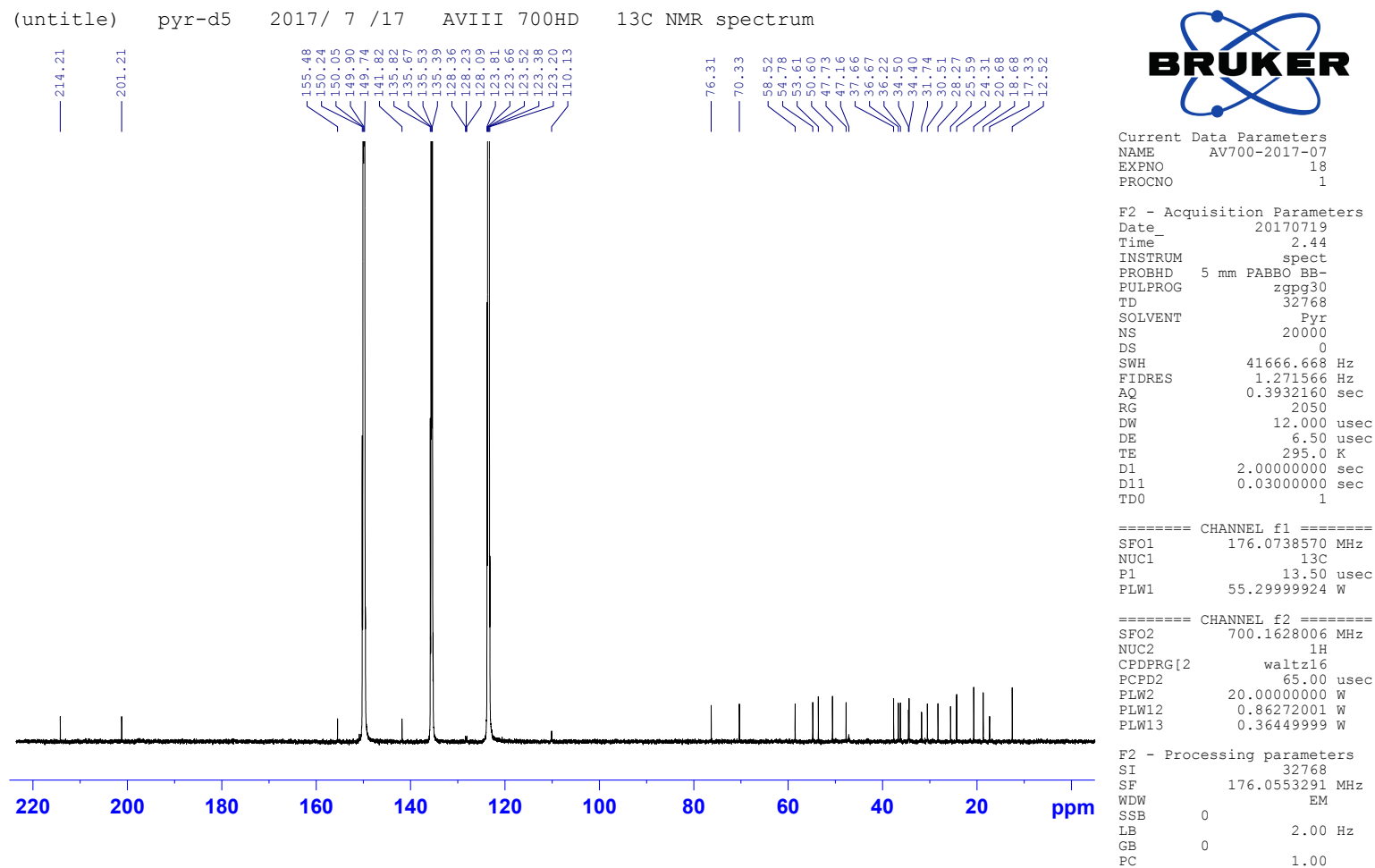


Figure S4. The ^{13}C -NMR (700 MHz, Pyridine- d_5) spectrum of compound (2).

(untitled) pyr-d5 2017/ 7 /26 AVIII 700HD HMBC NMR spectrum



Current Data Parameters
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 PROCNO 1

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 SOLVENT Pyr
 NS 48
 DS 16
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 DW 55.000 usec
 DE 6.50 usec
 TE 295.0 K
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 CNST13 10.0000000
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 D2 0.00344828 sec
 D6 0.05000000 sec
 D16 0.00020000 sec
 IN0 0.00001170 sec

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 NUC1 1H
 P1 13.50 usec
 P2 27.00 usec
 PLW1 15.89999962 W

===== CHANNEL f2 =====
 SFO2 176.0756184 MHz
 NUC2 13C
 P3 13.50 usec
 PLW2 55.00000000 W

===== GRADIENT CHANNEL =====
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 GPNAM[2] SMSQ10.100
 GPNAM[3] SMSQ10.100
 GPZ1 50.00 %
 GPZ2 30.00 %
 GPZ3 40.10 %
 P16 1000.00 usec

F1 - Acquisition parameters
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 FIDRES 333.867523 Hz
 SW 242.708 ppm
 F1MODE QF

F2 - Processing parameters
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 WDW 0
 SSB SINE
 LB 0 Hz
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F1 - Processing parameters
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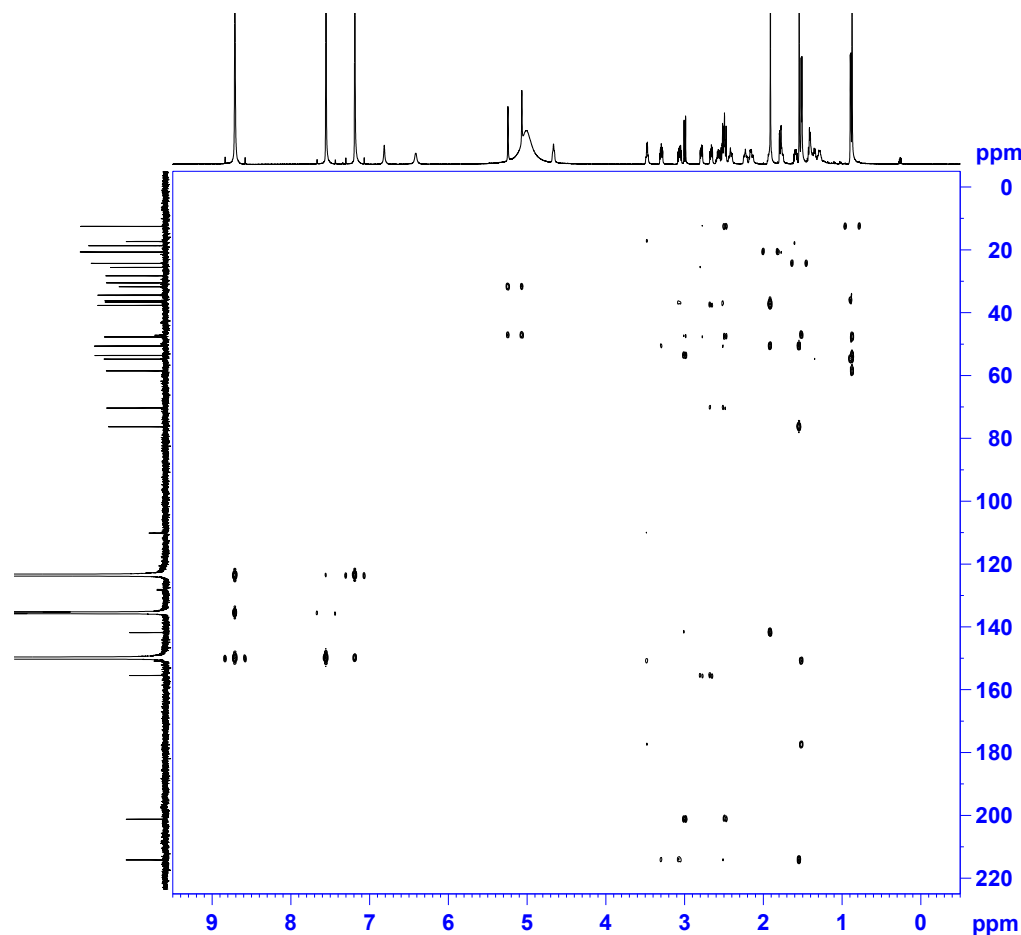


Figure S5. The HMBC (700 MHz, Pyridine-d5) spectrum of compound (2).

(untitled) pyr-d5 2017/ 7 /26 AVIII 700HD HSQC NMR spectrum

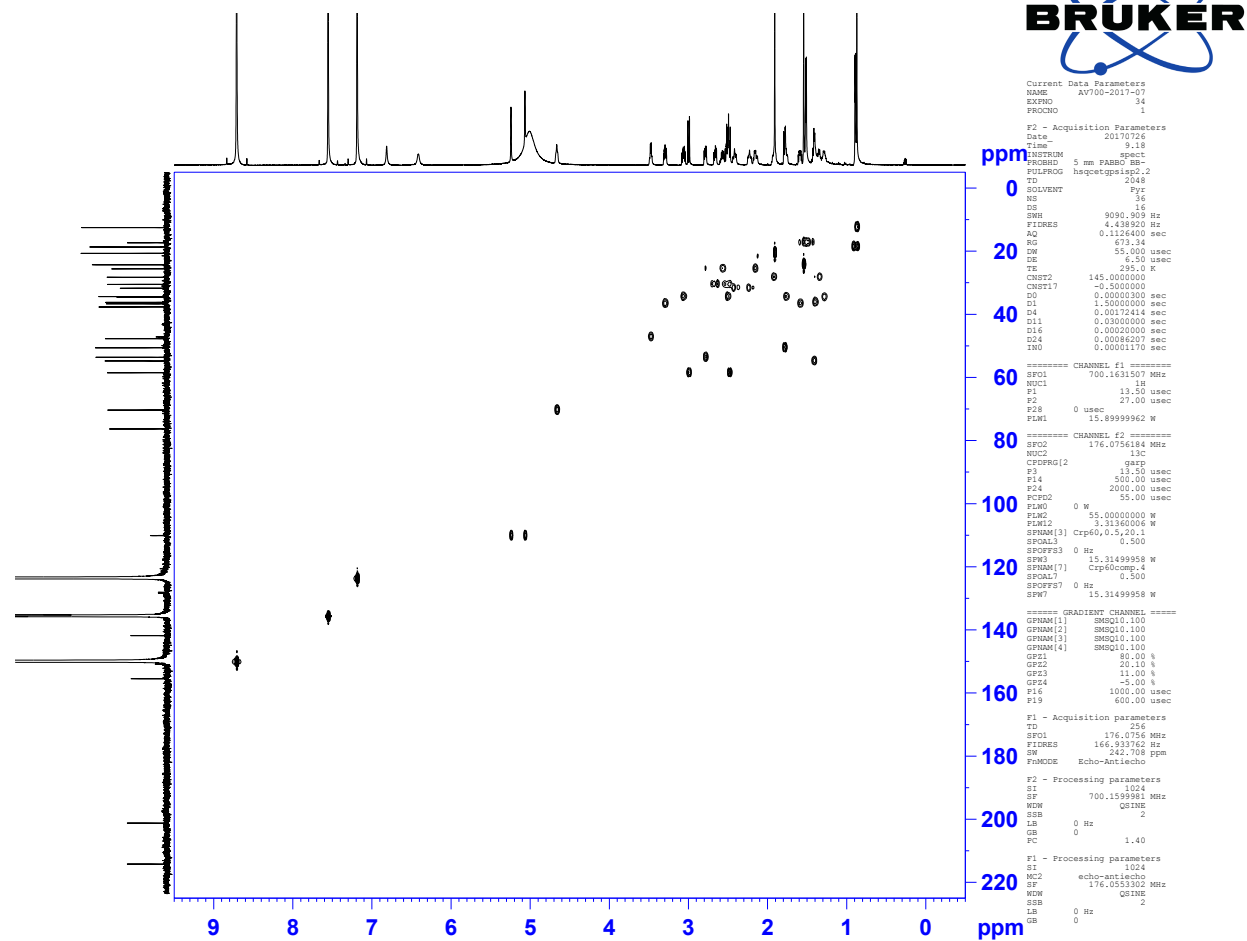


Figure S6. The HSQC (700 MHz, Pyridine-d5) spectrum of compound (2).

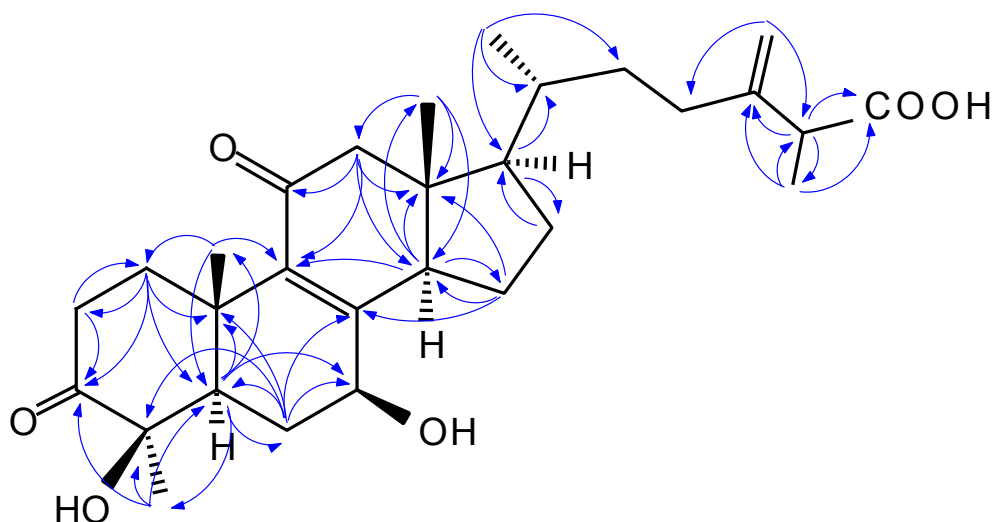


Figure S7. The key HMBC correlations of compound (1)/(2).

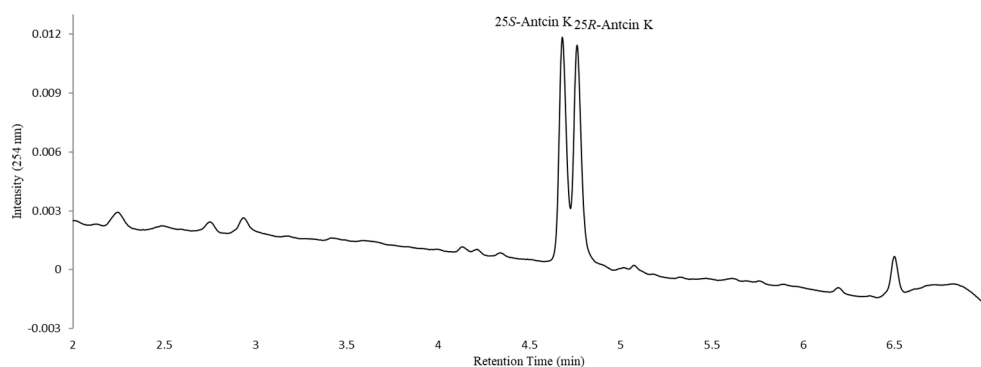


Figure S8. Biotransformation of antcin K by *B. megaterium* ATCC 14581 strain. The strain was cultivated in LB media containing both 25S- and 25R-antcin K. The fermentation broth with cultivation of 72-h was analyzed by UPLC. The UPLC operation conditions were described in Materials and Methods.

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