

## Supporting Information

# Indole Derivatives Produced by the Metagenome Genes of the Escherichia coli-Harboring Marine Sponge Discodermia calyx

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## List of Supporting Information

<b>S1.</b> Comparative data of indole trimer production in the clones.....	3
<b>S2.</b> LC-MS data of compound <b>1</b> .....	3
<b>S3.</b> Chiral HPLC analysis of compound <b>1</b> .....	3
<b>S4.</b> HR-ESI-MS data of compound <b>1</b> .....	4
<b>S5.</b> NMR spectrum of <b>1</b> .....	5

## S1. Comparative data of indole trimmer production in the clones

The culture of negative control (means *E. coli* carrying void vector) (1.5 L) and pDC115 (1.5 L) were subjected to solid phase extraction using HP-20 resin, respectively. The methanol extracts were further separated by ODS column chromatography (Cosmosil 75C18-PREP, Nacalai Tesque) eluted with a stepwise gradient system from water to methanol to afford four fractions. The 100% methanol fractions from pDC115 and NC cultures were subjected to DAD-HPLC analysis. HPLC analysis was performed on ODS column (Cosmosil 5C18 PAQ waters, 4.6 x 250 mm) with a mixture of H<sub>2</sub>O and MeCN, both containing 0.05% trifluoroacetic acid: 0–30 min, 5-100% MeCN; 30–50 min, 100% MeCN; 50–55 min, 100-5% MeCN; 55–60 min, 5% MeCN. Flow rate: 0.8 mL/min. DAD profile were measured with the Shimadzu HPLC System: LC-20AD and SPD-20A Prominence Diode Array Detector.

## S2. LC-MS data of compound 1

LC-MS (Agilent 1100 series-Bruker Esquire 4000, positive ESI.) analysis was performed on ODS column (TSK-Gel ODS-80Ts, 4.6 x 150 mm) with a mixture of H<sub>2</sub>O and MeOH. Flow rate: 0.2mL/min. Detection wavelength: 405 nm.

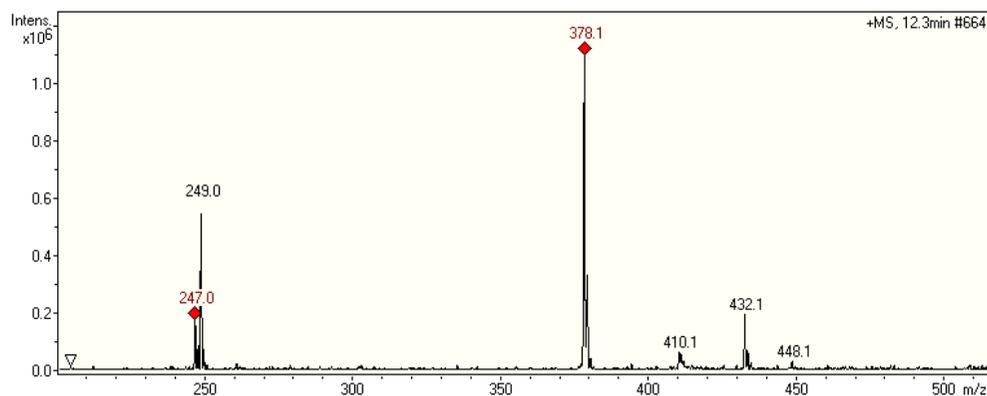


Figure S2. LC-MS (pos.) data of compound 1

### S3. Chiral HPLC analysis of compound 1

Chiral HPLC analysis was performed on ODS-RH column (5  $\mu$ m, 150 x 4.6 mm, Daicel, city, Japan) with 80% MeCN in H<sub>2</sub>O. Flow rate: 0.3mL/min, column pressure: 3 MPa. DAD profile were measured with the Shimadzu HPLC System: LC-20AD and SPD-20A Prominence Diode Array Detector.

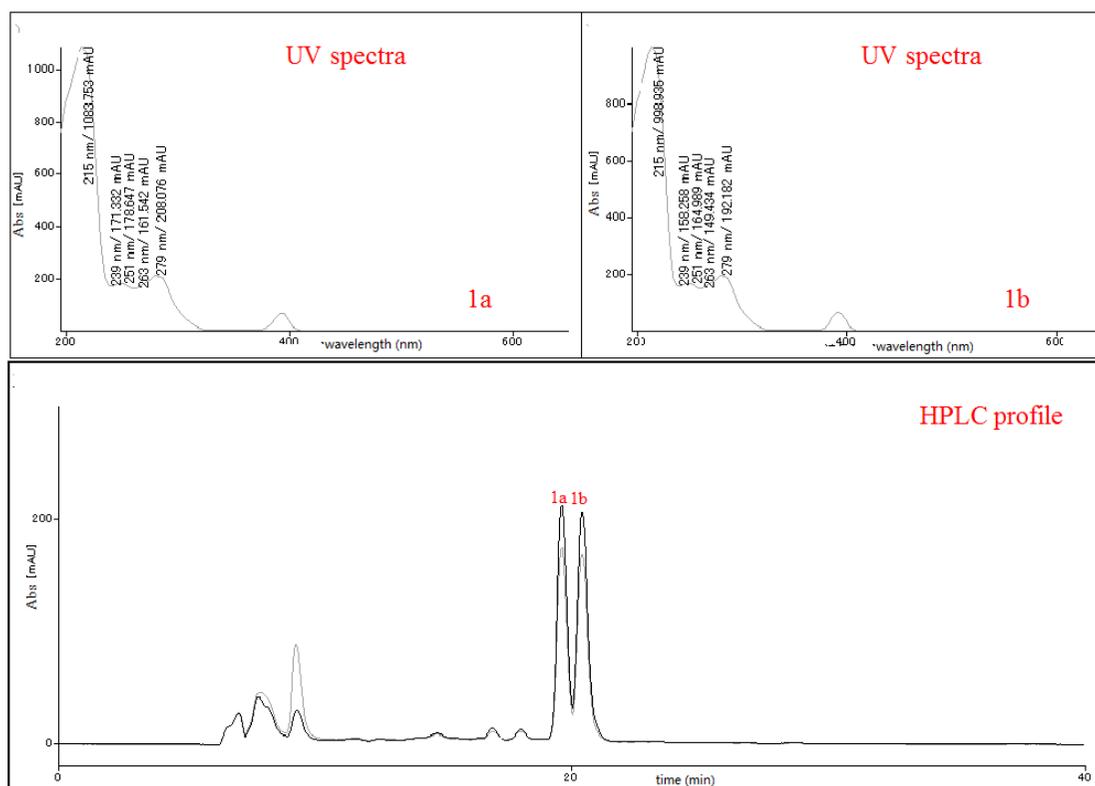
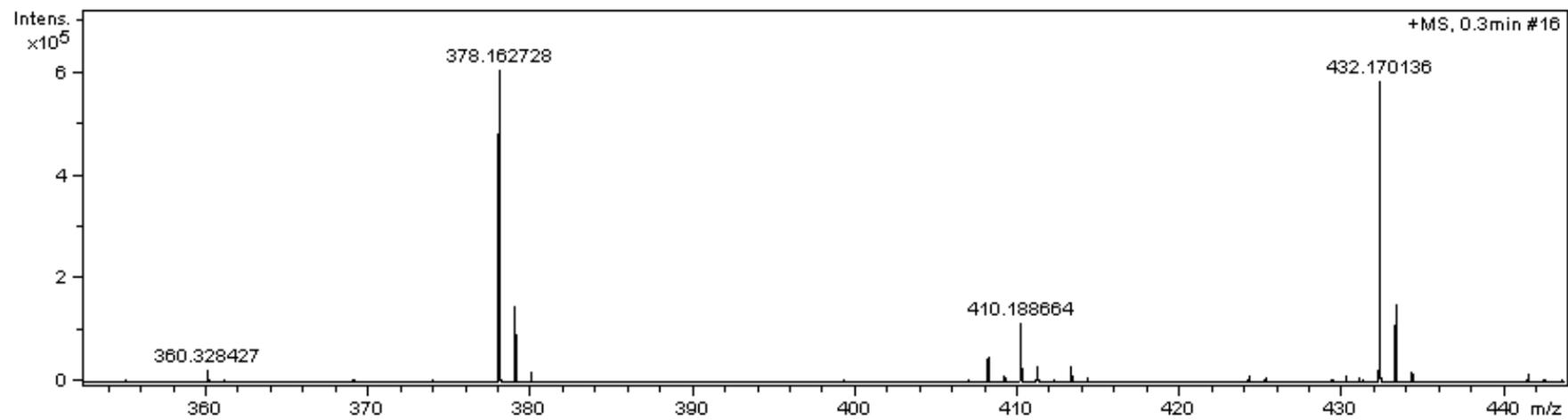
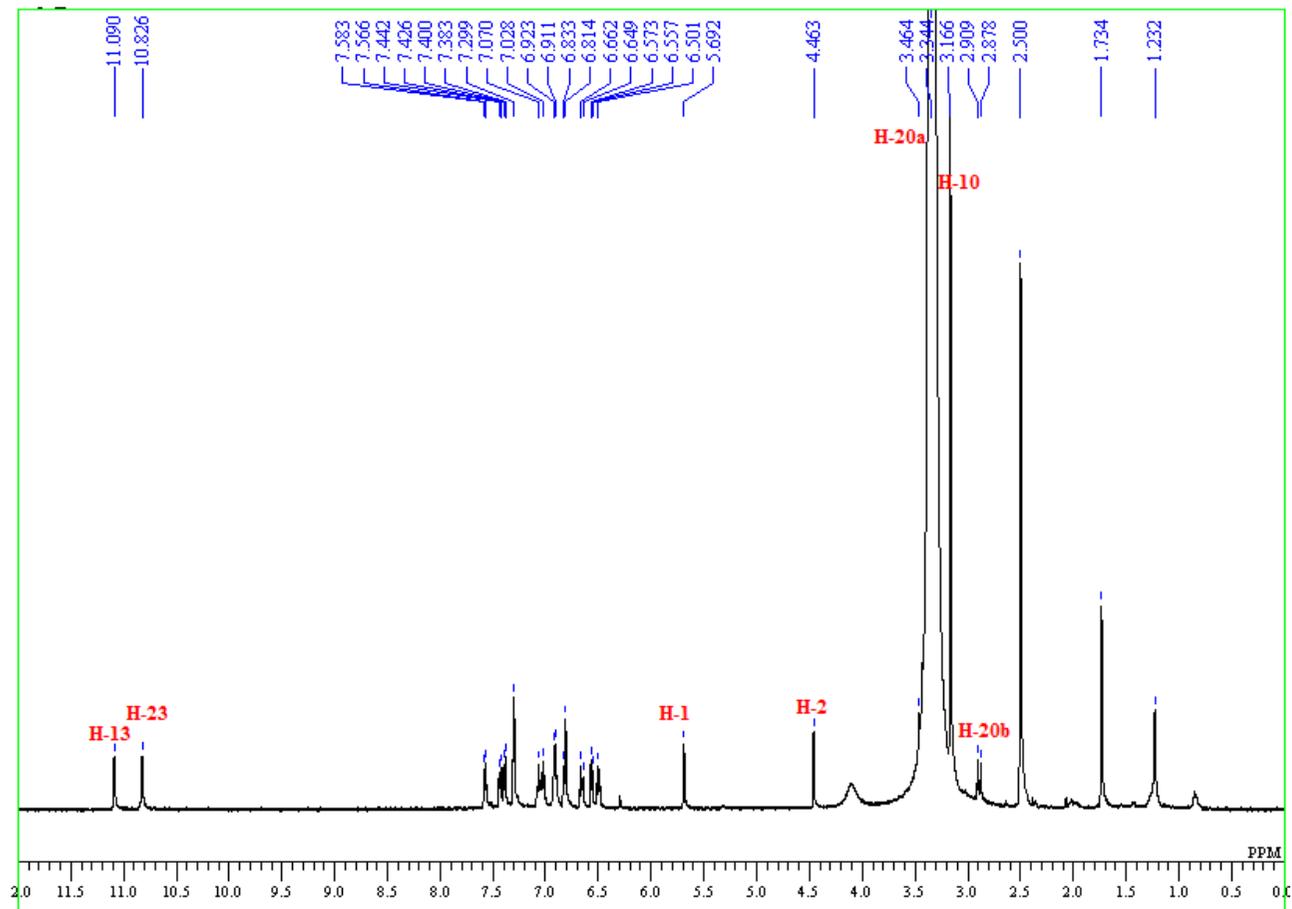


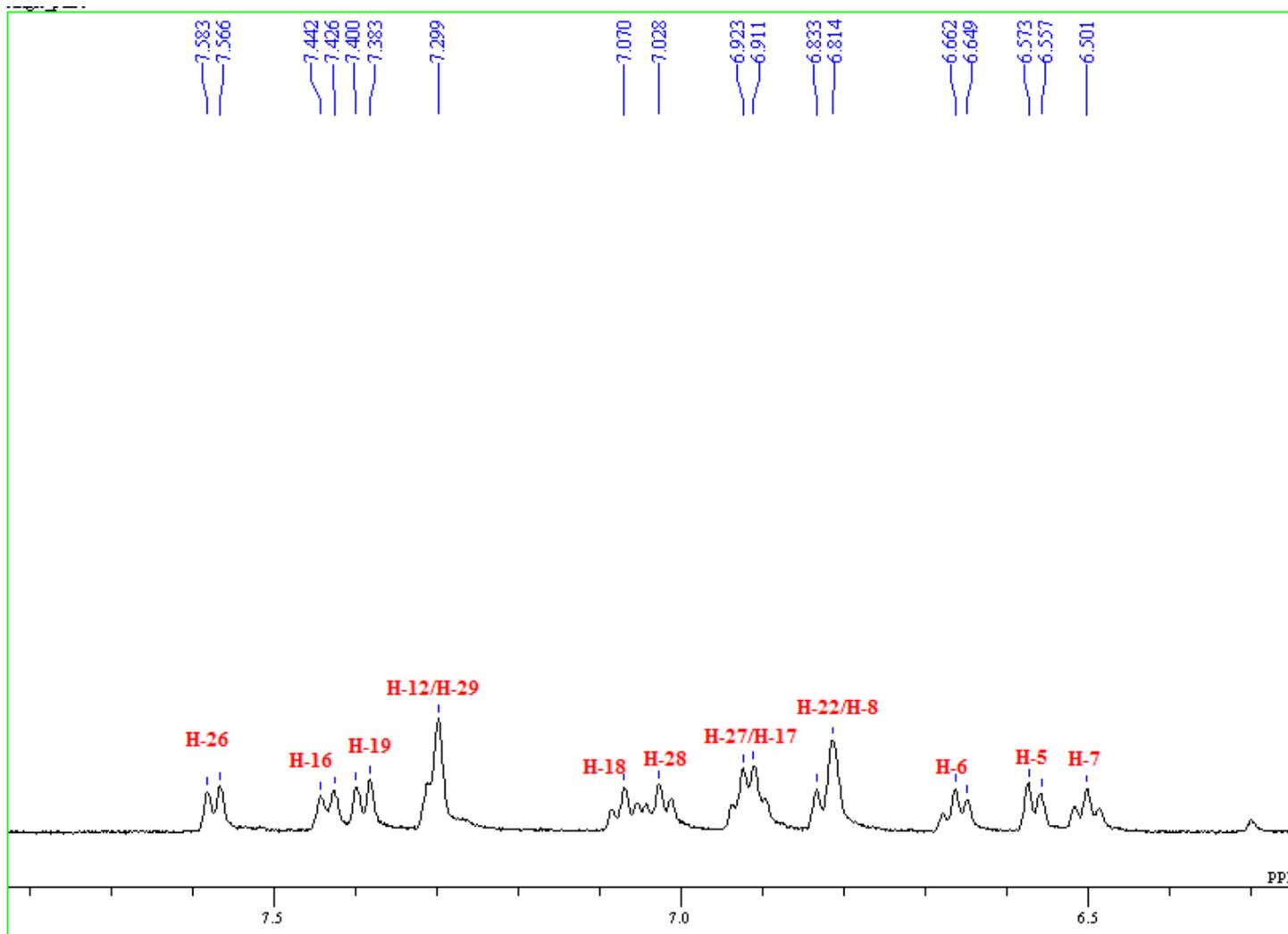
Figure S3. Chiral HPLC analysis of compound 1 and UV spectra for peaks 1a and 1b



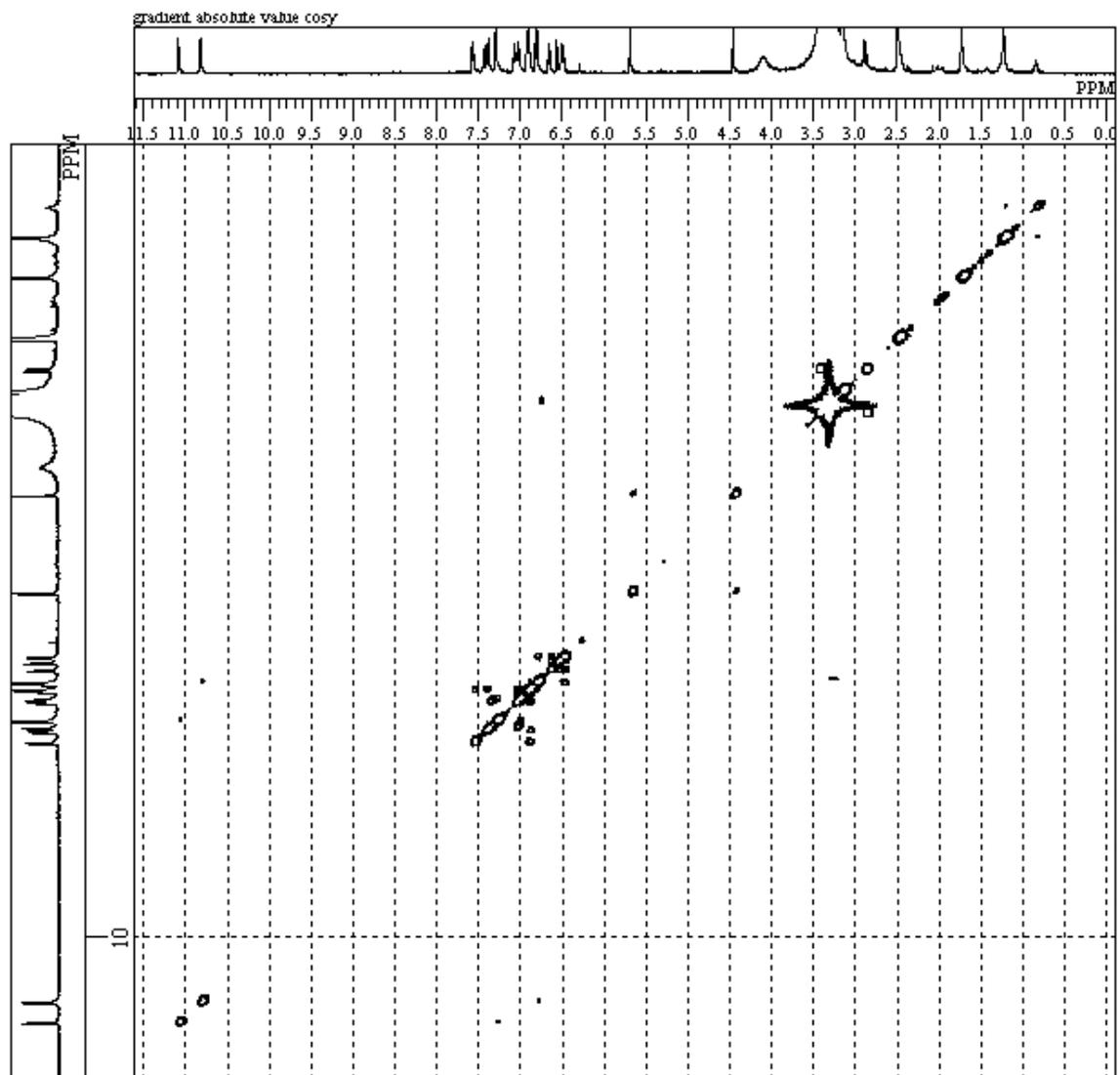
**Figure S4.** HR-ESI-MS (positive model) of compound **1**

### S5. NMR spectrum of compound 1





**Figure S5-1.** <sup>1</sup>H-NMR spectrum of **1** (500 MHz, DMSO-d<sub>6</sub>)



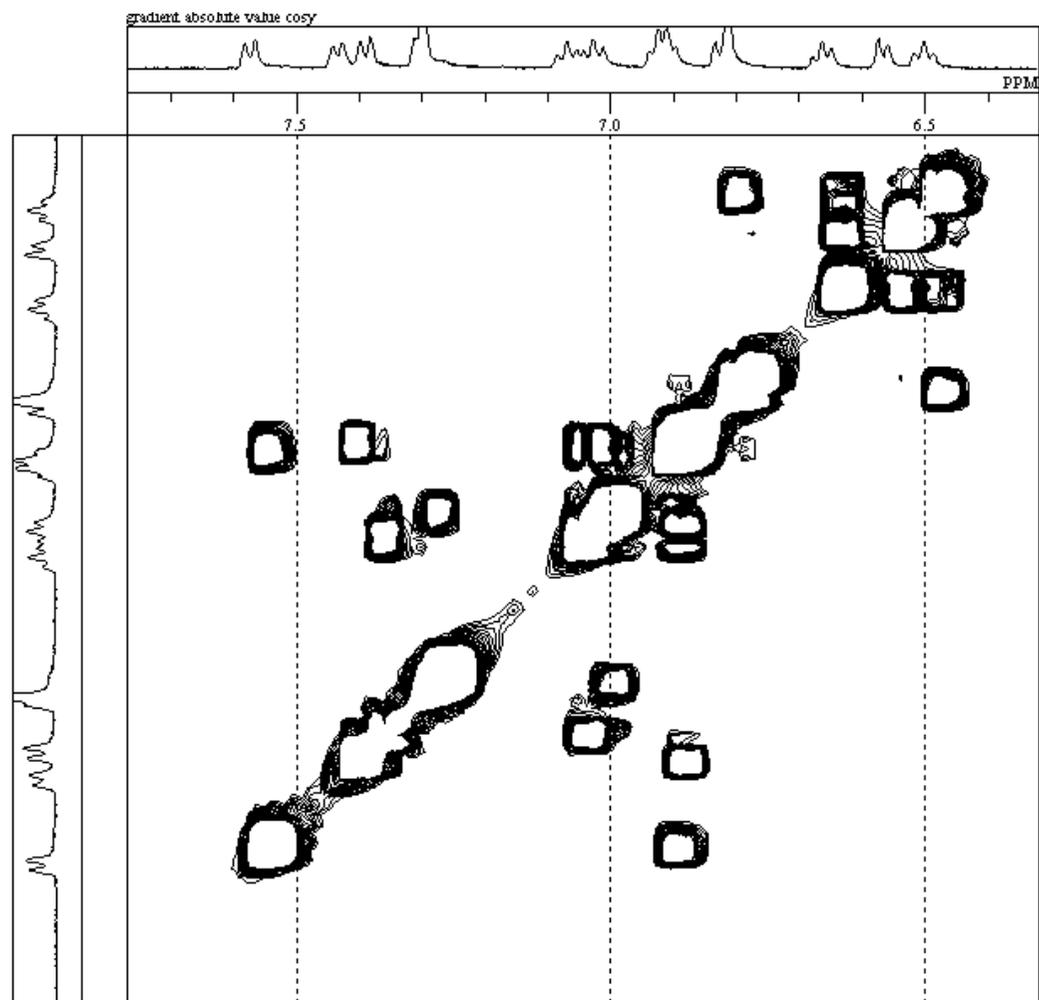
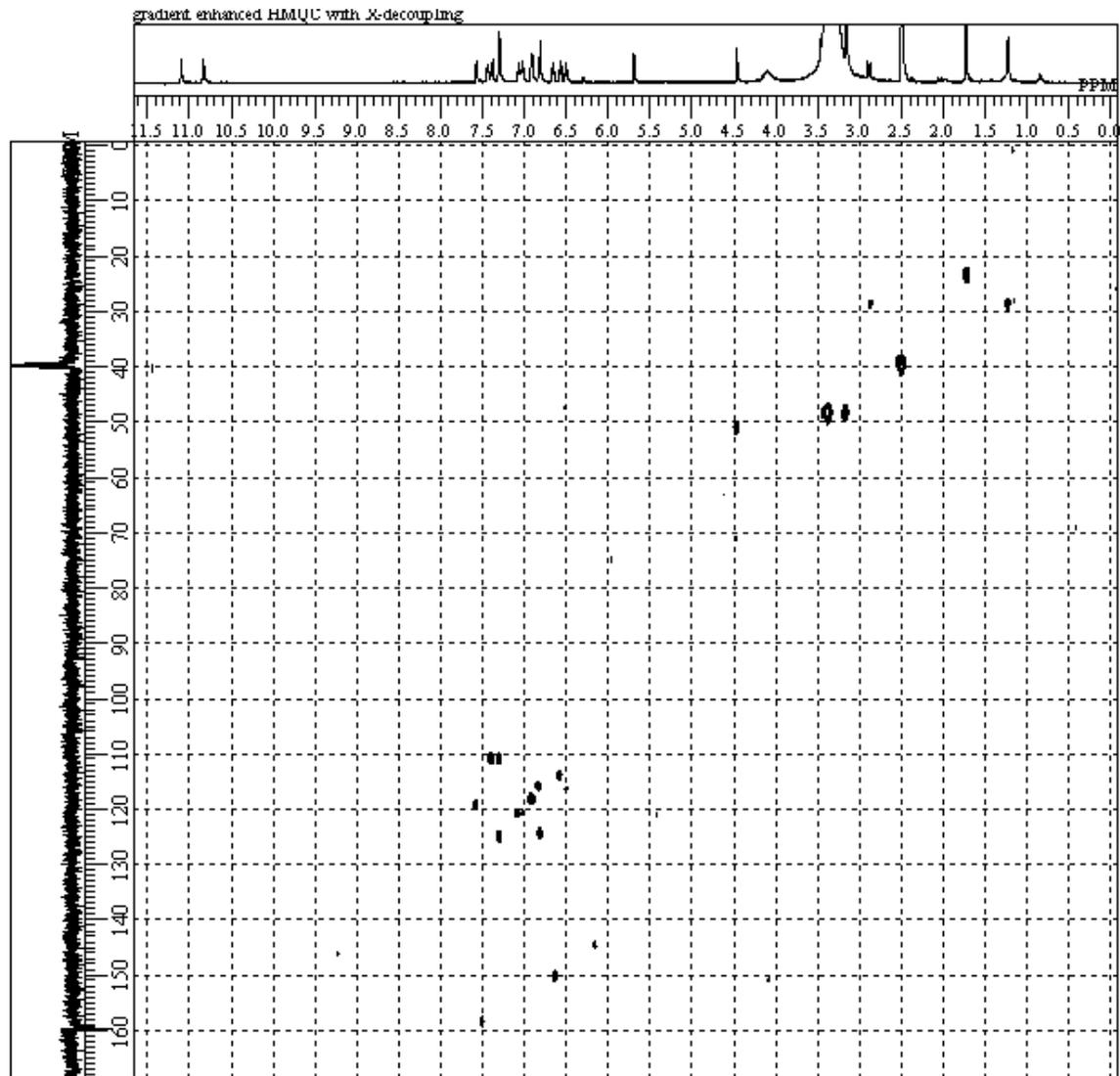
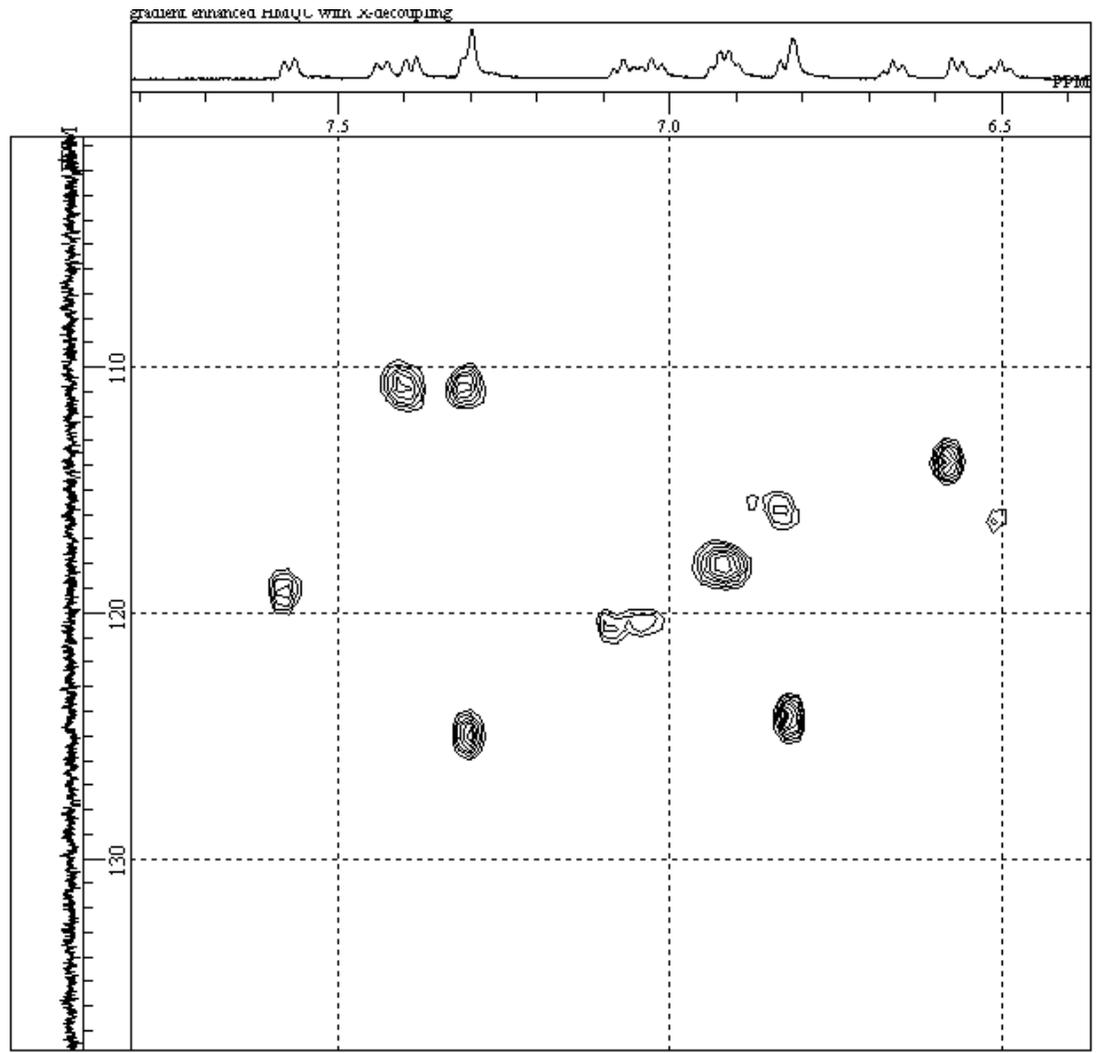


Figure S5-2.  $^1\text{H}$ ,  $^1\text{H}$ -COSY spectrum of **1**





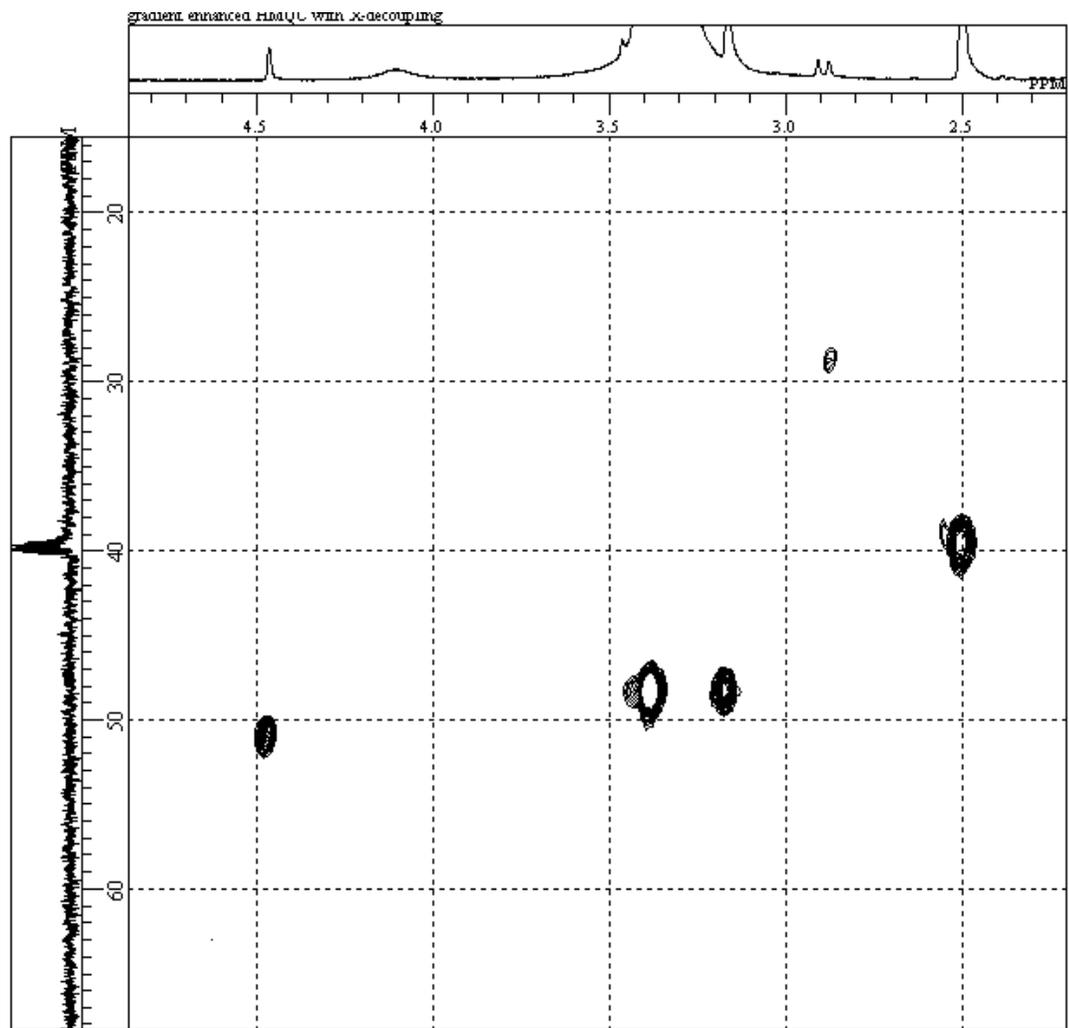
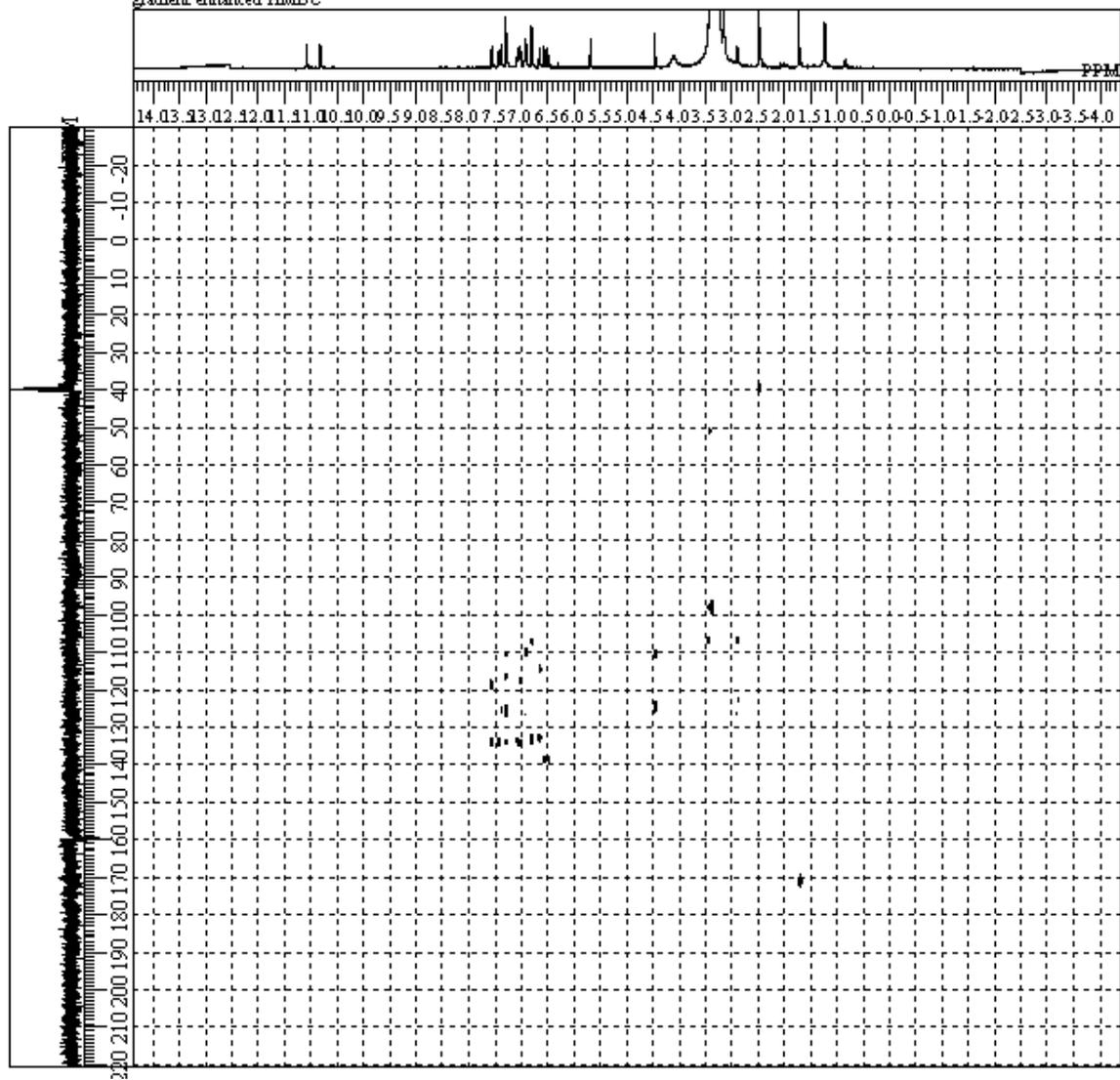
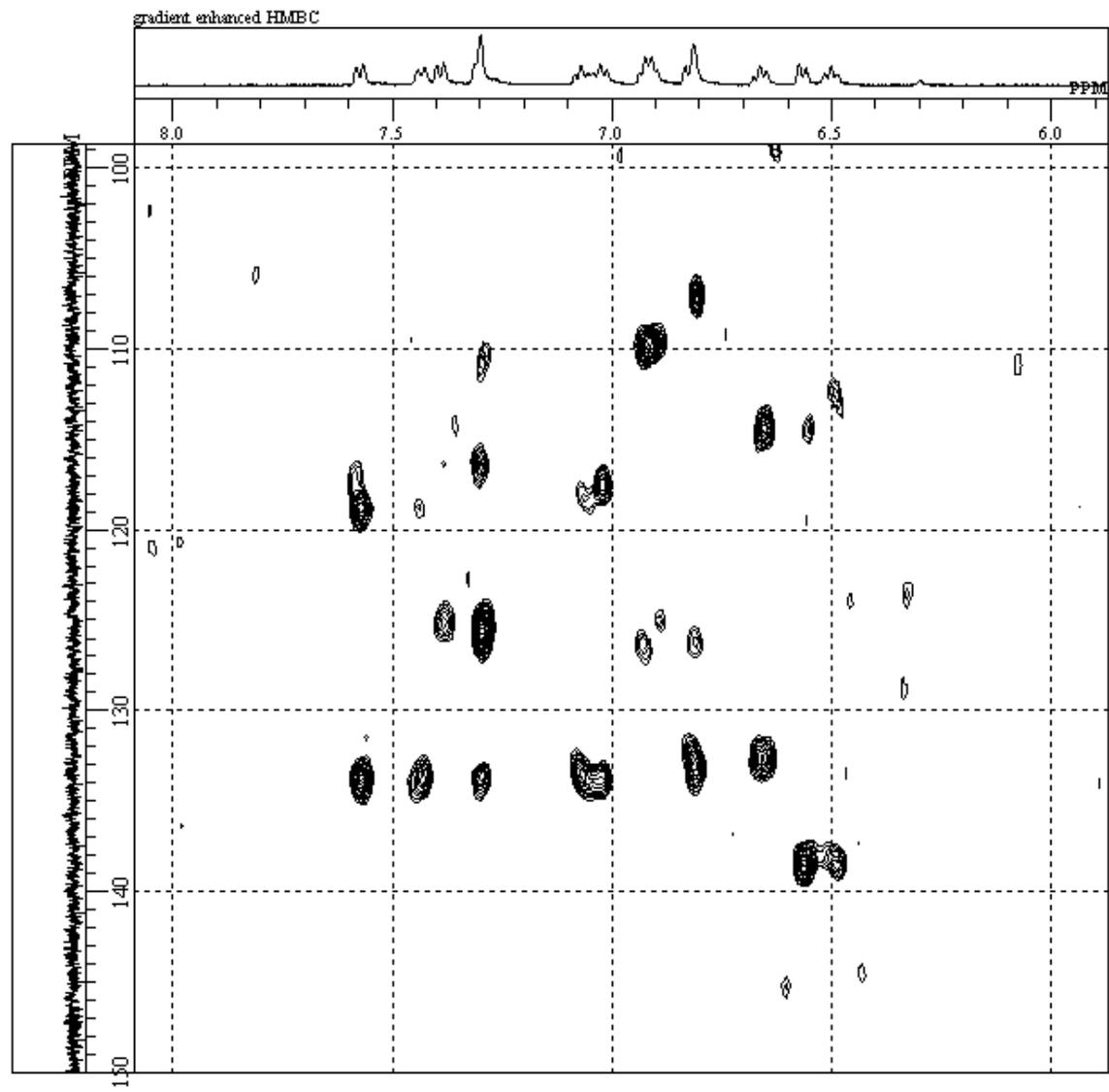
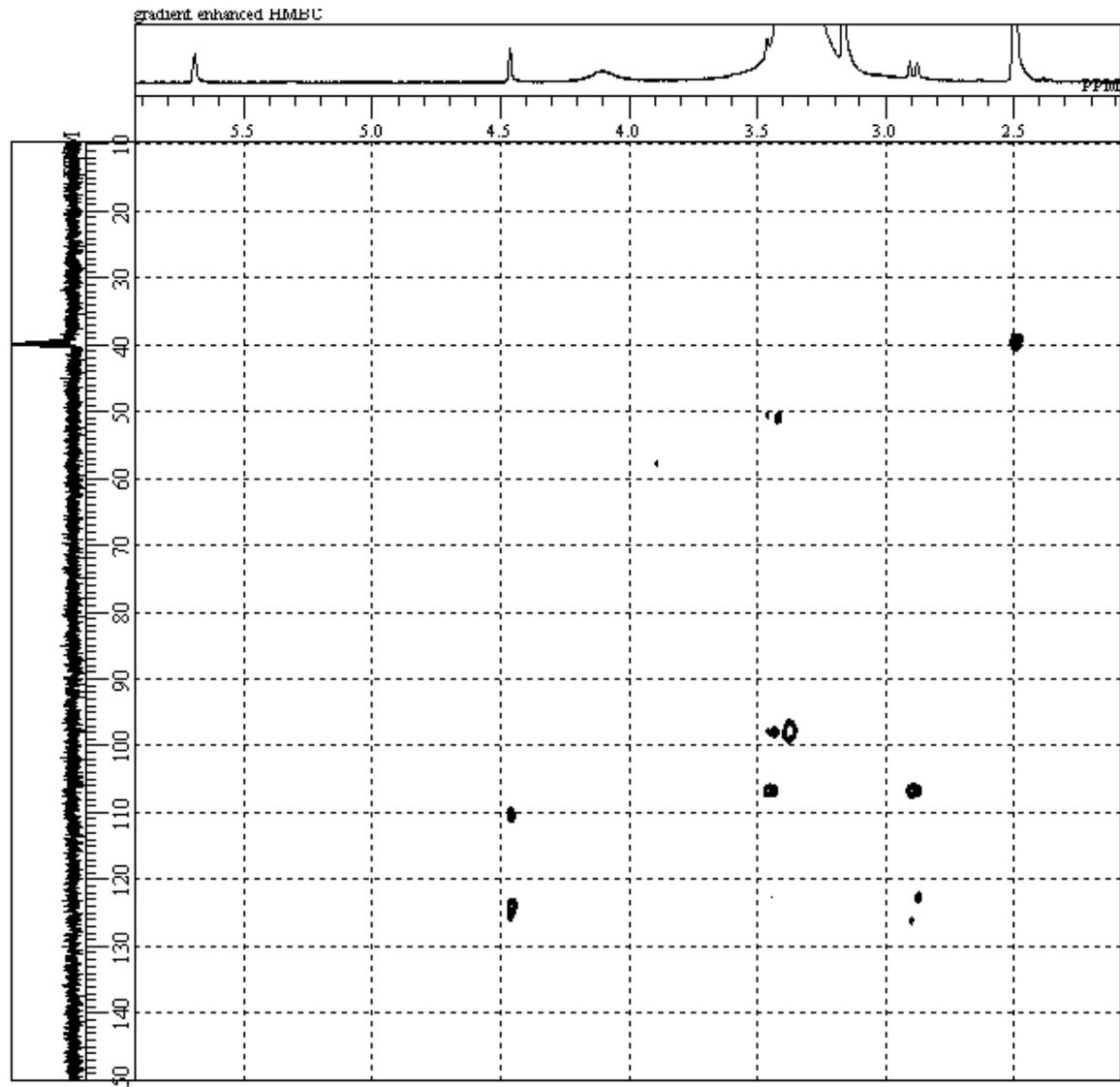


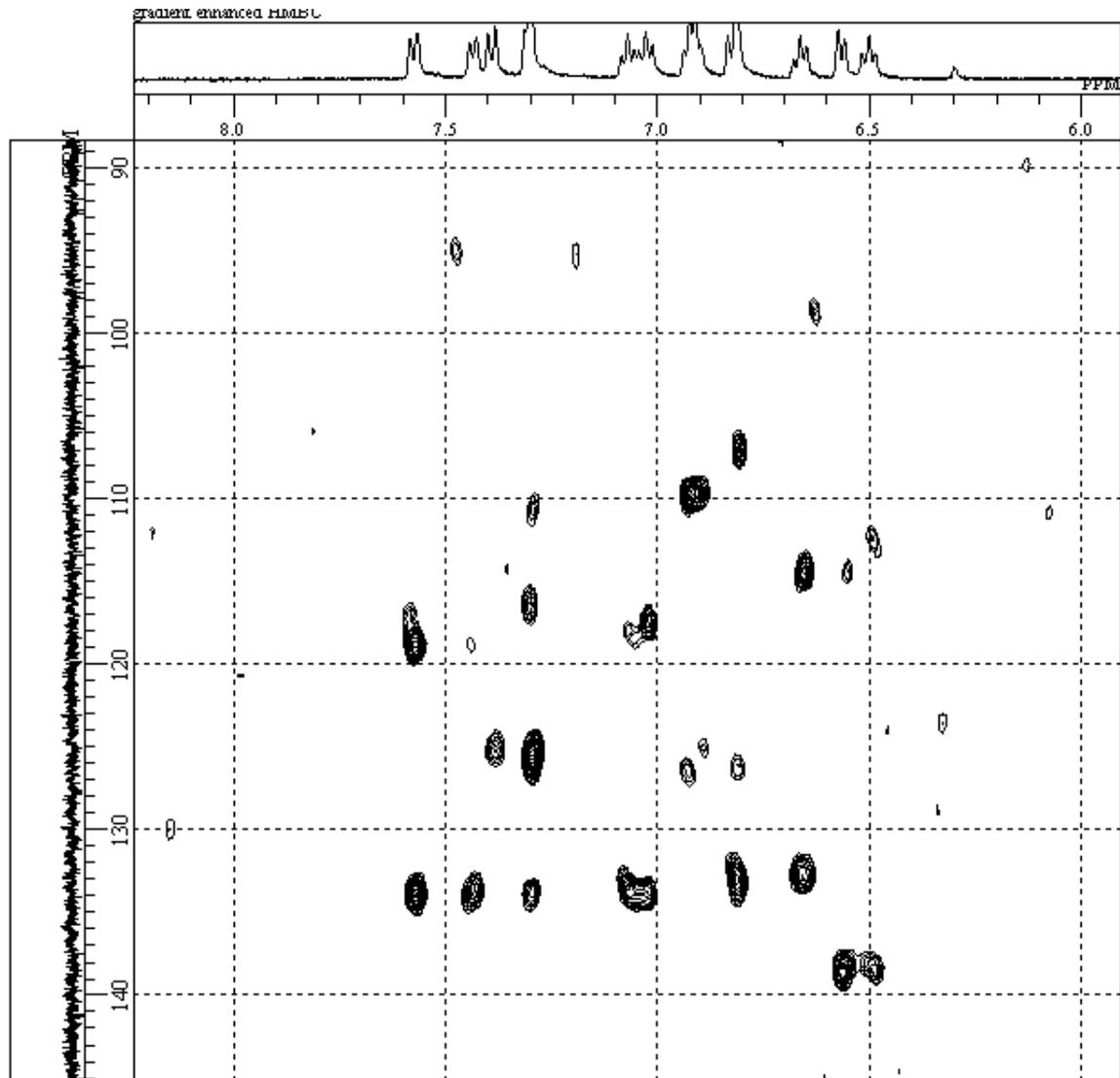
Figure S5-3. HSQC spectrum of **1**

gradient enhanced HMB









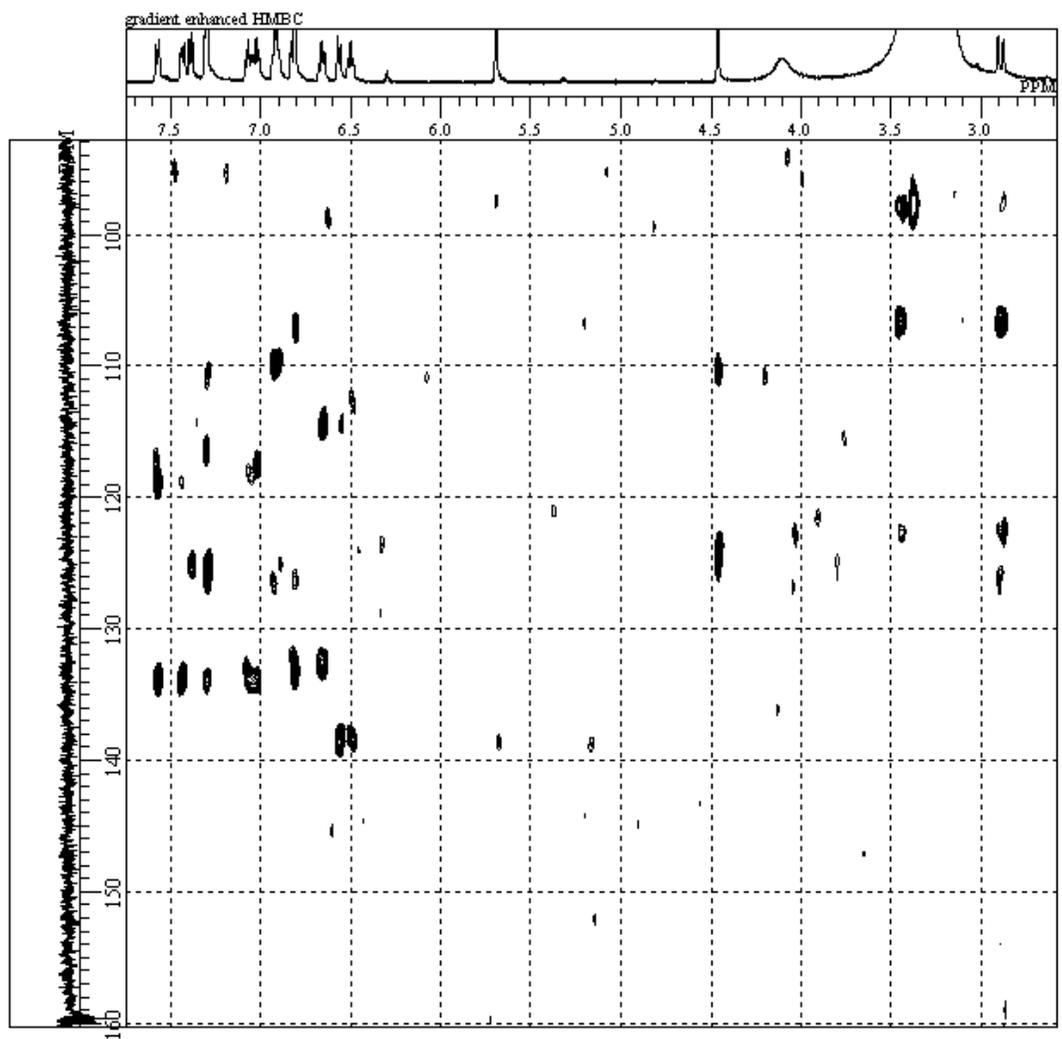


Figure S5-4. HMBC spectrum of **1**