

Supporting Information

Cottoquinazoline A and Cotteslosins A-B: Metabolites from an Australian Marine-Derived Strain of *Aspergillus versicolor*

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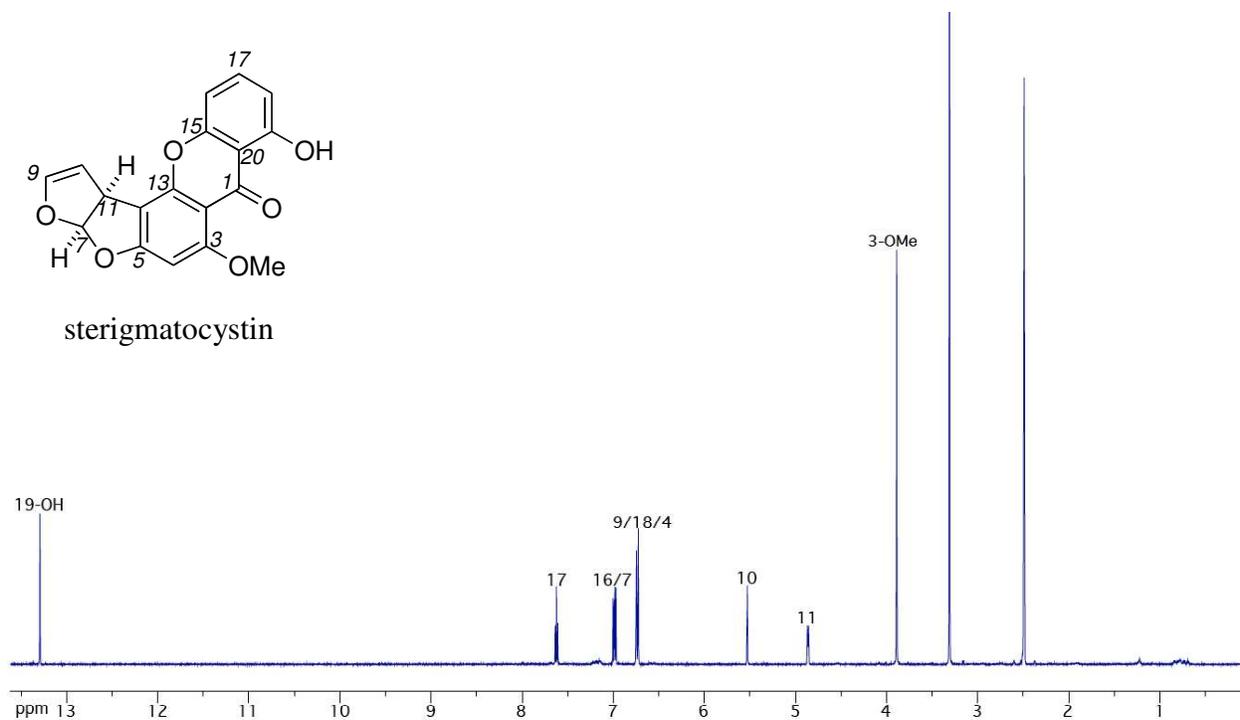


Figure S1: ^1H NMR (DMSO- d_6 , 600 MHz) spectrum for sterigmatocystin

Table S1: NMR data (DMSO- d_6 , 600 MHz) for sterigmatocystin

Position	δ_{H} (m, J in Hz)	δ_{C}	COSY	HMBC (^1H - ^{13}C)
1		180.4		
2		106.4		
3		162.8		
3-OMe	3.89 (s)	56.4		C-3
4	6.73 (s)*	90.7		C-2, C-5, C-12
5		164.4		
7	6.97 (d, 7.0)	112.7	10, 11	C-5, C-9, C-11
9	6.74 (m)*	145.1	10	C-7, C-10, C-11
10	5.52 (t, 2.6)	102.3	9	C-7, C-9, C-11
11	4.86 (ddd, 7.0, 2.4, 2.2)	46.9	7	C-9, C-10, C-12
12		106.5		
13		153.3		
15		154.4		
16	6.99 (d, 8.3)	106.1	17	C-15, C-18, C-20
17	7.62 (t, 8.3)	135.8	16, 18	C-15, C-19
18	6.73 (m)*	110.5	17	C-16, C-20
19		161.2		
19-OH	13.29 (s)			C-18, C-19, C-20
20		108.3		

* overlapping signals

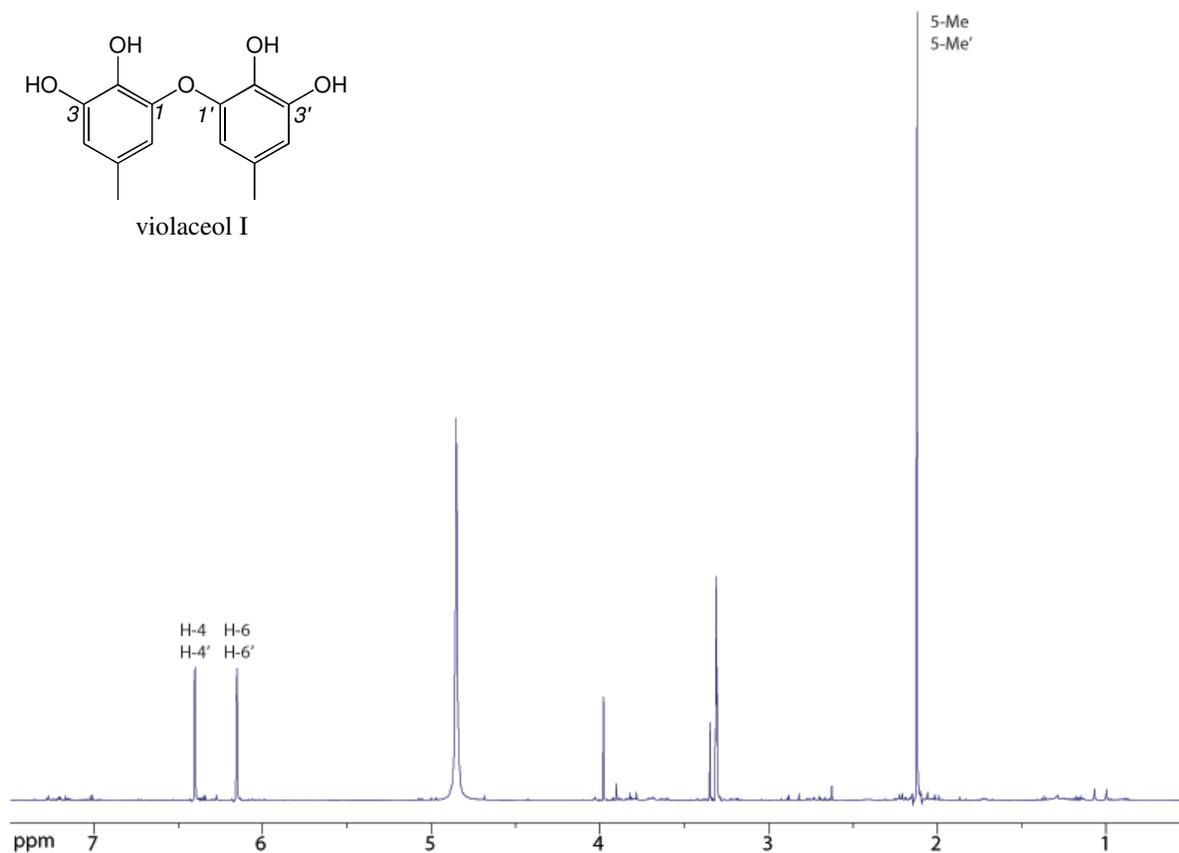
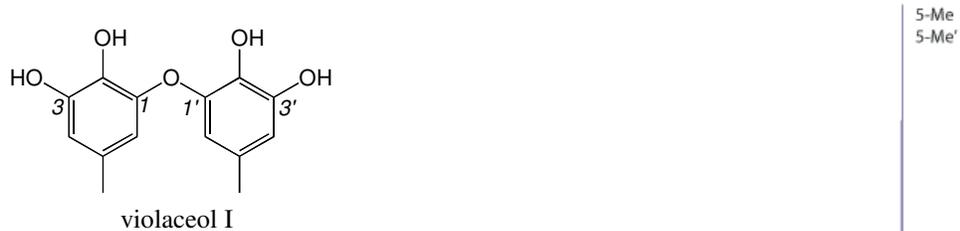


Figure S2: ^1H NMR (MeOH- d_4 , 600 MHz) spectrum for violaceol I

Table S2: NMR data (MeOH- d_4 , 600 MHz) for violaceol I

Position	δ_{H} (m)	δ_{C}	TOCSY	HMBC (^1H - ^{13}C)
1 / 1'		146.7		
2 / 2'		135.0		
3 / 3'		147.6		
4 / 4'	6.40 (m)	112.6	6/6', 5-Me/5-Me'	C-2/2', C-3/3', C-6/6', 5-Me/5-Me'
5 / 5'		130.1		
6 / 6'	6.15 (m)	111.8	4/4', 5-Me/5-Me'	C-1/1', C-3/3', C-4/4', 5-Me/5-Me'
5-Me / 5-Me'	2.12 (s)	21.2	4/4', 6/6'	C-4/4', C-5/5', C-6/6'

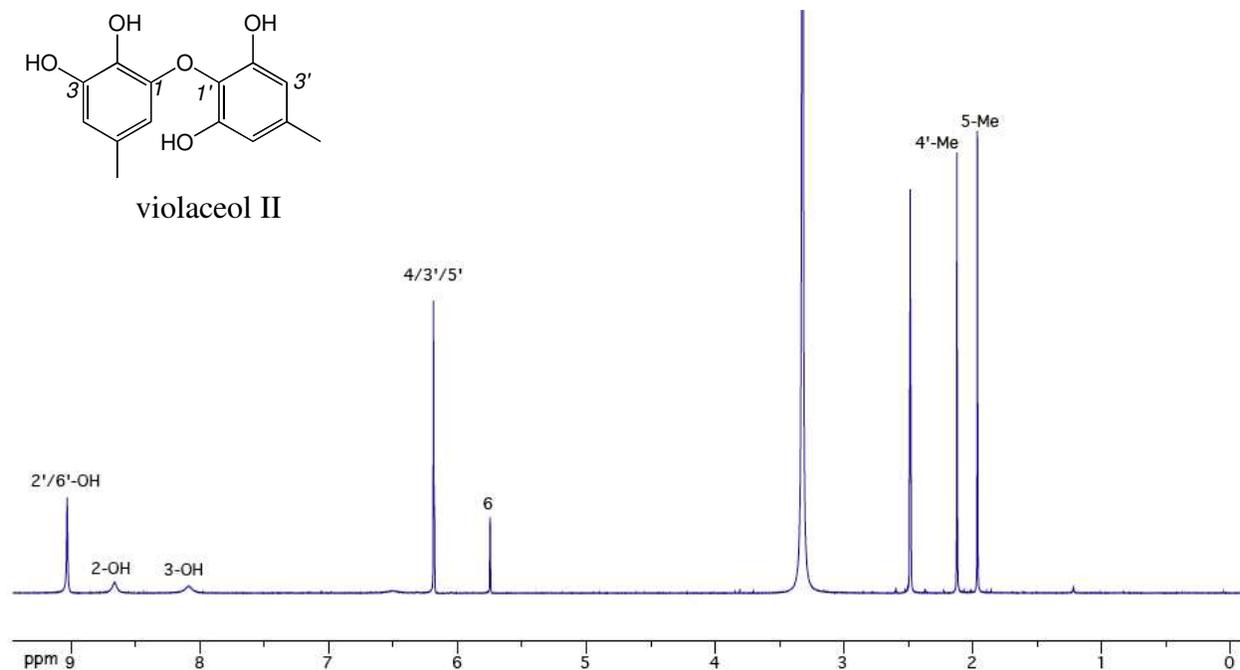


Figure S3: ^1H NMR (MeOH- d_4 , 600 MHz) spectrum for violaceol II

Table S3: NMR data (DMSO- d_6 , 600 MHz) for violaceol II

Position	δ_{H} (m, J in Hz)	δ_{C}	TOCSY	HMBC (^1H - ^{13}C)
1		146.0		
2		131.6		
3		147.1		
4	6.20 (m)	109.8	6, 5-Me	C-1, C-2, C-6, 5-Me
5		126.6		
6	5.77 (d, 1.5)	105.6	4, 5-Me	C-2, C-3, C-4, 5-Me
2'-OH	8.67 (brs)			
3'-OH	8.09 (brs)			
5-Me	1.98 (s)	20.8		
1'		128.1		
2'		150.5		
3'	6.20 (m)	108.2	4'-Me	C-1', C-2', 4'-Me
4'		134.1		
5'	6.20 (m)	108.2	4'-Me	C-1', C-2', 4'-Me
6'		150.5		
2'-OH	9.04 (s)			C-1', C-2'/6', C-3'/5'
6'-OH	9.04 (s)			C-1', C-2'/6', C-3'/5'
4'-Me	2.14 (s)	21.0	3'/5'	C-1', C-2', C-3'/5', C-4'

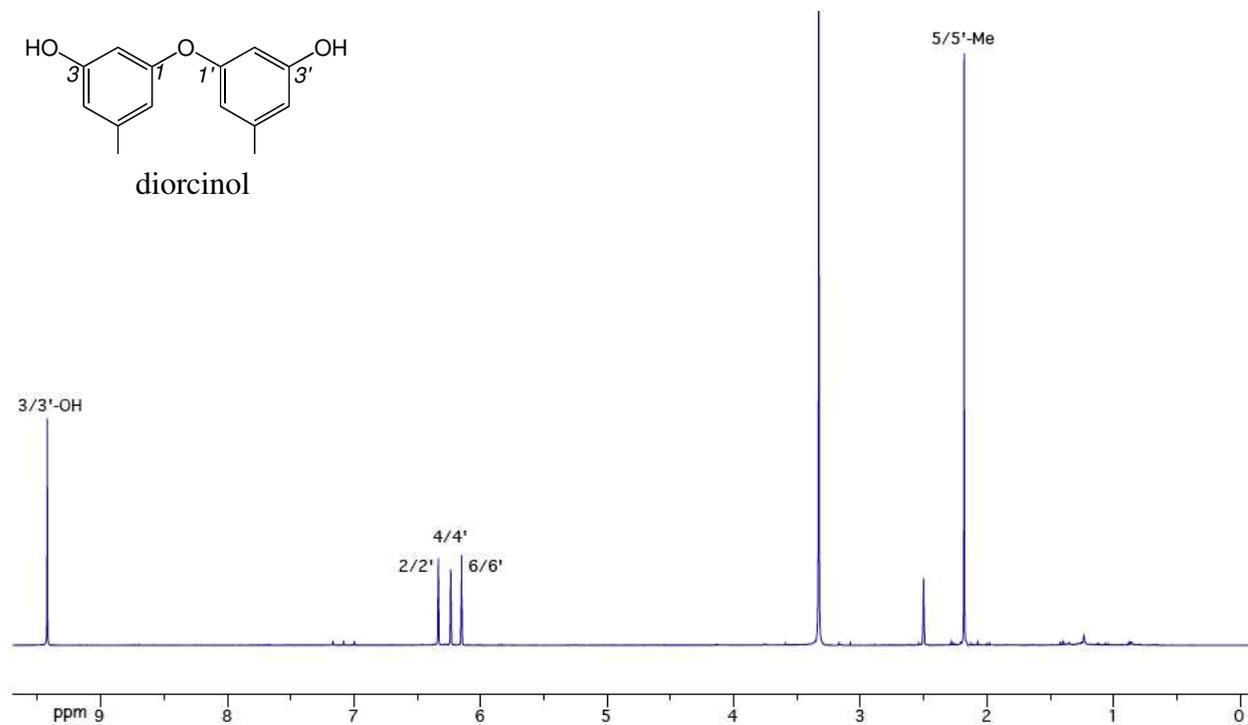


Figure S4: ¹H NMR (DMSO-*d*₆, 600 MHz) spectrum for diorcinol

Table S4: NMR data (DMSO-*d*₆, 600 MHz) for diorcinol

Position	δ_{H} (m, <i>J</i> in Hz)	δ_{C}	TOCSY	HMBC (¹ H- ¹³ C)
1 / 1'		157.6		
2 / 2'	6.45 (t, 2.0)	102.9	4/4', 6/6', 3/3'-OH, 5/5'-Me	C-1/1', C-3/3', C-4/4', C-6/6'
3 / 3'		158.4		
4 / 4'	6.33 (m)	111.1	2/2', 6/6', 3/3'-OH, 5/5'-Me	C-2/2', C-3/3', C-6/6', 5/5'-Me
5 / 5'		140.0		
6 / 6'	6.24 (m)	110.0	2/2', 4/4', 3/3'-OH, 5/5'-Me	C-1/1', C-2/2', C-4/4', 5/5'-Me
3 / 3'-OH	9.45 (s)		2/2', 4/4', 6/6', 5/5'-Me	C-2/2', C-3/3', C-4/4'
5 / 5'-Me	2.18 (s)	21.1	2/2', 4/4', 6/6', 3/3'-OH	C-4/4', C-5/5', C-6/6'

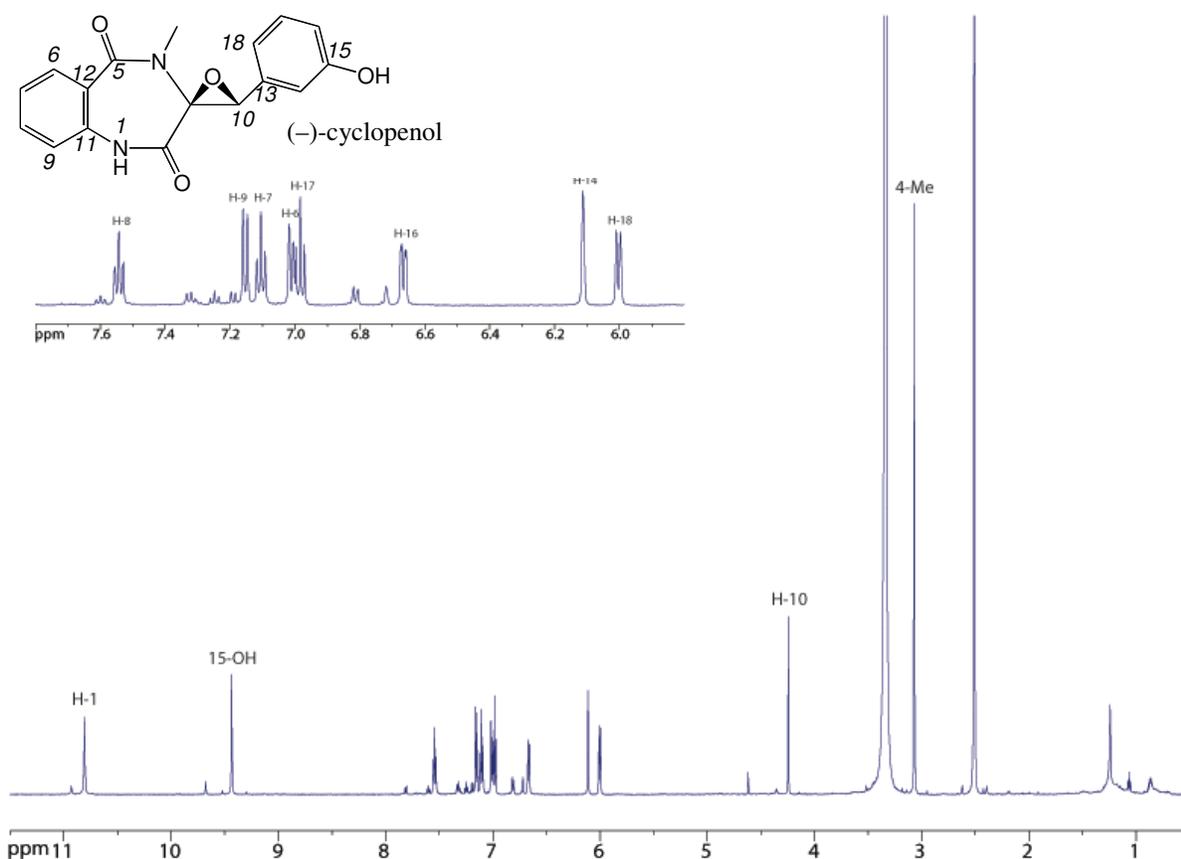


Figure S5: ¹H NMR (DMSO-*d*₆, 600 MHz) spectrum for (-)-cyclophenol

Table S5: NMR data (DMSO-*d*₆, 600 MHz) for (-)-cyclophenol

Pos	δ_{H} (m, J in Hz)	δ_{C}	COSY	TOCSY	HMBC (¹ H- ¹³ C)
1	10.80 (brs)				C-3
2		166.4			
3		70.6			
4					
5		165.8			
6	7.01 (dd, 7.8, 1.5)	130.9	7	7, 8, 9	C-5, C-8
7	7.09 (m)	124.7	6, 8	6, 8, 9	C-9, C-12
8	7.53 (m)	132.9	7, 9	6, 7, 9	C-6, C-11
9	7.15 (d, 8.2)	121.5	8	6, 7, 8	C-7, C-12
10	4.24 (s)	64.2			C-13, C-14, C-18
11		135.6			
12		126.9			
13		132.8			
14	6.10 (t, 1.9)	113.2		16, 17, 18	C-13, C-16, C-18
15		157.4			
16	6.60 (d, 8.0, 1.9)	116.1	17	14, 17, 18	C-14, C-18
17	6.97 (t, 7.8)	129.4	16, 18	14, 16, 18	C-13, C-15
18	6.00 (m)	117.4	17	14, 16, 17	C-13, C-14, C-16
4-Me	3.06 (s)	31.3			C-3
15-OH	9.42 (s)				C-14, C-15, C-16

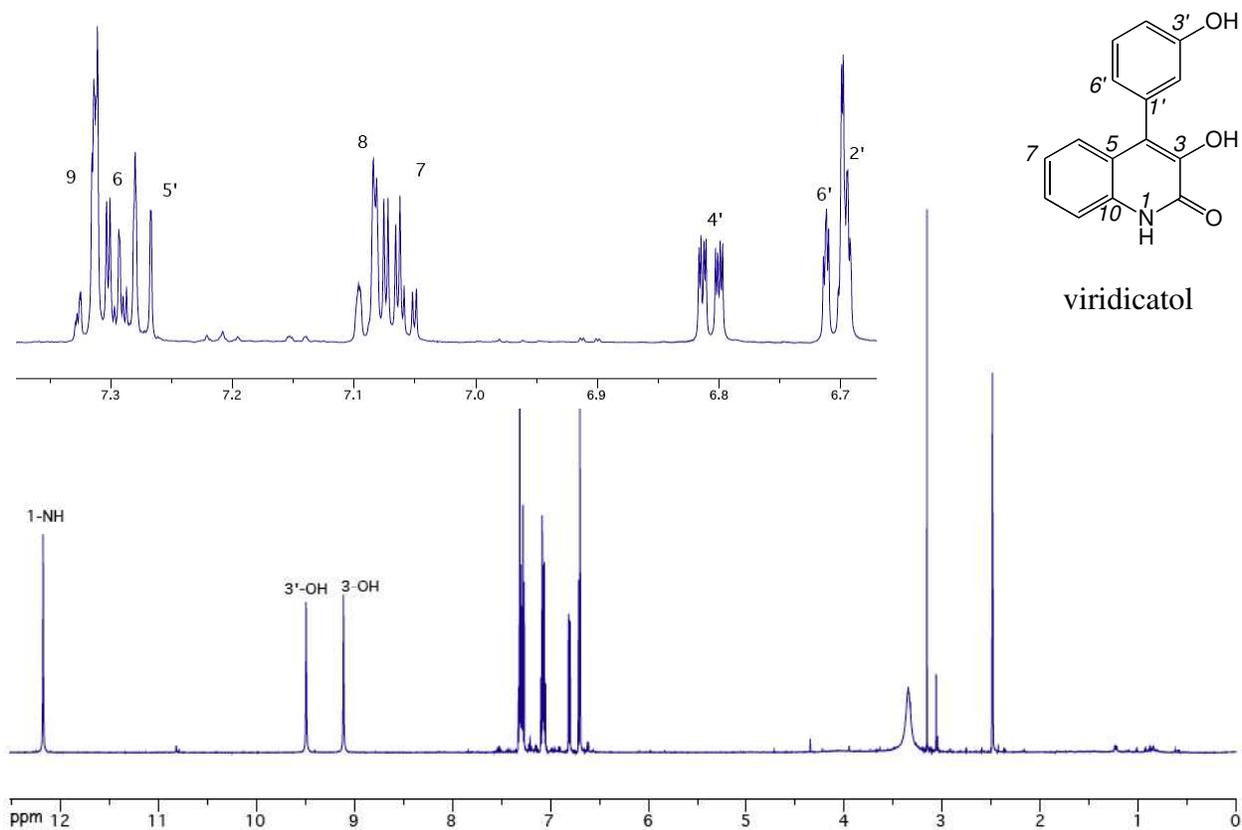


Figure S6: ^1H NMR (DMSO- d_6 , 600 MHz) spectrum for viridicatol

Table S6: NMR data (DMSO- d_6 , 600 MHz) for viridicatol

Pos	δ_{H} (m, J in Hz)	δ_{C}	COSY	TOCSY	HMBC (^1H - ^{13}C)
1-NH	12.19 (s)				C-5, C-9, C-10
2		158.3			
3		124.0			
4		133.1			
5		120.9			
6	7.31 (m)	126.4	7	7, 8	C-4, C-8
7	7.08 (ddd, 8.1, 6.0, 1.9)	122.1	6, 8	6, 8, 9	C-5, C-6, C-9
8	7.11 (m)	124.4	7, 9	6, 7, 9	C-6, C-10
9	7.33 (m)	115.2	8	6, 7, 8	C-5, C-7
10		142.2			
1'		134.9			
2'	6.71 (m)	116.7			C-3', C-4', C-6'
3'		157.3			
4'	6.83 (ddd, 8.2, 2.3, 1.1)	114.6	5'	5', 6'	C-2', C-3', C-6'
5'	7.30 (t, 7.6)	129.3	4', 6'	4', 6'	C-1', C-2', C-3'
6'	6.72 (m)	120.3	5'	4', 5'	C-2', C-4'
3-OH	9.13 (s)				C-2, C-3
3'-OH	9.51 (s)				C-2', C-3', C-4'

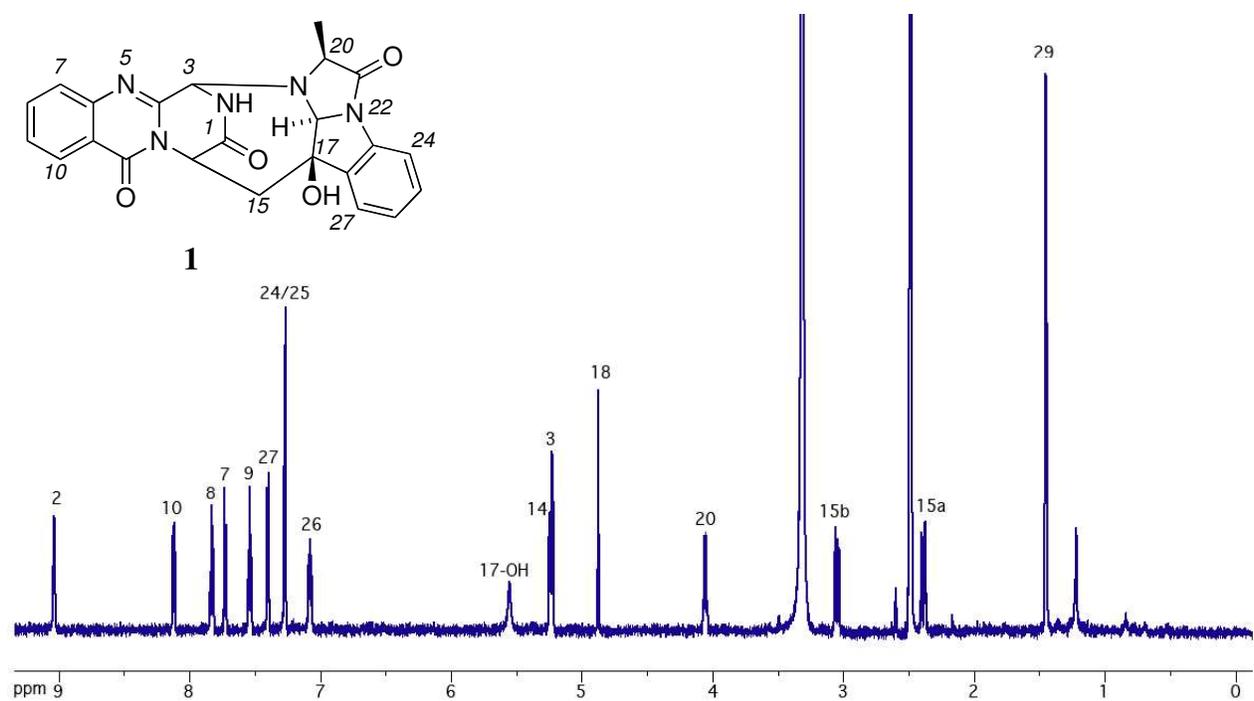


Figure S7: ^1H NMR ($\text{DMSO-}d_6$, 600 MHz) spectrum for cottoquinazoline A (**1**)

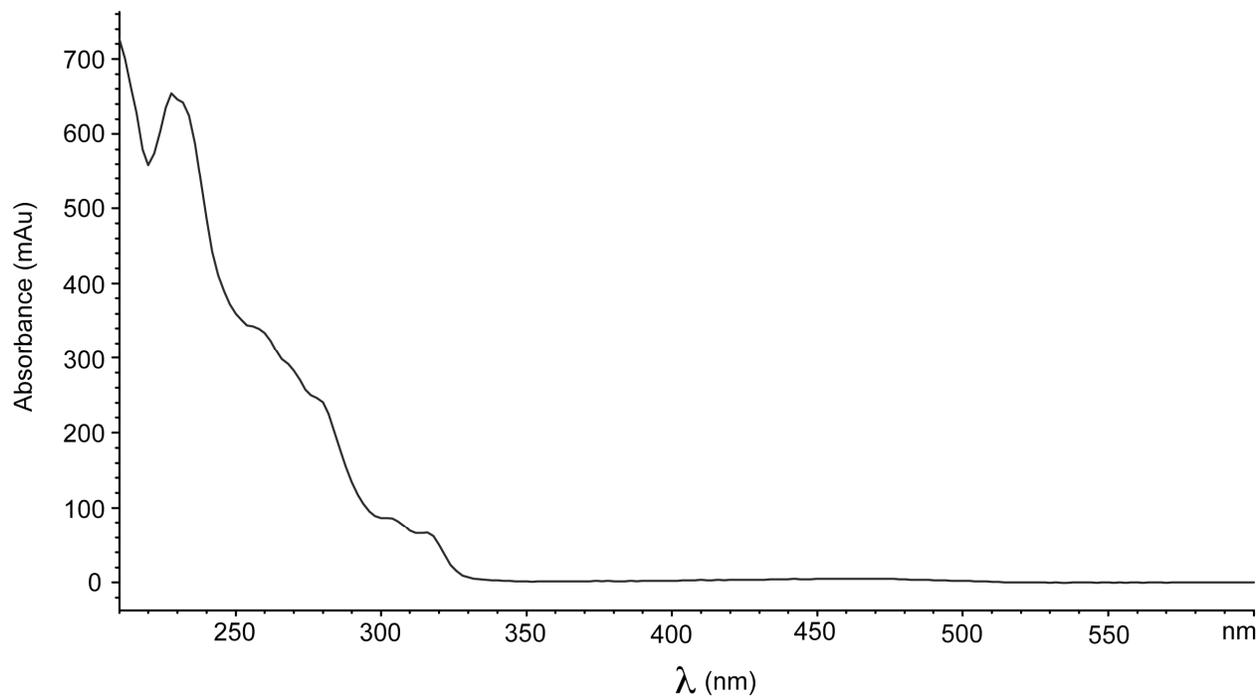


Figure S8: UV-Vis spectrum of cottoquinazoline A (**1**) in 1:1 MeCN:H₂O

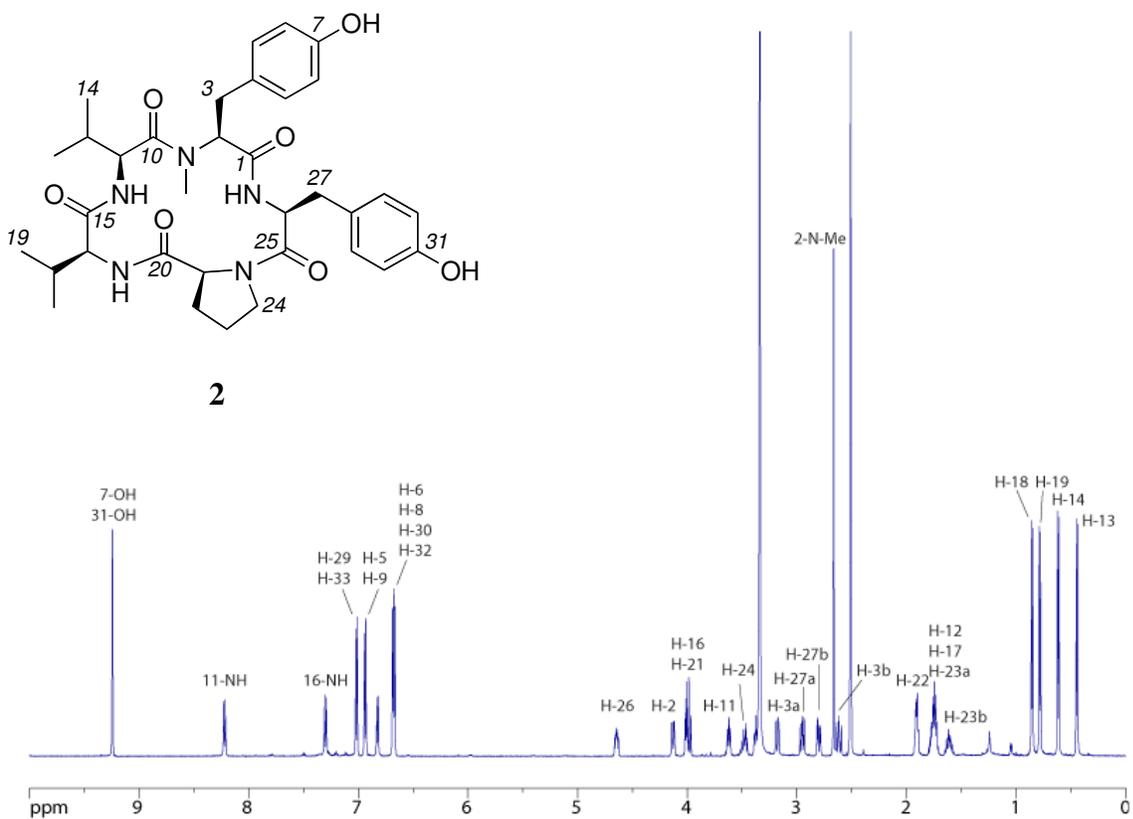


Figure S9: ^1H NMR (DMSO- d_6 , 600 MHz) spectrum for cotteslosin A (2).

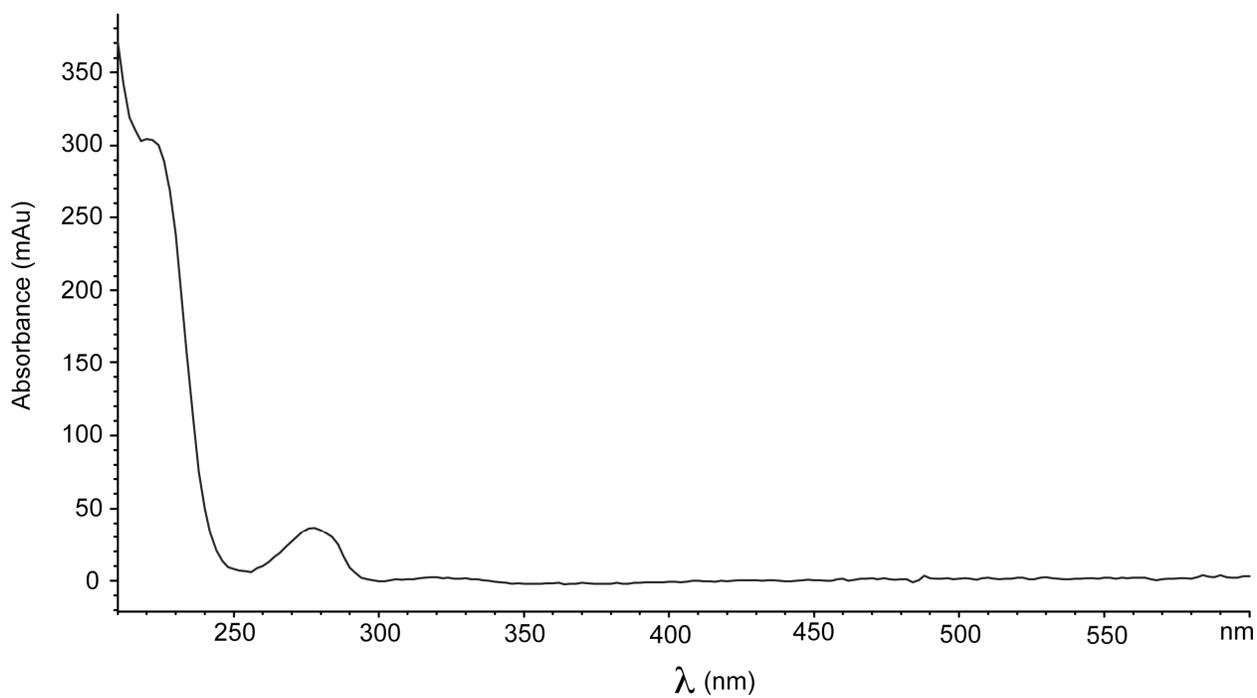


Figure S10: UV-Vis spectrum of cotteslosin A (2) in 1:1 MeCN:H₂O

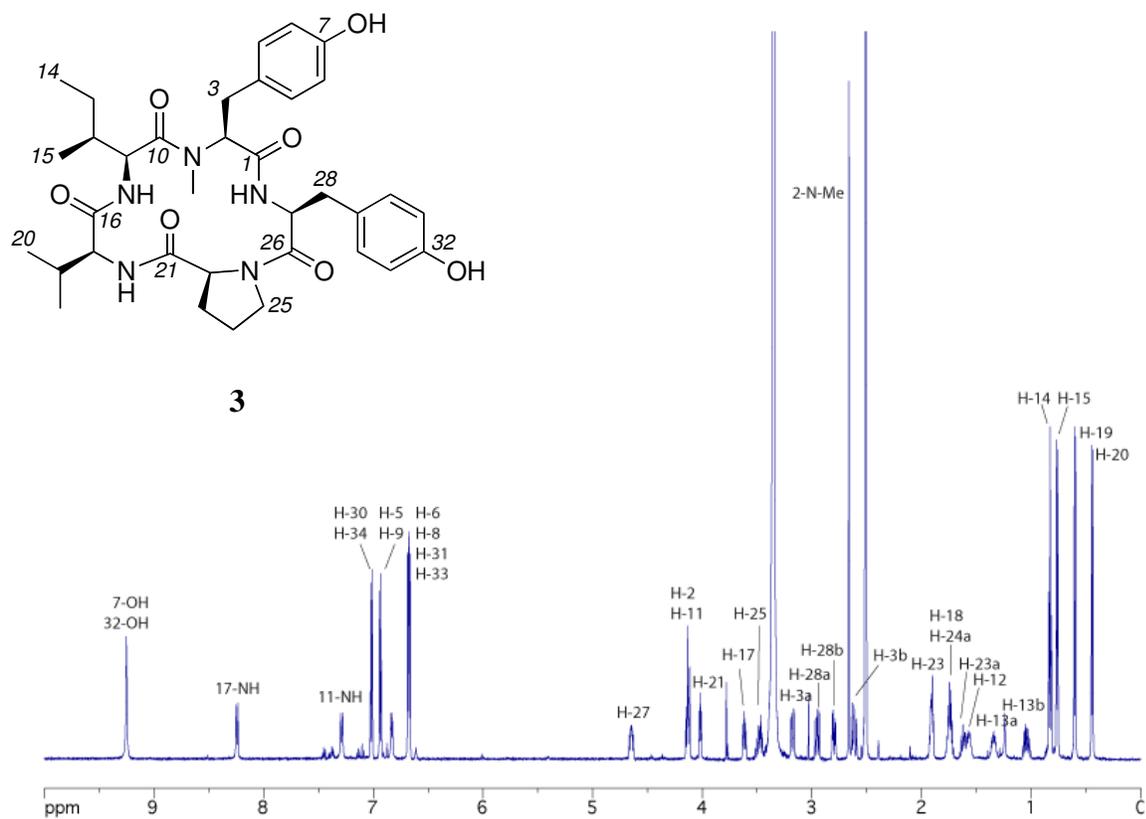


Figure S11: ¹H NMR (DMSO-*d*₆, 600 MHz) spectrum for cotteslosin B (3)

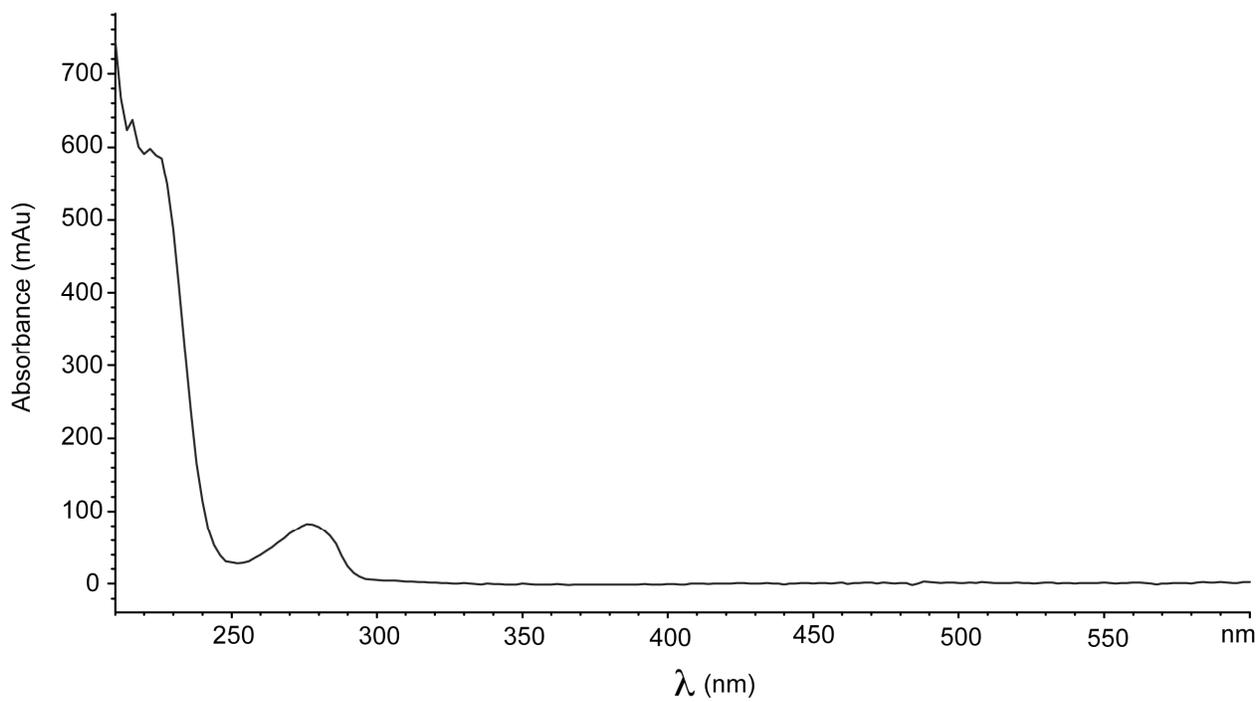


Figure S12: UV-Vis spectrum of cotteslosin B (3) in 1:1 MeCN:H₂O