

Supporting Information
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New Sulfureous Diketopiperazine from Roots of *Moringa oleifera*

Tran Van Hien^{1,2}, Nguyen Thi Hong Anh², Nguyen Thi Luyen², Le Thi Phuong Quynh³, Nguyen Thi Thuy Hang⁴, Nguyen Thi Thu Thuy^{1,5}, Do Hoang Giang^{2,*} and Nguyen Tien Dat^{2,*}

¹ Graduate University of Science and Technology, Vietnam Academy of Science and Technology (VAST), 18-Hoang Quoc Viet, Cau Giay, Hanoi, Vietnam

² Center for High Technology Research and Development, VAST, 18-Hoang Quoc Viet, Cau Giay, Hanoi, Vietnam

³ Institute of Natural Product Chemistry, VAST, 18-Hoang Quoc Viet, Cau Giay, Hanoi, Vietnam;

⁴ Institute of Chemistry, VAST, 18-Hoang Quoc Viet, Cau Giay, Hanoi, Vietnam

⁵ Joint Vietnam-Russia Tropical Science and Technology Research Center, Nguyen Van Huyen, Cau Giay, Hanoi, Vietnam

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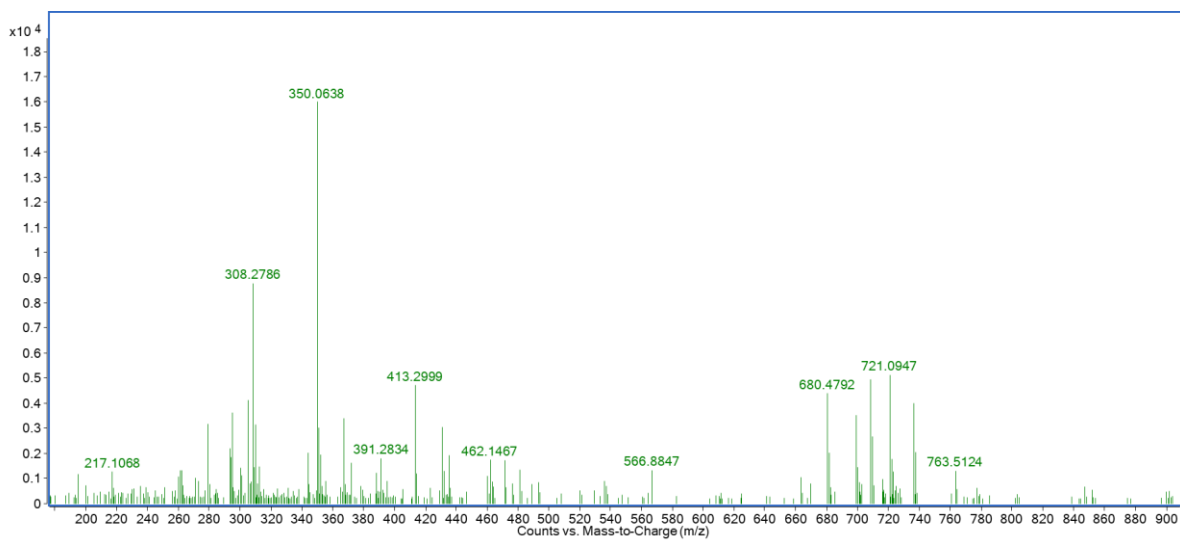


Figure S1:HRESIMS spectrum of compound (1)

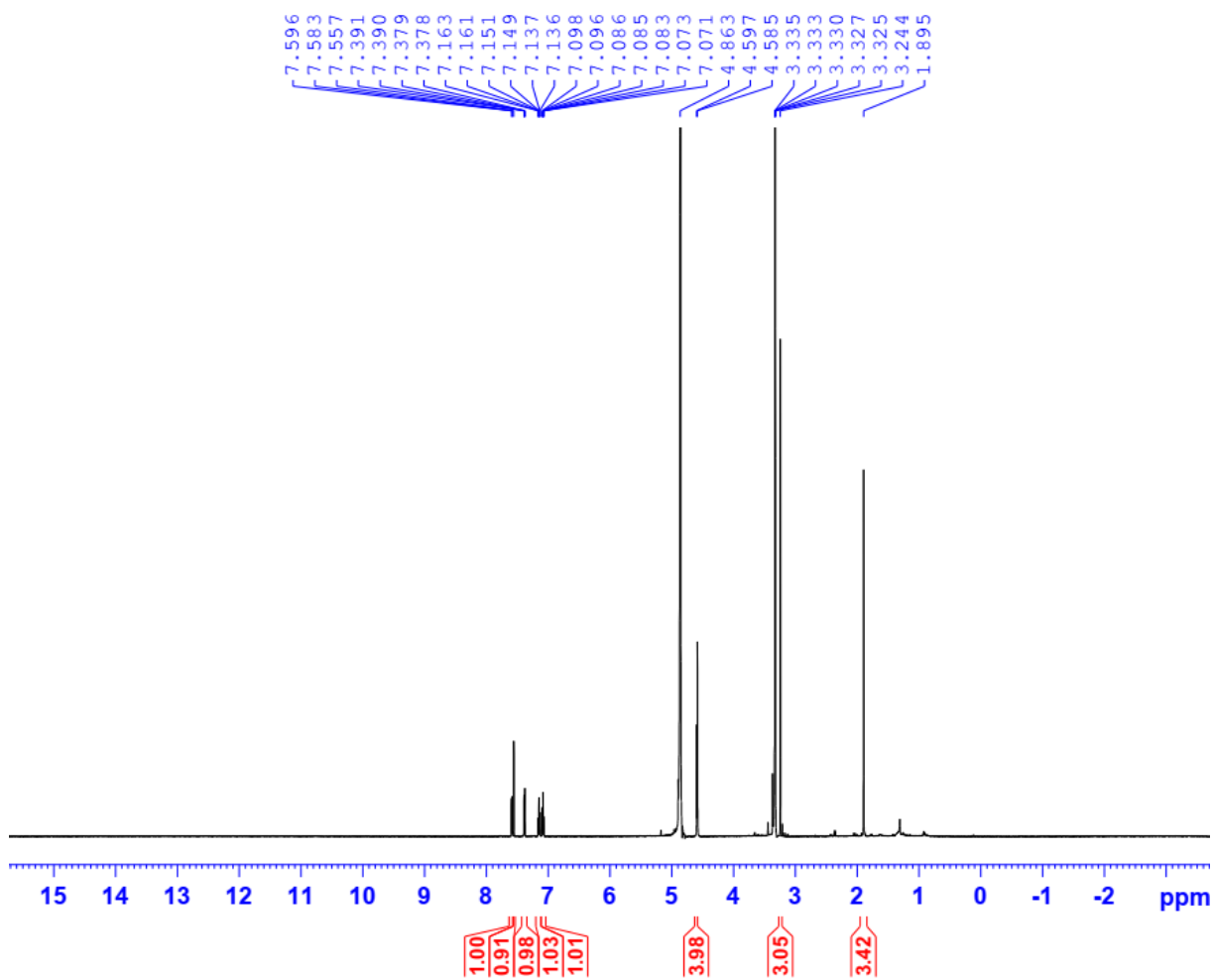


Figure S2:¹H NMR spectrum of compound (1). Measured in CD₃OD, 600 MHz

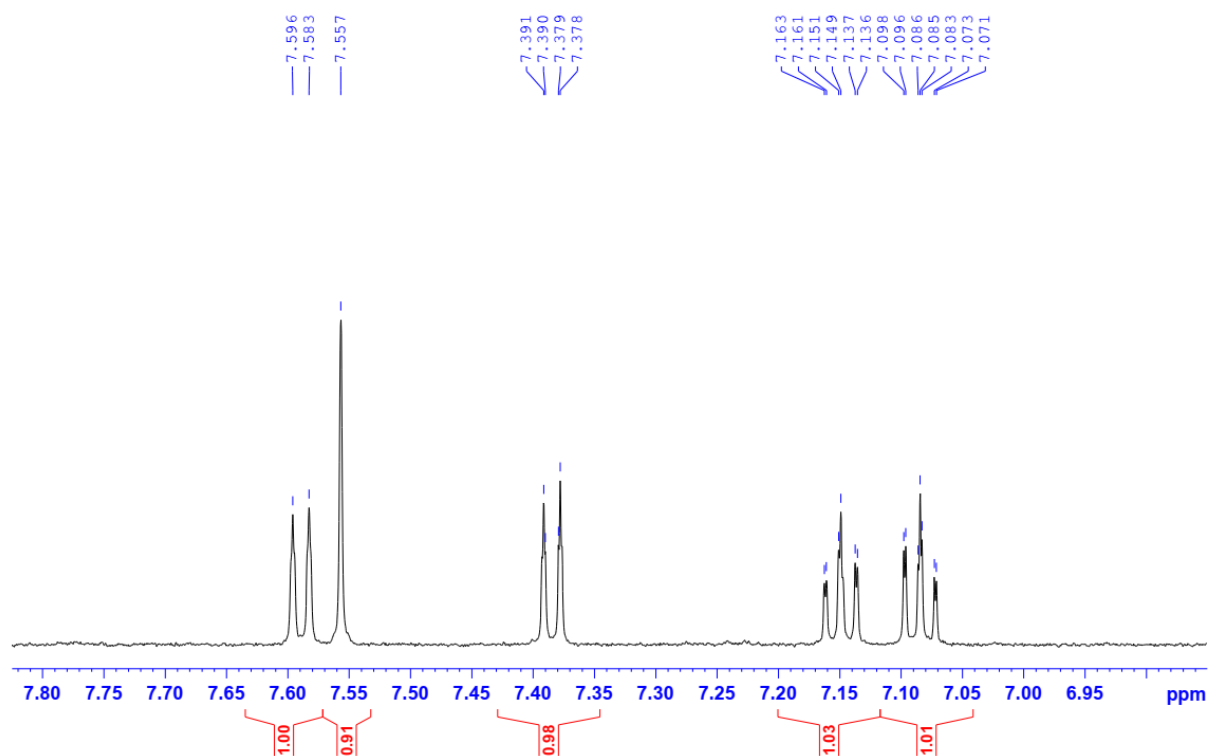


Figure S3: ^1H NMR spectrum (6.8-7.8 ppm) of compound (**1**). Measured in CD_3OD , 600 MHz

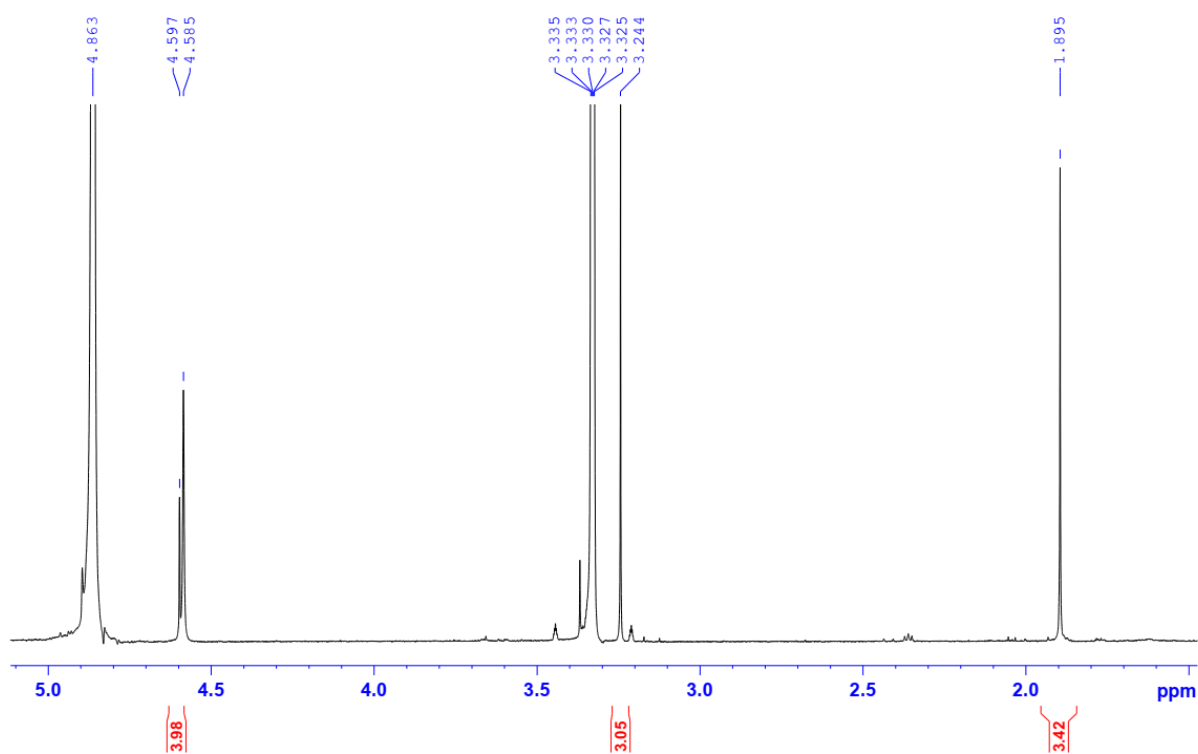


Figure S4: ^1H NMR spectrum (1.5-5.0 ppm) of compound (**1**). Measured in CD_3OD , 600 MHz

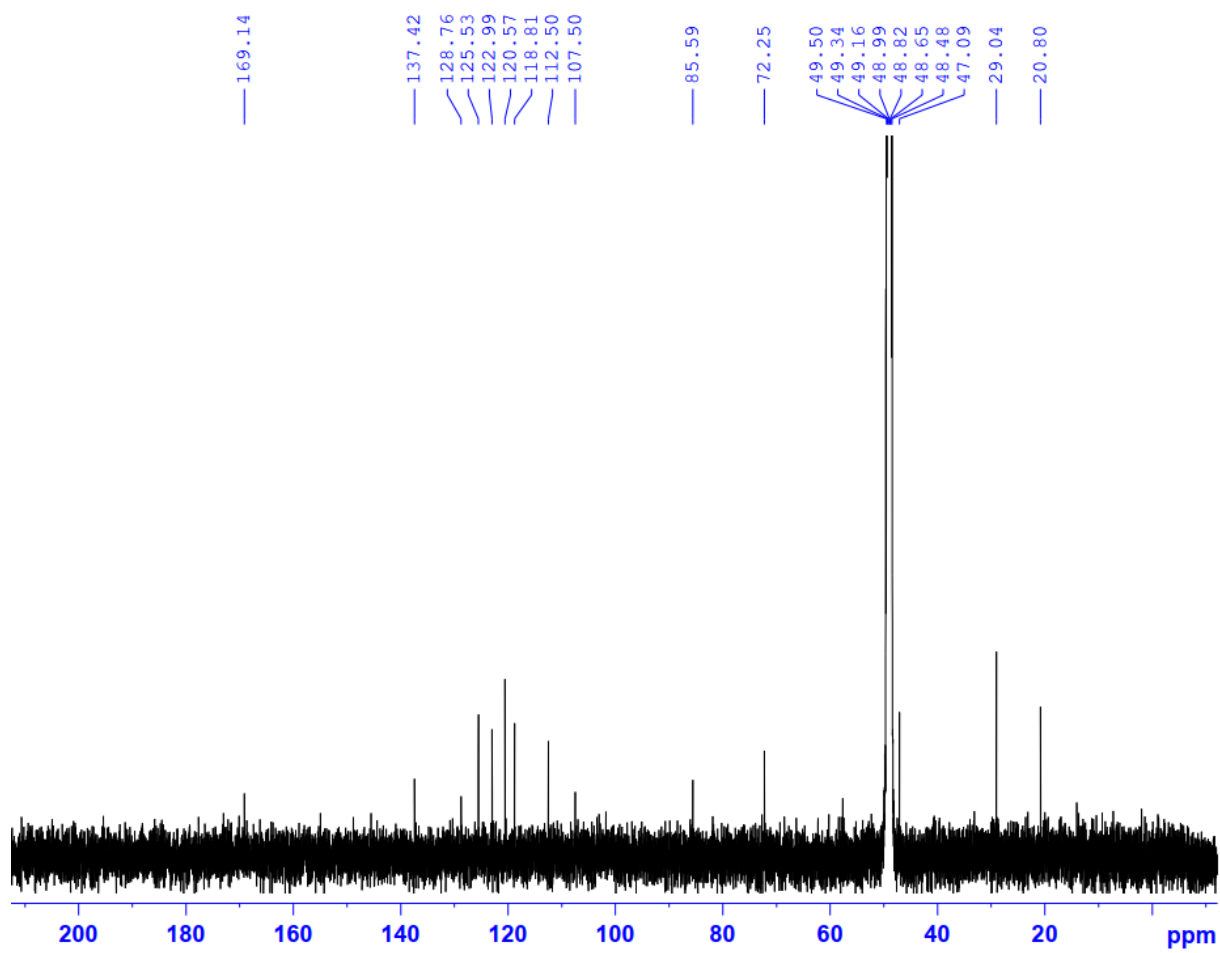


Figure S5: ^{13}C NMR spectrum of compound (**1**). Measured in CD_3OD , 150 MHz

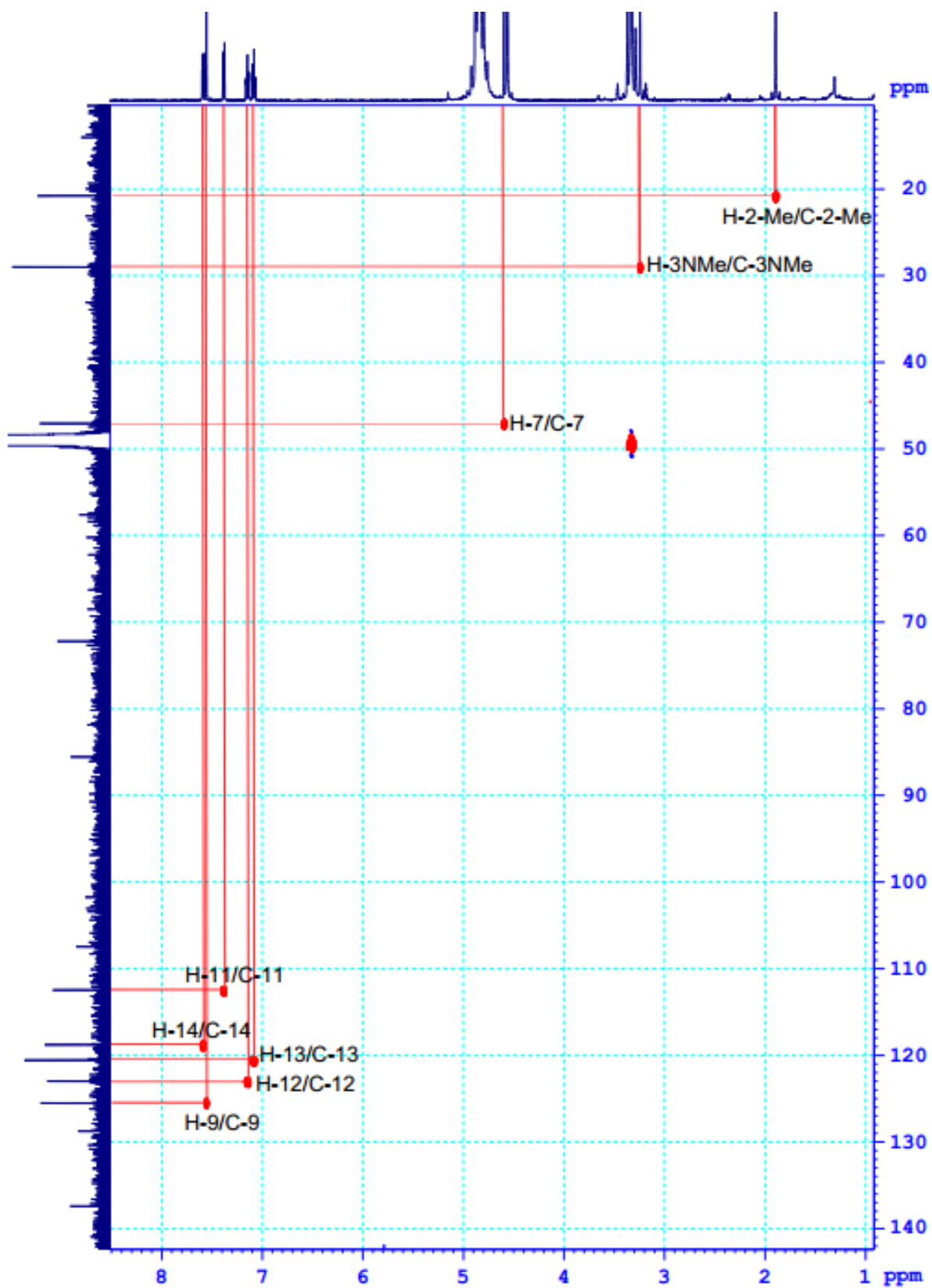


Figure S6:HSQC NMR spectrum of compound (1). Measured in CD₃OD

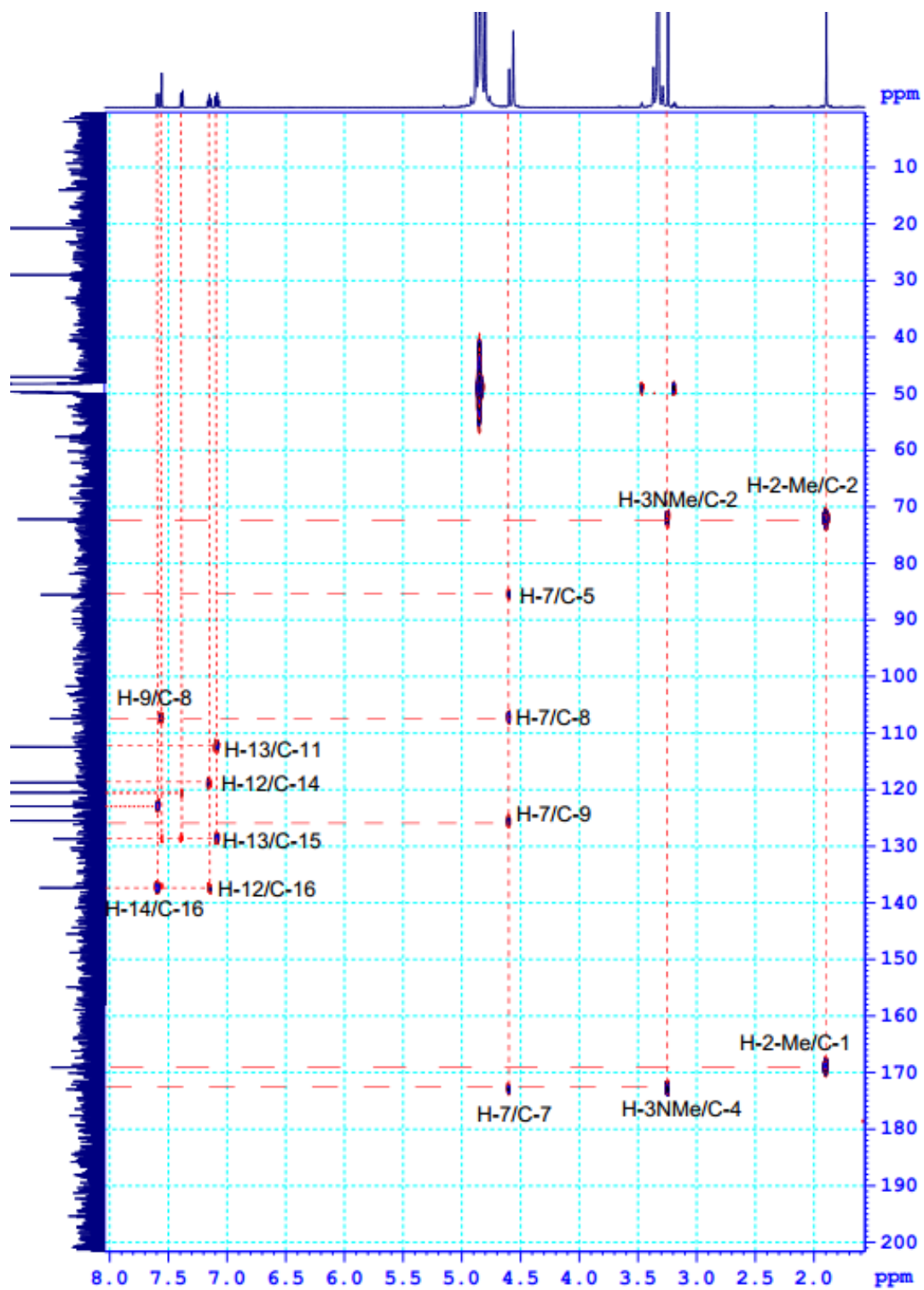
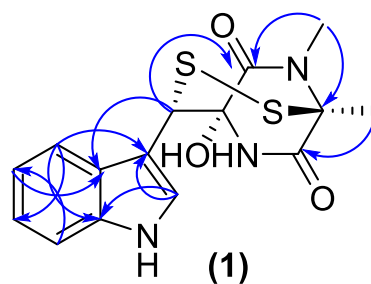


Figure S7:HMBC NMR spectrum of compound (1). Measured in CD₃OD
Key HMBC → correlations

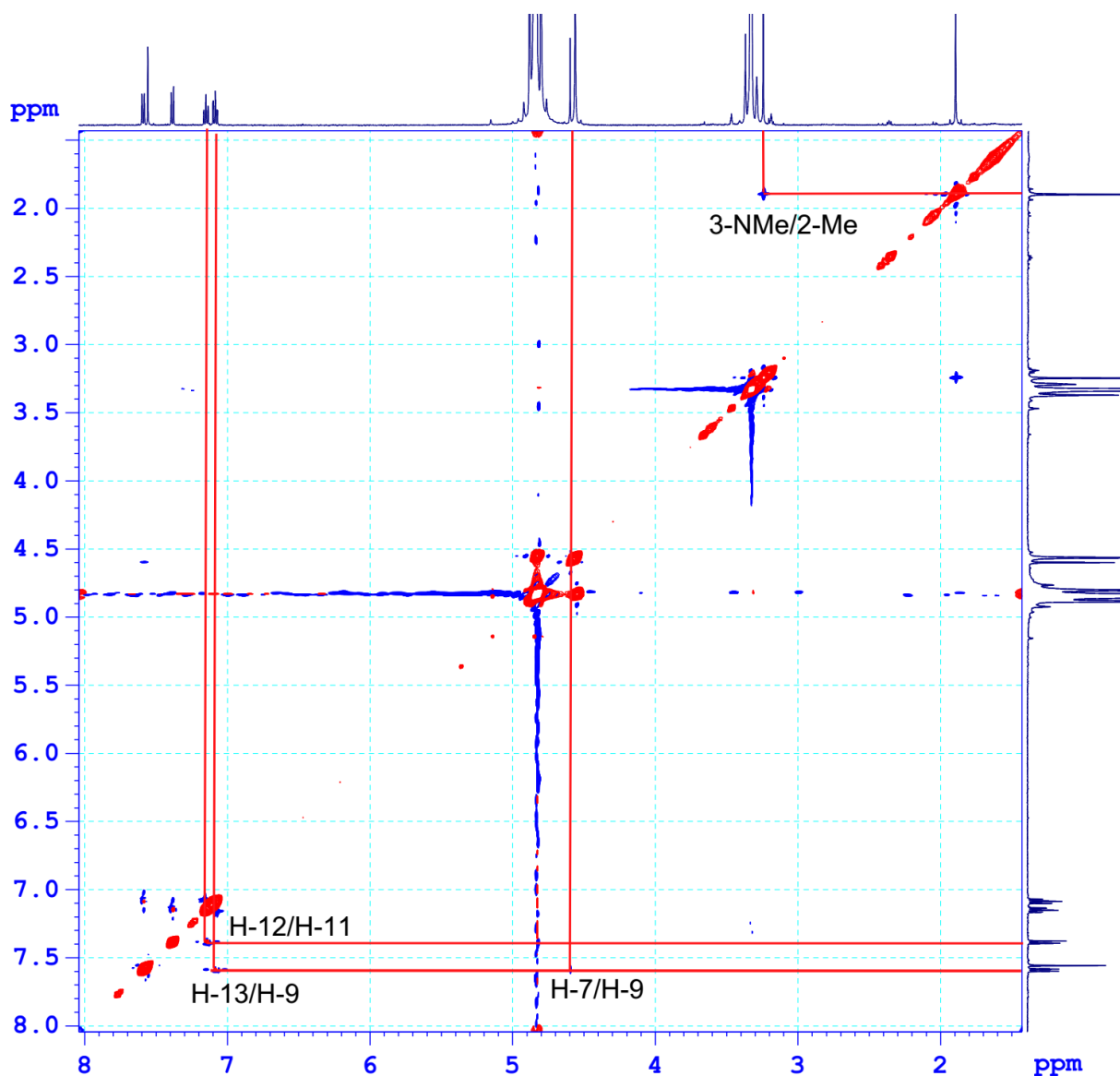


Figure S8:NOESY NMR spectrum of compound (1). Measured in CD₃OD

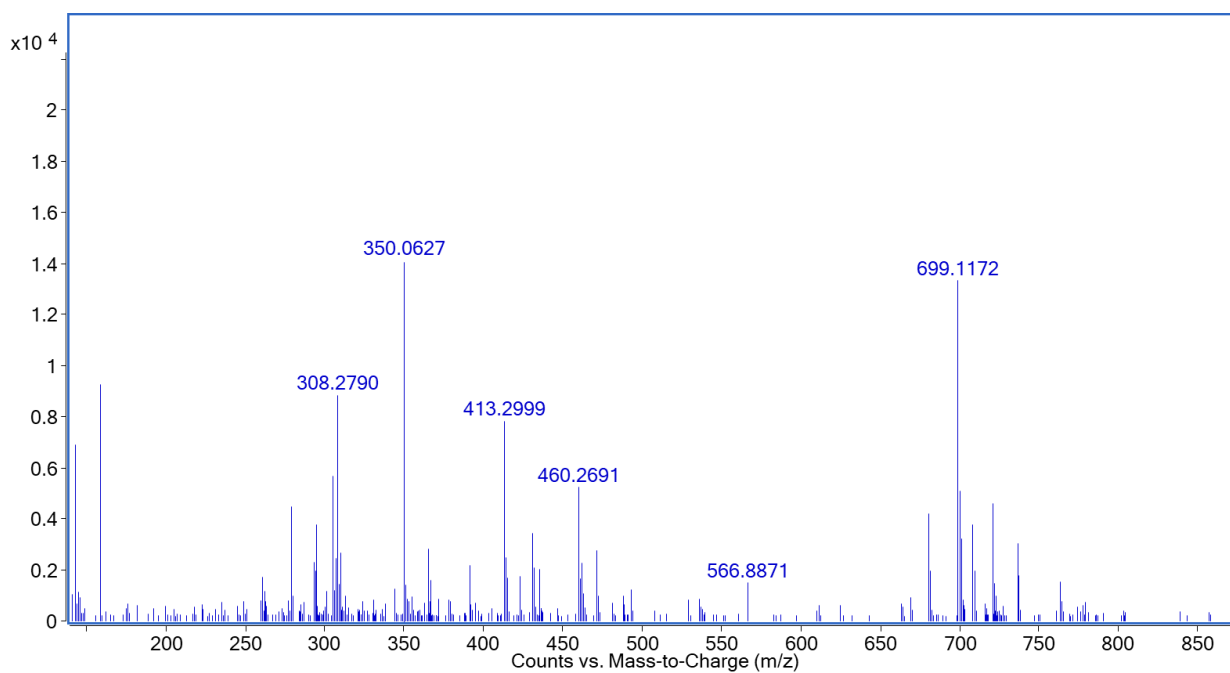


Figure S9:HRESIMS spectrum of compound (2)

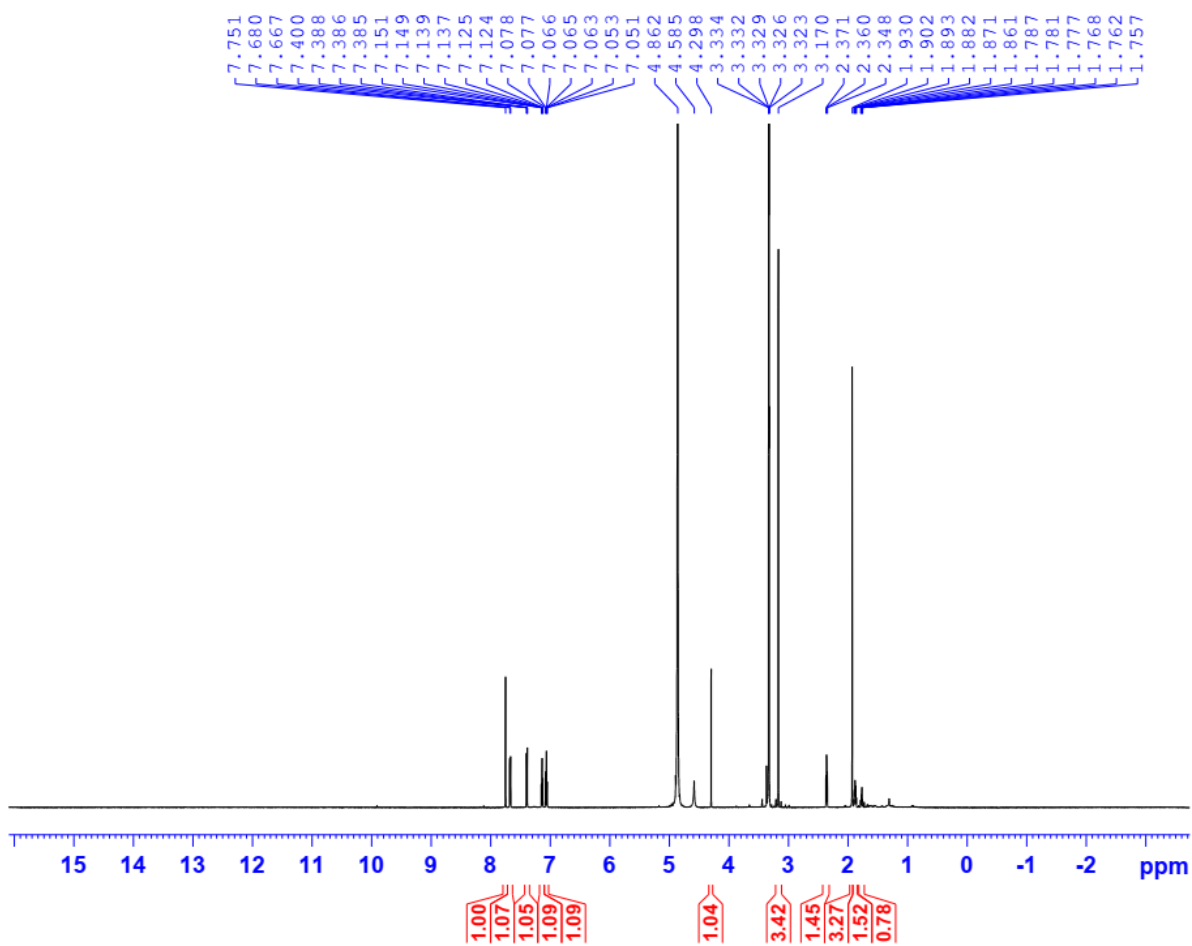


Figure S10: ^1H NMR spectrum of compound (2). Measured in CD_3OD , 600 MHz

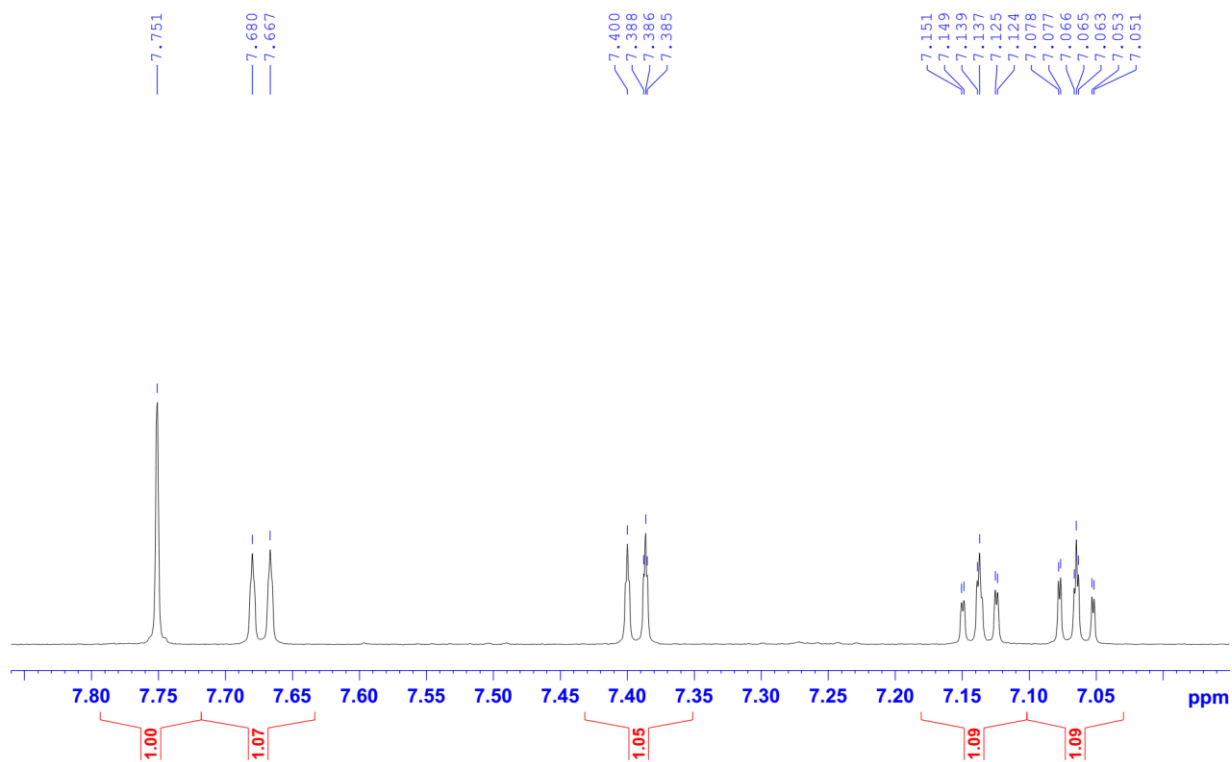


Figure S11: ^1H NMR spectrum (7.0-7.9 ppm) of compound **(2)**. Measured in CD_3OD , 600 MHz

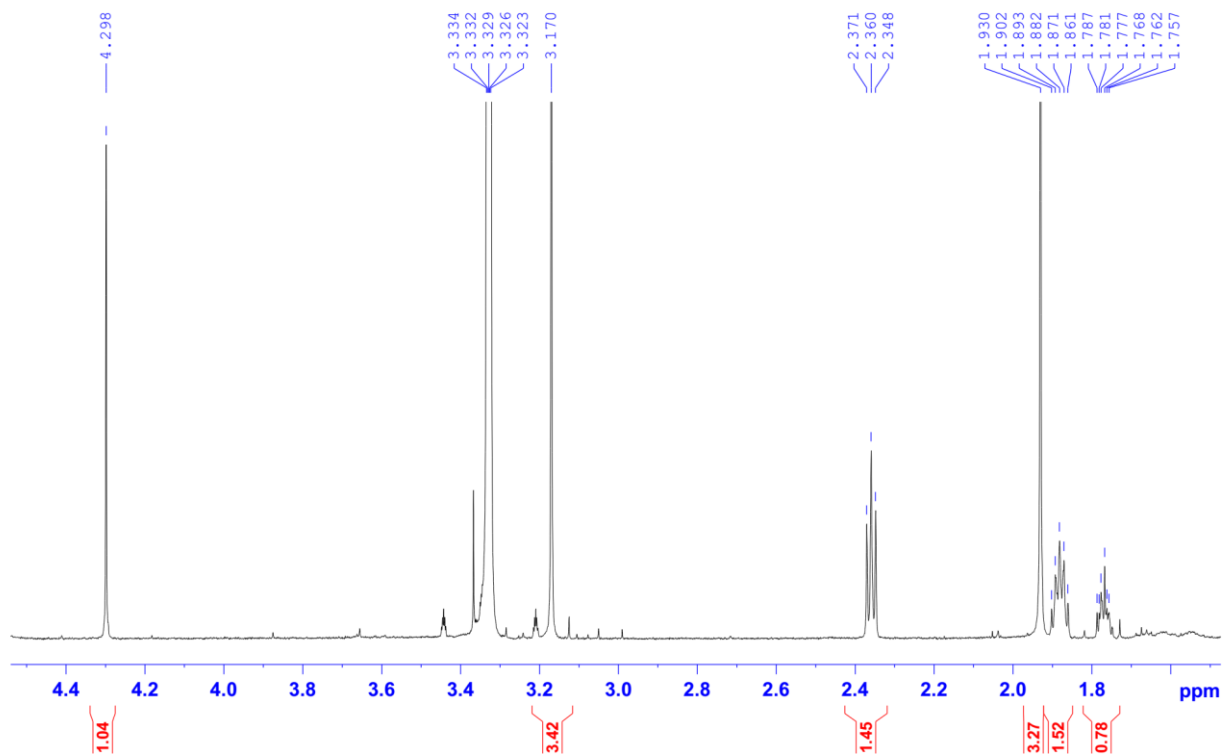


Figure S12: ^1H NMR spectrum (1.6 - 4.5 ppm) of compound **(2)**. Measured in CD_3OD , 600 MHz

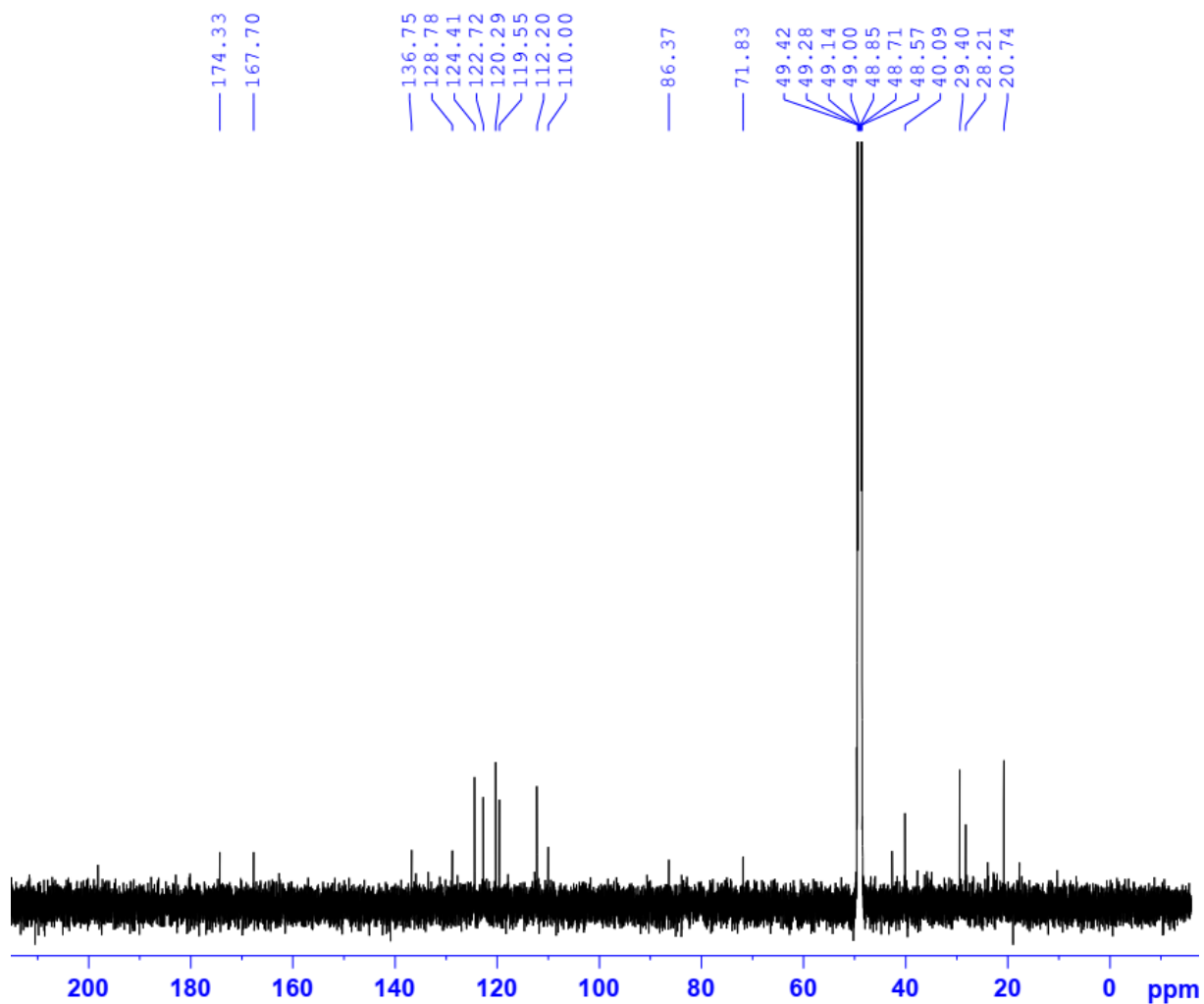


Figure S13: ^{13}C NMR spectrum of compound (2). Measured in CD_3OD , 150 MHz

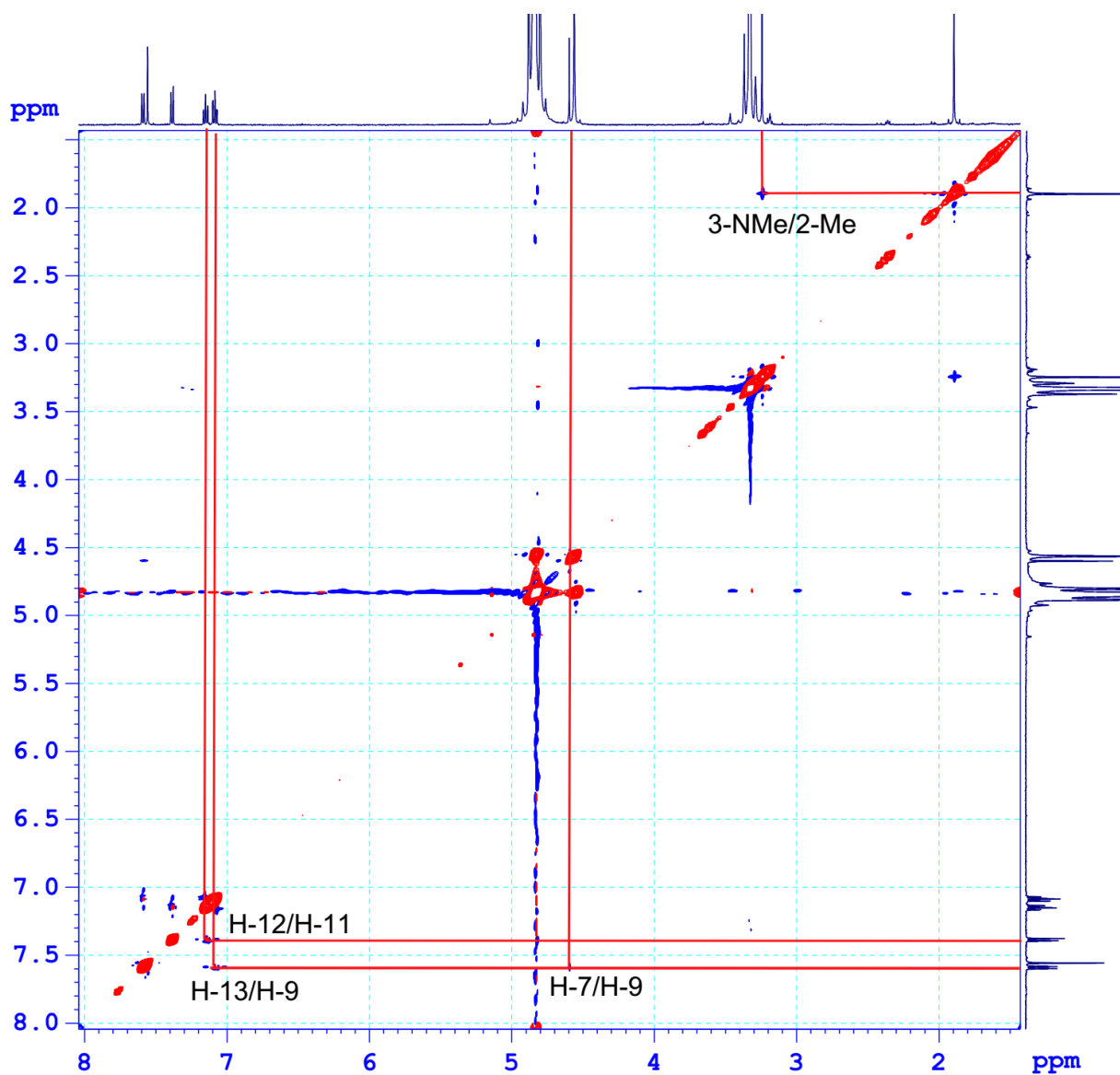


Figure S14:NOESY NMR spectrum of compound (2). Measured in CD₃OD

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

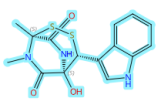
Filter Behavior
Filter by Exclude

a)

1 Result View: Full

1

1574569-27-9



Absolute stereochemistry shown, Rotation (+)

C₁₅H₁₅N₃O₃S₂
(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 ³	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	10.14±0.70	Most Acidic Temp: 25 °C

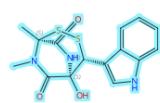
References Reactions Suppliers

b)

2 Results Sort: Relevance View: Full

1 100

1574569-27-9



Absolute stereochemistry shown, Rotation (-)

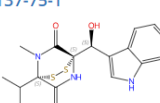
C₁₅H₁₅N₃O₃S₂
(1S,4R,5S)-5-Hydroxy-4-(1H-indol-3-yl)-1,8-dimethyl-2,3-dithia-6,8-diazabicyclo[3.2.2]nonane-7,9-dione

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 ³	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	10.14±0.70	Most Acidic Temp: 25 °C

References Reactions Suppliers

2 80

2640137-75-1



Absolute stereochemistry shown, Rotation (-)

C₁₇H₁₉N₃O₃S₂
(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 ³	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	10.22±0.60	Most Acidic Temp: 25 °C

Reference Reactions Suppliers

Search Within Results

Similarity

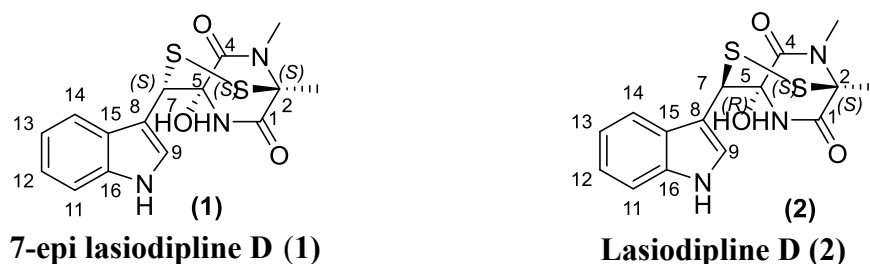
- >=99 (1)
- 80-84 (1)
- 70-74 (17)
- 65-69 (329)
- 60-64 (3,840)

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** (*2S,5S,7R* configuration) was found, meanwhile, compound **1** (*2S,5S,7S* 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)

[#] Measure in CD₃OD, ^a 150 MHz; ^b 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 (μ M)	NO production inhibition (%)	Cell viability (%)
1	10	15.36 \pm 2.44	99.53 \pm 3.15
	50	45.54 \pm 3.87	96.41 \pm 5.64
2	10	11.78 \pm 1.67	95.77 \pm 6.39
	50	42.79 \pm 6.28	97.71 \pm 7.11
3	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