Supplementary Information

Xanthones and Anthraquinones from the soil fungus Penicillium *sp*. DWS10-P-6

Ya-jing Wang ^a, Nan Ma ^a, Chun-yue Liu ^a, Yi-xuan Feng ^a, Feng-xiang Zhang ^d, Chang Li ^{a,*}, and Yue-hu Pei ^{a, b*}

 ^a Department of Medicinal Chemistry and Natural Medicine Chemistry, College of Pharmacy, HarBin Medical University, HarBin 150081, People's Republic of China;
 ^b Shenyang Pharmaceutical University, Shenyang 110016, People's Republic of China;
 ^cThe first Affiliated Hospital of Jinan University, GuangZhou 510632, People's Republic of China.

* E mail: lichang661@126.com; peiyueh@vip.163.com.

* To whom correspondence should be addressed.

Contents

1	. The spectra of penicillone A (1)	5
	Figure S1. The UV spectrum of compound 1	5
	Figure S2. The IR spectrum of compound 1	5
	Figure S3. The HR-ESI-MS spectrum of compound 1	6
	Figure S4. The ¹ H-NMR spectrum of compound 1	6
	Figure S5. The ¹³ C-NMR spectrum of compound 1	7
	Figure S6. The HSQC spectrum of compound 1	7
	Figure S7. The HMBC spectrum of compound 1	8
	Figure S8. The NOESY spectrum of compound 1	8
2.	The spectra of penicillone B (2)	9
	Figure S9. The UV spectrum of compound 2	9
	Figure S10. The IR spectrum of compound 2	9
	Figure S11. The HR-ESI-MS spectrum of compound 2	.10
	Figure S12. The ¹ H-NMR spectrum of compound 2	.10
	Figure S13. The ¹³ C-NMR spectrum of compound 2	.11
	Figure S14. The HSQC spectrum of compound 2	.11
	Figure S15. The HMBC spectrum of compound 2	.12
	Figure S16. The NOESY spectrum of compound 2	.12
3.	The spectra of penicillone C (3)	.13
	Figure S17. The UV spectrum of compound 3	.13
	Figure S18. The IR spectrum of compound 3	.13
	Figure S19. The HR-ESI-MS spectrum of compound 3	.14
	Figure S20. The ¹ H-NMR spectrum of compound 3	.14
	Figure S21. The ¹³ C-NMR spectrum of compound 3	.15
	Figure S22. The HSQC spectrum of compound 3	.15
	Figure S23. The HMBC spectrum of compound 3	.16
	Figure S24. The NOESY spectrum of compound 3	.16
4.	The spectra of penicillone D (4)	.17

Figure S25. The UV spectrum of compound 4	17
Figure S26. The IR spectrum of compound 4	17
Figure S27. The HR-ESI-MS spectrum of compound 4	
Figure S28. The ¹ H-NMR spectrum of compound 4	
Figure S29. The ¹³ C-NMR spectrum of compound 4	19
Figure S30. The HSQC spectrum of compound 4	19
Figure S31. The HMBC spectrum of compound 4	20
Figure S32. The NOESY spectrum of compound 4	20
5. The spectra of compound 5	21
Figure S33. The ¹ H-NMR spectrum of compound 5	21
Figure S34. The ¹³ C-NMR spectrum of compound 5	21
6. The spectra of compound 6	22
Figure S35. The ¹ H-NMR spectrum of compound 6	22
Figure S36. The ¹³ C-NMR spectrum of compound 6	
7. The spectra of compound 7	23
Figure S37. The ¹ H-NMR spectrum of compound 7	23
Figure S38. The ¹³ C-NMR spectrum of compound 7	23
8. The spectra of compound 8	24
Figure S39. The ¹ H-NMR spectrum of compound 8	24
Figure S40. The ¹³ C-NMR spectrum of compound 8	24
9. The spectra of compound 9	25
Figure S41. The ¹ H-NMR spectrum of compound 9	25
Figure S42. The ¹³ C-NMR spectrum of compound 9	25
10. The spectra of compound 10	26
Figure S43. The ¹ H-NMR spectrum of compound 10	26
Figure S44. The ¹³ C-NMR spectrum of compound 10	26
11. The spectra of compound 11	27
Figure S45. The ¹ H-NMR spectrum of compound 11	27
Figure S46. The ¹³ C-NMR spectrum of compound 11	27
12. The spectra of compound 12	

Figure S47. The ¹ H-NMR spectrum of compound 12	
Figure S48. The ¹³ C-NMR spectrum of compound 12	
13. The spectra of compound 13	29
Figure S49. The ¹ H-NMR spectrum of compound 13	29
Figure S50. The ¹³ C-NMR spectrum of compound 13	29
14. The spectra of compound 14	30
Figure S51. The ¹ H-NMR spectrum of compound 14	30
Figure S52. The ¹³ C-NMR spectrum of compound 14	
15. The spectra of compound 15	31
Figure S53. The ¹ H-NMR spectrum of compound 15	31
Figure S54. The ¹³ C-NMR spectrum of compound 15	31
16. The spectra of compound 16	32
Figure S55. The ¹ H-NMR spectrum of compound 16	32
Figure S56. The ¹³ C-NMR spectrum of compound 16	32

1. The spectra of penicillone A (1)



Figure S1. The UV spectrum of compound 1







Figure S3. The HR-ESI-MS spectrum of compound 1

Figure S4. The ¹H-NMR spectrum of compound 1













Figure S7. The HMBC spectrum of compound 1

Figure S8. The NOESY spectrum of compound 1



2. The spectra of penicillone B (2)



Figure S9. The UV spectrum of compound 2

Figure S10. The IR spectrum of compound 2



Figure S11. The HR-ESI-MS spectrum of compound 2

Analysis Info								A	cquisition	Date 5	/29/2018	10:50:17	AM	
Analysis Name Method Sample Name Comment		D:\Data\20180529CEYANG\S-9.d 2017_tune_Low_Neg.m S-9							O	Operator Instrument / Ser#		Bruker Customer micrOTOF-Q 125		
Acquisition	Pa	rameter						201		10000	un en			
Source Type Focus Scan Begin Scan End		ESI Active 50 m/z 3000 m/z		lon Polar Set Capil Set End Set Colli:		arity billary I Plate Offset lision Cell RF		Positive 4500 V -500 V 400.0 Vpp		Set Nebulizer Set Dry Heate Set Dry Gas Set Divert Valv		0.4 Bar 180 °C 4.0 l/min ve Source		
Intens. x10 ⁵ -													+MS, 0.4	4min #21
0.8-														
0.6-						.0970 I								
0.4-														
0.2-									3	66.0991		379	.0716	
0.0						353.25	34			1				
0.0	330)	340		350			360		.,.,.	370		380	m/z
Meas. m/z	#	Formula	m/z	err [pp m]	Me an err [pp m]	rdb	N- R ul e	e Conf	mSig ma	Std I	Std Mean m/z	Std I VarNo rm	Std m/z Diff	Std Comb Dev
357.0970	1	C 19 H 17 O 7	357.0969	-0.4	4.1	11.5	ok	even	44.69	0.0710	0.0032	0.0302	0.0063	0.8427
Intens. x10 ⁵												C 19	H 17 O 7	,357.10
0.8-														
0.6-							357.	.0969						
0.4-														
0.2-														
0.0	330) , , ,	340		350		-,-	360		, , 3	370		380	m/z
Meas. m/z	#	Form r ula	n/z err [ppm]	Mean err [ppm]		rdb I	N-Rul e	e Conf	mS n	na Std	I Sto Mean m/:	d Std n VarNo z rm	Std m/z Diff	Std Comb Dev

Mass Spectrum SmartFormula Report

Figure S12. The ¹H-NMR spectrum of compound 2











Figure S15. The HMBC spectrum of compound 2

Figure S16. The NOESY spectrum of compound 2



3. The spectra of penicillone C (3)



Figure S17. The UV spectrum of compound 3







Figure S19. The HR-ESI-MS spectrum of compound 3

Figure S20. The ¹H-NMR spectrum of compound 3



Figure S21. The ¹³C-NMR spectrum of compound 3



Figure S22. The HSQC spectrum of compound 3





Figure S23. The HMBC spectrum of compound 3

Figure S24. The NOESY spectrum of compound 3



4. The spectra of penicillone D (4)



Figure S25. The UV spectrum of compound 4

Figure S26. The IR spectrum of compound 4



Figure S27. The HR-ESI-MS spectrum of compound 4



Figure S28. The ¹H-NMR spectrum of compound 4



Figure S29. The ¹³C-NMR spectrum of compound 4



Figure S30. The HSQC spectrum of compound 4





Figure S31. The HMBC spectrum of compound 4

Figure S32. The NOESY spectrum of compound 4

AV-600-NOESY Sample: RUKÉR BI (NAME EXPNO PROCNO SF7-2Dppm 1 20170707 10.22 spect PABBO BB-0 8 0 5 DMS 2 3 .0611400 000 Ô 0 -10 1 DÓ 59 4 0.00004547 2.00000000 0.60000002 0.00011920 5 P 100 Mº: 01 CHANNEL f1 === IH 11.10 -4.00 34.70265579 600.1342009 1 NUC1 P1 PL1 PL1 PL1 SF01 SF01 FIDRES SW SF01 FIDRES SF WDW SSB LB GB GB SSB LB SSB LB GG SSB LB GG GG GG 6 Ø 7 1 128 600.1342 65.541222 13.979 States-TPPI 1024 600.1300000 8 9 10 QSINE 0.00 1.00 11 1024 States-TPPI 600.1300000 QSINE 2 0.00 0 12 12 11 10 7 0 ppm 9 8 6 5 4 3 2 1





Figure S34. The ¹³C-NMR spectrum of compound 5





20160527 spect O BB/

5 mm





Figure S36. The ¹³C-NMR spectrum of compound 6









Figure S39. The ¹H-NMR spectrum of compound 8

Figure S40. The ¹³C-NMR spectrum of compound 8





Figure S41. The ¹H-NMR spectrum of compound 9

Figure S42. The ¹³C-NMR spectrum of compound 9





Figure S43. The ¹H-NMR spectrum of compound 10

Figure S44. The ¹³C-NMR spectrum of compound 10





Figure S45. The ¹H-NMR spectrum of compound 11

 1510
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 15000
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500
 1500









Figure S49. The ¹H-NMR spectrum of compound 13



Figure S51. The ¹H-NMR spectrum of compound 14

Figure S52. The ¹³C-NMR spectrum of compound 14





Figure S53. The ¹H-NMR spectrum of compound 15

NAME EXPNO PROCNO Date_ Time INSTRUM PROBHD PULPROG SOLVENT NS SOLVENT NS SWH FIDRES AQ RG RG DW DE E D1 TE D11 TD0 6.50 2.00000000 0.03000000 1000000 s IANNEL f1 100.6228293 MI 13C 9.40 u: 32768 100.6128119 MI 0 1.00 H: 0 1.40 SF01 NUC1 P1 SI SF WDW SSB LB GB PC 190 180 170 160 150 140 130 120 110 100 30 20 10 ppm 90 80 40 70 60 50



