

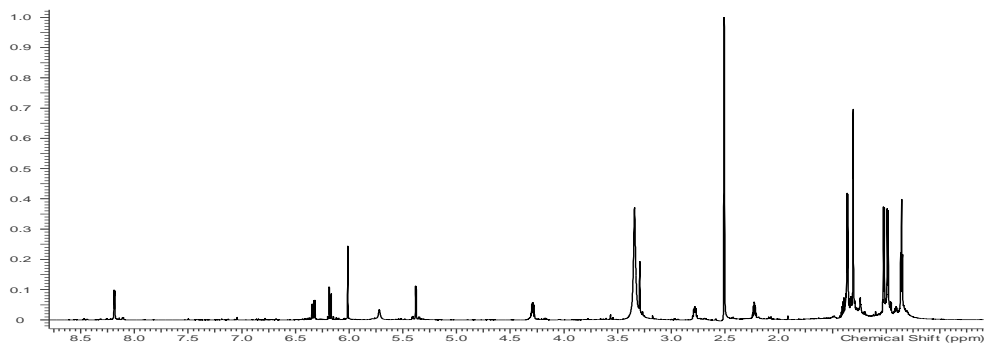
2 **Chlorinated azaphilone pigments with antimicrobial**
3 **and cytotoxic activities isolated from the deep sea**
4 **derived Fungus *Chaetomium* sp. NA-S01-R1**

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6 Maolin Gao ¹, Zongze Shao ¹, Jianming Chen ^{3,*} and Fang Li ^{1,*}

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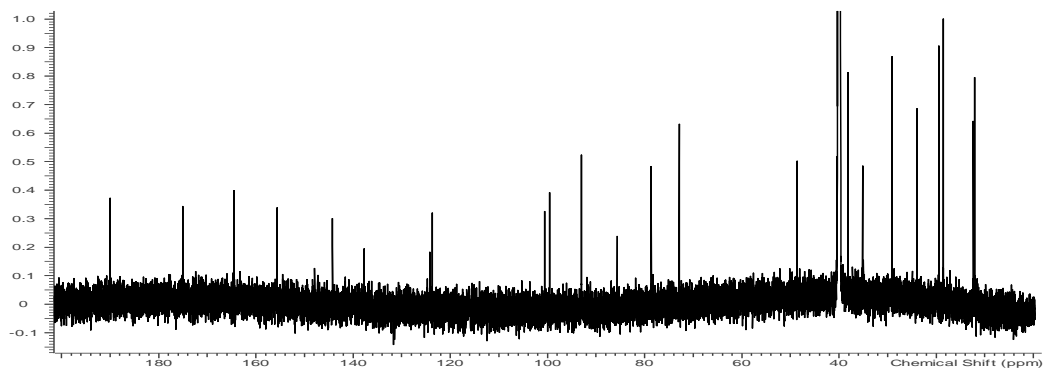


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Figure S1. ¹H NMR spectrum of compound 1

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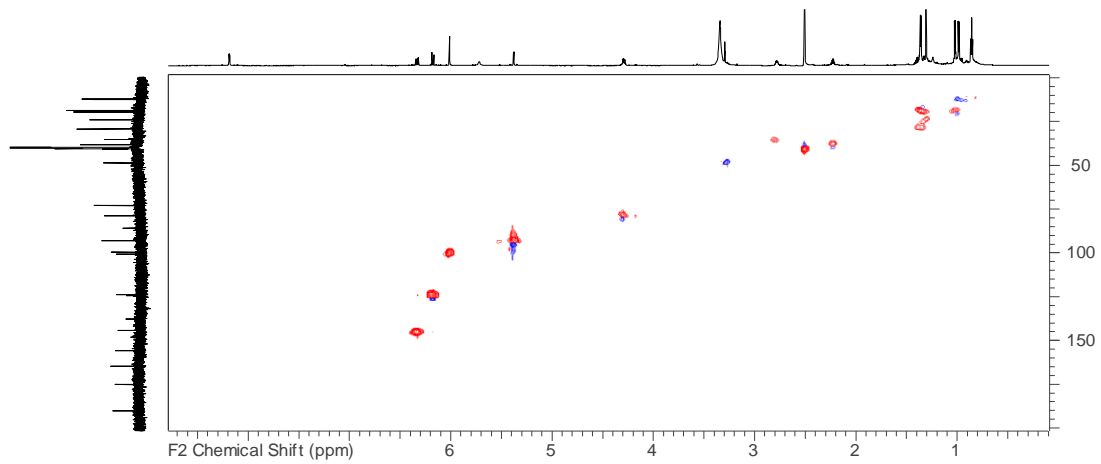


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Figure S2. ¹³C NMR spectrum of compound 1

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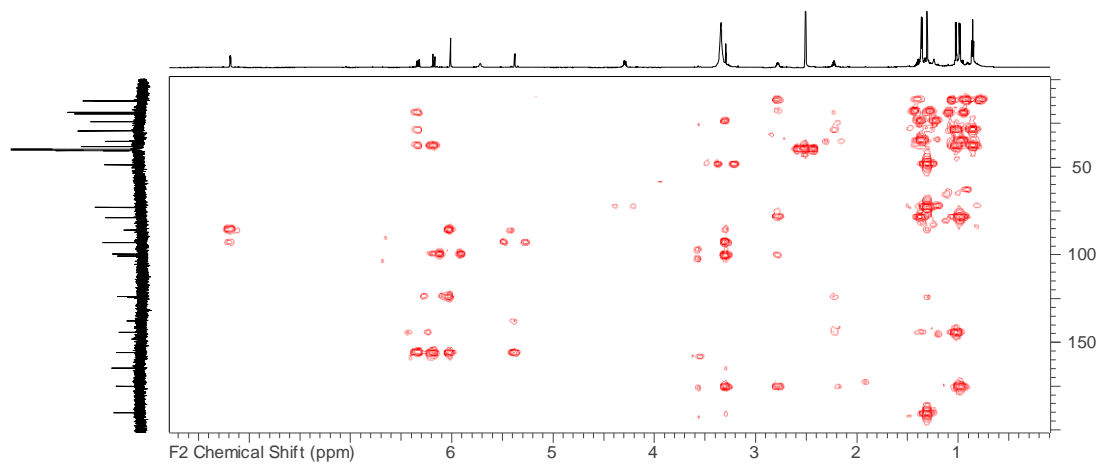


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Figure S3. HSQC spectrum of compound 1

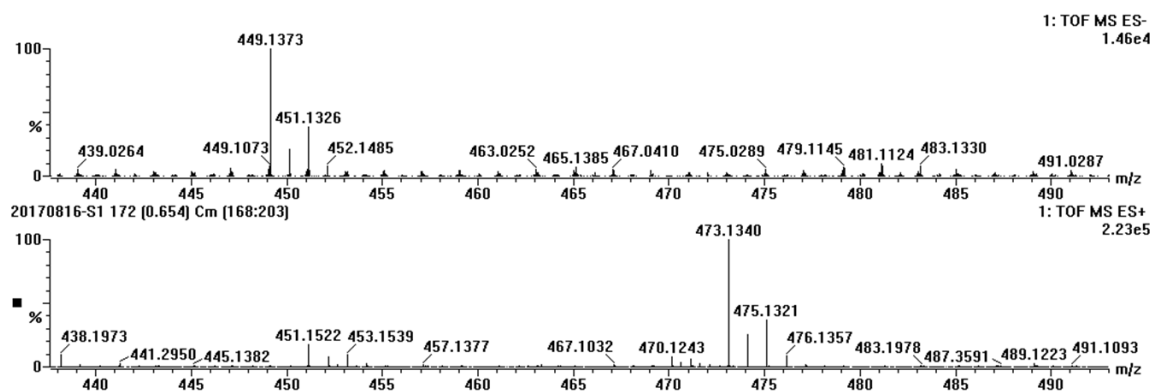
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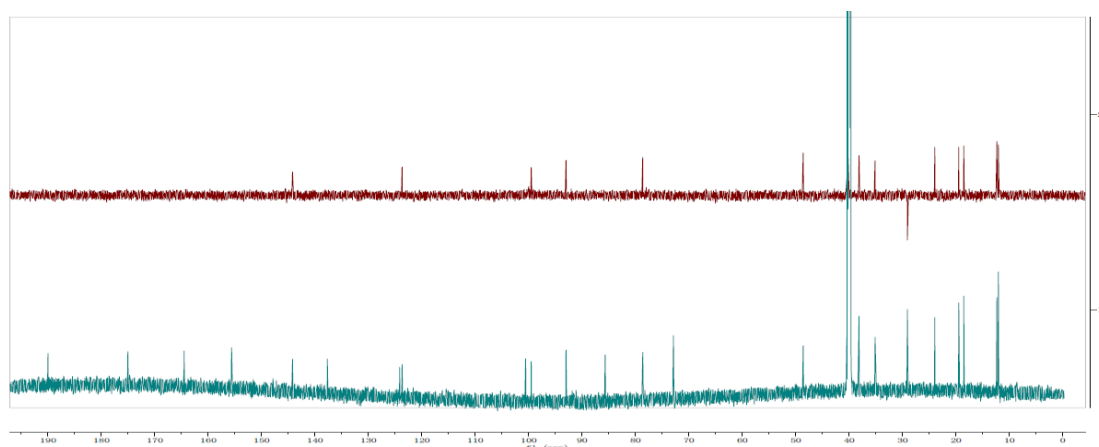
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Figure S4. HMBC spectrum of compound 1



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Figure S5. HRESIMS spectrum of compound 1



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Figure S6. $^{13}\text{C}/\text{DEPT}$ spectrum of compound 1

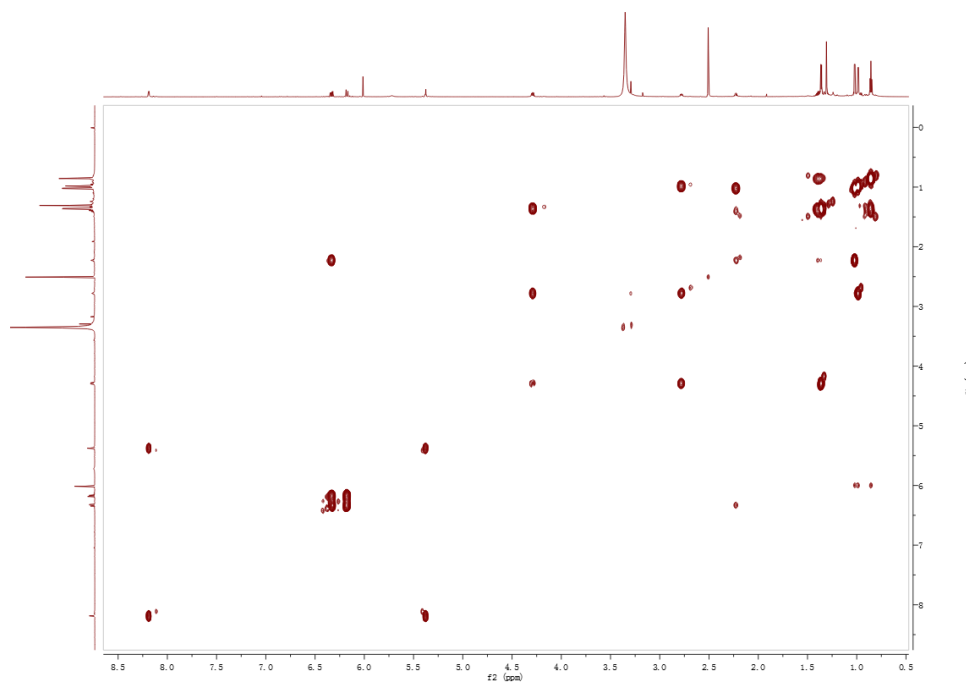


Figure S7. ^1H - ^1H COSY spectrum of compound 1

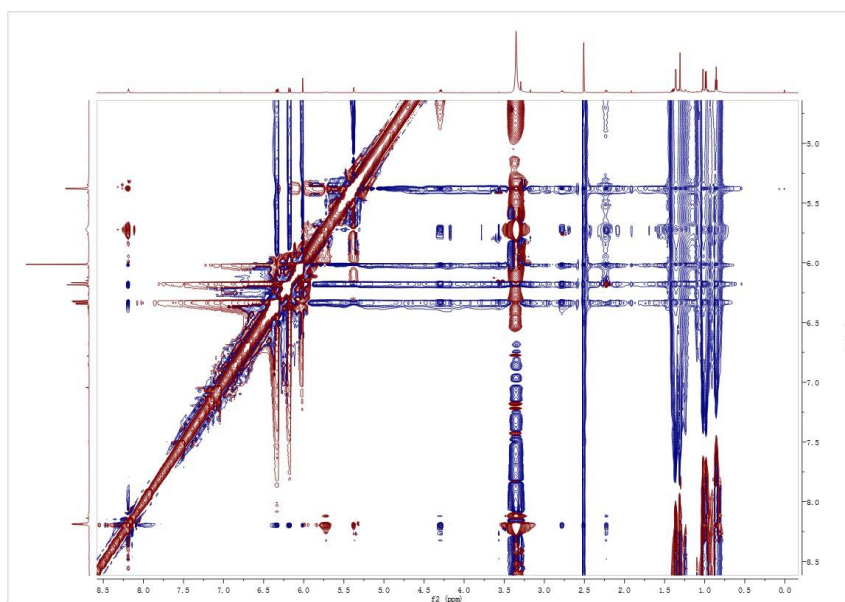


Figure S8. Selected NOESY spectrum of compound 1

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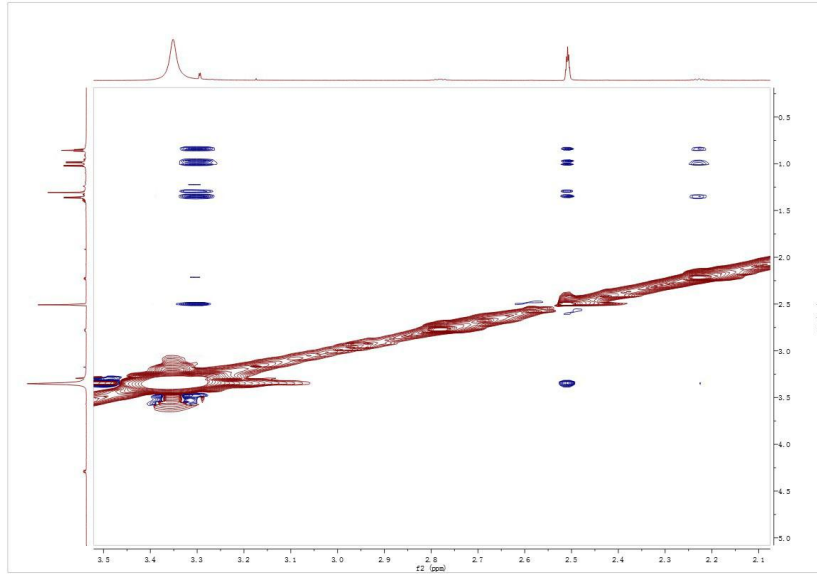


Figure S9. Selected NOESY spectrum of compound 1

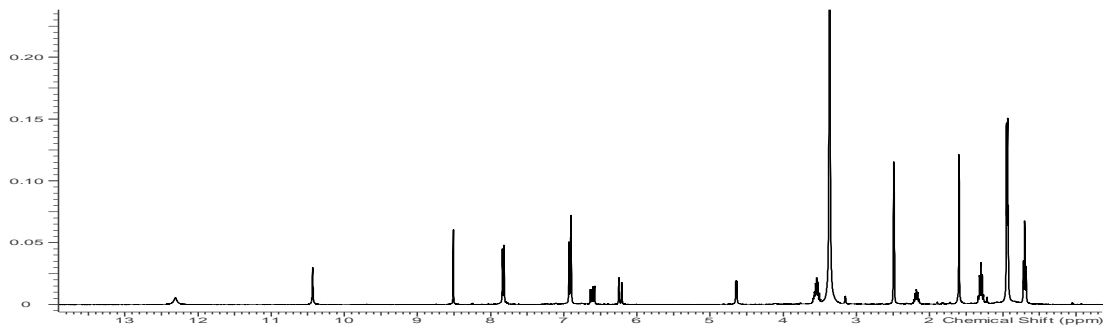


Figure S10. ¹H NMR spectrum of compound 2

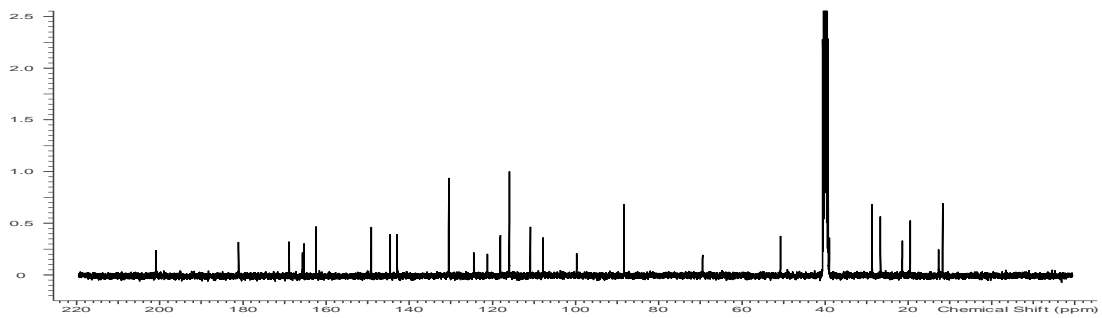


Figure S11. ¹³C NMR spectrum of compound 2

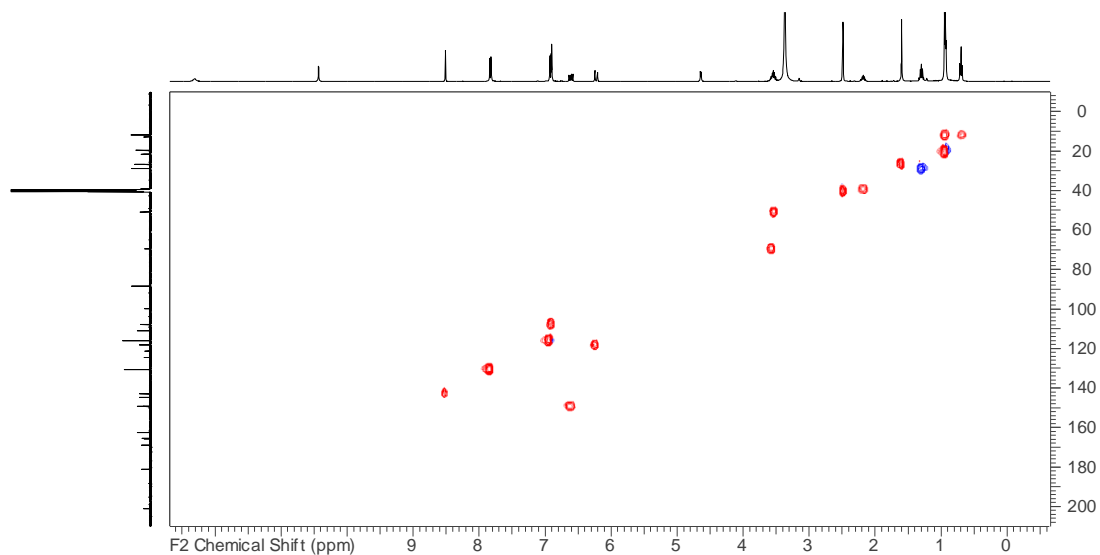


Figure S12. HSQC spectrum of compound 2

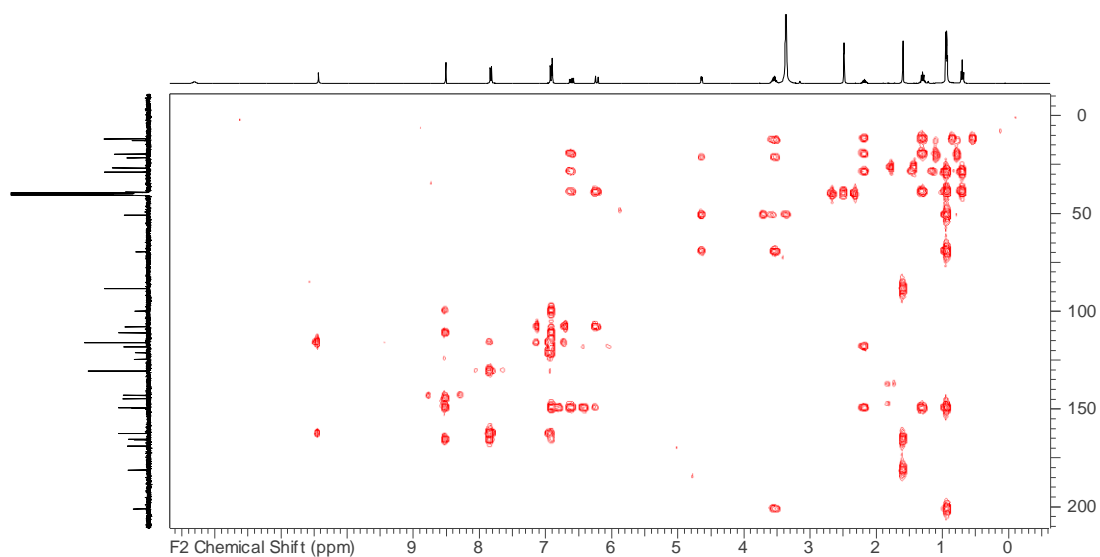


Figure S13. HMBC spectrum of compound 2

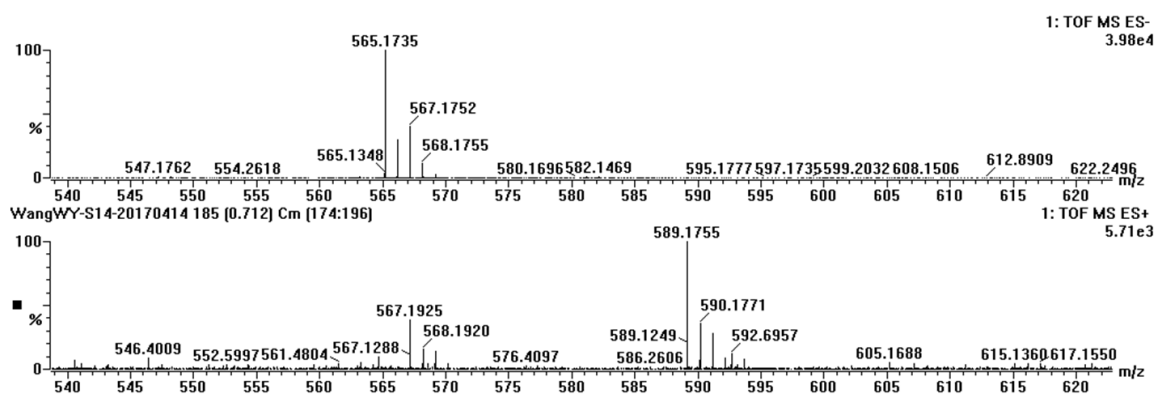
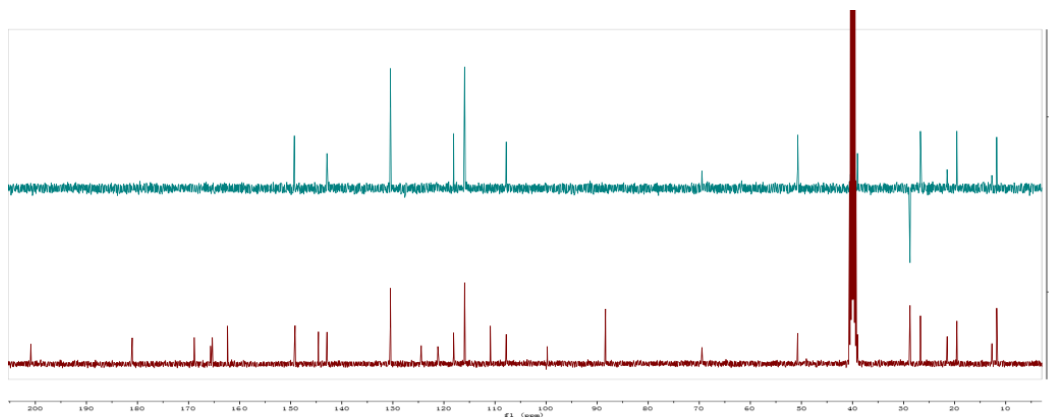


Figure S14. HRESIMS spectrum of compound 2

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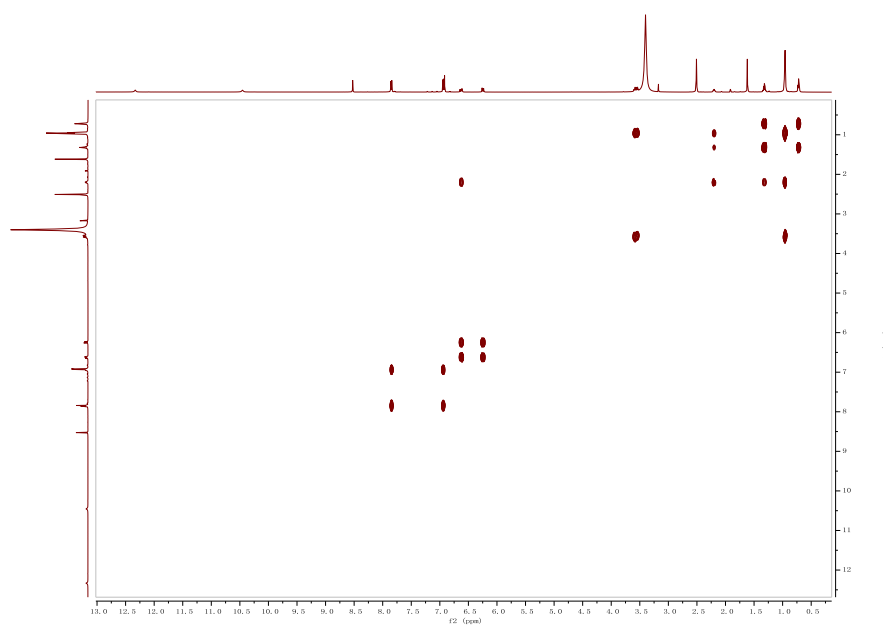
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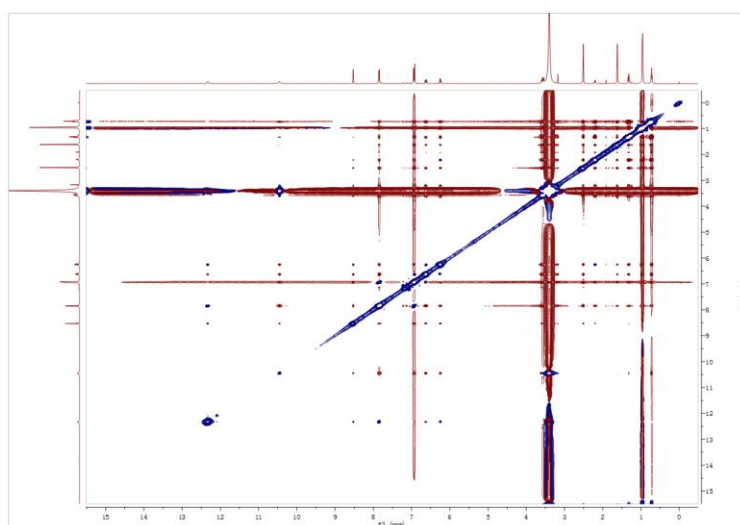
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Figure S15. $^{13}\text{C}/\text{DEPT}$ spectrum of compound 2



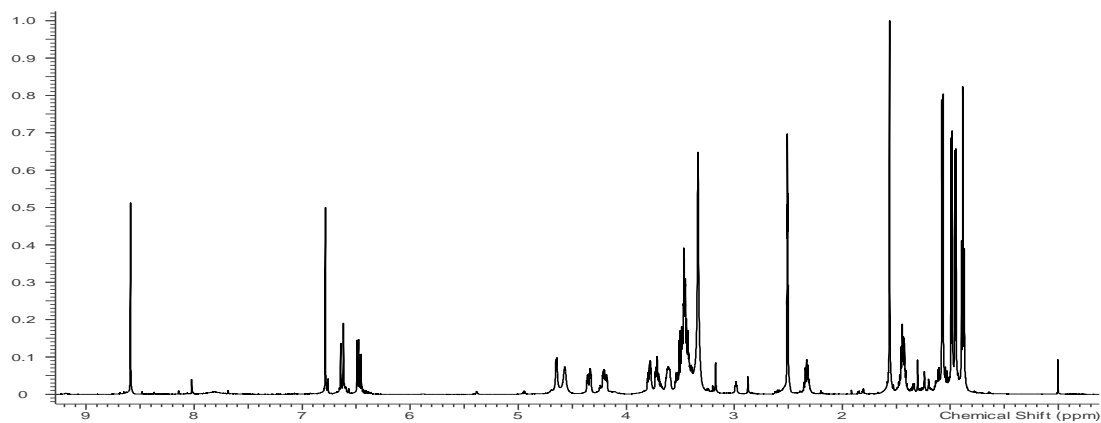
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Figure S16. $^1\text{H}-^1\text{H}$ COSY spectrum of compound 2



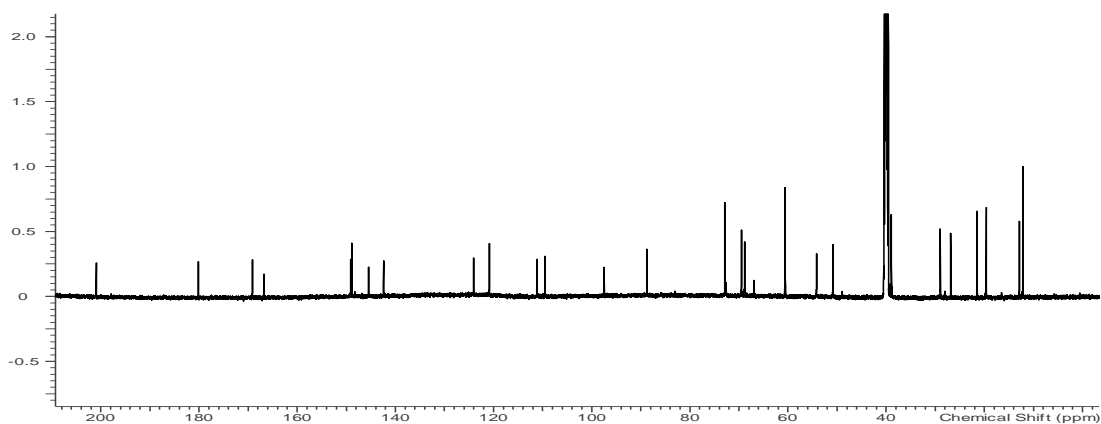
90
91

Figure S17. NOESY spectrum of compound 2



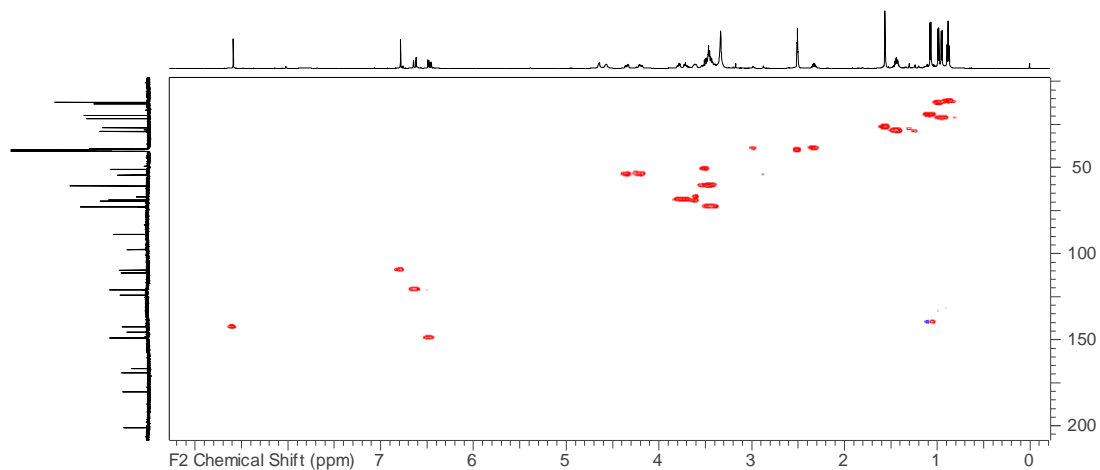
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93
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Figure S18. ^1H NMR spectrum of compound 3



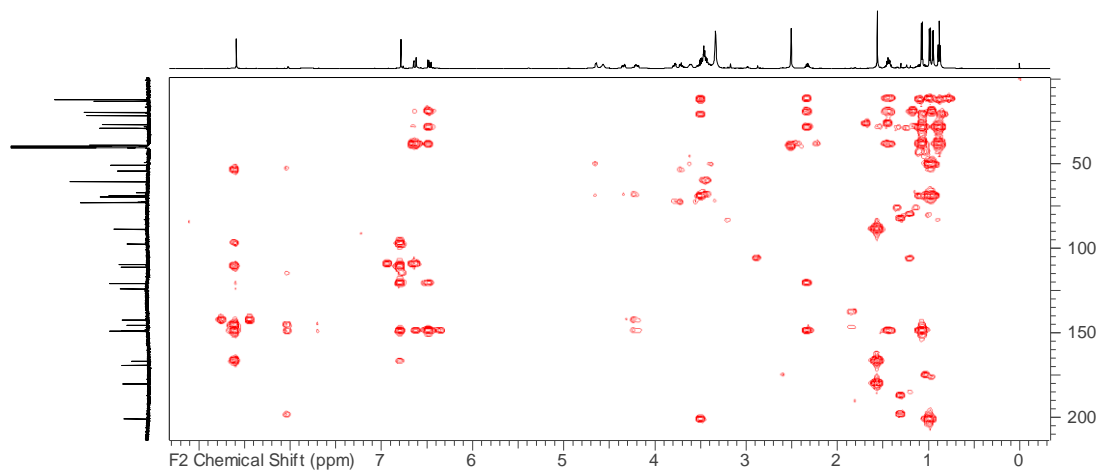
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Figure S19. ^{13}C NMR spectrum of compound 3



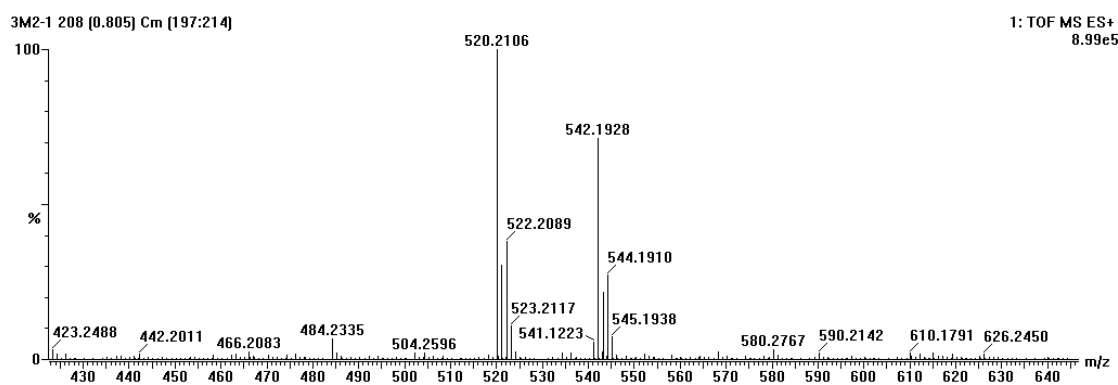
98
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Figure S20. HSQC spectrum of compound 3



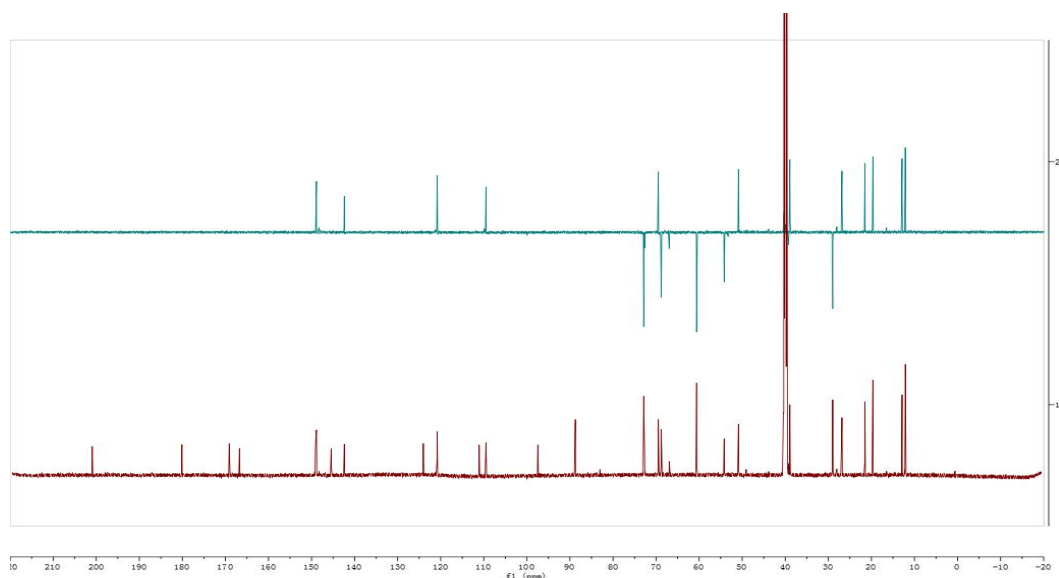
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Figure S21. HMBC spectrum of compound 3



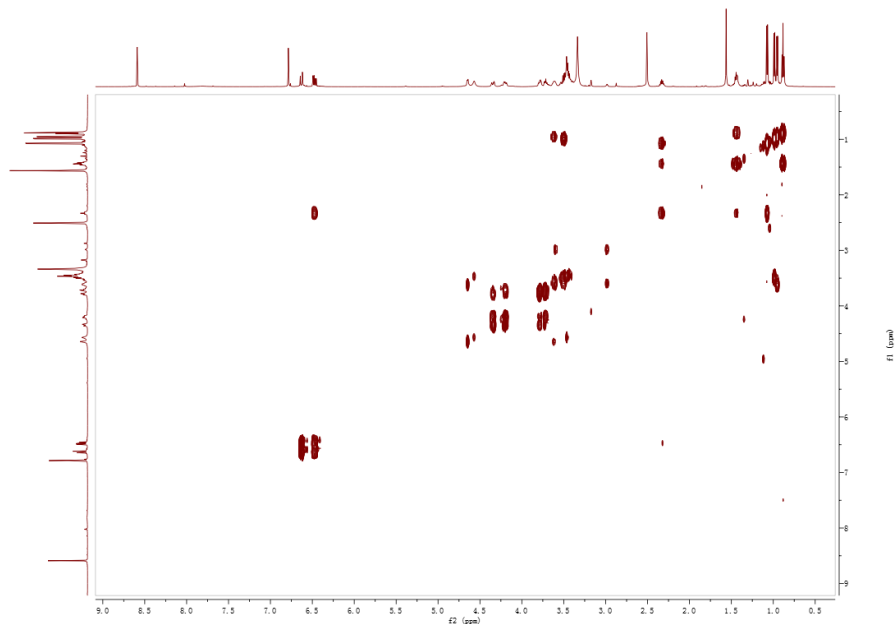
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Figure S22. HRESIMS spectrum of compound 3



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Figure S23. $^{13}\text{C}/\text{DEPT}$ spectrum of compound 3

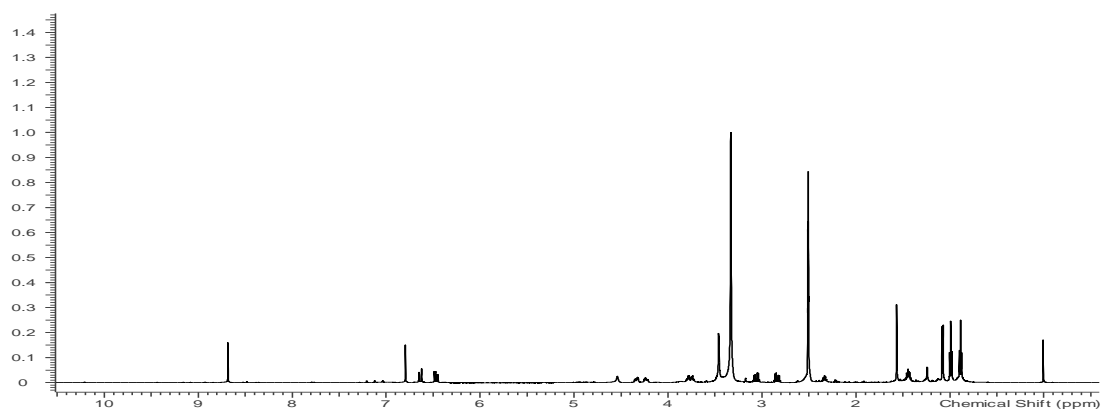


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Figure S24. ^1H - ^1H COSY spectrum of compound 3

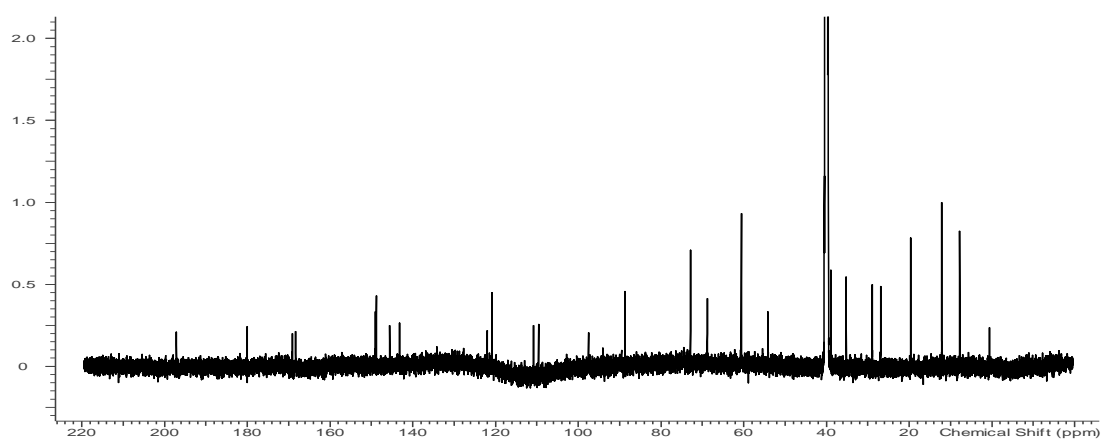


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Figure S25. ^1H NMR spectrum of compound 4

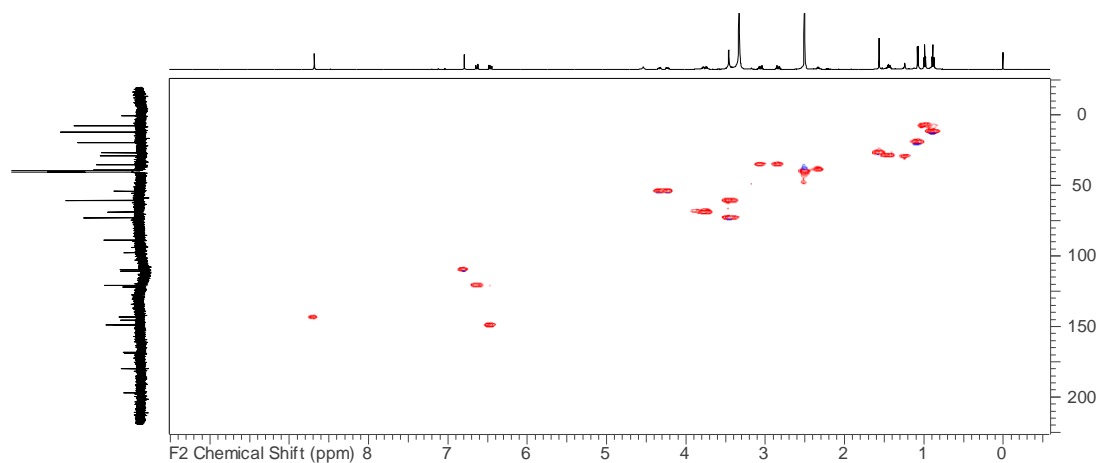


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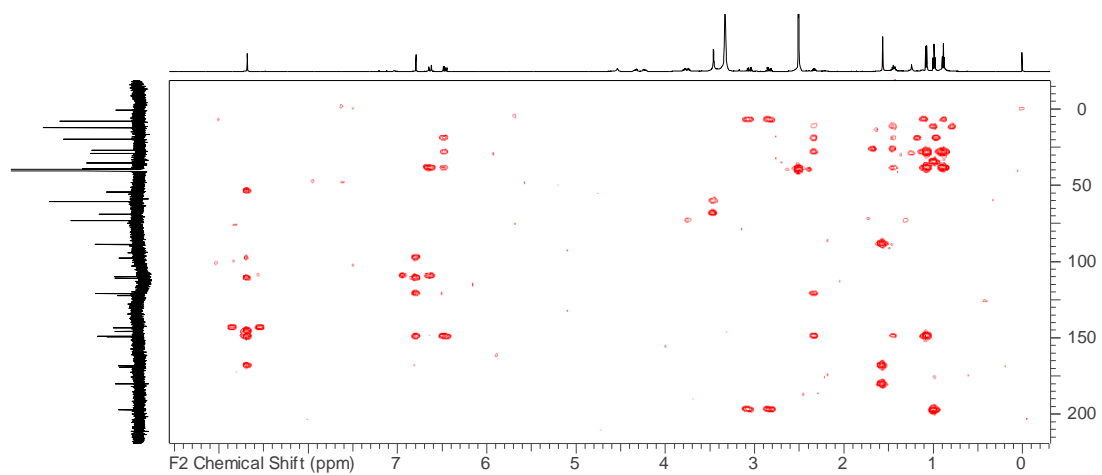
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Figure S26. ^{13}C NMR spectrum of compound 4



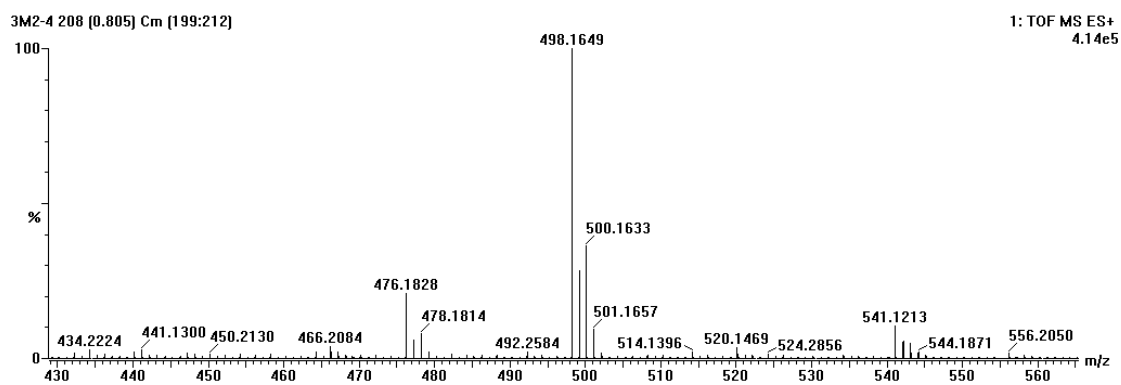
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Figure S27. HSQC spectrum of compound 4



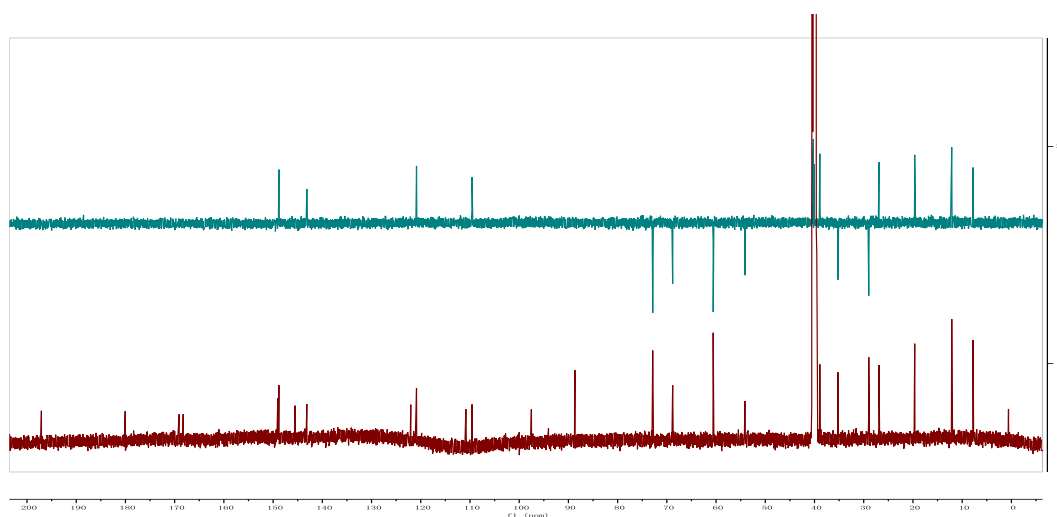
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Figure S28. HMBC spectrum of compound 4



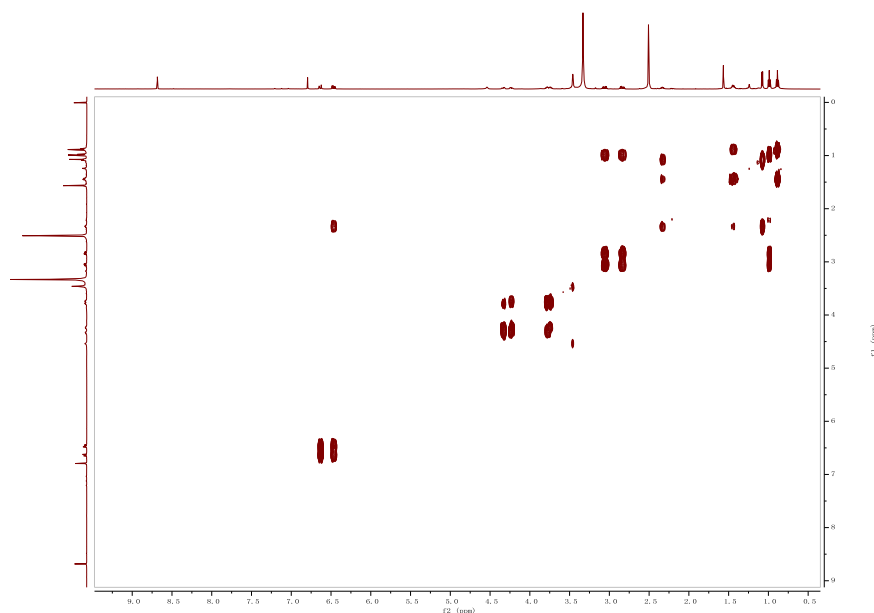
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Figure S29. HRESIMS spectrum of compound 4



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Figure S30. $^{13}\text{C}/\text{DEPT}$ spectrum of compound 4



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Figure S31. $^1\text{H}-^1\text{H}$ COSY spectrum of compound 4

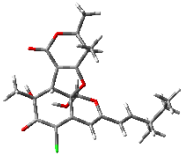
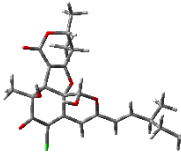
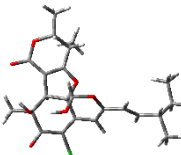
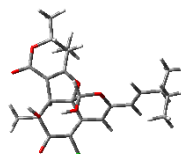
Table S1. Energies of the dominative conformers at MMFF94 force field of compound 1

Configuration	Conformer	Energy (kcal/mol)
(1 <i>R</i> , 7 <i>R</i> , 8 <i>S</i> , 8 <i>aR</i> , 11 <i>S</i> , 4' <i>R</i> , 5' <i>S</i>)-1	1	131.80
	2	133.62
	3	133.64
	4	133.71
(1 <i>S</i> , 7 <i>S</i> , 8 <i>R</i> , 8 <i>aS</i> , 11 <i>S</i> , 4' <i>S</i> , 5' <i>R</i>)-1	1	134.38
	2	135.20
	3	135.64
	4	135.94
	5	135.95
	6	136.04

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Table S2. Energies of the conformers at B3LYP/6-311G** of compound 1 in methanol.

Configuration	Conformer	Structure	E (Hartree)	E (kcal/mol)	Population (%)
(1R, 7R, 8S, 8aR, 11S, 4'R, 5'S)-1	3		-1879.82988243	-1179611.05	100.00
(1S, 7S, 8R, 8aS, 11S, 4'S, 5'R)-1	1		-1879.82899701	-1179610.50	26.34
(1S, 7S, 8R, 8aS, 11S, 4'S, 5'R)-1	2		-1879.82633158	-1179608.82	1.57
(1S, 7S, 8R, 8aS, 11S, 4'S, 5'R)-1	4		-1879.82994775	-1179611.09	72.10

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Text S1: ITS1-5.8S-ITS2 rDNA sequence (MG786198) of strain *Chaetomium* sp. NA-S01-R1

LOCUS Seq 568 bp DNA linear PLN 11-JAN-2018

DEFINITION 1 *Chaetomium* sp. NA-S01-R1 18S ribosomal RNA gene, partial sequence; internal transcribed spacer 1, 5.8S ribosomal RNA gene, and internal transcribed spacer 2, complete sequence; and 28S ribosomal RNA gene, partial sequence.

ACCESSION Seq

VERSION

KEYWORDS .

SOURCE *Chaetomium* sp.ORGANISM *Chaetomium* sp.

Eukaryota; Fungi; Dikarya; Ascomycota; Pezizomycotina;

Sordariomycetes; Sordariomycetidae; Sordariales; Chaetomiaceae;

Chaetomium.

REFERENCE 1 (bases 1 to 568)

AUTHORS Wang, W.

TITLE Chlorinated azaphilone pigments with antimicrobial and cytotoxic

156 activities isolated from the deep sea derived Fungus Chaetomium sp.
 157 NA-S01-R1
 158 JOURNAL Unpublished
 159 REFERENCE 2 (bases 1 to 568)
 160 AUTHORS Wang, W.
 161 TITLE Direct Submission
 162 JOURNAL Submitted (11-JAN-2018) Key Laboratory of Marine Biogenetic
 163 Resources, Third Institute of Oceanography, State Oceanic
 164 Administration, 178 Daxue Road, Xiamen, Fujian 361005, China
 165 COMMENT Bankit Comment: ALT EMAIL:wywang_cas@163.com.
 166 Bankit Comment: TOTAL # OF SEQS:1.
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 169 Sequencing Technology :: Sanger dideoxy sequencing
 170 ##Assembly-Data-END##
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 185 and internal transcribed spacer 2, complete sequence; and
 186 28S ribosomal RNA gene, partial sequence"
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 188 ORIGIN
 189 1 ctggcggctct ctactttcc gaggtcacct tgggttaaaa ggtggttaa cggccggaac
 190 61 ccgcgcgcg accagagcga gatgatgct actacgctcg gtgcgacagc gagcccgcca
 191 121 ctgctttca gggcctgcgg cagccgagg tcccaaacac aagcccgggg gcttgatggt
 192 181 tgaatgacg ctcaatagg catgccgcc agaatgctgg cggcgcaat gtgcgtcaa
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