
Supplementary Materials for

Aromatic Polyketides from a Symbiotic Strain *Aspergillus fumigatus* D and Characterization of Their Biosynthetic Gene *D8.t287*

Yi Hua ¹, Rui Pan ¹, Xuelian Bai ², Bin Wei ¹, Jianwei Chen ¹, Hong Wang ^{1,*} and Huawei Zhang ^{1,*}

Figure S1. Isolation procedure of compounds 1-8	1
Figure S2. Screening resistance marker of strain D	1
Figure S3. PCR verification of target genes LB and RB in constructed vector	1
Figure S4. Colony morphology of positive transformant and PCR verification	1
Figure S5. PCR identification results of mutant strain Δ HY44	2
Figure S6. ¹ H NMR Spectrum of compound 1 in CDCl ₃	3
Figure S7. ¹ H NMR Spectrum of compound 2 in DMSO- <i>d</i> ₆	4
Figure S8. ¹ H NMR Spectrum of compound 3 in CDCl ₃	5
Figure S9. ¹ H NMR Spectrum of compound 4 in CDCl ₃	6
Figure S10. ¹ H NMR Spectrum of compound 5 in CDCl ₃	7
Figure S11. ¹ H NMR Spectrum of compound 6 in CDCl ₃	8
Figure S12. ¹ H NMR Spectrum of compound 7 in CDCl ₃	9
Figure S13. ¹ H NMR Spectrum of compound 8 in CDCl ₃	11
Table S1. Primers and its sequences of PCR	2
Table S2. Conditions of PCR reaction	2
Table S3. Comparison of ¹ H NMR spectral data of compound 1	3
Table S4. Comparison of ¹ H NMR spectral data of compound 2	4
Table S5. Comparison of ¹ H NMR spectral data of compound 3	5
Table S6. Comparison of ¹ H NMR spectral data of compound 4	6
Table S7. Comparison of ¹ H NMR spectral data of compound 5	7

Table S8. Comparison of ^1H NMR spectral data of compound 6	8
Table S9. Comparison of ^1H NMR spectral data of compound 7	10
Table S10. Comparison of ^1H NMR spectral data of compound 8	11

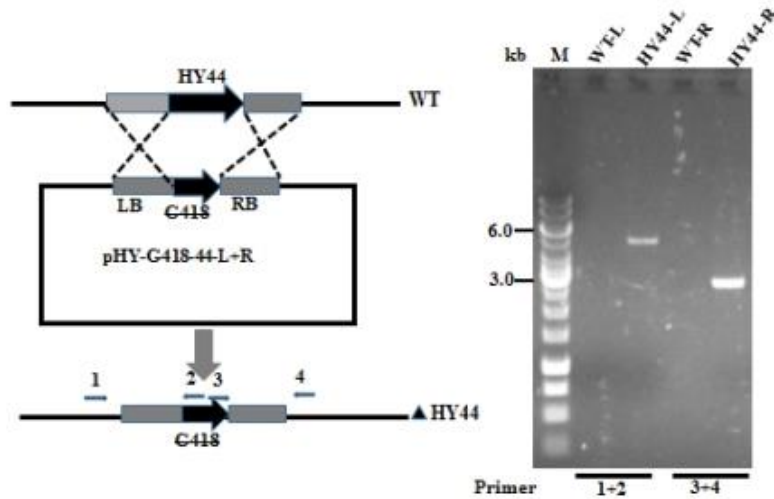


Figure S5. PCR identification of mutant strain Δ HY44
(M: Marker; WT: wild strain; Δ HY44: mutant strain)

Table S1. Conditions for PCR reaction

Reagent	V (μ L)
5 \times PCR Buffer	10
dNTP Mixture	4
P1/ P2 primers	1
Template	1
Primer STAR HS DNA polymerase	1
ddH ₂ O	33
Total	50

Table S2. Primers and their sequences for PCR verification

Primers	Sequences
HY44-L-1	TTGAACATCGCGCAGTAATGCC
HY44-L-2	GAATTAATGGTACCGAGCTCGAATTAGACACATTTGGGCAAAGTGCG
HY44-R-1	GTTTAGAGGTAATCCTCCC GGGACCTCGCTGTTGTGTGCTTTTG
HY44-R-2	CGATCCTAGAACTAGTGGATCCCGTATACTATCGCGAAGAGAAGC
P-check-F	GGCAGGATATATTGTGGTGTAAC
P-check-R	CTCTCAGTGCGGATCAGTC
P1	GGCAGGATATATTGTGGTGTAAC
P2	GCCTGCGTTC TACTACTAGCACG
P3	GCATTCGCCATT CAGGCTGC
P4	CGTGACCGATAGCTTCAACACC

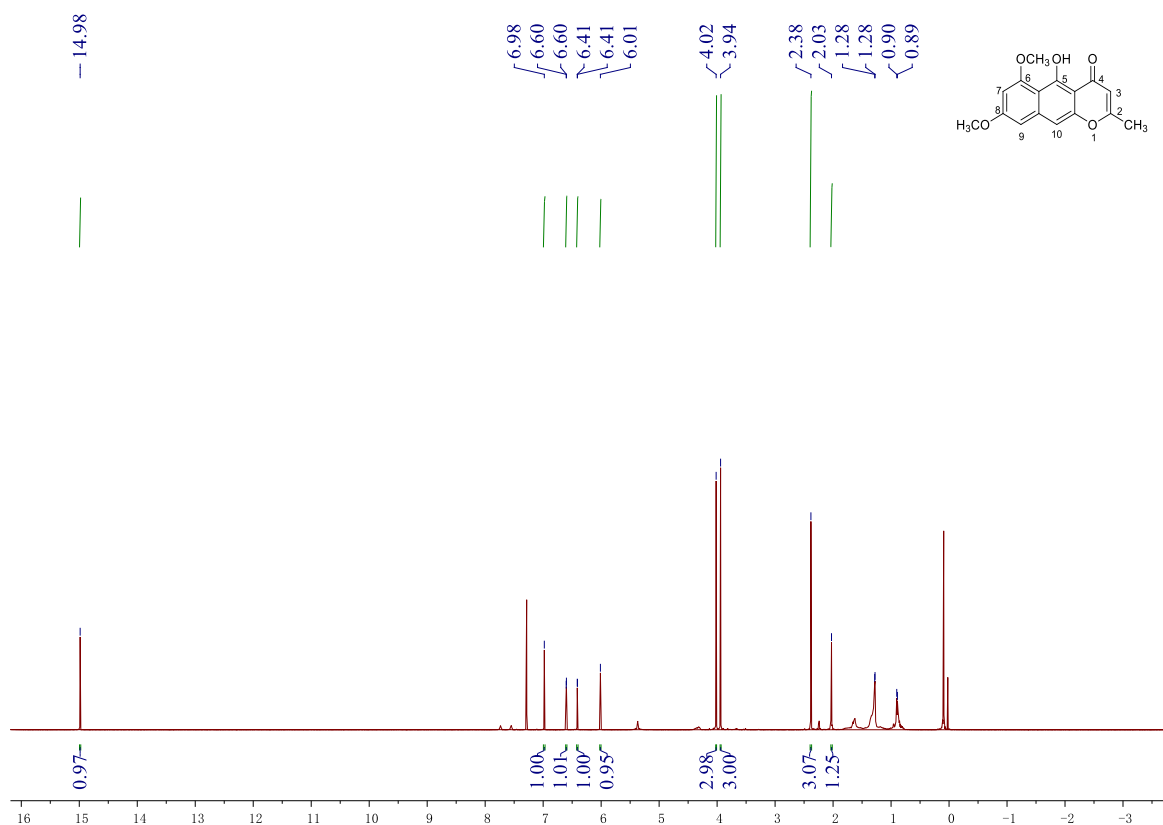


Figure S6. ¹H NMR spectrum of compound **1** in CDCl₃

Table S3. Comparison of ¹H NMR spectral data of compound **1** with reference (600 MHz, CDCl₃)

Position	δ _H	δ _H in reference [9]
2	/	/
2-CH ₃	2.38 (3H, s)	2.37 (3H, s)
3	6.01 (1H, s)	6.00 (1H, s)
4	/	/
5	14.98 (1H, s, 5-OH)	14.96 (1H, s, 5-OH)
6	/	/
6-OCH ₃	4.02 (3H, s)	4.00 (3H, s)
7	6.41 (1H, <i>d</i> , <i>J</i> = 2.35)	6.40 (1H, <i>d</i> , <i>J</i> = 2.20)
8	/	/
8-OCH ₃	3.94 (3H, s)	3.93 (3H, s)
9	6.60 (1H, <i>d</i> , <i>J</i> = 2.35)	6.59 (1H, <i>d</i> , <i>J</i> = 2.20)
10	6.98 (1H, s)	6.97 (1H, s)

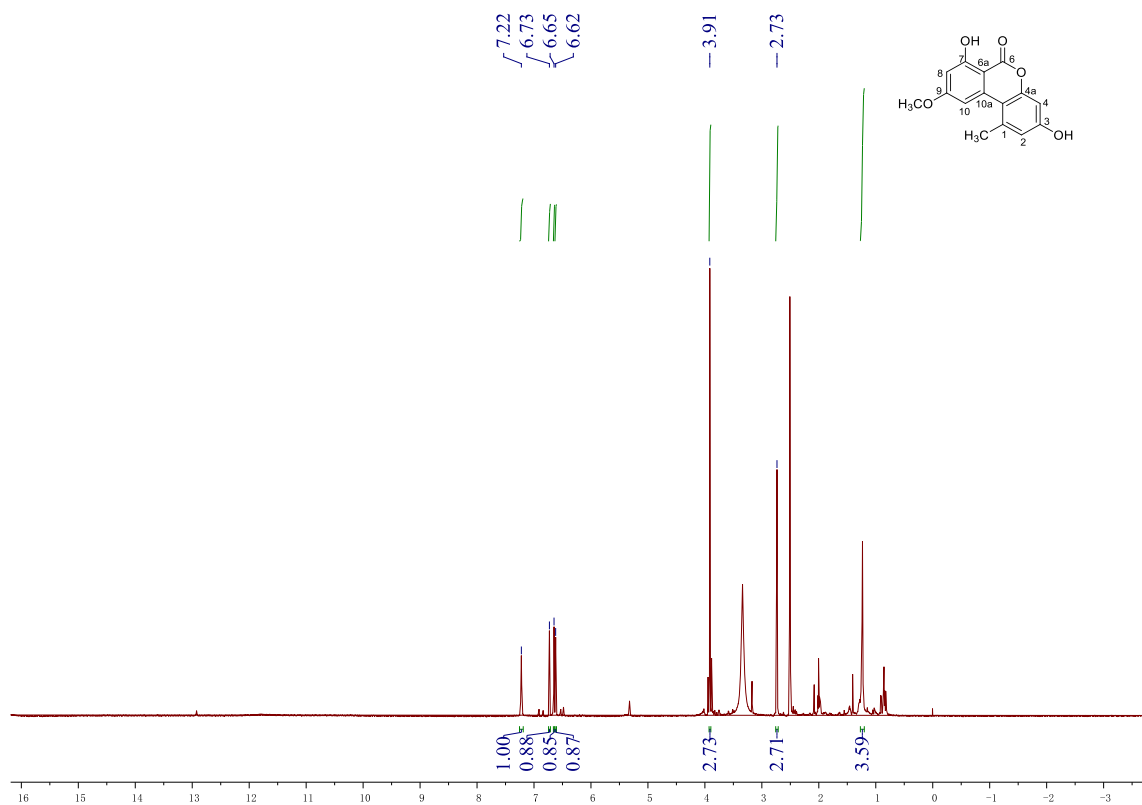


Figure S7. ^1H NMR spectrum of compound **2** in DMSO

Table S4. Comparison of ^1H NMR spectral data of compound **2** with reference (DMSO)

Position	δ_{H}	δ_{H} in reference [10]
	(<i>I</i> in Hz, 600 MHz)	(<i>I</i> in Hz, 500 MHz)
1	/	/
2	6.73 (1H, <i>d</i> , <i>J</i> = 2.30)	6.73 (1H, <i>d</i> , <i>J</i> = 2.30)
3	/	/
4	6.65 (1H, <i>d</i> , <i>J</i> = 2.30)	6.65 (1H, <i>d</i> , <i>J</i> = 2.30)
4a	/	/
6a	/	/
7	/	/
8	6.62 (1H, <i>d</i> , <i>J</i> = 1.90)	6.63 (1H, <i>d</i> , <i>J</i> = 1.90)
9	/	/
10	7.22 (1H, <i>d</i> , <i>J</i> = 1.90)	7.23 (1H, <i>d</i> , <i>J</i> = 1.90)
10a	/	/
10b	/	/
11	2.73 (3H, <i>s</i>)	2.74 (3H, <i>s</i>)
12	3.91 (3H, <i>s</i>)	3.91 (3H, <i>s</i>)

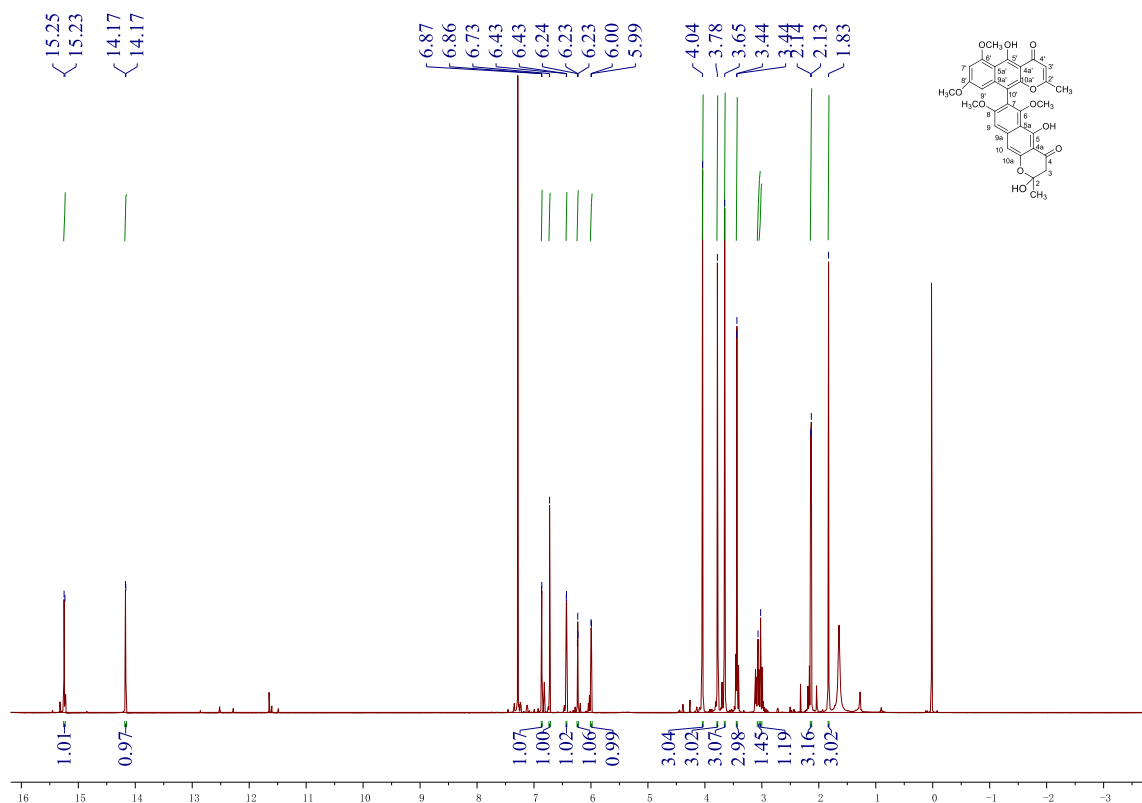


Figure S8. ^1H NMR spectrum of compound **3** in CDCl_3

Table S5. Comparison of ^1H NMR spectral data of compound **3** with reference (CDCl_3)

Position	δ_{H}	δ_{H} in reference [11, 12]
	(I in Hz, 600 MHz)	(I in Hz, 60 MHz)
2- CH_3	1.83 (3H, s)	1.78 (3H, s)
2'- CH_3	2.13 (3H, s)	2.11 (3H, s)
3	3.02/3.07 (1H, s)	3.01 (1H, s)
3'	6.00 (1H, <i>d</i> , $J = 4.08$)	5.98 (1H, <i>d</i>)
5-OH	14.17 (1H, s)	14.11 (1H, s)
5'-OH	15.24 (1H, s)	15.10 (1H, s)
6-OMe	3.44 (3H, s)	3.42 (3H, s)
6'-OMe	4.04 (3H, s)	4.00 (3H, s)
7'	6.43 (1H, <i>d</i> , $J = 2.09$)	6.42 (1H, <i>d</i> , $J = 2.50$)
8-OMe	3.78 (3H, s)	3.74 (3H, s)
8'-OMe	3.65 (3H, s)	3.63 (3H, s)
9	6.86 (1H, <i>d</i> , $J = 1.41$)	6.84 (1H, <i>d</i>)
9'	6.23 (1H, <i>d</i> , $J = 2.49$)	6.23 (1H, <i>d</i> , $J = 2.50$)
10	6.73 (1H, <i>d</i> , $J = 1.41$)	6.70 (1H, <i>d</i>)

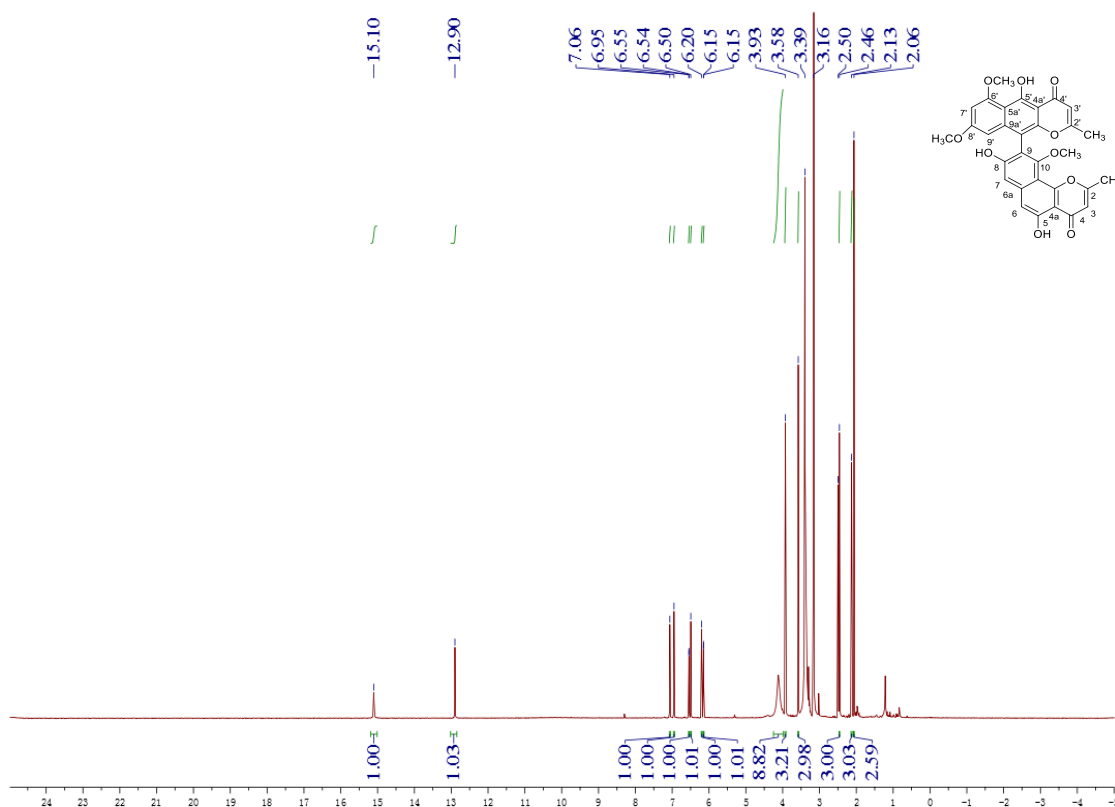


Figure S9. ^1H NMR spectrum of compound **4** in CDCl_3

Table S6. Comparison of ^1H NMR spectral data of compound **4** with reference (CDCl_3)

Position	δ_{H}	δ_{H} in reference [13]
	(<i>I</i> in Hz, 600 MHz)	(<i>I</i> in Hz, 500MHz)
2- CH_3	2.48 (3H, s)	2.46 (3H, s)
2'- CH_3	2.10 (3H, s)	2.13 (3H, s)
3	6.50 (1H, s)	6.50 (1H, s)
3'	6.20 (1H, s)	6.19 (1H, s)
5-OH	12.90 (1H, s)	12.90 (1H, s)
5'-OH	15.10 (1H, s)	15.10 (1H, s)
6	6.95 (1H, s)	6.96 (1H, s)
7	7.06 (1H, s)	7.07 (1H, s)
7'	6.55 (1H, <i>d</i> , $J = 2.28$)	6.55 (1H, <i>d</i> , $J = 2.30$)
6'-OMe	3.93 (3H, s)	3.93 (3H, s)
8'-OMe	3.58 (3H, s)	3.58 (3H, s)
9'	6.14 (1H, <i>d</i> , $J = 2.29$)	6.14 (1H, <i>d</i> , $J = 2.30$)
10-OMe	3.39 (3H, s)	3.39 (3H, s)

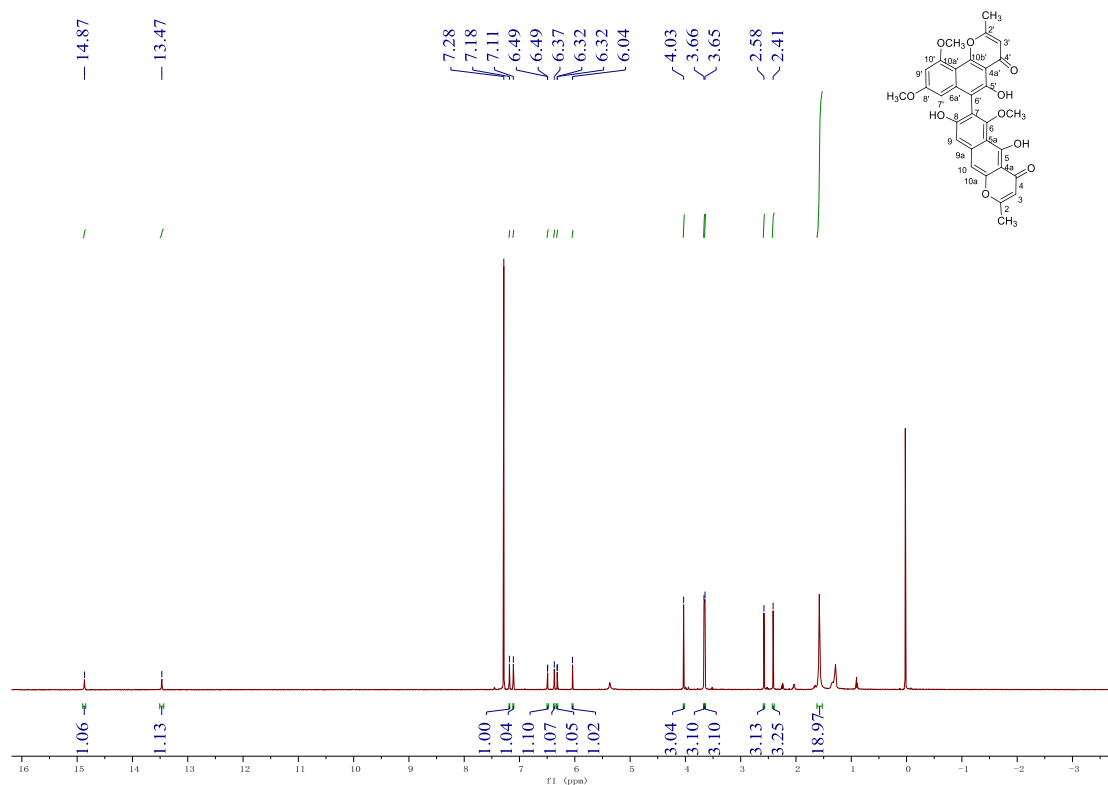


Figure S10. ¹H NMR spectrum of compound 5 in CDCl₃

Table S7. Comparison of ¹H NMR spectral data of compound 5 with reference (CDCl₃)

Position	δ_{H} (<i>I</i> in Hz, 600 MHz)	δ_{H} in reference [14] (<i>I</i> in Hz, 500 MHz)
2-CH ₃	2.41 (3H, s)	2.37 (3H, s)
2'-CH ₃	2.58 (3H, s)	2.54 (3H, s)
3	6.04 (1H, s)	6.00 (1H, s)
3'	6.37 (1H, s)	6.33 (1H, s)
5-OH	14.87 (1H, s)	14.80 (1H, s)
5'-OH	13.47 (1H, s)	13.40 (1H, s)
6-OCH ₃	3.66 (3H, s)	3.62 (3H, s)
7'	6.32 (1H, <i>d</i> , <i>J</i> = 2.21)	6.27 (1H, <i>d</i> , <i>J</i> = 2.20)
8'-OMe	3.65 (3H, s)	3.60 (3H, s)
9	7.18 (1H, s)	7.14 (1H, s)
9'	6.49 (1H, <i>d</i> , <i>J</i> = 2.21)	6.45 (1H, <i>d</i> , <i>J</i> = 2.20)
10	7.11 (1H, s)	7.07 (1H, s)
10'-OMe	4.03 (3H, s)	3.99 (3H, s)

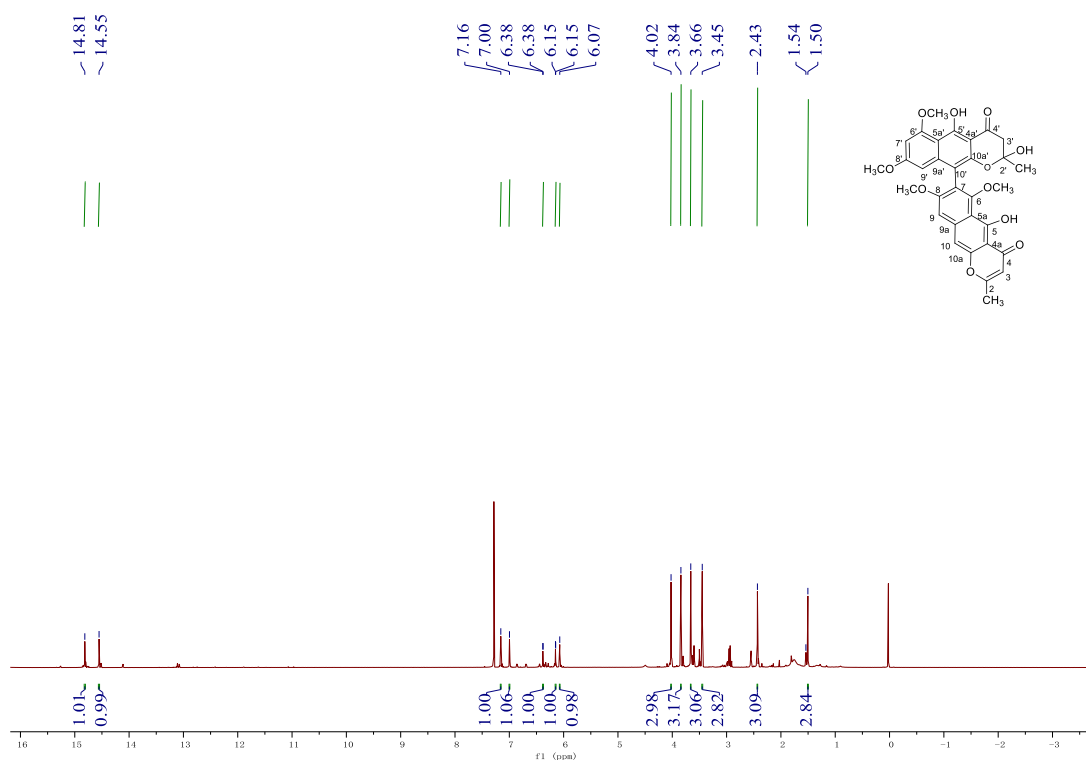


Figure S11. ^1H NMR spectrum of compound **6** in CDCl_3

Table S8. Comparison of ^1H NMR spectral data of compound **6** with reference (CDCl_3)

Position	δ_{H} (<i>I</i> in Hz, 600 MHz)	δ_{H} in reference [11] (<i>I</i> in Hz, 60 MHz)
2- CH_3	2.43 (3H, s)	2.39 (3H, s)
2'- CH_3	1.50 (3H, s)	1.49 (3H, s)
3	6.07 (1H, s)	6.01 (1H, s)
3'	3.50 (1H, s)	2.91 (1H, s)
5-OH	14.81 (1H, s)	14.70 (1H, s)
5'-OH	14.55 (1H, s)	14.40 (1H, s)
6-OMe	3.45 (3H, s)	3.43 (3H, s)
6'-OMe	4.02 (3H, s)	3.98 (3H, s)
7'	6.38 (1H, <i>d</i> , $J = 2.21$)	6.35 (1H, <i>d</i> , $J = 2.50$)
8-OMe	3.84 (3H, s)	3.80 (3H, s)
8'-OMe	3.66 (3H, s)	3.62 (3H, s)
9	7.00 (1H, s)	6.95 (1H, s)
9'	6.15 (1H, <i>d</i> , $J = 2.21$)	6.13 (1H, <i>d</i> , $J = 2.50$)
10	7.15 (1H, s)	7.10 (1H, s)

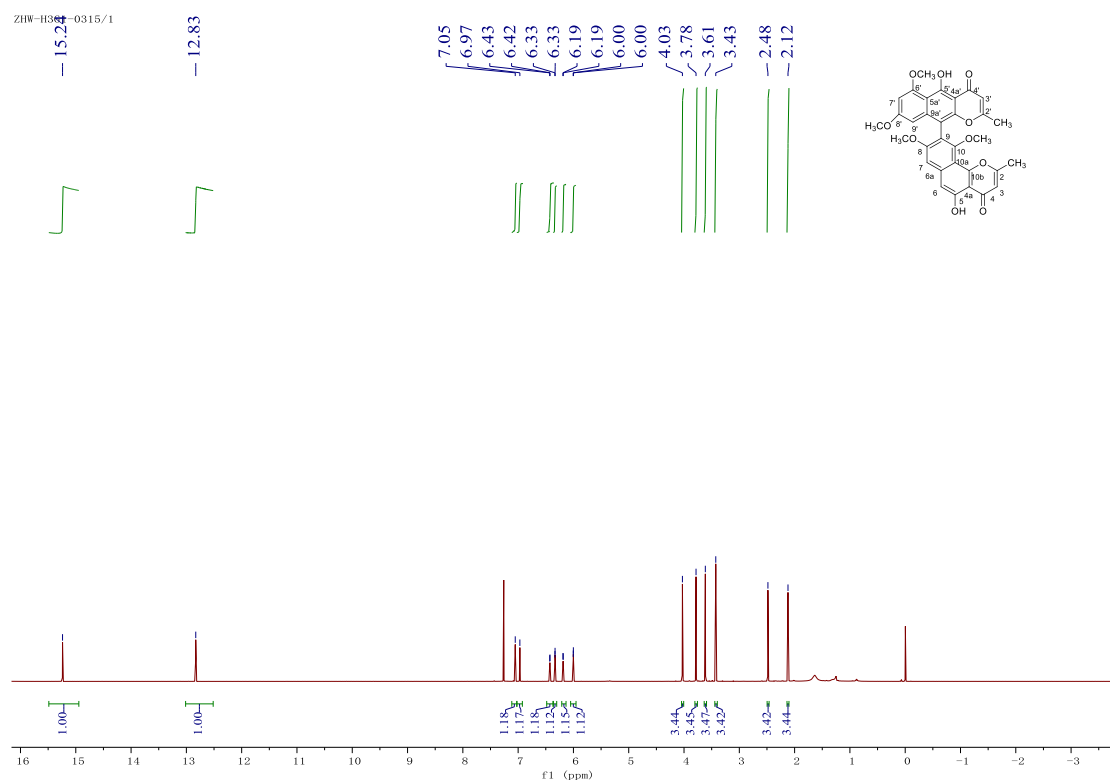


Figure S12. ^1H NMR spectrum of compound **7** in CDCl_3

Table S9. Comparison of ^1H NMR spectral data of compound **7** with reference (CDCl_3)

Position	δ_{H}	δ_{H} in reference [15]
	(<i>I</i> in Hz, 600 MHz)	(<i>I</i> in Hz, 400 MHz)
2	/	/
2-CH ₃	2.48 (3H, s)	2.49 (3H, s)
2'	/	/
2'-CH ₃	2.12 (3H, s)	2.13 (3H, s)
3	6.33 (1H, s)	6.34 (1H, s)
3'	6.00 (1H, s)	6.01 (1H, s)
4	/	/
4'	/	/
4a	/	/
4a'	/	/
5-OH	12.83 (1H, s)	12.85 (1H, s)
5'-OH	15.24 (1H, s)	15.27 (1H, s)
5a'	/	/
6	7.05 (1H, s)	7.06 (1H, s)
6'	/	/
6'-OMe	4.03 (3H, s)	4.04 (3H, s)
6a	/	/
7	6.97 (1H, s)	6.97 (1H, s)
7'	6.43 (1H, <i>d</i> , <i>J</i> = 2.20)	6.43 (1H, <i>d</i> , <i>J</i> = 2.20)
8	/	/
8-OMe	3.78 (3H, s)	3.79 (3H, s)
8'	/	/
8'-OMe	3.61 (3H, s)	3.63 (3H, s)
9	/	/
9'	6.19 (1H, <i>d</i> , <i>J</i> = 2.20)	6.19 (1H, <i>d</i> , <i>J</i> = 2.20)
9a'	/	/
10	/	/
10-OMe	3.43 (3H, s)	3.44 (3H, s)
10a	/	/
10b	/	/
10'	/	/
10a'	/	/

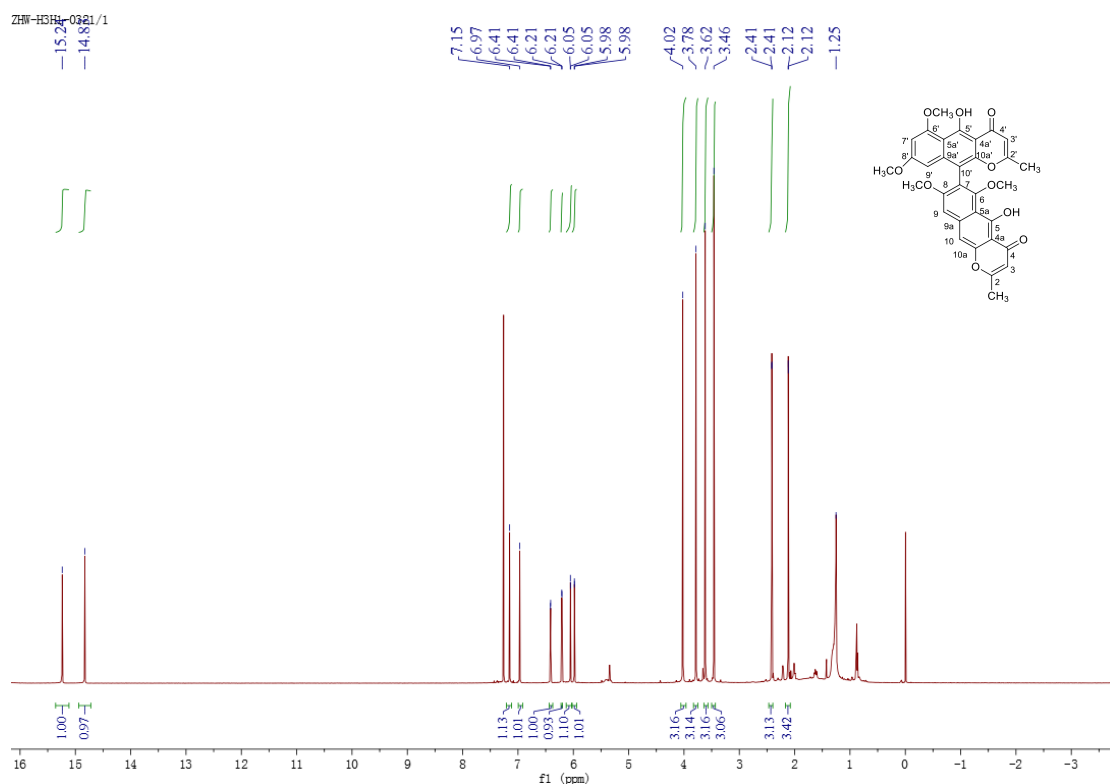


Figure S13. ^1H NMR spectrum of compound **8** in CDCl_3

Table S10. Comparison of ^1H NMR spectral data of compound **8** with reference (CDCl_3)

Position	δ_{H}	δ_{H} in reference [16]
	(J in Hz, 600 MHz)	(J in Hz, 400 MHz)
2- CH_3	2.41 (3H, s)	2.42 (3H, s)
2'- CH_3	2.12 (3H, s)	2.12 (3H, s)
3	6.05 (1H, s)	6.06 (1H, s)
3'	5.98 (1H, s)	5.98 (1H, s)
5-OH	14.83 (1H, s)	14.84 (1H, s)
5'-OH	15.24 (1H, s)	15.26 (1H, s)
6-OMe	3.46 (1H, s)	3.46 (1H, s)
6'-OMe	4.02 (3H, s)	4.03 (3H, s)
7'	6.41 (1H, <i>d</i> , $J = 2.27$)	6.41 (1H, <i>d</i> , $J = 2.20$)
8-OMe	3.78 (3H, s)	3.79 (3H, s)
8'-OMe	3.62 (3H, s)	3.62 (3H, s)
9	6.97 (1H, s)	6.97 (1H, s)
9'	6.20 (1H, <i>d</i> , $J = 2.27$)	6.20 (1H, <i>d</i> , $J = 2.20$)
10	7.15 (1H, s)	7.16 (1H, s)