

## Supplementary Information

# Cytotoxic Polyketide Metabolites from a Marine Mesophotic Zone Chalinidae Sponge-Associated Fungus *Pleosporales* sp. NBUF144

Jing Zhou <sup>1</sup>, Hairong Zhang <sup>1</sup>, Jing Ye <sup>2</sup>, Xingxin Wu <sup>2</sup>, Weiyi Wang <sup>3</sup>, Houwen Lin <sup>4</sup>, Xiaojun Yan <sup>1</sup>, J. Enrico H. Lazaro <sup>5</sup>, Tingting Wang <sup>1,\*</sup>, C. Benjamin Naman <sup>1</sup>, Shan He <sup>1,\*</sup>

<sup>1</sup> Li Dak Sum Marine Biopharmaceutical Research Center, Department of Marine Pharmacy, College of Food and Pharmaceutical Sciences, Ningbo University, Ningbo, Zhejiang, 315800, China

<sup>2</sup> State Key Laboratory of Pharmaceutical Biotechnology, School of Life Sciences, Nanjing University, Nanjing, 210023, China

<sup>3</sup> Key Laboratory of Marine Biogenetic Resources, Third Institute of Oceanography, Ministry of Natural Resources, Xiamen, 361005, China

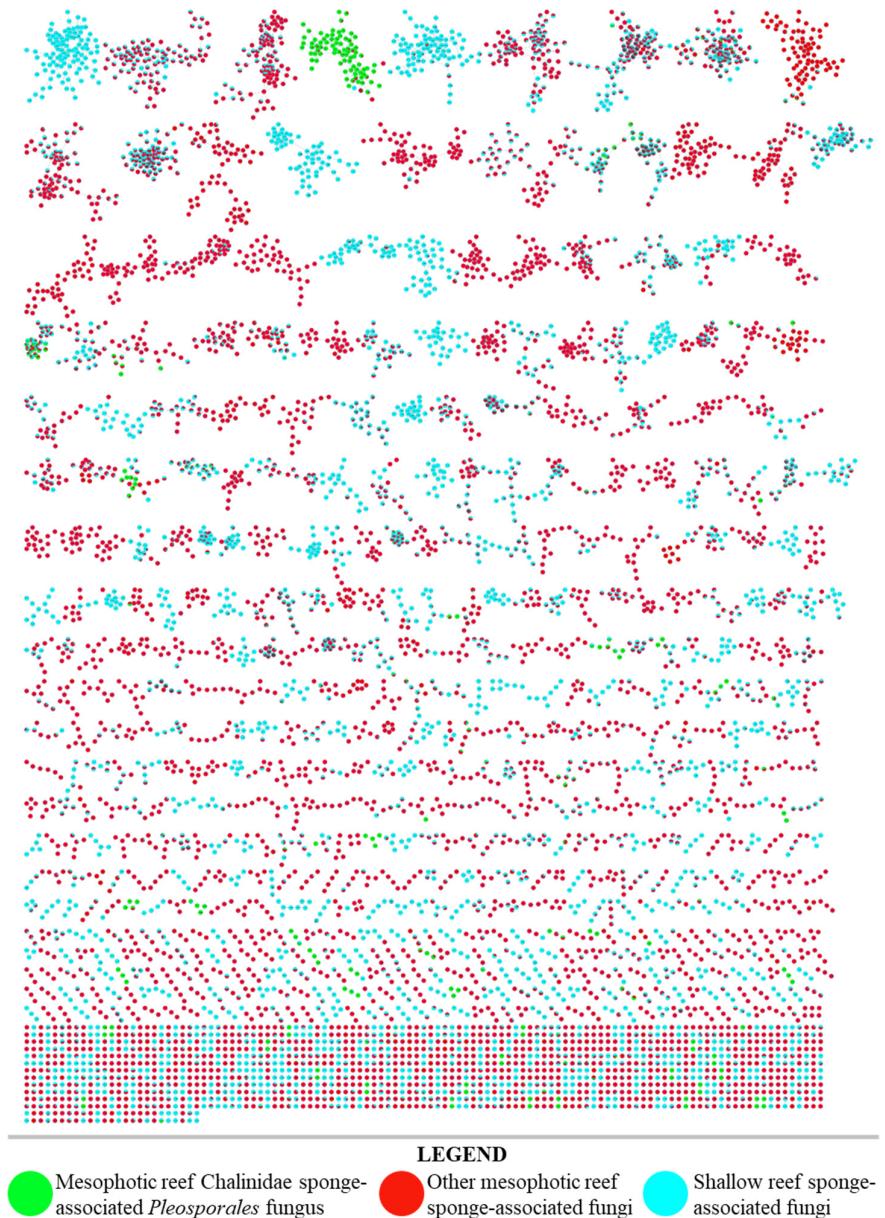
<sup>4</sup> Research Center for Marine Drugs, State Key Laboratory of Oncogene and Related Genes, Department of Pharmacy, Ren Ji Hospital, School of Medicine, Shanghai Jiao Tong University, Shanghai 200127, China

<sup>5</sup> National Institute of Molecular Biology and Biotechnology, University of the Philippines Diliman, Quezon, 1101, Philippines

\* Correspondence: wangtingting1@nbu.edu.cn (T.W.); heshan@nbu.edu.cn (S.H.)

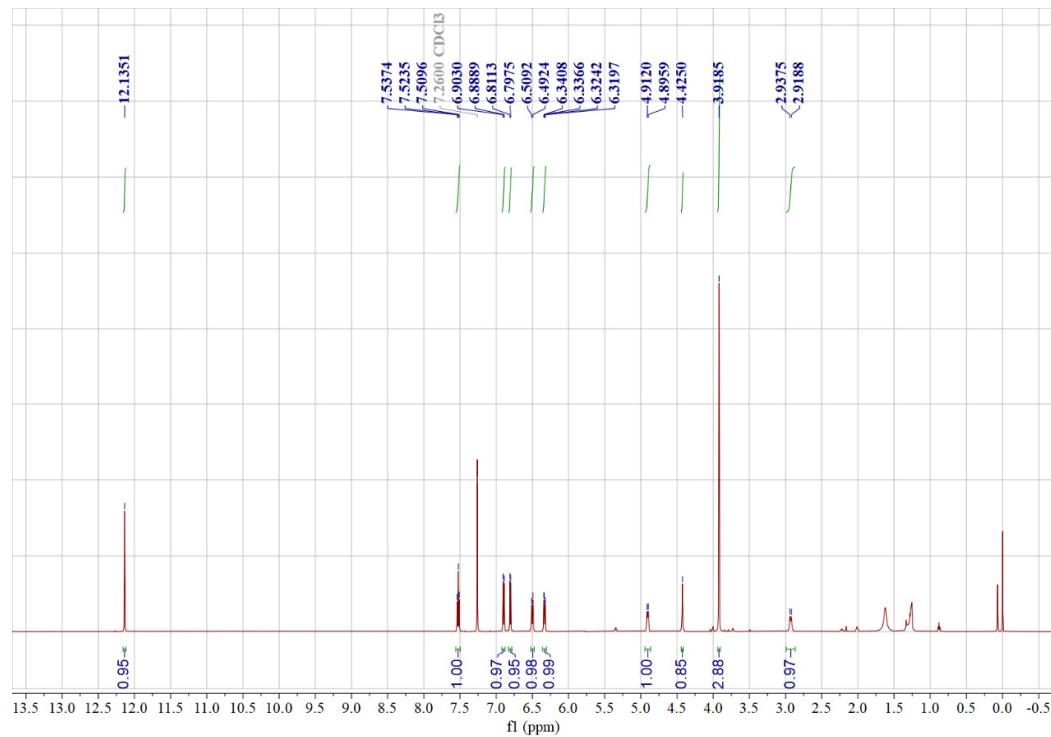
## Contents

Figure S1. LC-MS/MS derived molecular network of organic extracts produced from 80 fungal cultures (40 from shallow reef sponges, 40 from mesophotic zone sponges). Single node clusters, or self-loop nodes, were excluded for brevity. ....	2
Figure S2 <sup>1</sup> H NMR spectrum of compound <b>1</b> (600 MHz, CDCl <sub>3</sub> ).....	3
Figure S3 <sup>13</sup> C NMR spectrum of compound <b>1</b> (150 MHz, CDCl <sub>3</sub> ) .....	4
Figure S4 DEPT135 spectrum of compound <b>1</b> (150 MHz, CDCl <sub>3</sub> ).....	5
Figure S5 <sup>1</sup> H- <sup>1</sup> H COSY spectrum of compound <b>1</b> .....	6
Figure S6 HSQC spectrum of compound <b>1</b> .....	7
Figure S7 HMBC spectrum of compound <b>1</b> .....	8
Figure S8 NOESY spectrum of compound <b>1</b> .....	9
Figure S9 <sup>1</sup> H NMR spectrum of compound <b>2</b> (600 MHz, CDCl <sub>3</sub> ).....	11
Figure S10 <sup>13</sup> C NMR spectrum of compound <b>2</b> (150 MHz, CDCl <sub>3</sub> ).....	12
Figure S11 DEPT135 spectrum of compound <b>2</b> (150 MHz, CDCl <sub>3</sub> ) .....	13
Figure S12 <sup>1</sup> H- <sup>1</sup> H COSY spectrum of compound <b>2</b> .....	14
Figure S13 HSQC spectrum of compound <b>2</b> .....	15
Figure S14 HMBC spectrum of compound <b>2</b> .....	16
Figure S15 NOESY spectrum of compound <b>2</b> .....	17

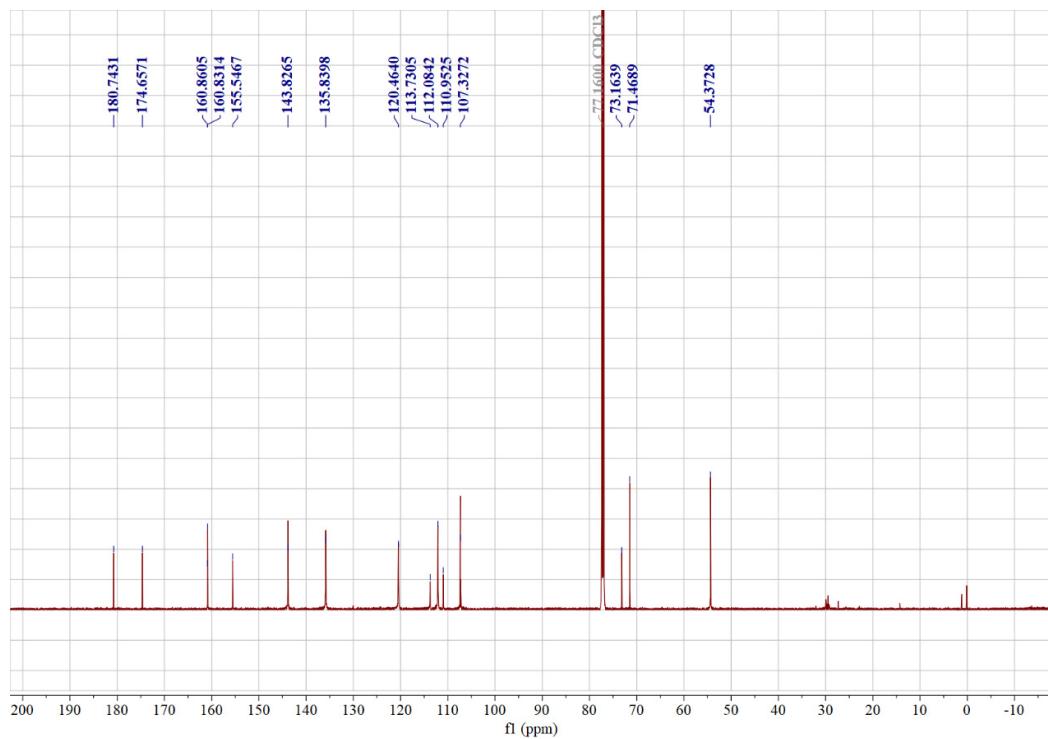


**Figure S1. LC-MS/MS derived molecular network of organic extracts produced from 80 fungal cultures (40 from shallow reef sponges, 40 from mesophotic zone sponges). Single node clusters, or self-loop nodes, were excluded for brevity.**

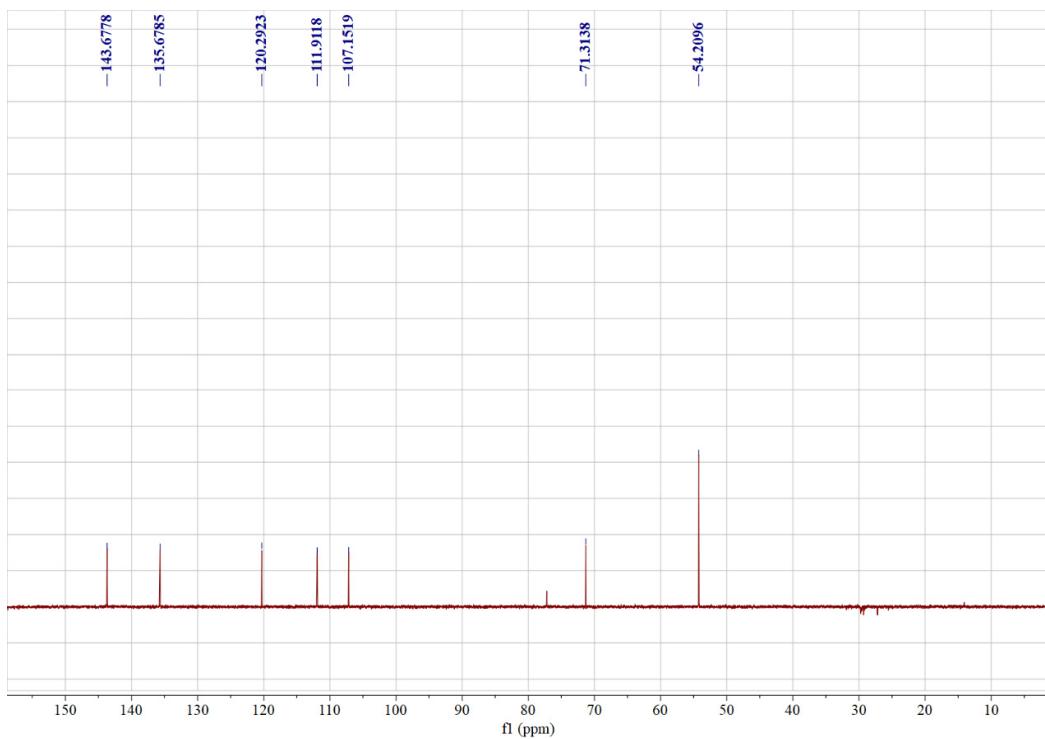
**Figure S2**  $^1\text{H}$  NMR spectrum of compound **1** (600 MHz,  $\text{CDCl}_3$ )



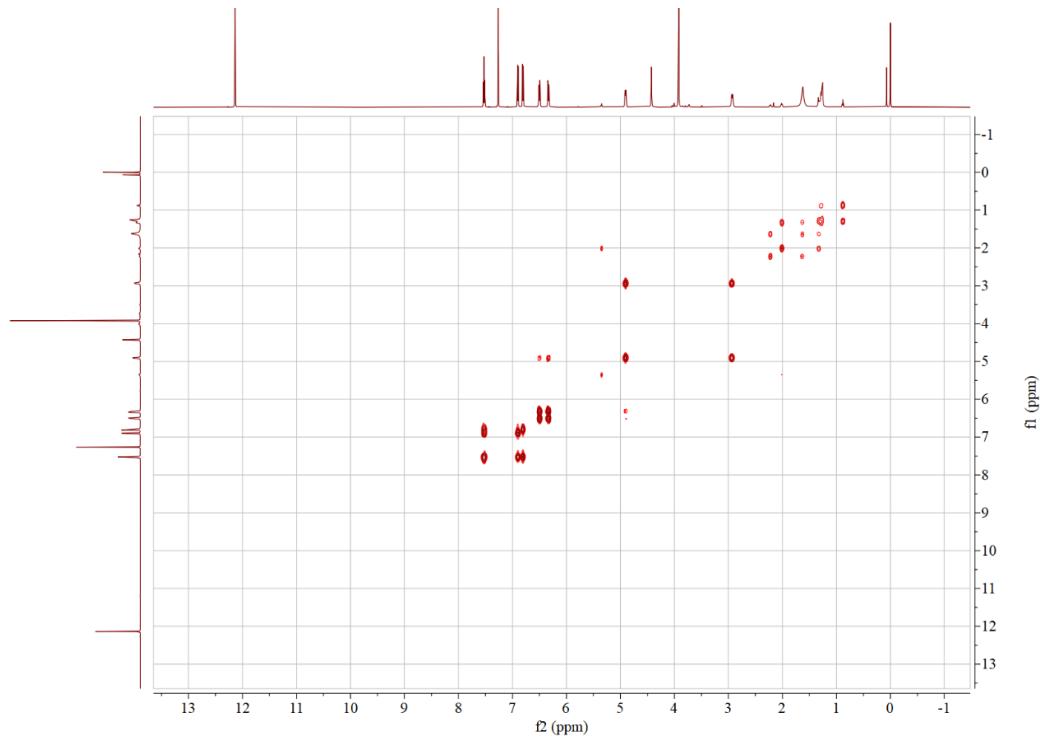
**Figure S3**  $^{13}\text{C}$  NMR spectrum of compound **1** (150 MHz,  $\text{CDCl}_3$ )



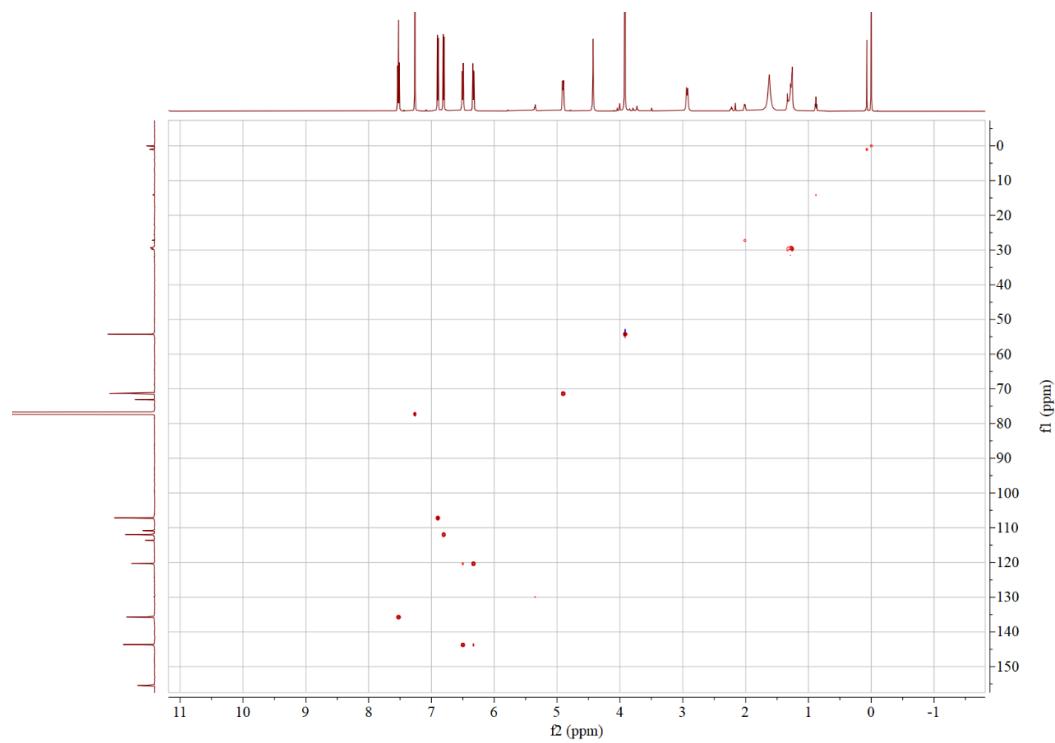
**Figure S4** DEPT135 spectrum of compound **1** (150 MHz, CDCl<sub>3</sub>)



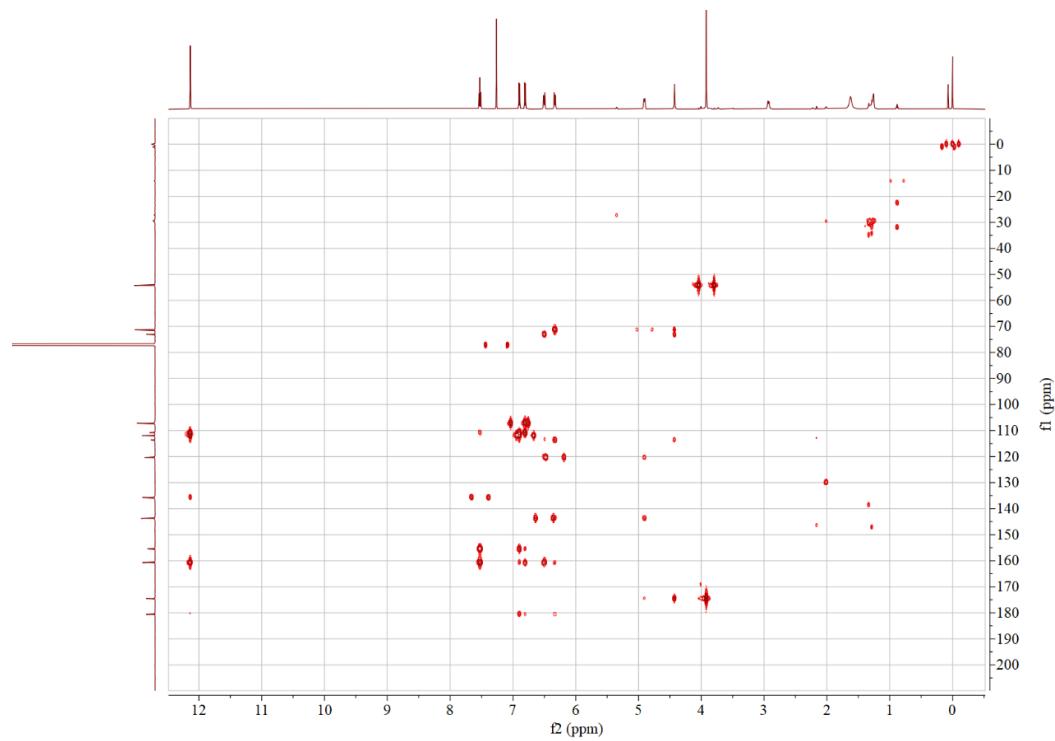
**Figure S5**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **1**



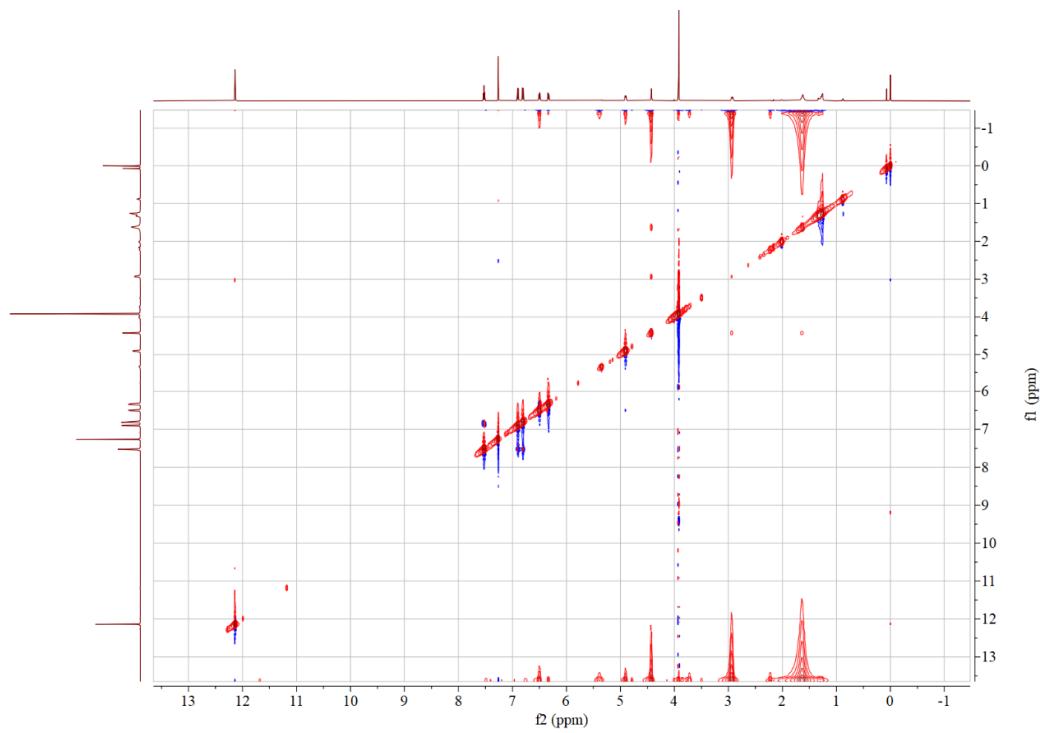
**Figure S6** HSQC spectrum of compound 1



**Figure S7** HMBC spectrum of compound **1**

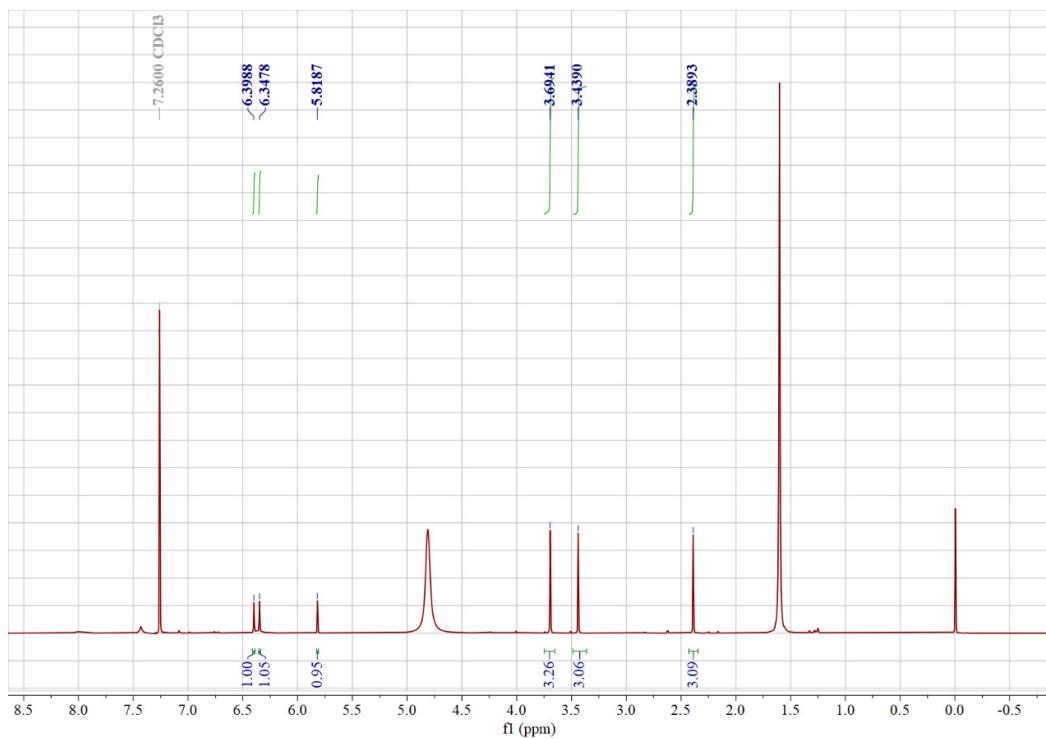


**Figure S8** NOESY spectrum of compound 1

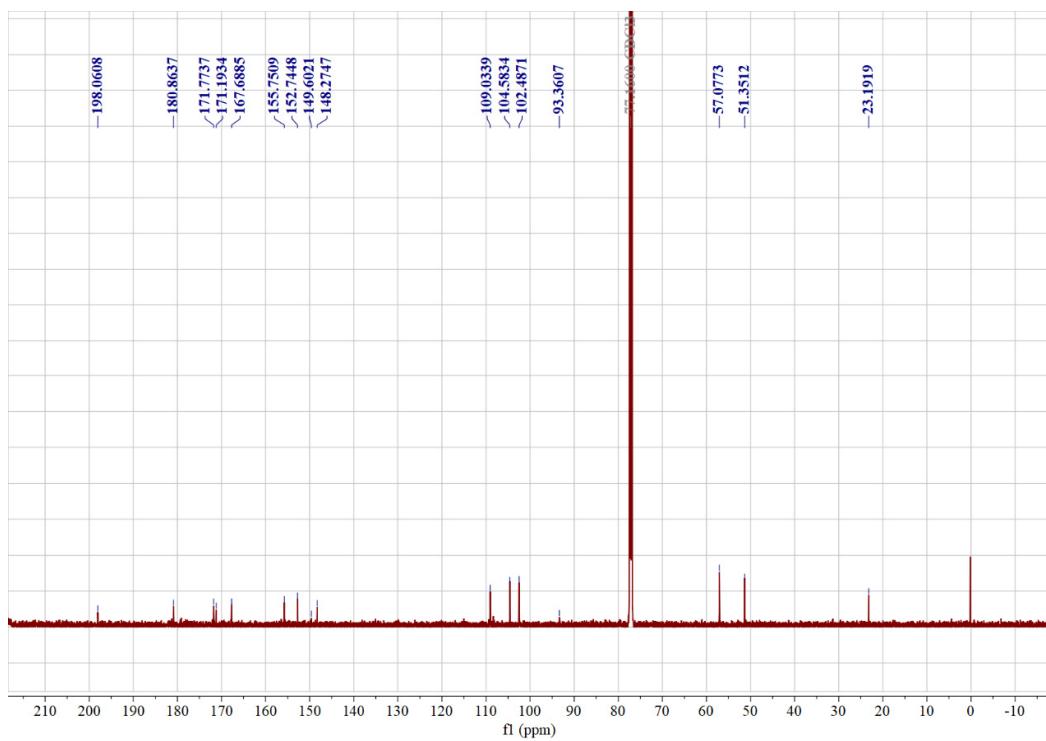




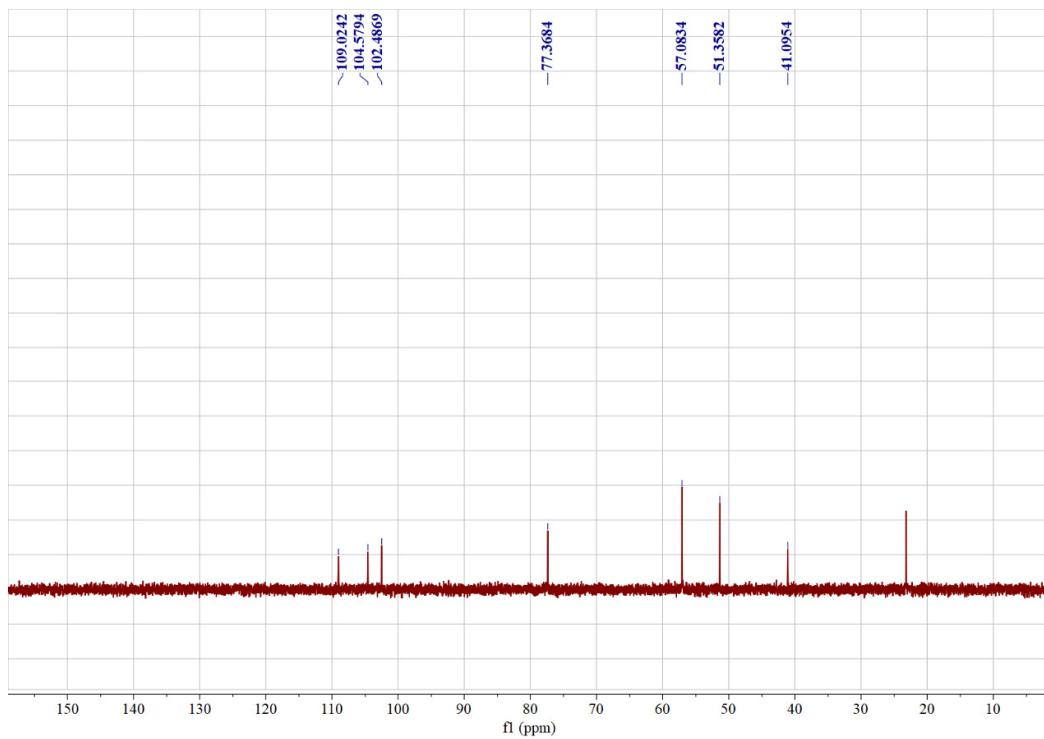
**Figure S9**  $^1\text{H}$  NMR spectrum of compound **2** (600 MHz,  $\text{CDCl}_3$ )



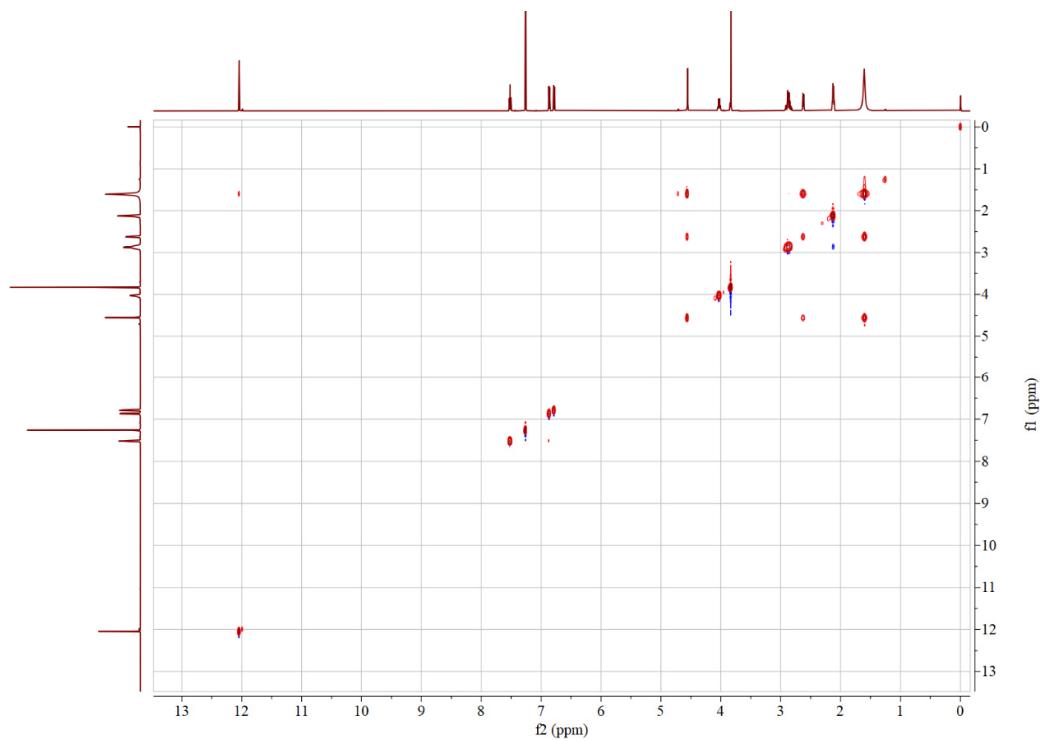
**Figure S10**  $^{13}\text{C}$  NMR spectrum of compound **2** (150 MHz,  $\text{CDCl}_3$ )



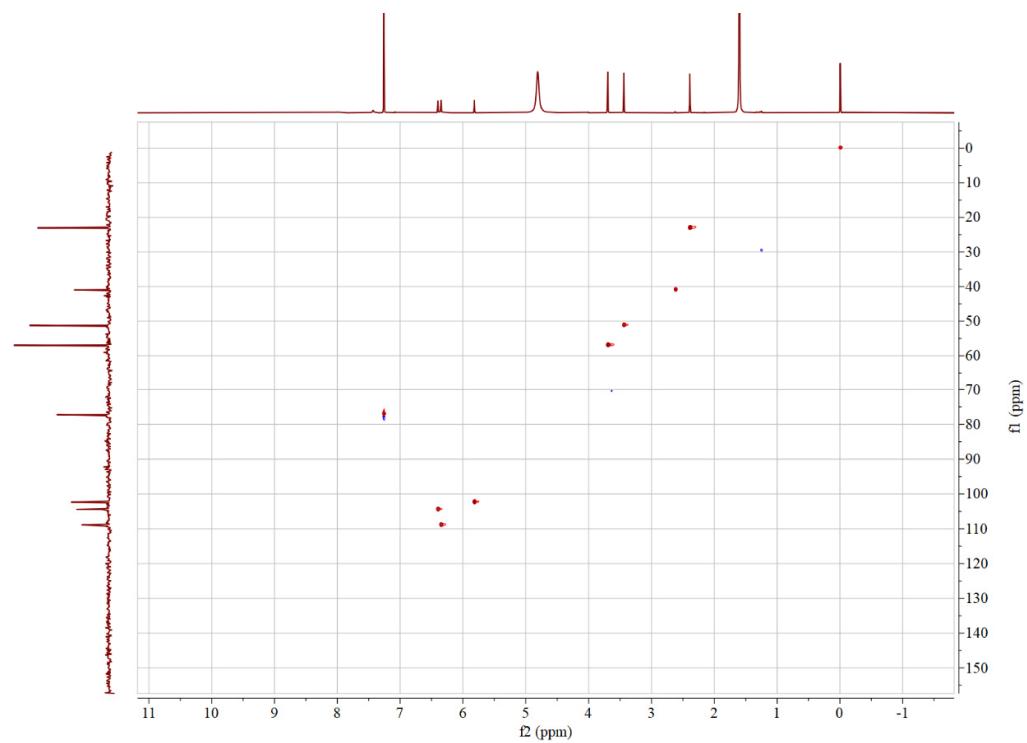
**Figure S11** DEPT135 spectrum of compound **2** (150 MHz, CDCl<sub>3</sub>)



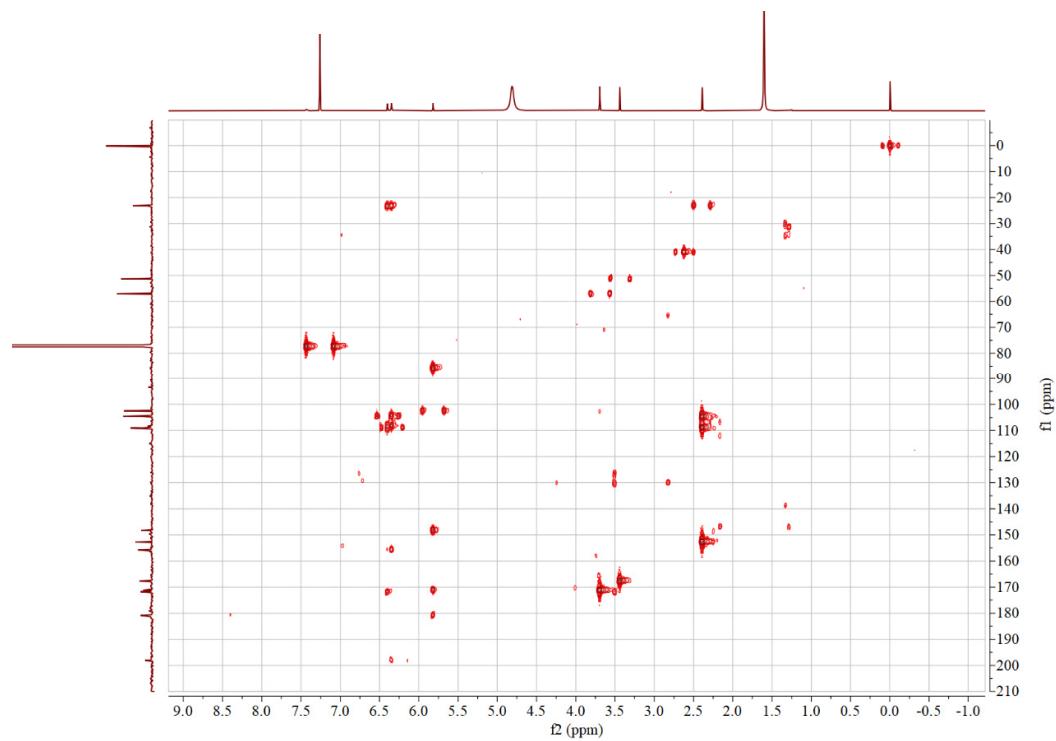
**Figure S12**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound 2



**Figure S13** HSQC spectrum of compound 2



**Figure S14** HMBC spectrum of compound 2



**Figure S15** NOESY spectrum of compound 2

