

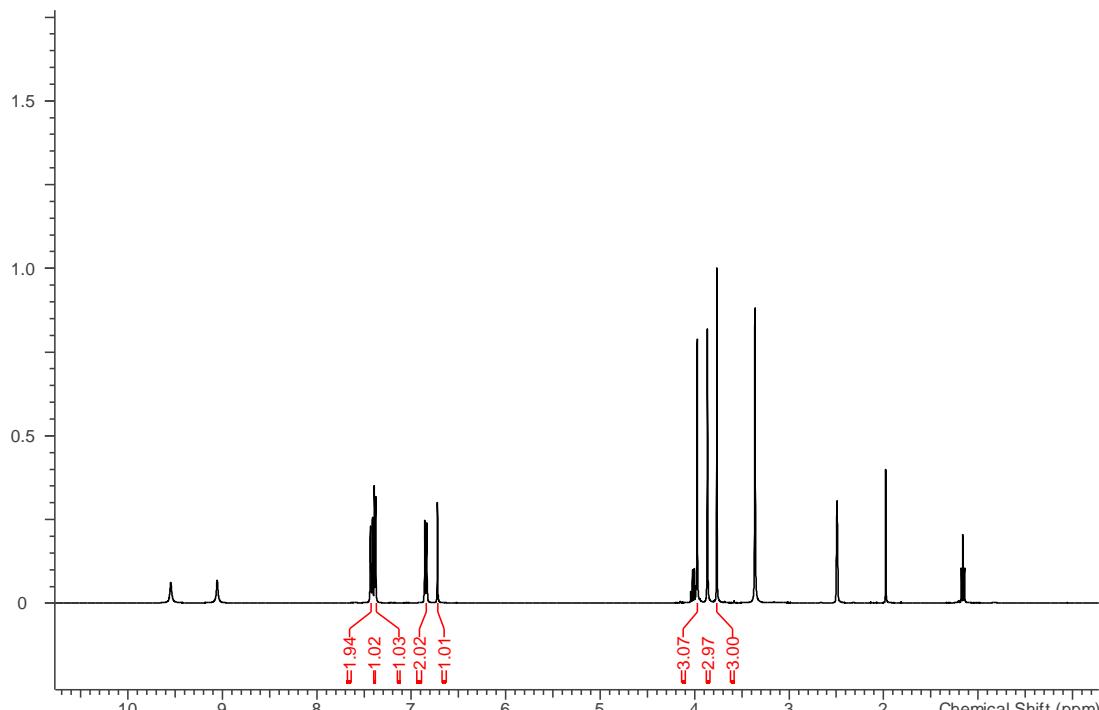
1 *Supplementary Files*

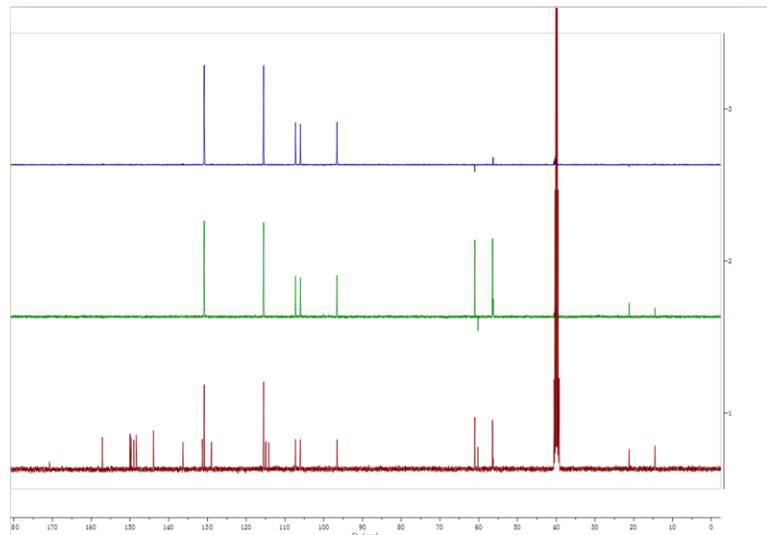
2 **Cytotoxic and Antibacterial Compounds from the 3 Coral-Derived Fungus *Aspergillus tritici* SP2-8-1**

4 **Weiyi Wang ^{1,2,3,†}, Yanyan Liao ^{1,2,4,†}, Chao Tang ^{1,2,4}, Xiaomei Huang ^{1,2,4}, Zhuhua Luo ³, Jianming
5 Chen ^{3,5,*}, Peng Cai ^{1,2,4,*}**

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Text S1: ITS1-5.8S-ITS2 rDNA sequence of strain SP2-8-1



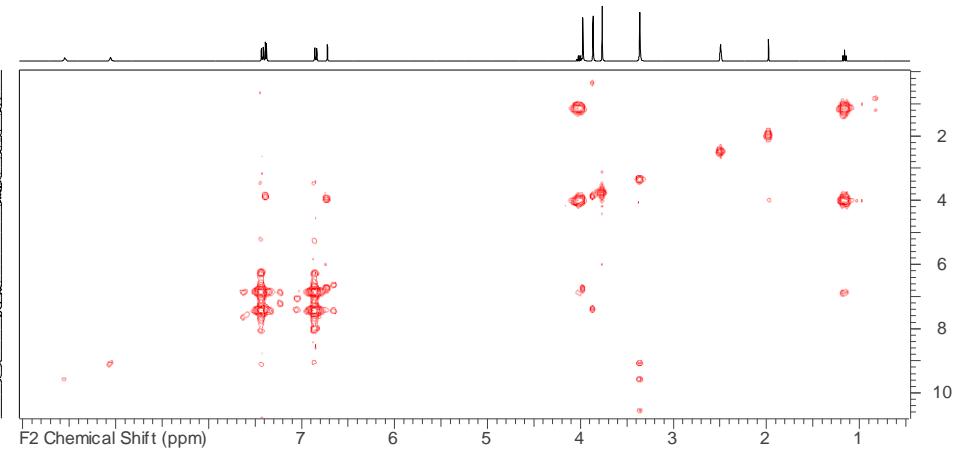


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Figure S3. ^{13}C /DEPT spectrum of compound 1

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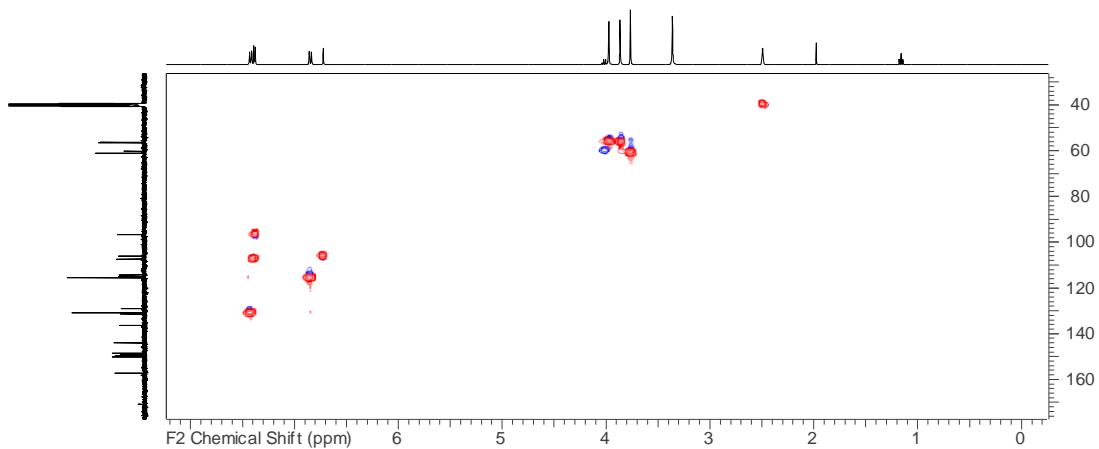


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Figure S4. ^1H - ^1H COSY spectrum of compound 1

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Figure S5. HSQC spectrum of compound 1

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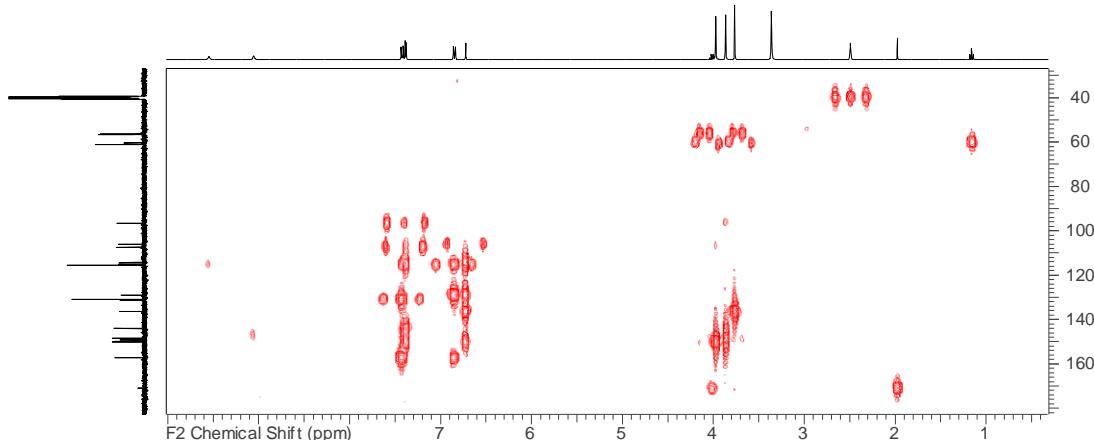


Figure S6. HMBC spectrum of compound 1

Acquisition Parameter

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	24	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3900.0 V	MALDI Plate	290.0 V
Broadband High Mass	3000.0 m/z	Capillary Entrance	4400.0 V	Imaging Spot Diameter	2000.0 μ m
Acquisition Mode	Single MS	Skimmer 1	36.0 V	Calibration Date	Tue Aug 11 09:48:49 2015
Pulse Program	basic	Drying Gas Temperature	200.0 °C		
Source Accumulation	0.1 sec	Drying Gas Flow Rate	4.0 L/min		
Ion Accumulation Time	0.0 sec	Nebulizer Gas Flow Rate	1.0 L/min		
Flight Time to Acq. Cell	0.0 sec				

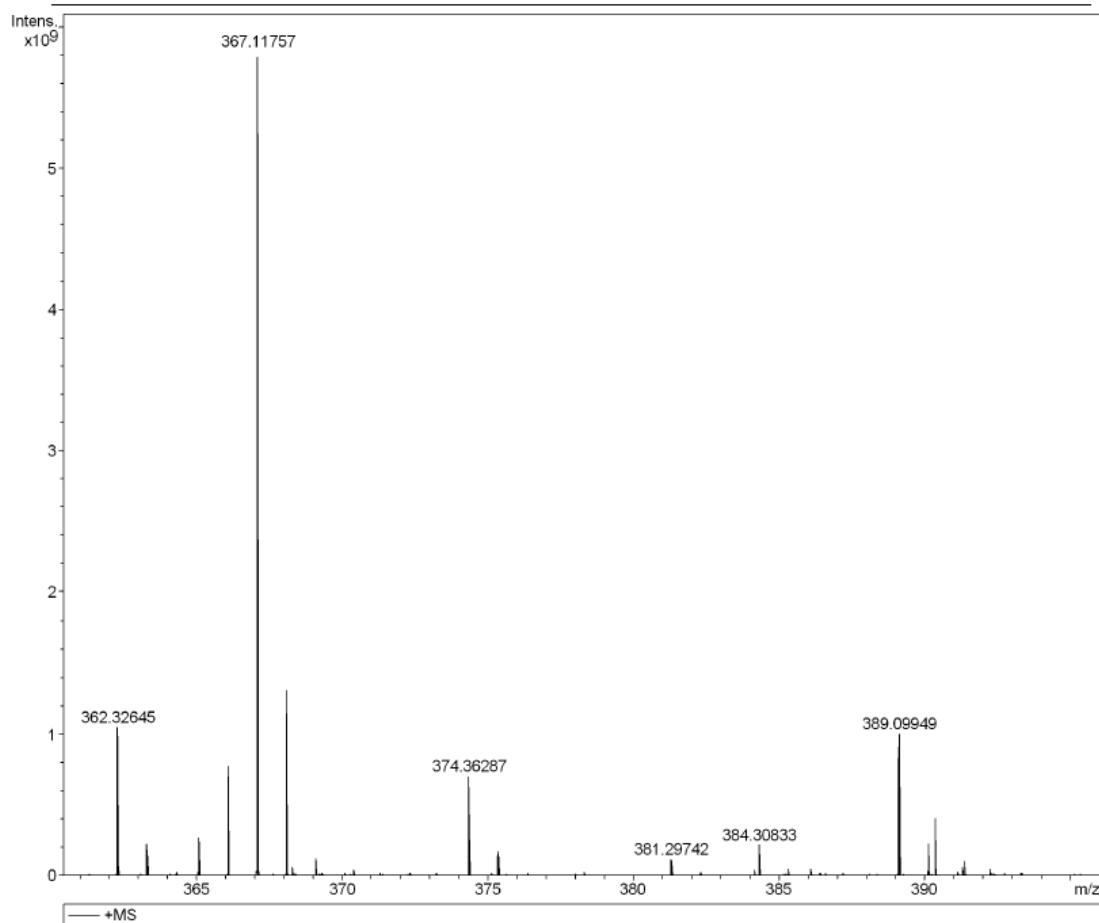


Figure S7. HRESIMS spectrum of compound 1

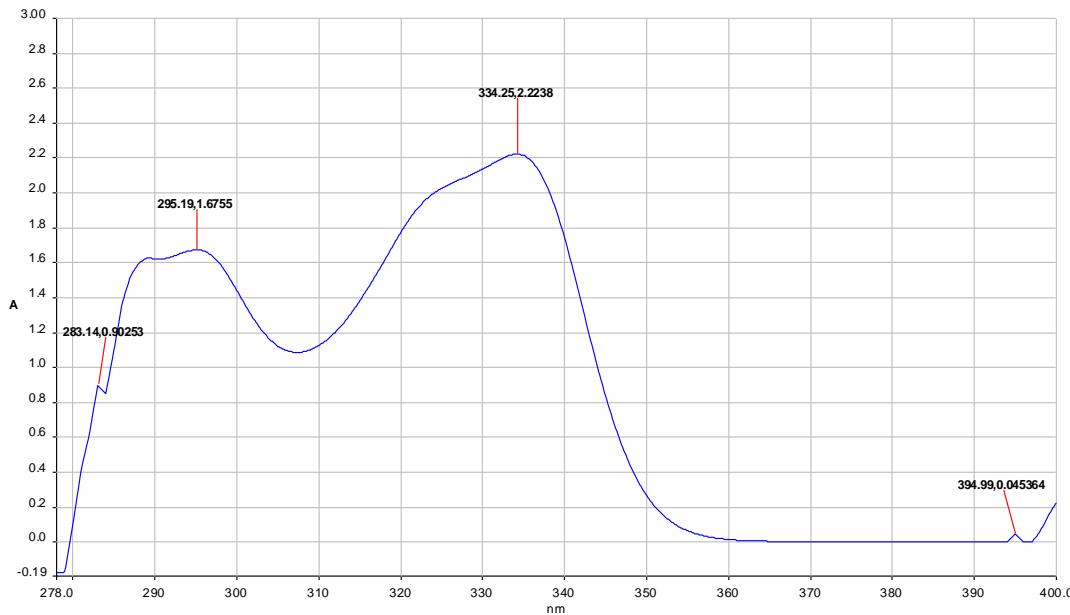
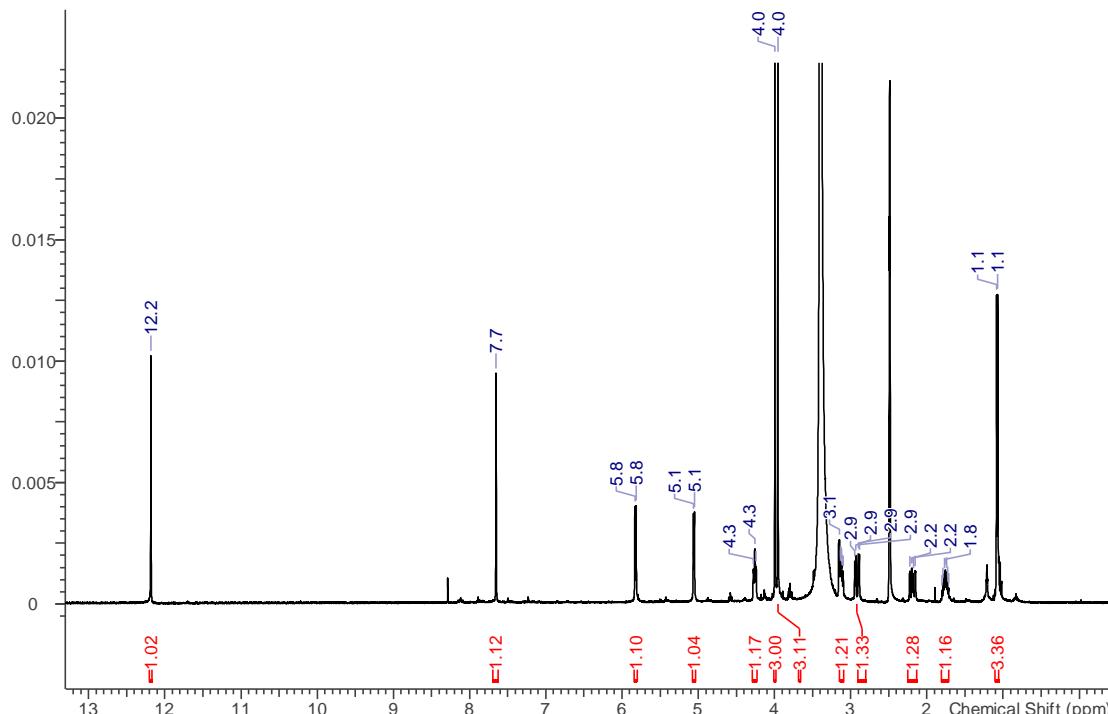
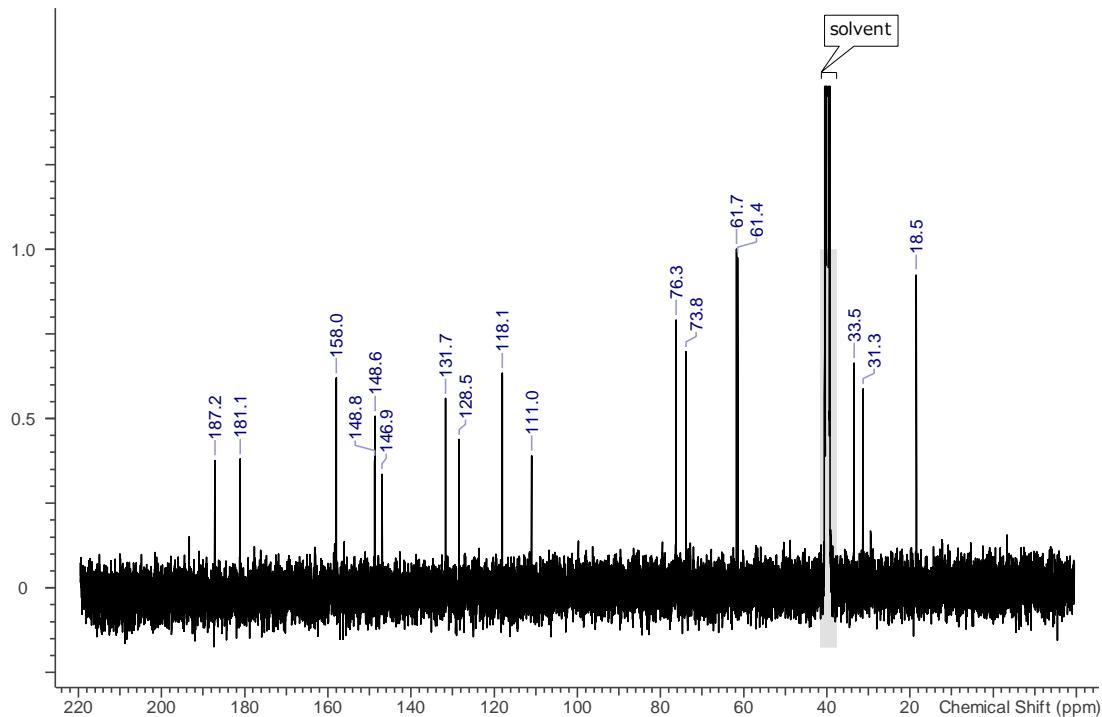


Figure S8. UV spectrum of compound 1

Figure S9. ^1H NMR spectrum of compound 2



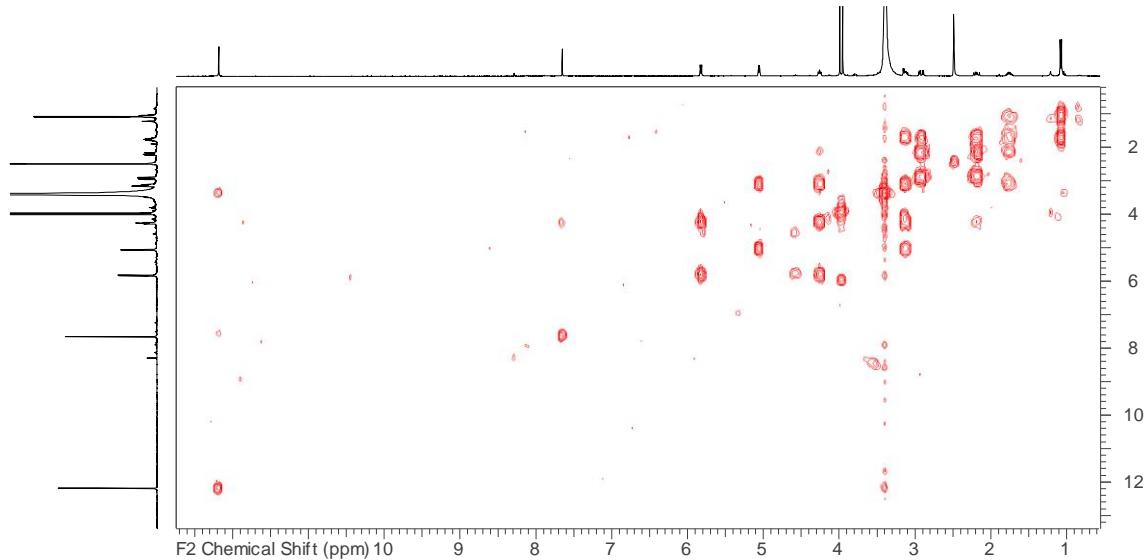
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Figure S10. ^{13}C NMR spectrum of compound 2

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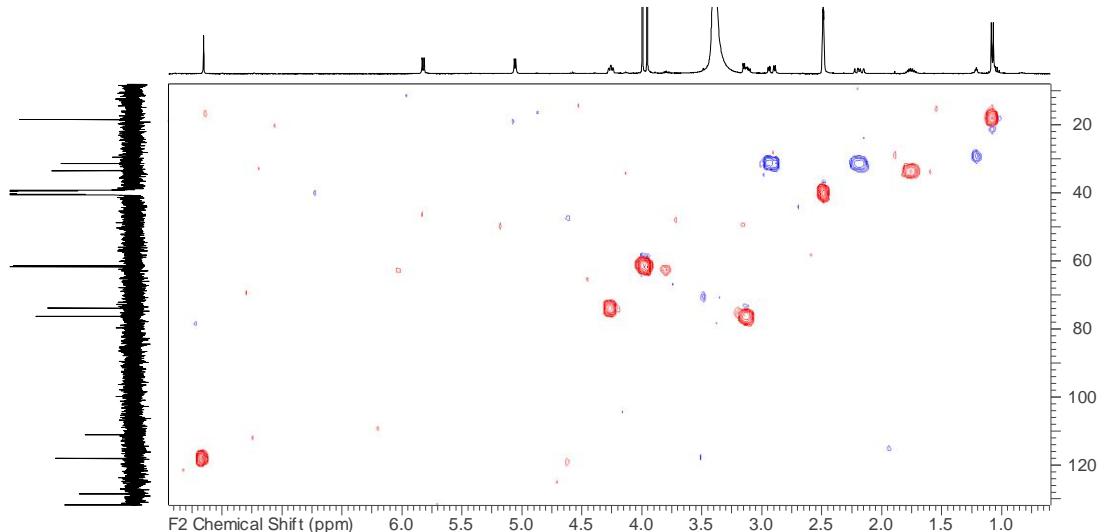
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Figure S11. ^1H - ^1H COSY spectrum of compound 2

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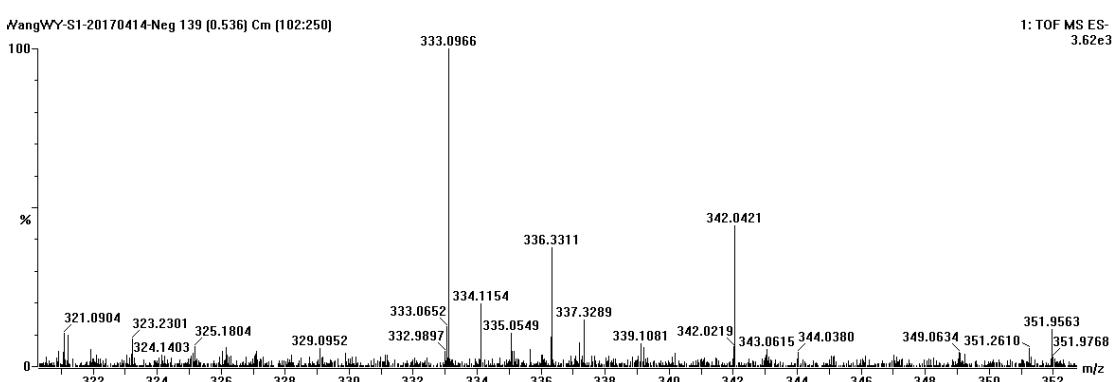
Figure S12. HSQC spectrum of compound 2



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Figure S13. HMBC spectrum of compound 2



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Figure S14. HRESIMS spectrum of compound 2

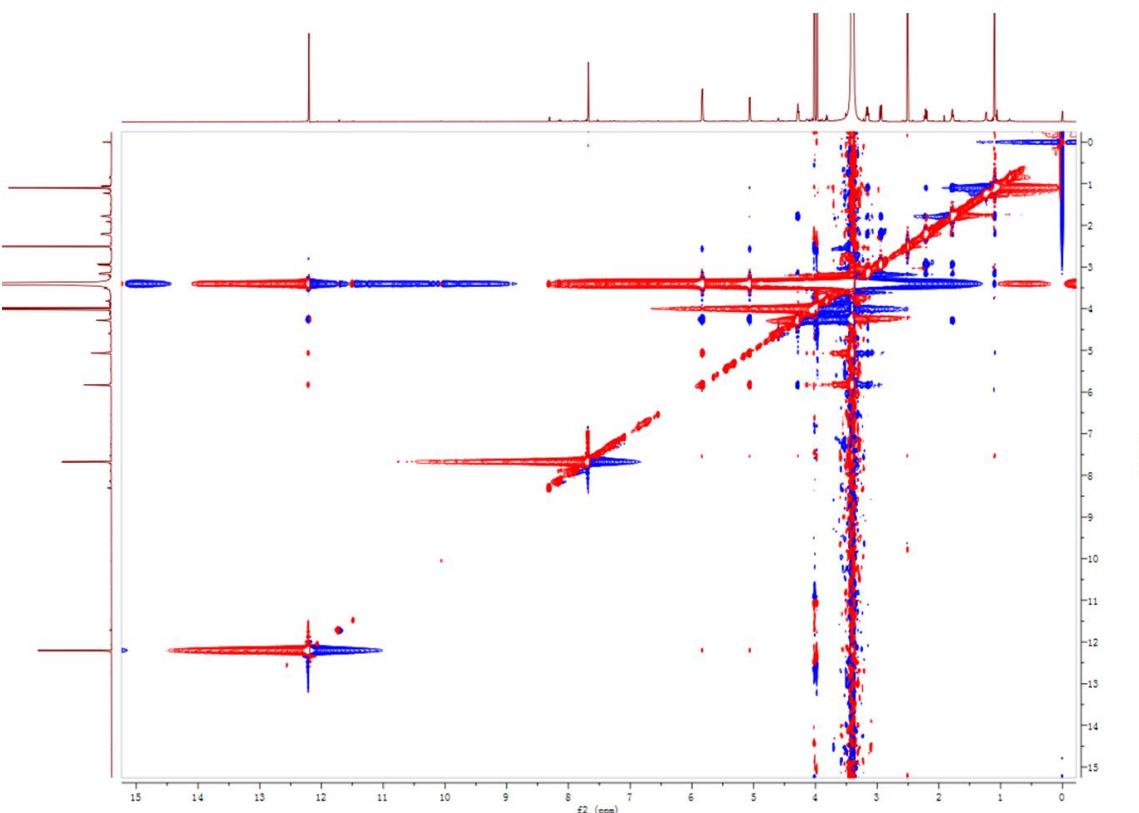


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Figure S15. UV spectrum of compound 2

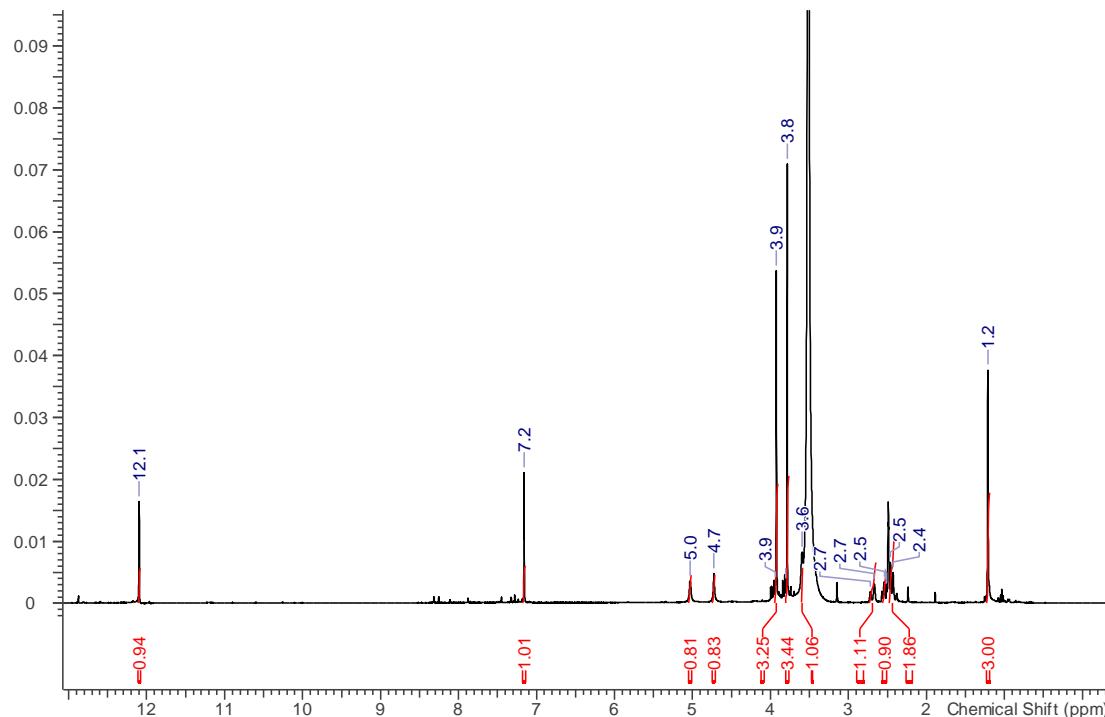
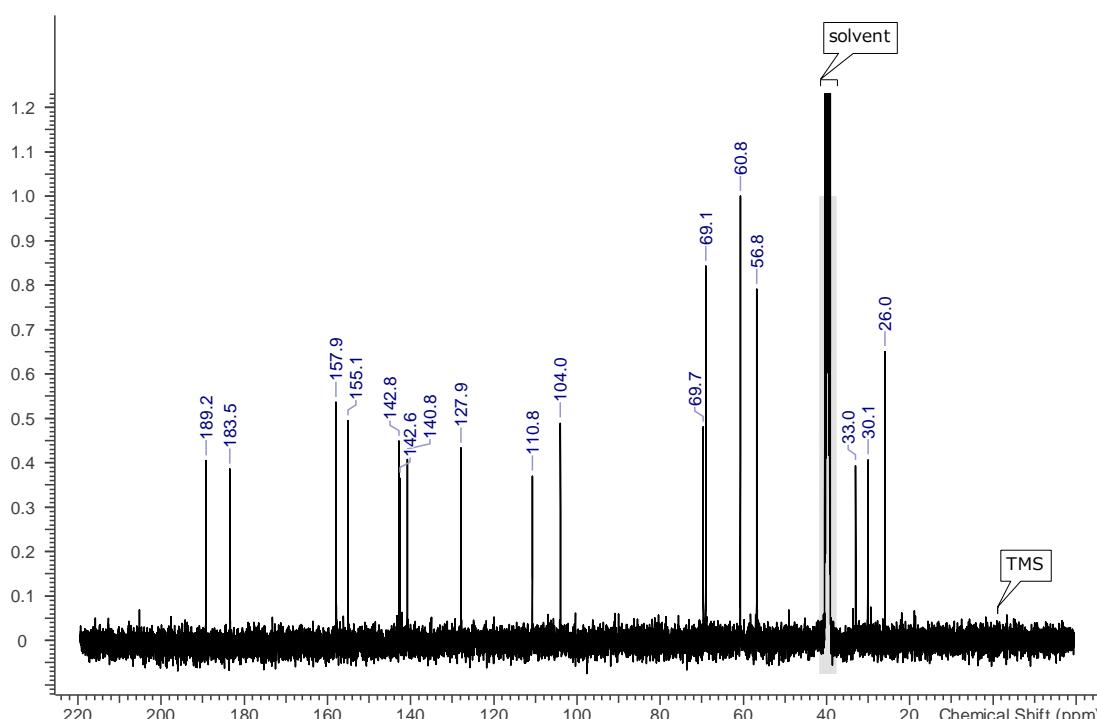


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Figure S16. NOESY spectrum of compound 2

Figure S17. ¹H NMR spectrum of compound 3Figure S18. ¹³C NMR spectrum of compound 3

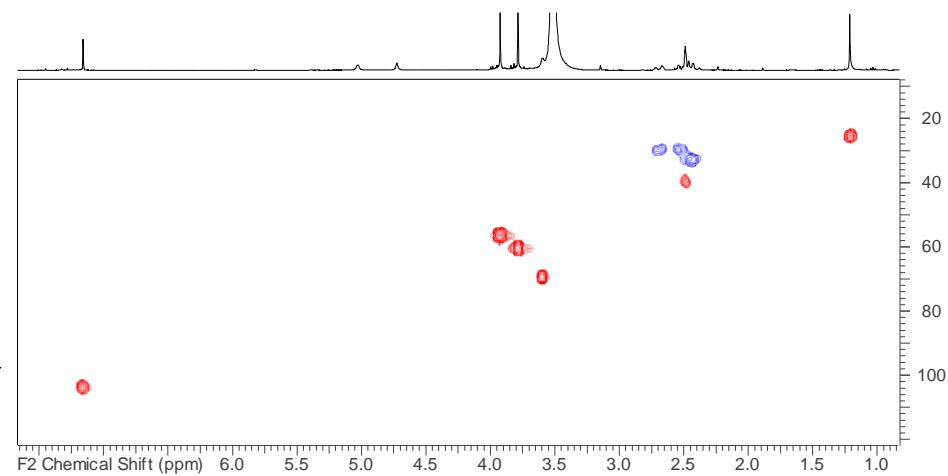
63
64
65Figure S19. ^1H - ^1H COSY spectrum of compound 366
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Figure S20. HSQC spectrum of compound 3

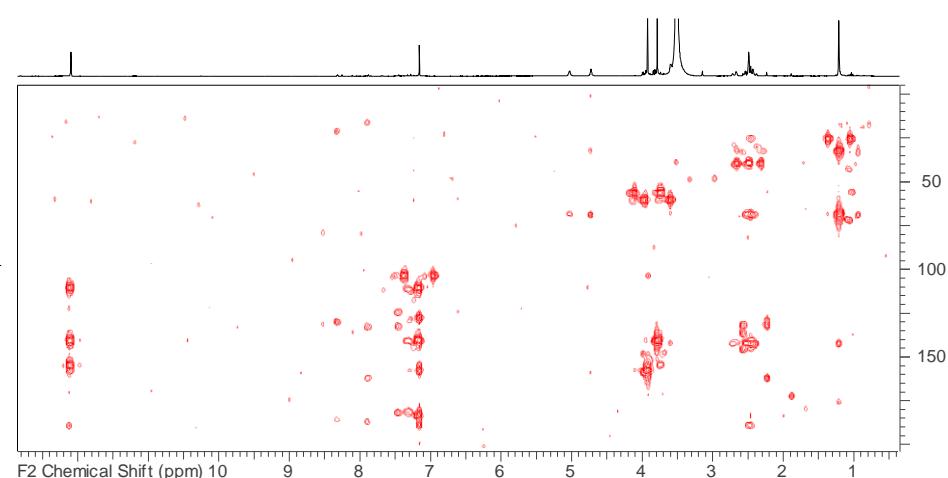
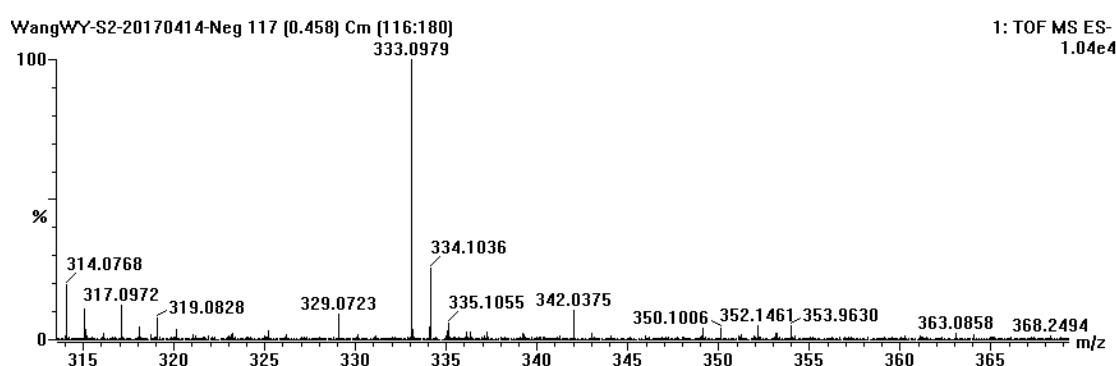
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Figure S21. HMBC spectrum of compound 3

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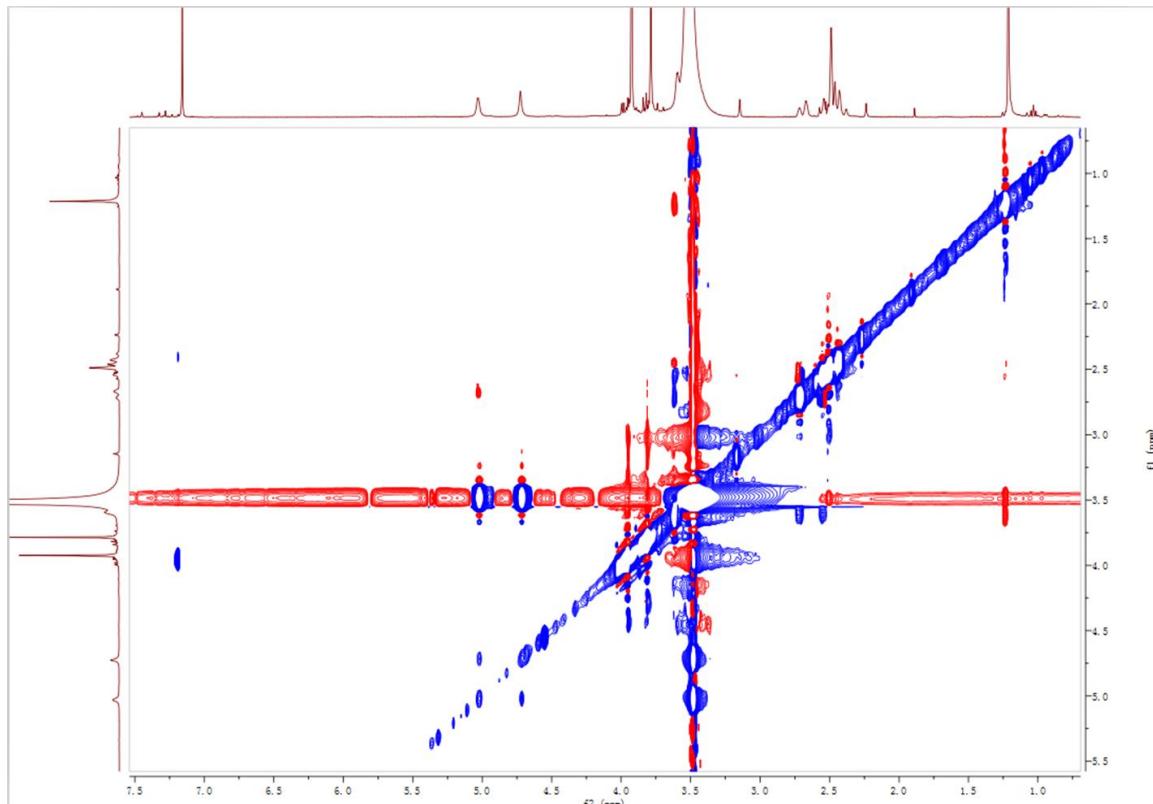
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Figure S22. HRESIMS spectrum of compound 3



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Figure S23. UV spectrum of compound 3



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Figure S24. NOESY spectrum of compound 3

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Table S1. Energies of the dominative conformers at MMFF94 force field of compound 2 & 3

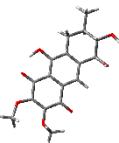
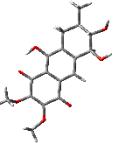
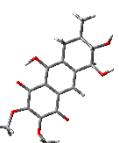
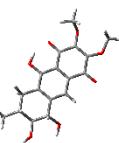
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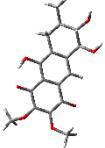
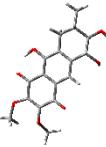
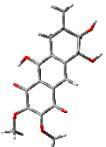
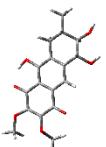
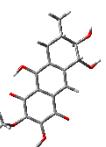
Configuration	Conformer	Energy(kcal/mol)
1S, 2S, 3R-2	1	137.97
	2	149.21
	3	149.92
	4	156
	5	163.91
1R, 2R, 3S-2	1	141.2
	2	152.77
	3	154.9
	4	159.02
	5	166.91
2R, 3S-3	1	90.07
	2	90.69
	3	90.76
	4	91.24
2S, 3R-3	1	89.92
	2	90.08
	3	90.54
	4	90.70

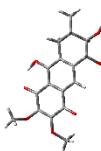
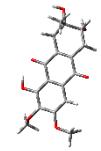
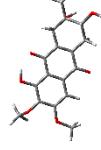
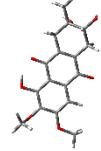
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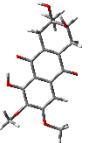
94

Table S2. Energies of the conformers at B3LYP/6-311G** of compound 2 & 3 in methanol

Configuration	Conformatio n	Structure	E (Hartree)	E (kcal/mol)	Population (%)
1S, 2S, 3R-2	1		-1185.52017	-743925.1326	39.19
	2		-1185.519535	-743924.7341	19.99
	3		-1185.519373	-743924.6322	16.82
	4		-1185.519576	-743924.7594	20.86

	5		-1185.51779	-743923.6389	3.14
1 <i>R</i> , 2 <i>R</i> , 3 <i>S</i> -2	1		-1185.52017	-743925.1326	39.19
	2		-1185.519535	-743924.7341	19.99
	3		-1185.519373	-743924.6322	16.82
	4		-1185.519576	-743924.7594	20.86

	5		-1185.51779	-743923.6389	3.14
2 <i>R</i> , 3 <i>S</i> -3	1		-1185.51779	-743923.6389	3.14
	2		-1183.866035	-742887.1467	38.1
	3		-1183.86602	-742887.1375	37.51
	4		-1183.86501	-742886.5041	12.86

2S, 3R-3	1		-1183.866032	-742887.1448	38.02
	2		-1183.866022	-742887.1388	37.63
	3		-1183.86501	-742886.5036	12.87
	4		-1183.864903	-742886.4363	11.48

95 Text S1: ITS1-5.8S-ITS2 rDNA sequence of strain SP2-8-1

96 GenBank flat file:

97 LOCUS MF716581 526 bp DNA linear PLN

98 21-AUG-2017

99 DEFINITION Aspergillus tritici strain sp2-8-1 18S ribosomal RNA gene, partial

100 sequence; and internal transcribed spacer 1, 5.8S ribosomal RNA

101 gene, and internal transcribed spacer 2, complete sequence.

102 ACCESSION MF716581

103 VERSION MF716581

104 KEYWORDS .

105 SOURCE Aspergillus tritici

106 ORGANISM Aspergillus tritici

107 Eukaryota; Fungi; Dikarya; Ascomycota; Pezizomycotina;

108 Eurotiomycetes; Eurotiomycetidae; Eurotiales; Aspergillaceae;

109 Aspergillus.

110 REFERENCE 1 (bases 1 to 526)

111 AUTHORS Wang,W. and Liao,Y.

112 TITLE Chemical compostion of a coral-derived Aspergillus tritici strain

113 sp2-8-1

114 JOURNAL Unpublished

115 REFERENCE 2 (bases 1 to 526)

116 AUTHORS Wang,W. and Liao,Y.

117 TITLE Direct Submission

118 JOURNAL Submitted (21-AUG-2017) Key Laboratory of Marine Biogenetic

119 Resources, Third Institute of Oceanography, State Oceanic

120 Administration, 178 Daxue Road, Xiamen, Fujian 361005, China

121 COMMENT ##Assembly-Data-START##

122 Sequencing Technology :: Sanger dideoxy sequencing

123 ##Assembly-Data-END##

124 FEATURES Location/Qualifiers

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131 /country="Malaysia"

132 /identified_by="Yanyan Liao"

133 misc_RNA <1..526

134 /note="contains 18S ribosomal RNA, internal transcribed

135 spacer 1, 5.8S ribosomal RNA, and internal transcribed

136 spacer 2"

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140 121 cccgggccccg cgcccgccga agaccccaac acgaacactg tctgaaaagt gcagtctgag

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