

**Supporting Information**  
**Rec. Nat. Prod. X:X (202X) XX-XX**  
**New sulfureous diketopiperazine from roots of *Moringa oleifera***

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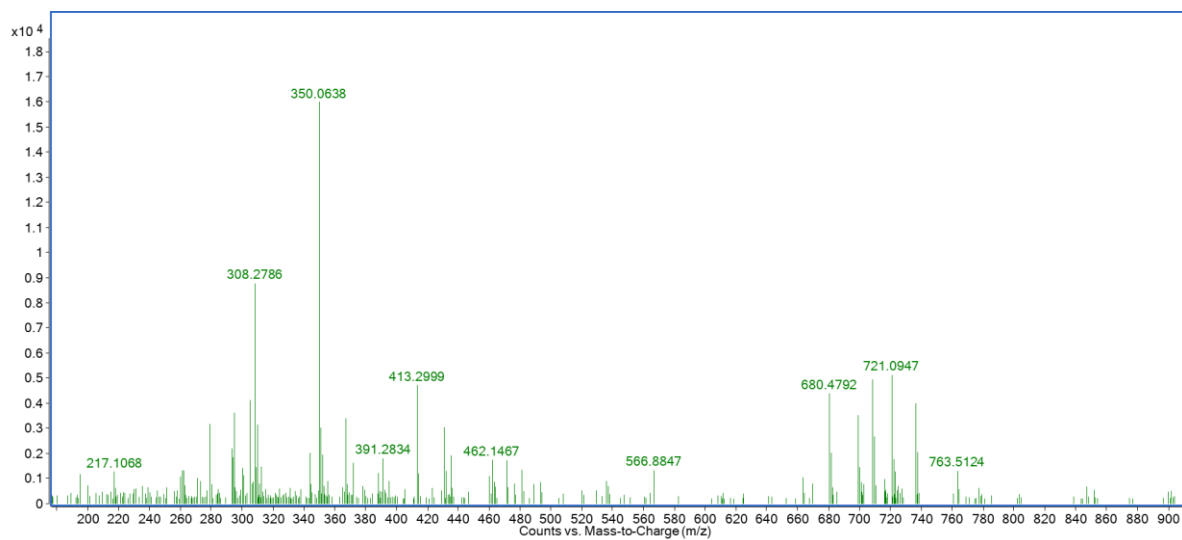
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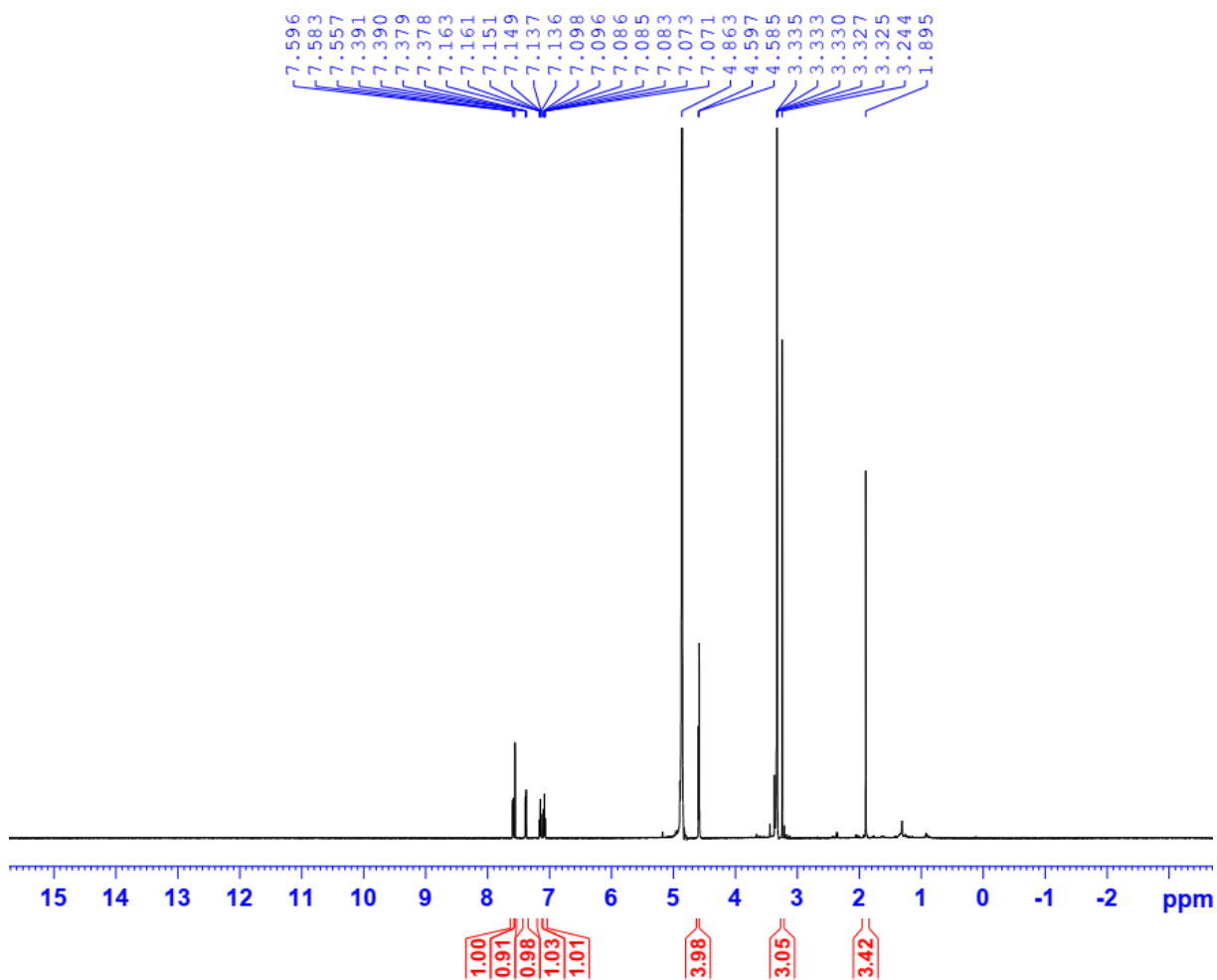
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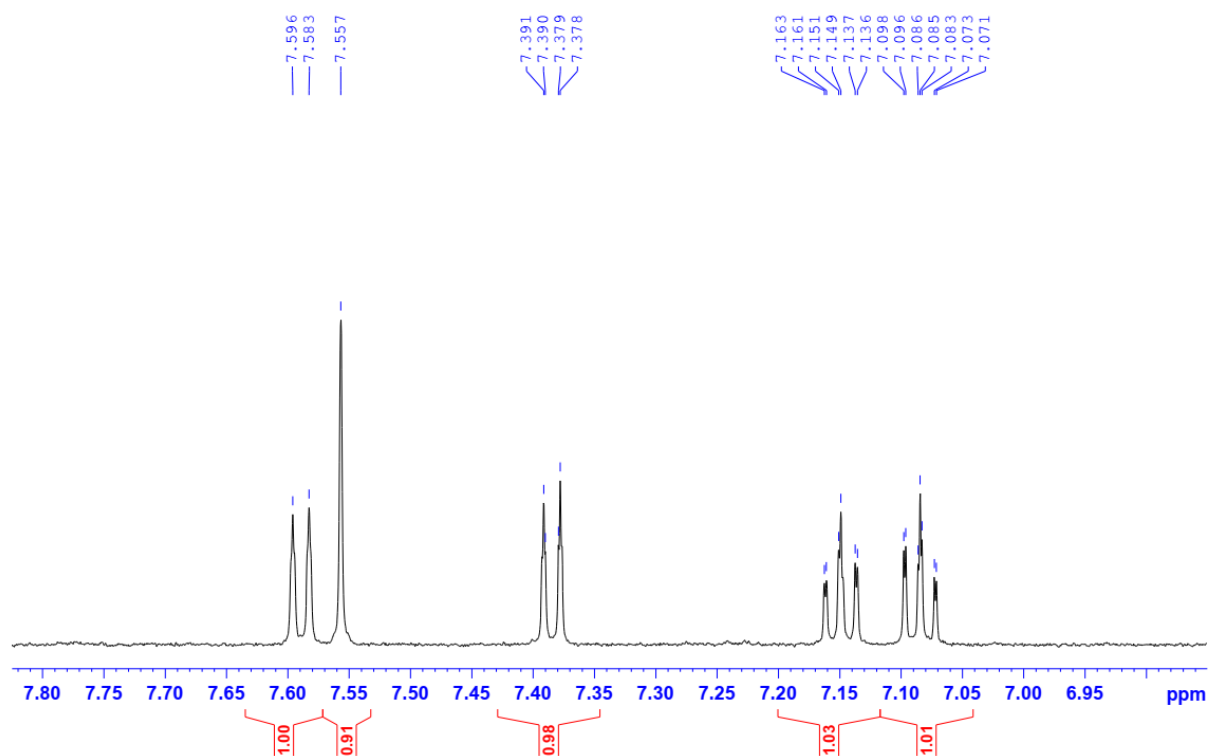
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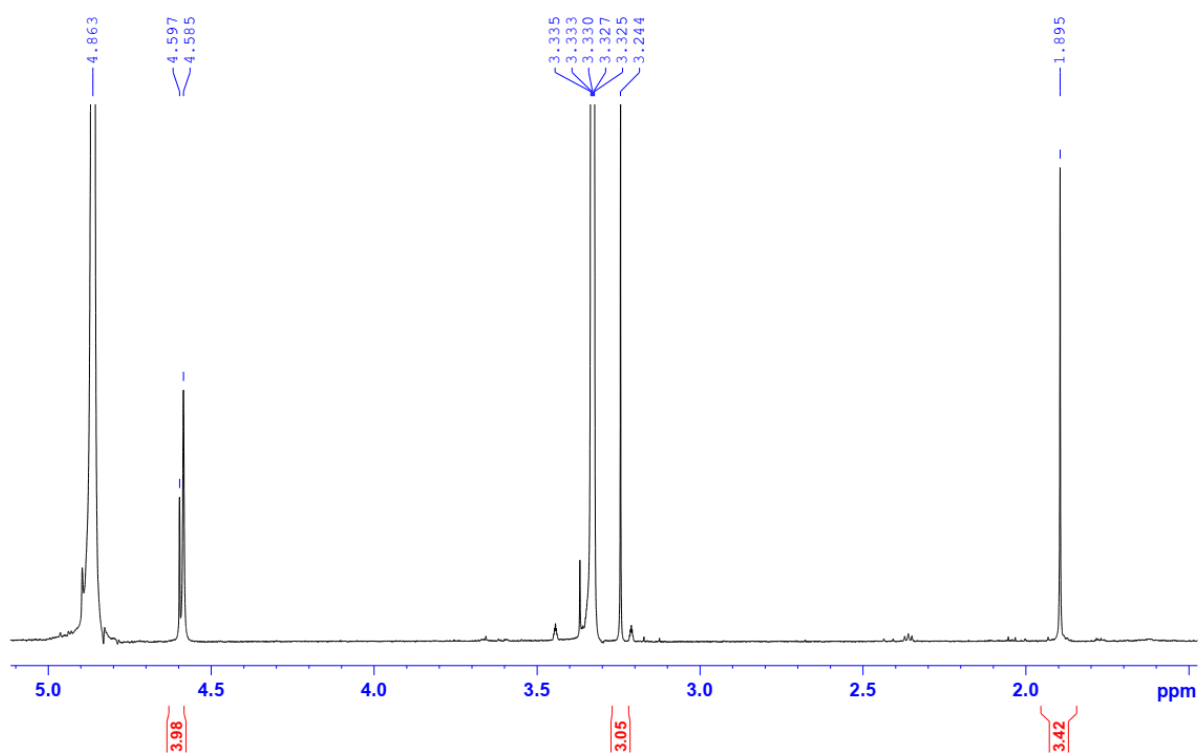
**Figure S1:**HRESIMS spectrum of compound (1)



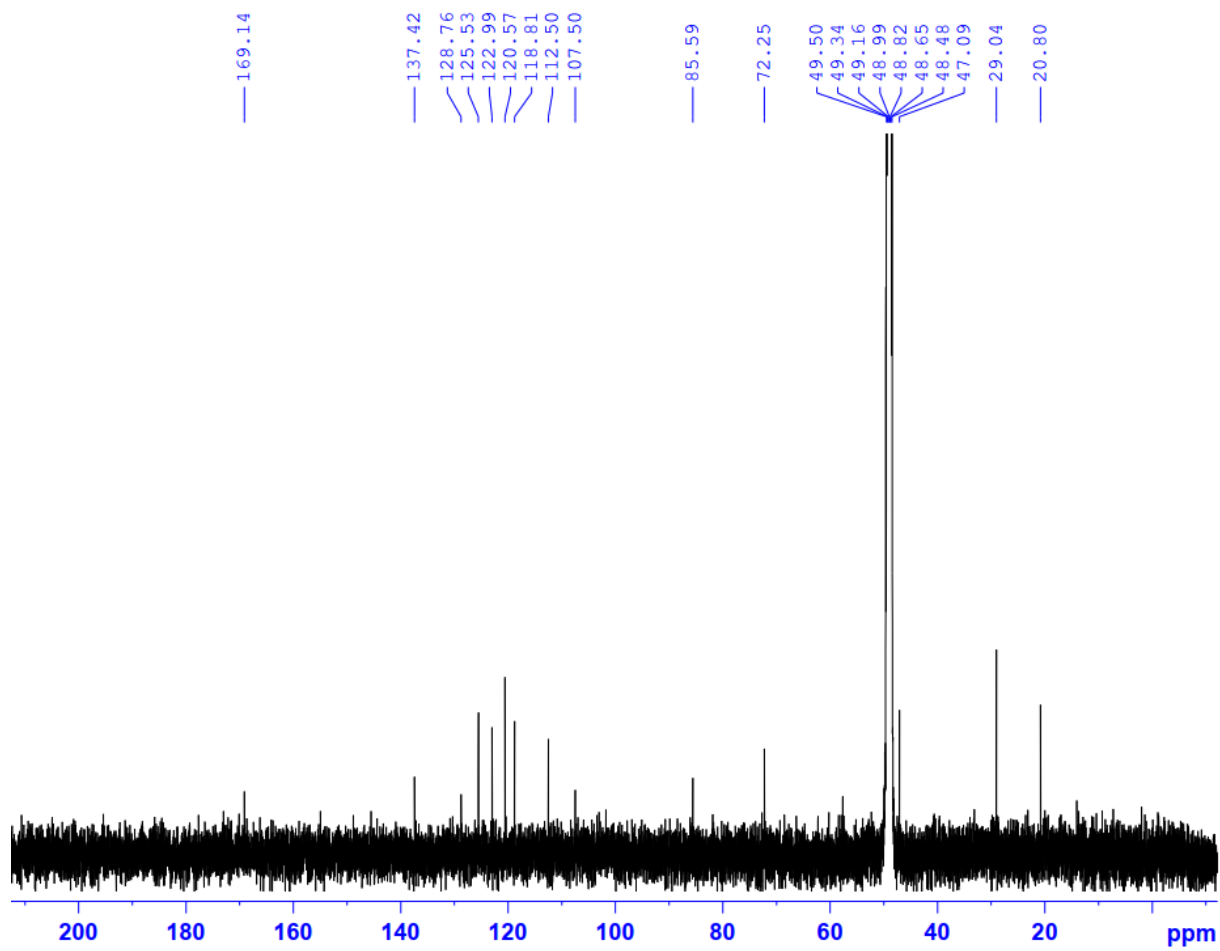
**Figure S2:** $^1\text{H}$  NMR spectrum of compound (1). Measured in  $\text{CD}_3\text{OD}$ , 600 MHz



**Figure S3:**  $^1\text{H}$  NMR spectrum (6.8-7.8 ppm) of compound (**1**). Measured in  $\text{CD}_3\text{OD}$ , 600 MHz



**Figure S4:**  $^1\text{H}$  NMR spectrum (1.5-5.0 ppm) of compound (**1**). Measured in  $\text{CD}_3\text{OD}$ , 600 MHz



**Figure S5:**  $^{13}\text{C}$  NMR spectrum of compound (1). Measured in  $\text{CD}_3\text{OD}$ , 150 MHz

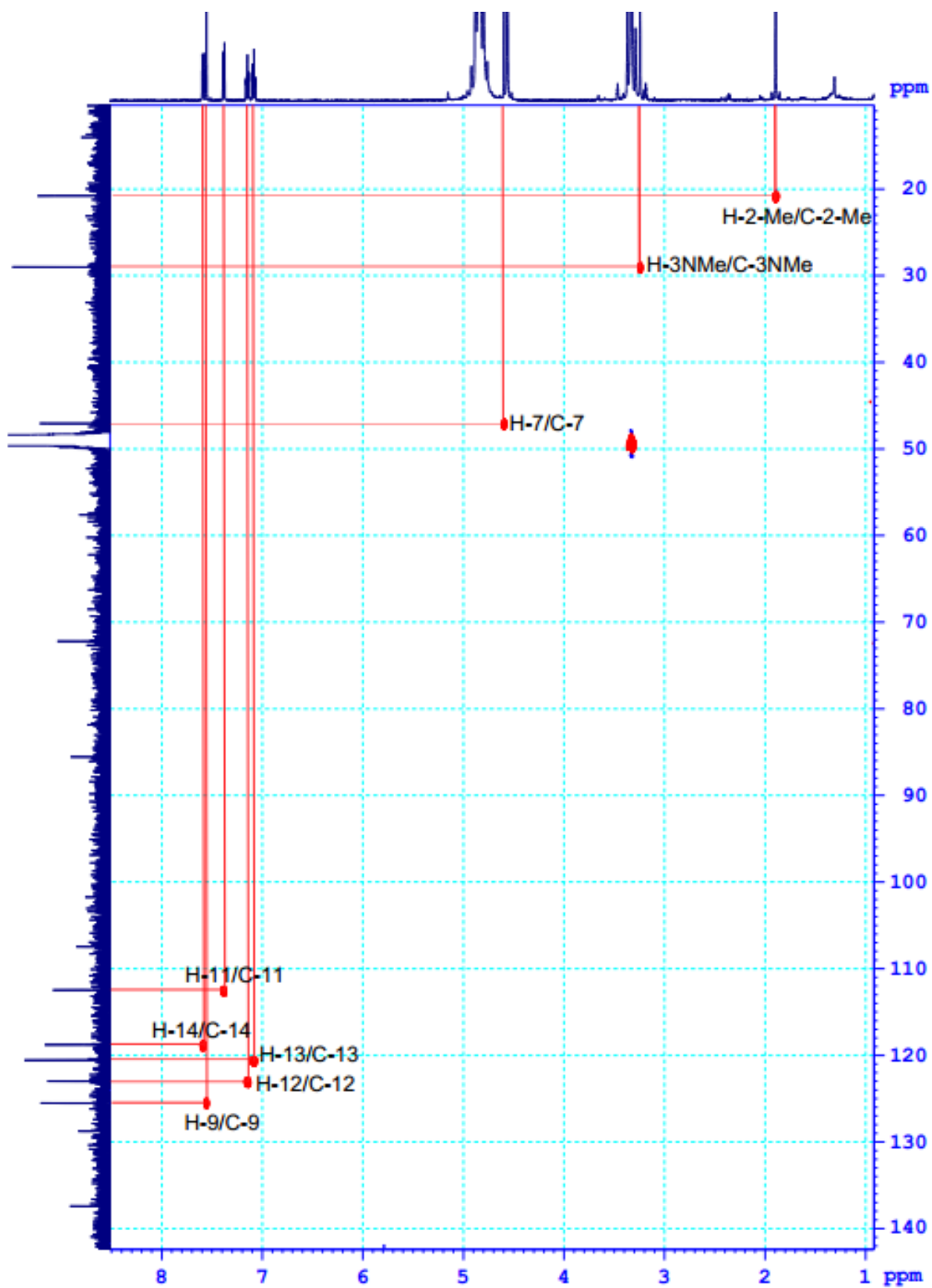


Figure S6:HSQC NMR spectrum of compound (1). Measured in CD<sub>3</sub>OD

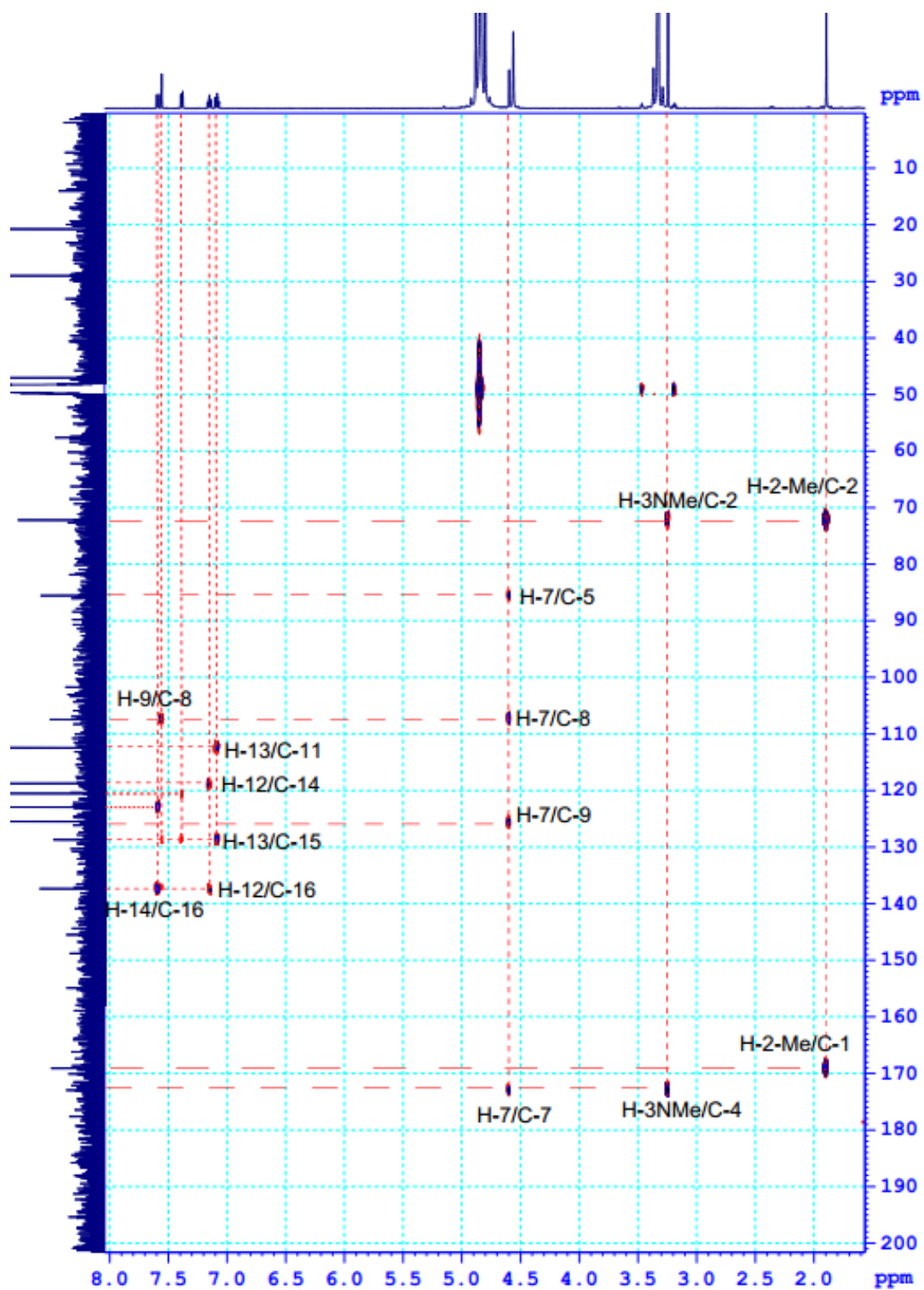
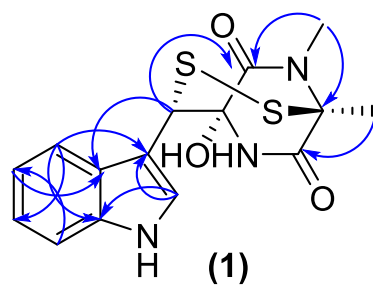
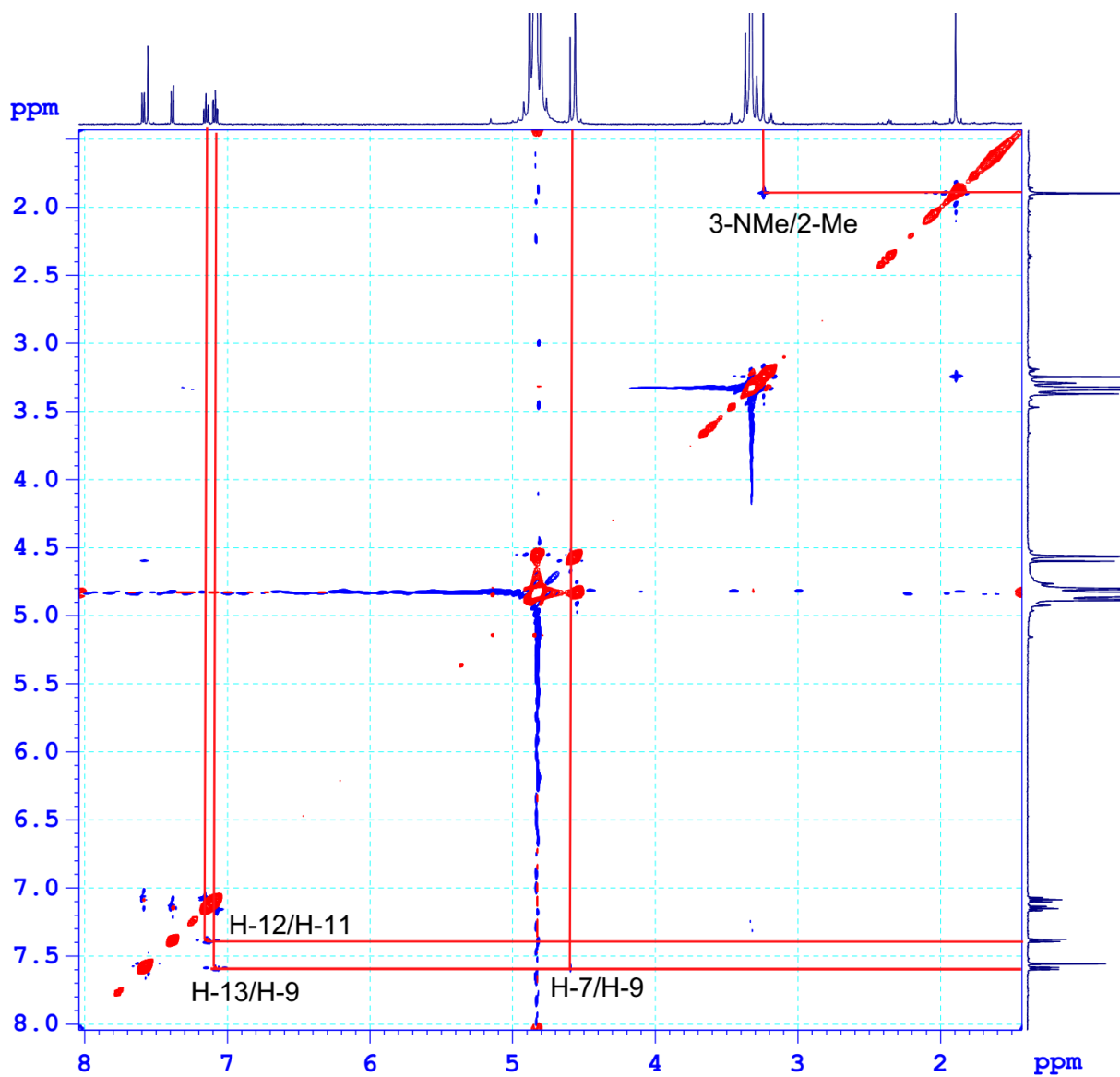
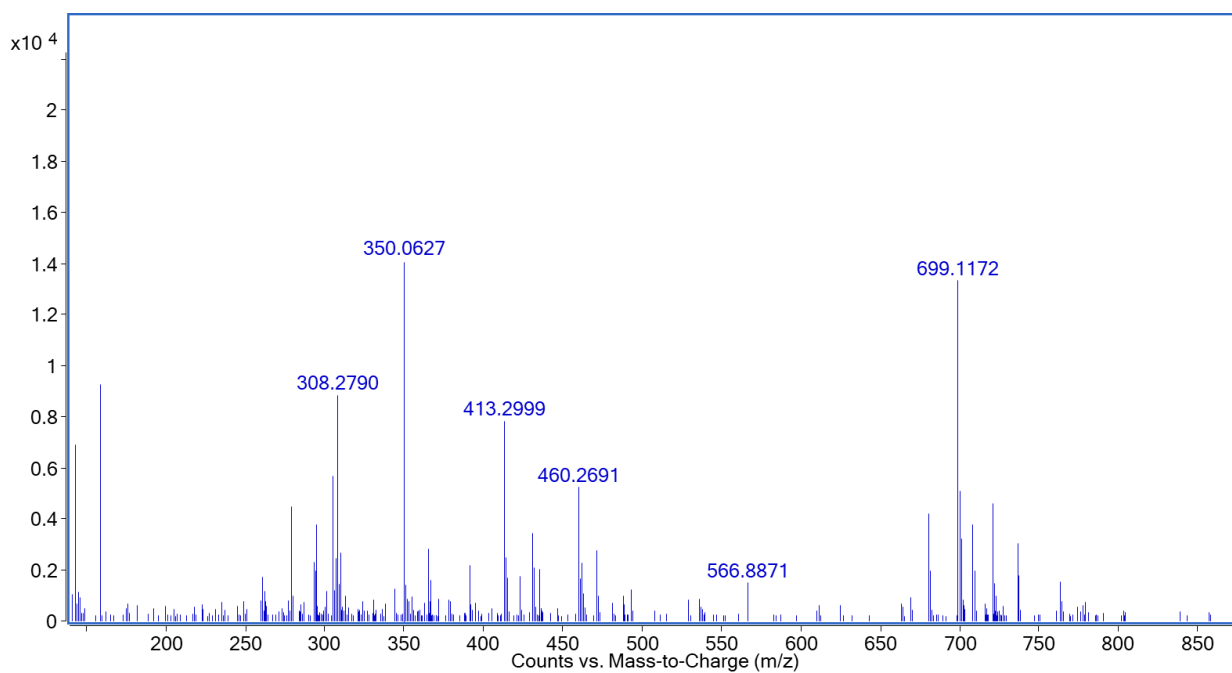


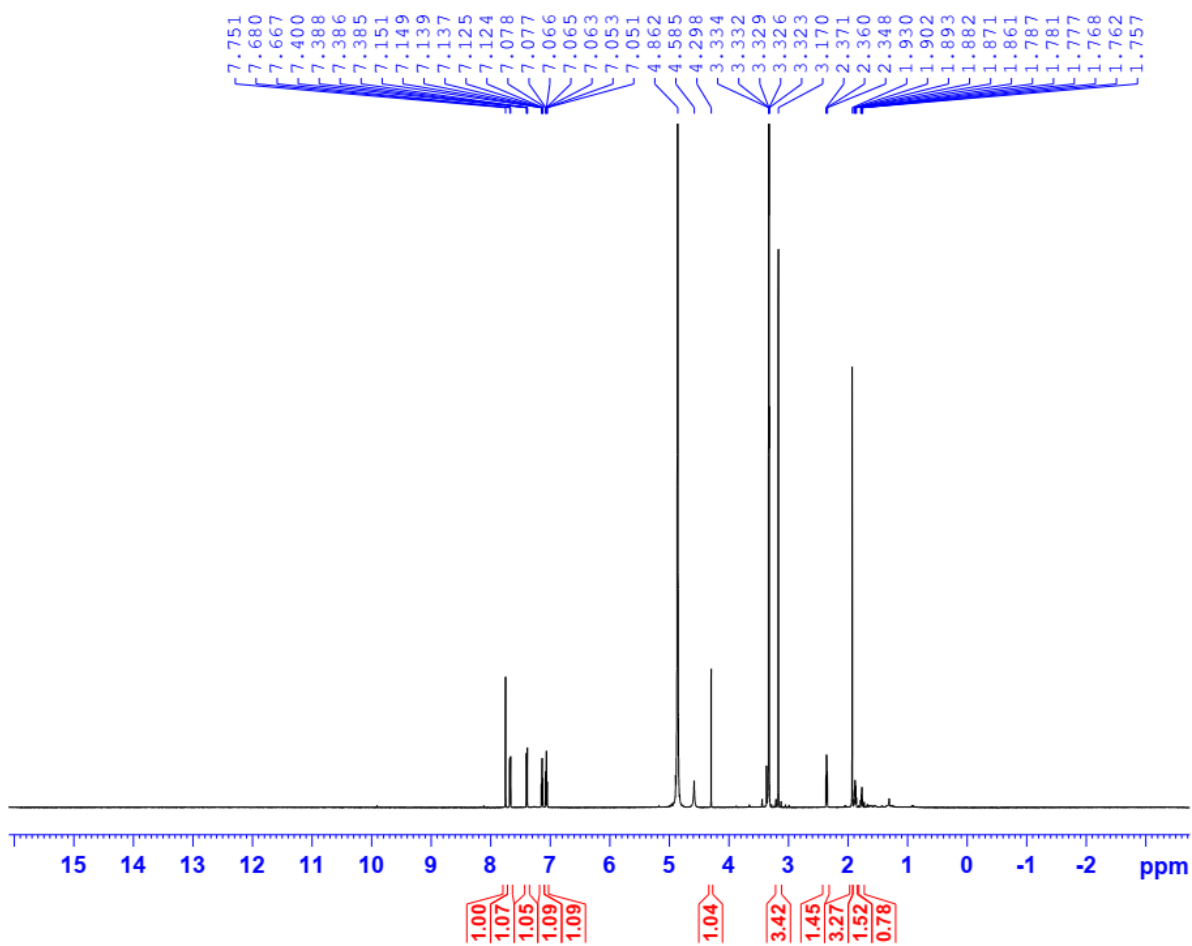
Figure S7:HMBC NMR spectrum of compound (1). Measured in CD<sub>3</sub>OD  
Key HMBC → correlations



**Figure S8:**NOESY NMR spectrum of compound (1). Measured in CD<sub>3</sub>OD

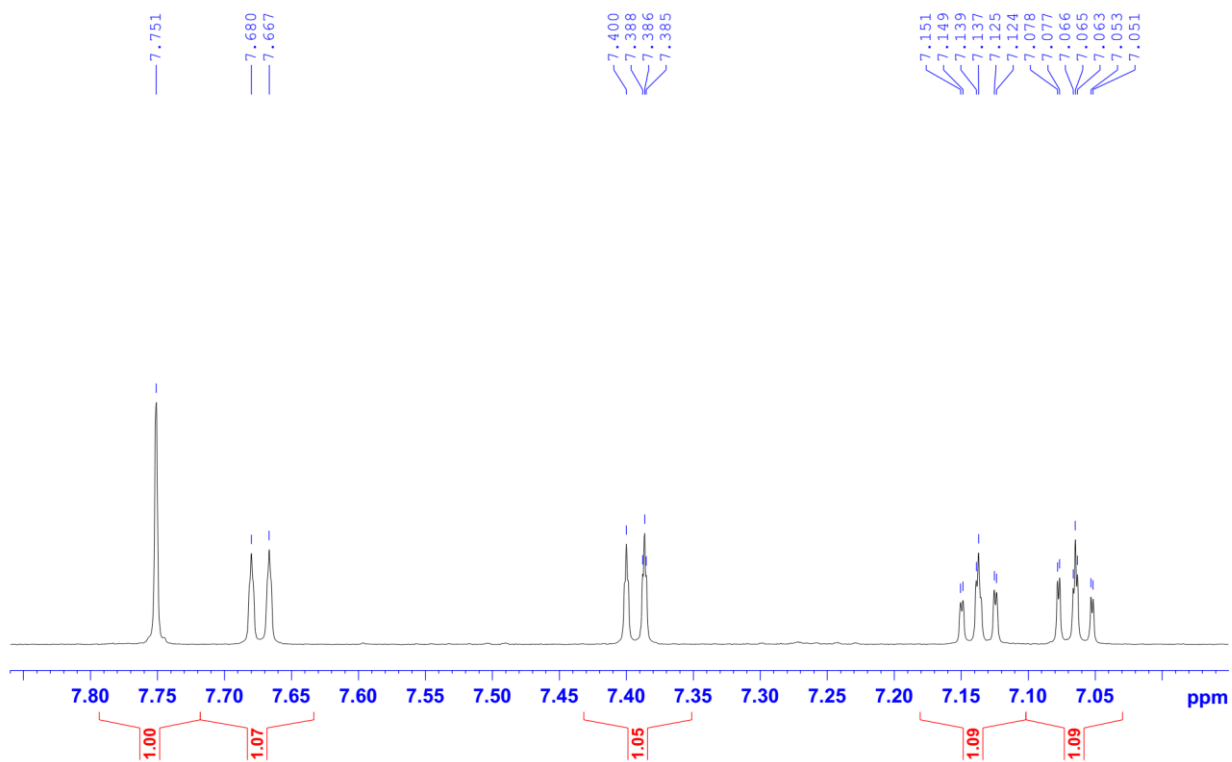


**Figure S9:**HRESIMS spectrum of compound (2)

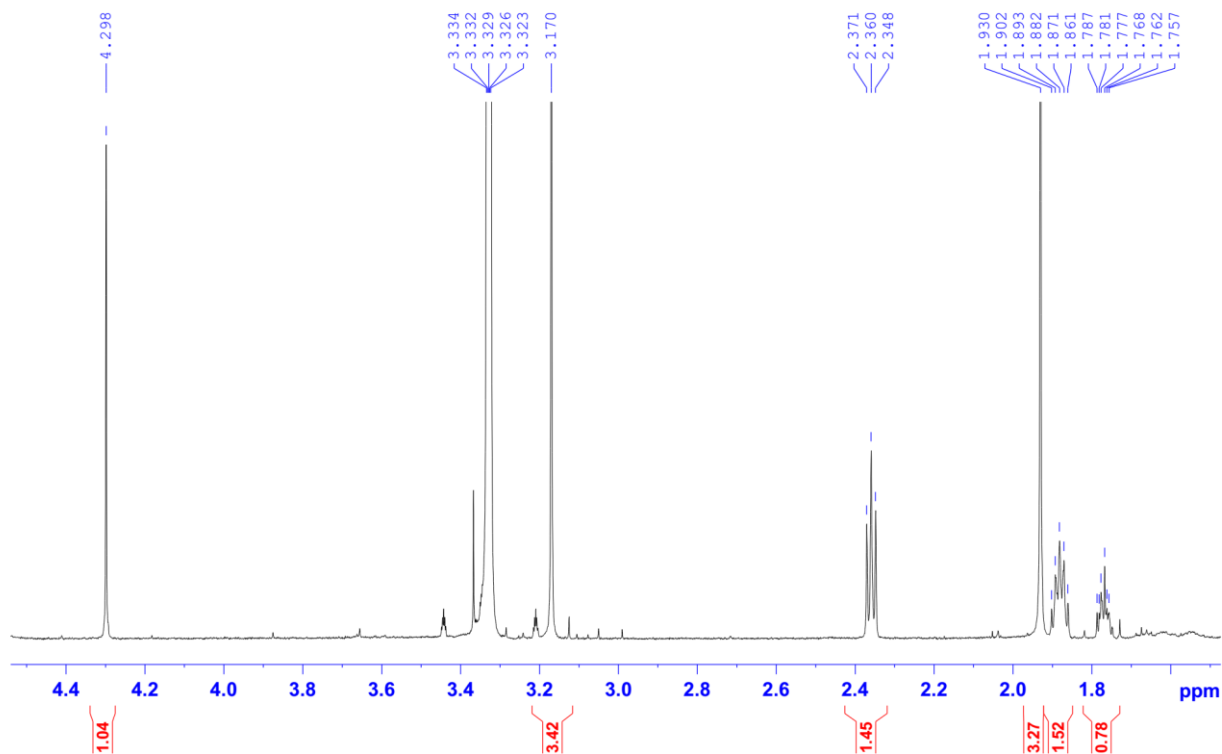


**Figure S10:** $^1\text{H}$  NMR spectrum of compound (2). Measured in  $\text{CD}_3\text{OD}$ , 600 MHz

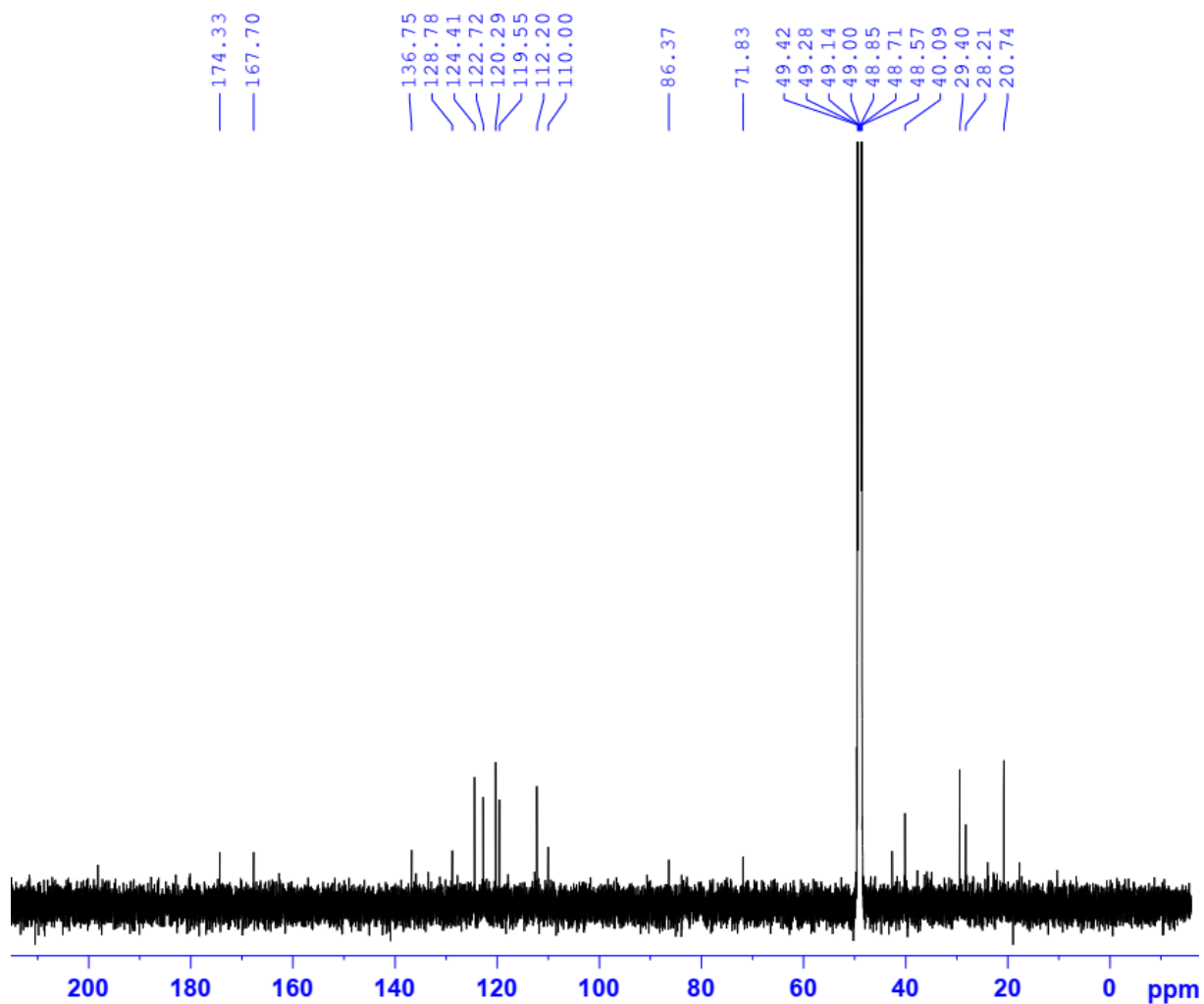




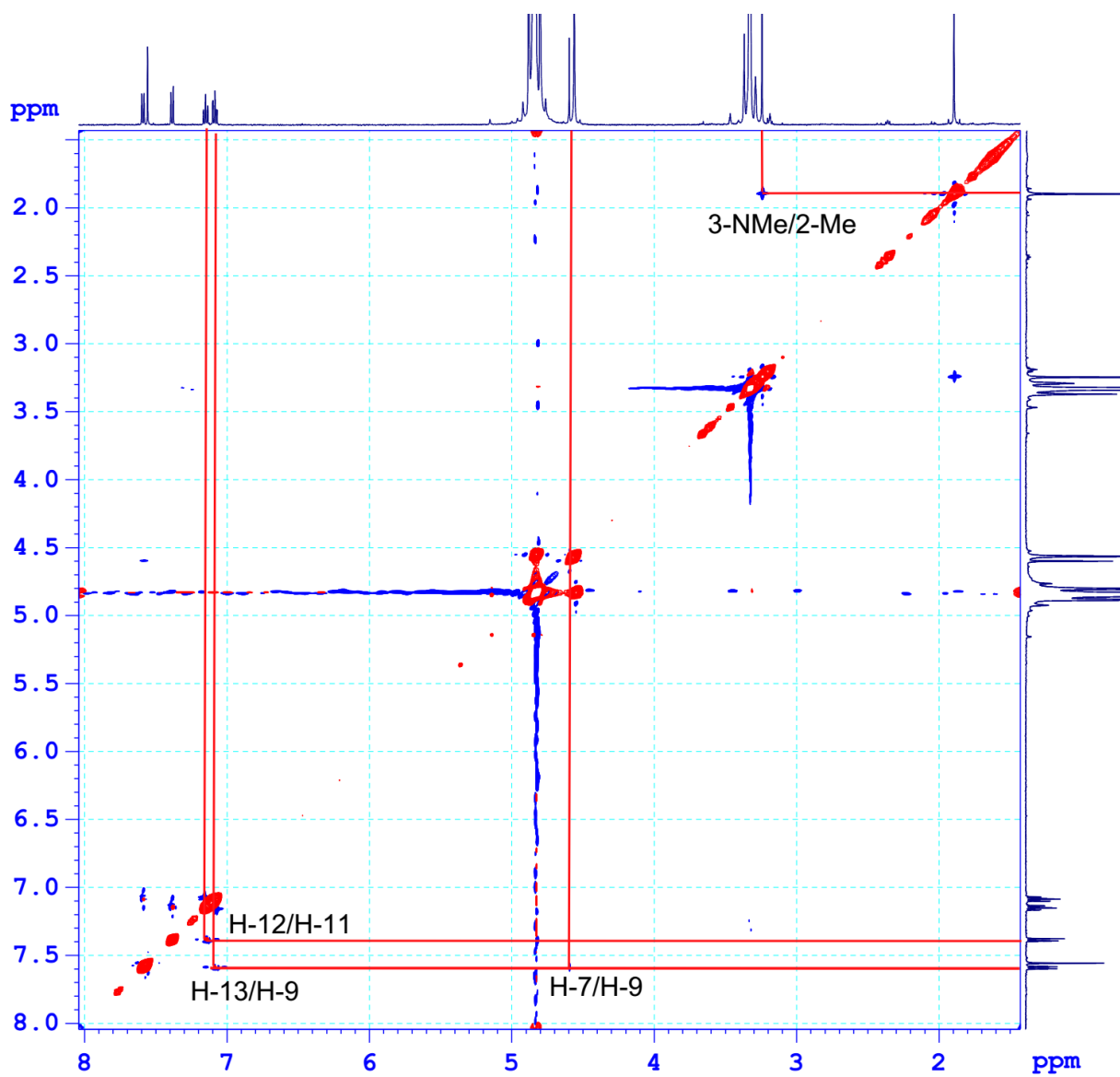
**Figure S11:**  $^1\text{H}$  NMR spectrum (7.0-7.9 ppm) of compound **(2)**. Measured in  $\text{CD}_3\text{OD}$ , 600 MHz



**Figure S12:**  $^1\text{H}$  NMR spectrum (1.6 - 4.5 ppm) of compound **(2)**. Measured in  $\text{CD}_3\text{OD}$ , 600 MHz



**Figure S13:**  $^{13}\text{C}$  NMR spectrum of compound **(2)**. Measured in  $\text{CD}_3\text{OD}$ , 150 MHz



**Figure S14:**NOESY NMR spectrum of compound (2). Measured in CD<sub>3</sub>OD

## Substances search for drawn structure

References Reactions Suppliers Save

**Structure Match**

As Drawn (1)  
Substructure (1)  
Similarity (4,237)  
Analyze Structure Precision

**Chemscape Analysis**  
Visually explore structure similarity with a powerful new tool. Learn more about Chemscape.  
Create Chemscape Analysis

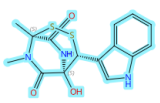
**Filter Behavior**  
Filter by Exclude

**a)**

1 Result View: Full

1

**1574569-27-9**



Absolute stereochemistry shown, Rotation (+)

**C<sub>15</sub>H<sub>15</sub>N<sub>3</sub>O<sub>3</sub>S<sub>2</sub>**  
(1S,4R,5S)-5-Hydroxy-4-(1H-indol-3-yl)-1,8-dimethyl-2,3-dithia-6,8-diazabicyclo[3.2.2]nonane-7,9-dione

Key Physical Properties	Value	Condition
Molecular Weight	349.43	-
Boiling Point (Predicted)	742.7±60.0 °C	Press: 760 Torr
Density (Predicted)	1.568±0.06 g/cm <sup>3</sup>	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	10.14±0.70	Most Acidic Temp: 25 °C

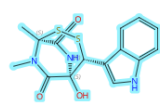
2 References 0 Reactions 0 Suppliers

**b)**

2 Results Sort: Relevance View: Full

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**1574569-27-9**



Absolute stereochemistry shown, Rotation (-)

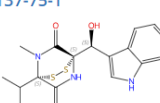
**C<sub>15</sub>H<sub>15</sub>N<sub>3</sub>O<sub>3</sub>S<sub>2</sub>**  
(1S,4R,5S)-5-Hydroxy-4-(1H-indol-3-yl)-1,8-dimethyl-2,3-dithia-6,8-diazabicyclo[3.2.2]nonane-7,9-dione

Key Physical Properties	Value	Condition
Molecular Weight	349.43	-
Boiling Point (Predicted)	742.7±60.0 °C	Press: 760 Torr
Density (Predicted)	1.568±0.06 g/cm <sup>3</sup>	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	10.14±0.70	Most Acidic Temp: 25 °C

2 References 0 Reactions 0 Suppliers

2 80

**2640137-75-1**



Absolute stereochemistry shown, Rotation (-)

**C<sub>17</sub>H<sub>19</sub>N<sub>3</sub>O<sub>3</sub>S<sub>2</sub>**  
(1S,4S)-1-[(5S)-Hydroxy-1H-indol-3-ylmethyl]-5-methyl-4-(1-methylethyl)-2,3-dithia-5,7-diazabicyclo[2.2.2]octane-6,8-dione

Key Physical Properties	Value	Condition
Molecular Weight	377.48	-
Boiling Point (Predicted)	716.2±60.0 °C	Press: 760 Torr
Density (Predicted)	1.494±0.06 g/cm <sup>3</sup>	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	10.22±0.60	Most Acidic Temp: 25 °C

1 Reference 0 Reactions 0 Suppliers

**Search Within Results**

Similarity

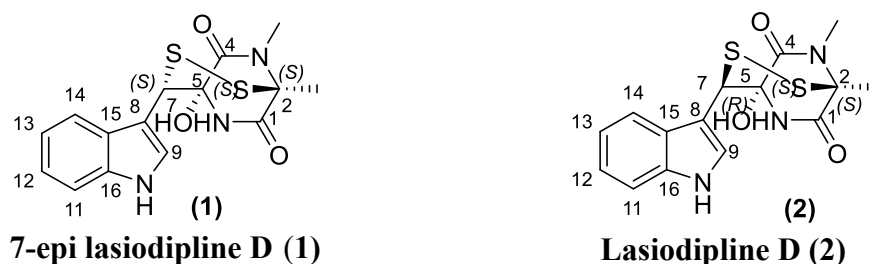
- >=99 (1)
- 80-84 (1)
- 70-74 (17)
- 65-69 (329)
- 60-64 (3,840)

Reference Role

- Biological Study (2)
- Biological Study, Unclassified (2)
- Natural Product Occurrence

**Figure S15:** The SciFinder search for compounds **1** and **2**

a) Search for the structure: only compound **2** (2*S*,5*S*,7*R* configuration) was found, meanwhile, compound **1** (2*S*,5*S*,7*S* configuration) was not in the database; b) Search for the compound at the similarity over 80%.

**Table S1:** Comparison of NMR data of compounds **1** and **2**

No.	$\delta_C^{\#,a}$	$\delta_H^{\#,b}$	$\delta_C^{\#,a}$	$\delta_H^{\#,b}$
1	169.1		167.7	
2	72.3		71.8	
4	173.0		174.3	
5	85.6		86.4	
7	47.1	4.60 (1H, s)	40.1	4.30 (1H, s)
8	107.5		110.0	
9	125.5	7.56 (1H, s)	124.4	7.75 (1H, brs)
11	112.5	7.39 (1H, d, $J = 7.8$ Hz)	112.2	7.39 (1H, d, $J = 7.8$ Hz)
12	123.0	7.15 (1H, td, $J = 7.8, 1.2$ Hz)	122.7	7.14 (1H, td, $J = 7.8, 1.2$ Hz)
13	120.6	7.08 (1H, td, $J = 7.8, 1.2$ Hz)	120.3	7.07 (1H, td, $J = 7.8, 1.2$ Hz)
14	118.8	7.59 (1H, d, $J = 7.8$ Hz)	119.6	7.67 (1H, d, $J = 7.8$ Hz)
15	128.8		128.8	
16	137.4		136.8	
2-Me	20.8	1.90 (3H, s)	20.7	1.81 (1H, s)
3-NMe	29.0	3.24 (3H, s)	29.4	3.03 (1H, s)

<sup>#</sup> Measure in CD<sub>3</sub>OD, <sup>a</sup> 150 MHz; <sup>b</sup> 600 MHz.

**Table S2:** NO production inhibition in LPS-induced RAW264.7 cells and cell viability of the compounds **1**, **2**, and **3**

Compound	Concentration ( $\mu$ M)	NO production inhibition (%)	Cell viability (%)
<b>1</b>	10	15.36 $\pm$ 2.44	99.53 $\pm$ 3.15
	50	45.54 $\pm$ 3.87	96.41 $\pm$ 5.64
<b>2</b>	10	11.78 $\pm$ 1.67	95.77 $\pm$ 6.39
	50	42.79 $\pm$ 6.28	97.71 $\pm$ 7.11
<b>3</b>	10	28.64 $\pm$ 1.29	94.29 $\pm$ 1.27
	50	40.38 $\pm$ 7.98	88.42 $\pm$ 1.55
Cardamonin	2.5	46.31 $\pm$ 3.30	99.95 $\pm$ 4.20
	10	83.87 $\pm$ 3.42	97.83 $\pm$ 3.83

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