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

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Table of Contents **Page**

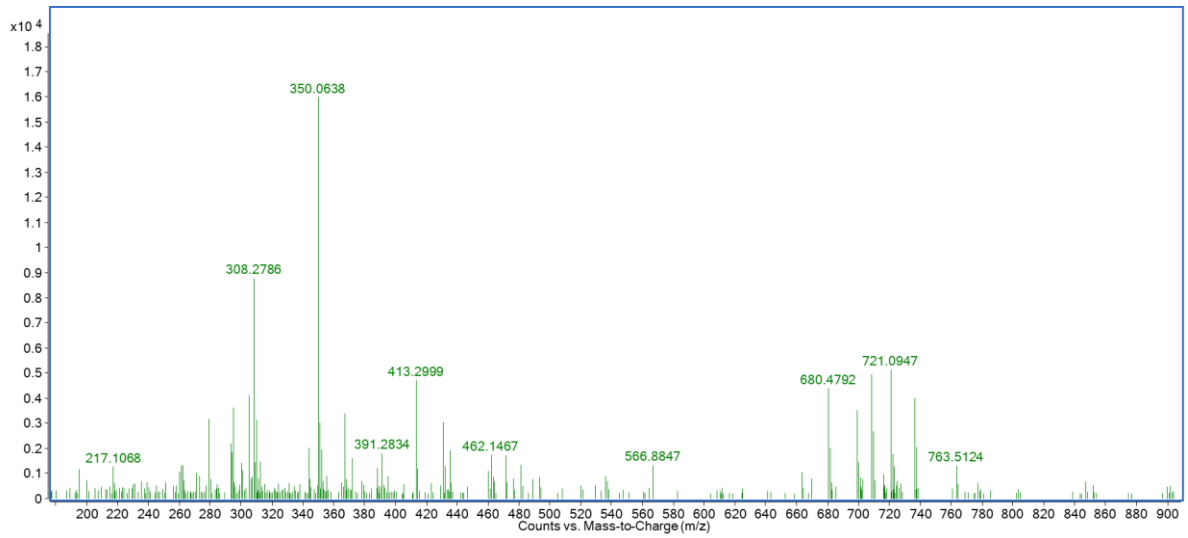


Figure S1:HRESIMS spectrum of compound **(1)**

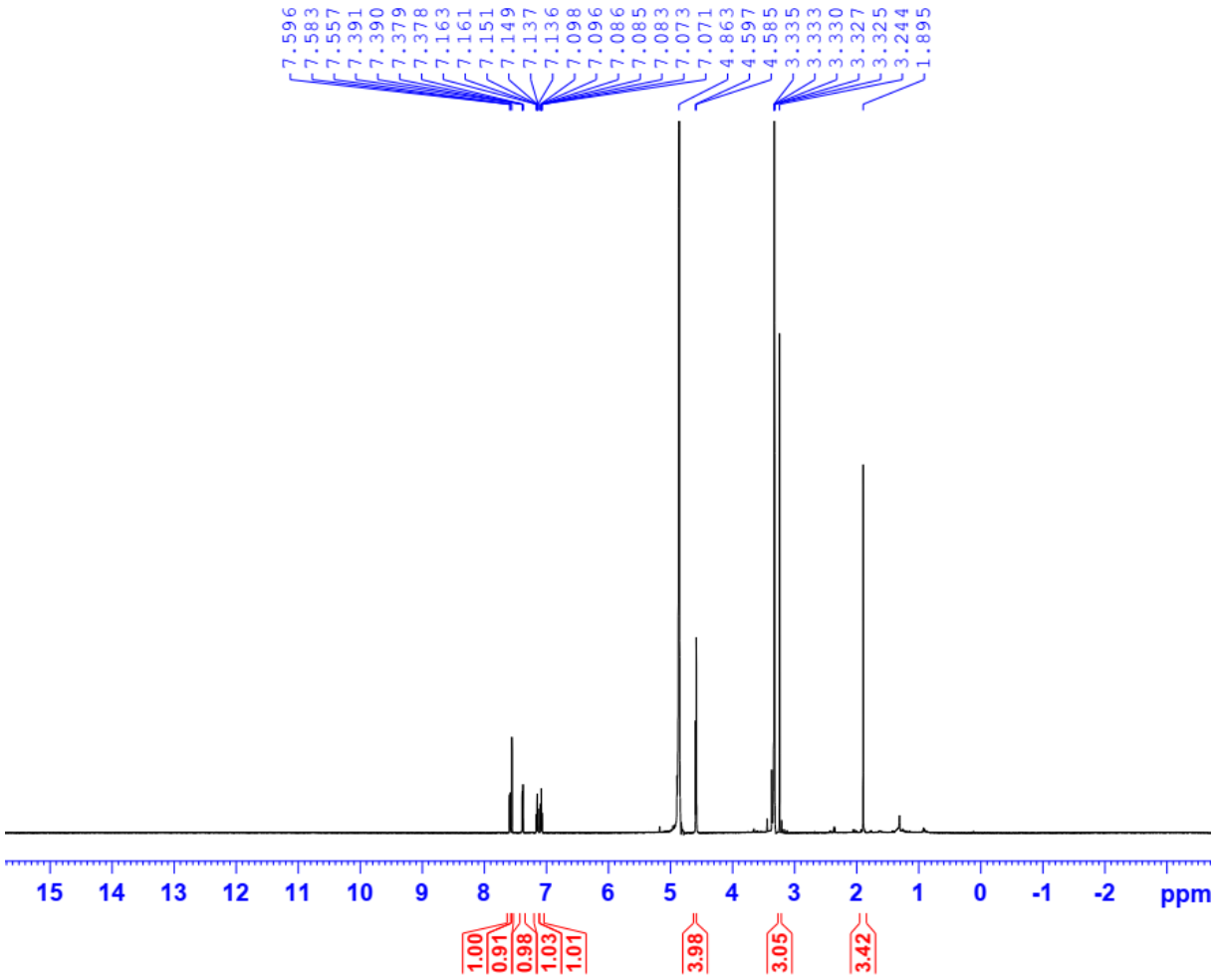


Figure S2:^{1}H NMR spectrum of compound **(1)**. Measured in CD_3OD, 600 MHz

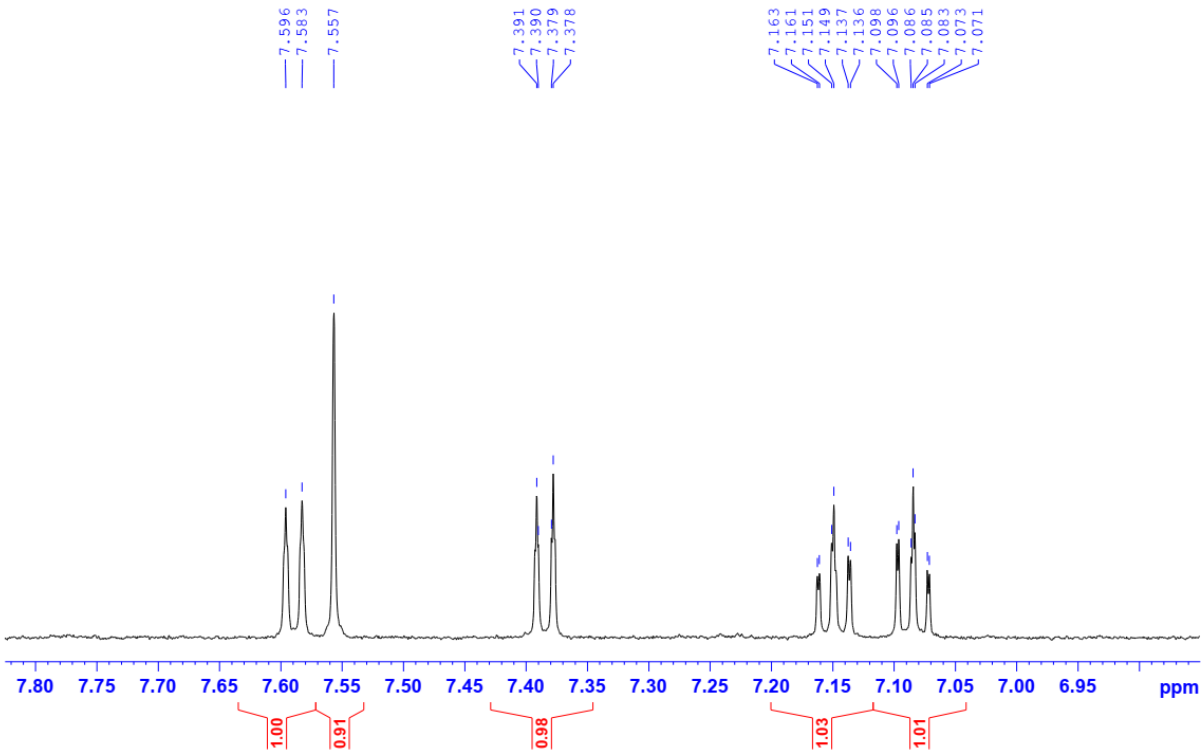


Figure S3: ^{1}H NMR spectrum (6.8-7.8 ppm) of compound **(1)**. Measured in CD_3OD, 600 MHz

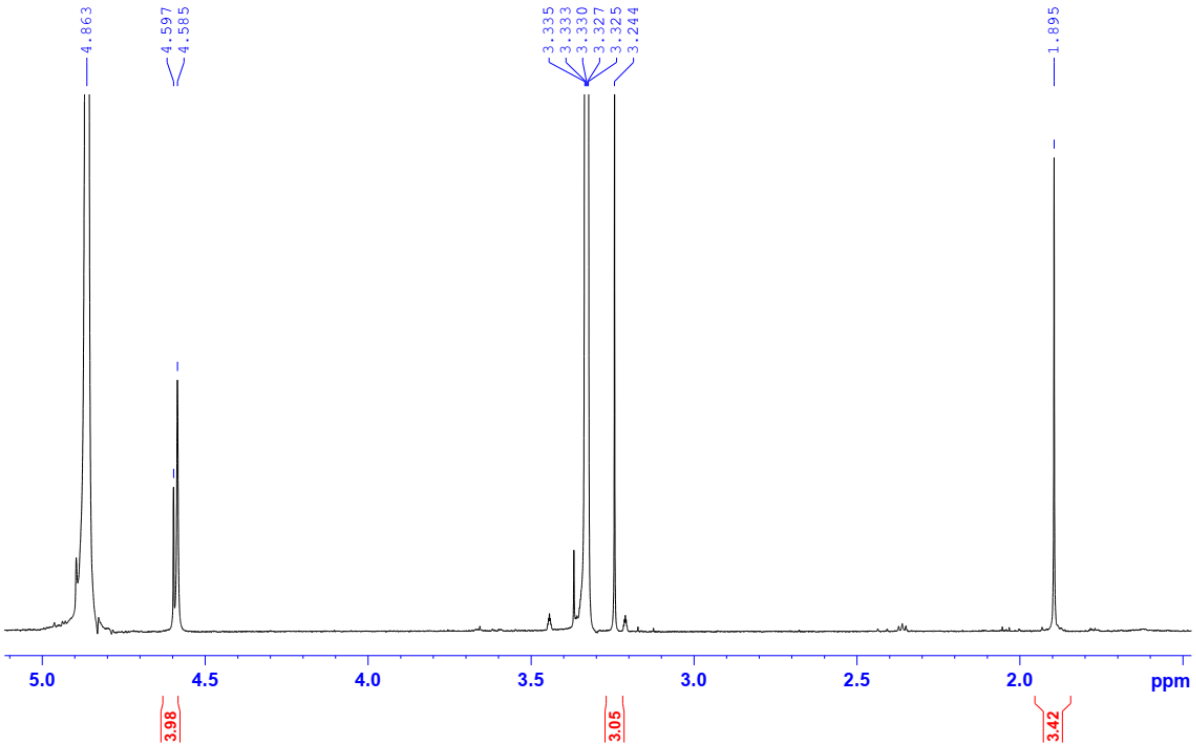


Figure S4: ^{1}H NMR spectrum (1.5-5.0 ppm) of compound **(1)**. Measured in CD_3OD, 600 MHz

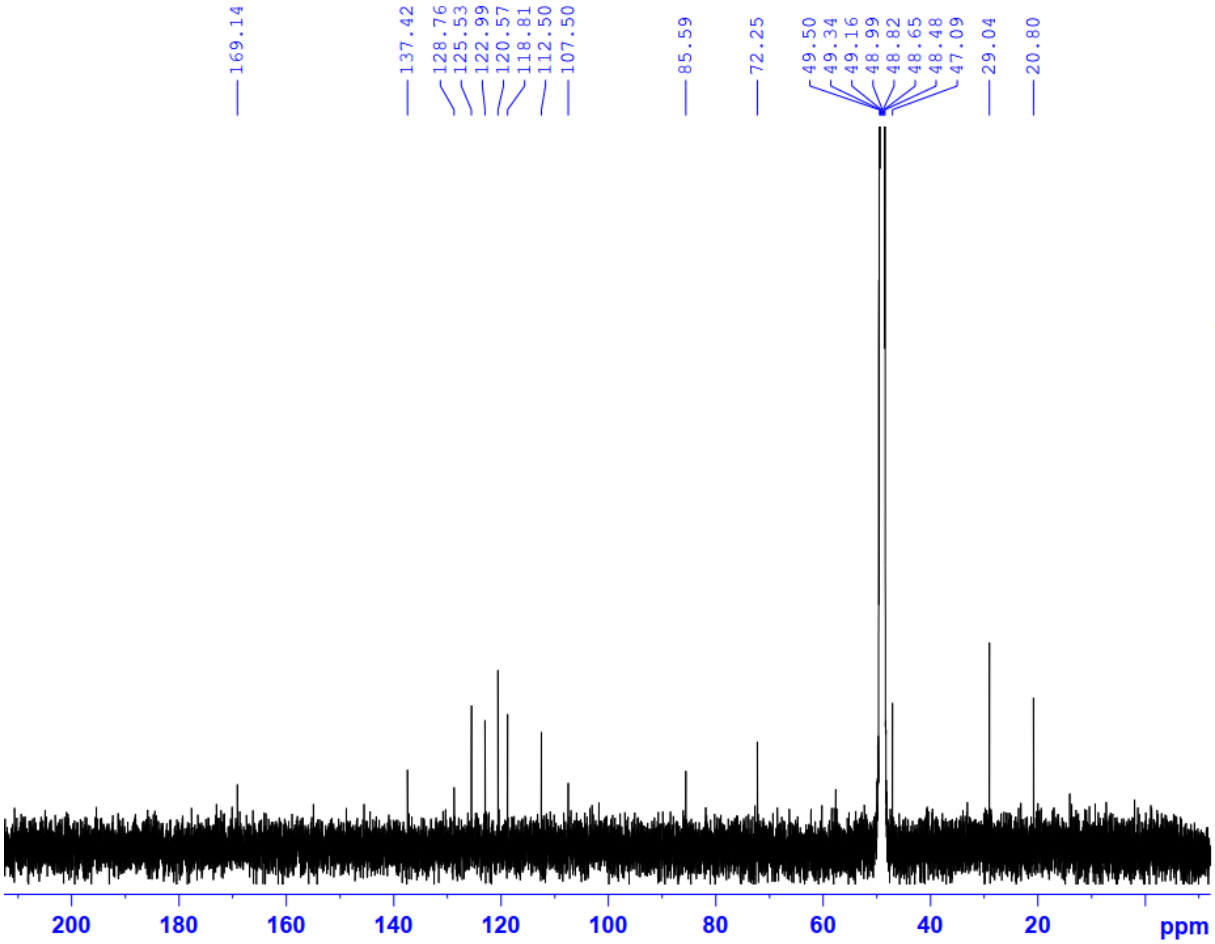


Figure S5: ^{13}C NMR spectrum of compound **(1)**. Measured in CD_3OD, 150 MHz

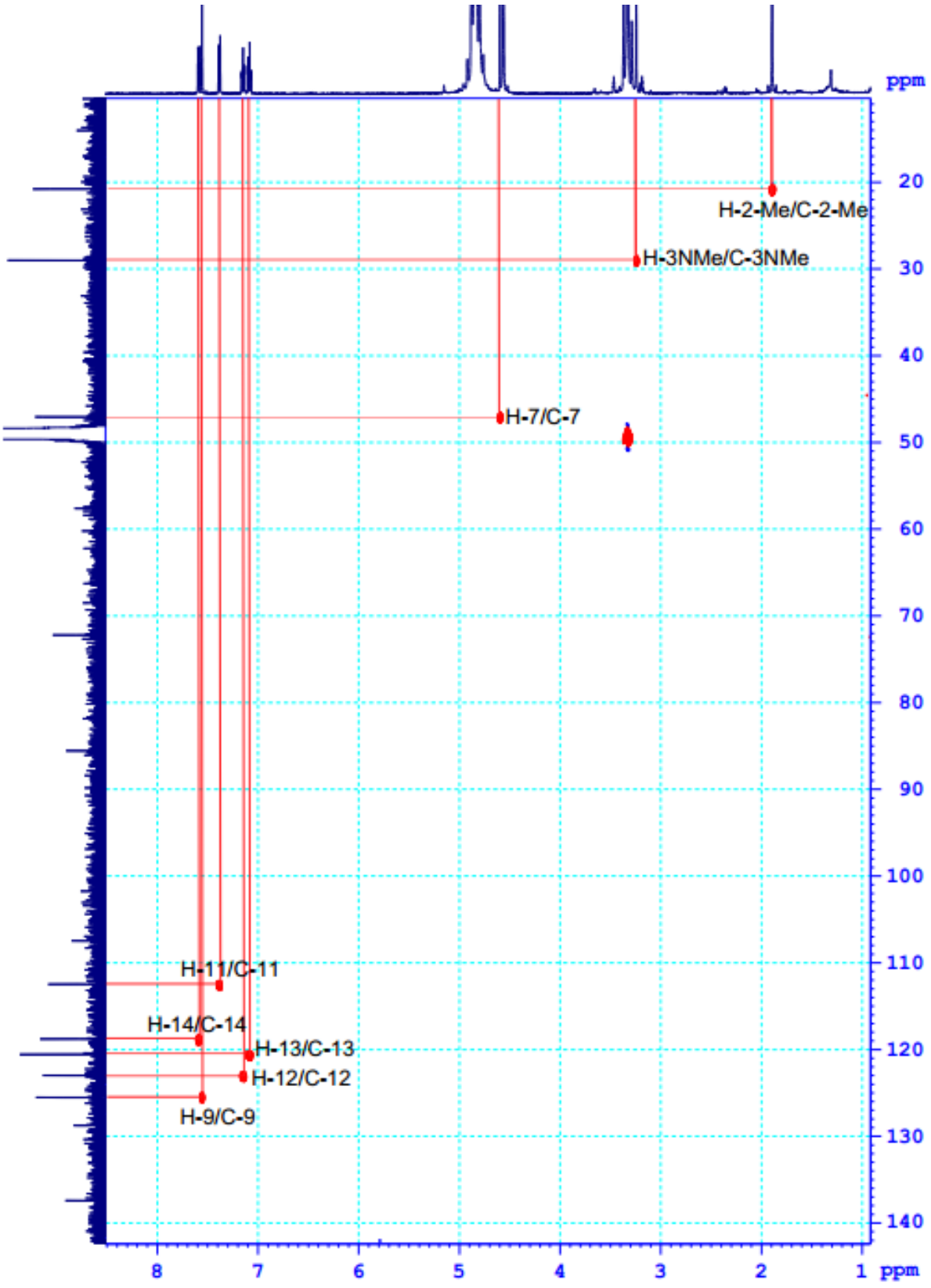
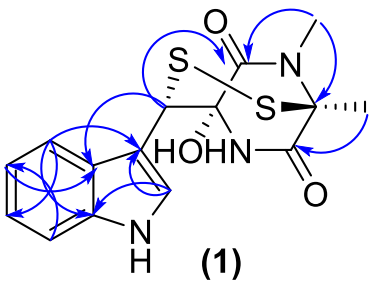


Figure S6:HSQC NMR spectrum of compound (**1**). Measured in CD_3OD



(1)

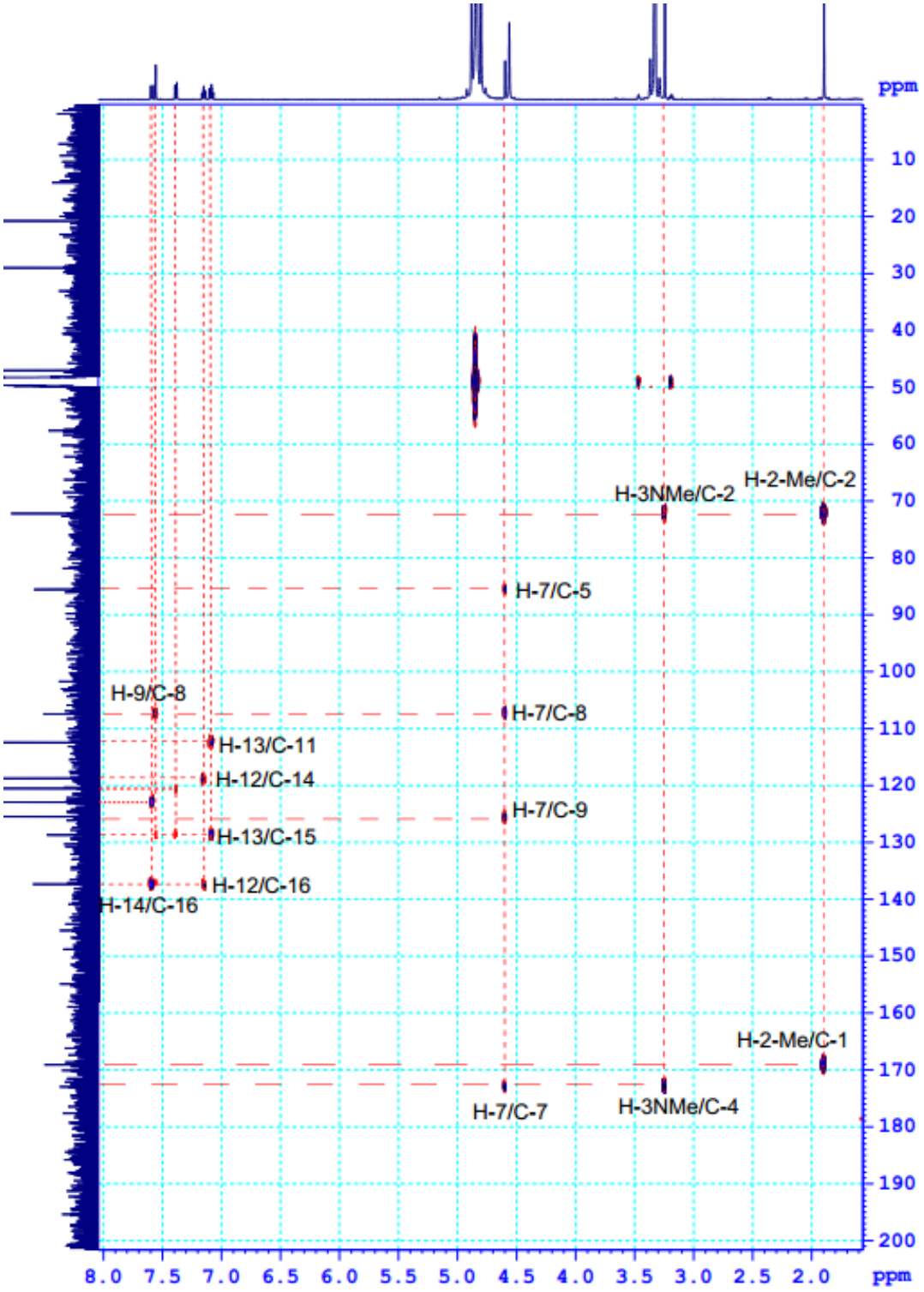


Figure S7:HMBC NMR spectrum of compound (**1**). Measured in CD_3OD
Key HMBC ⟶ correlations

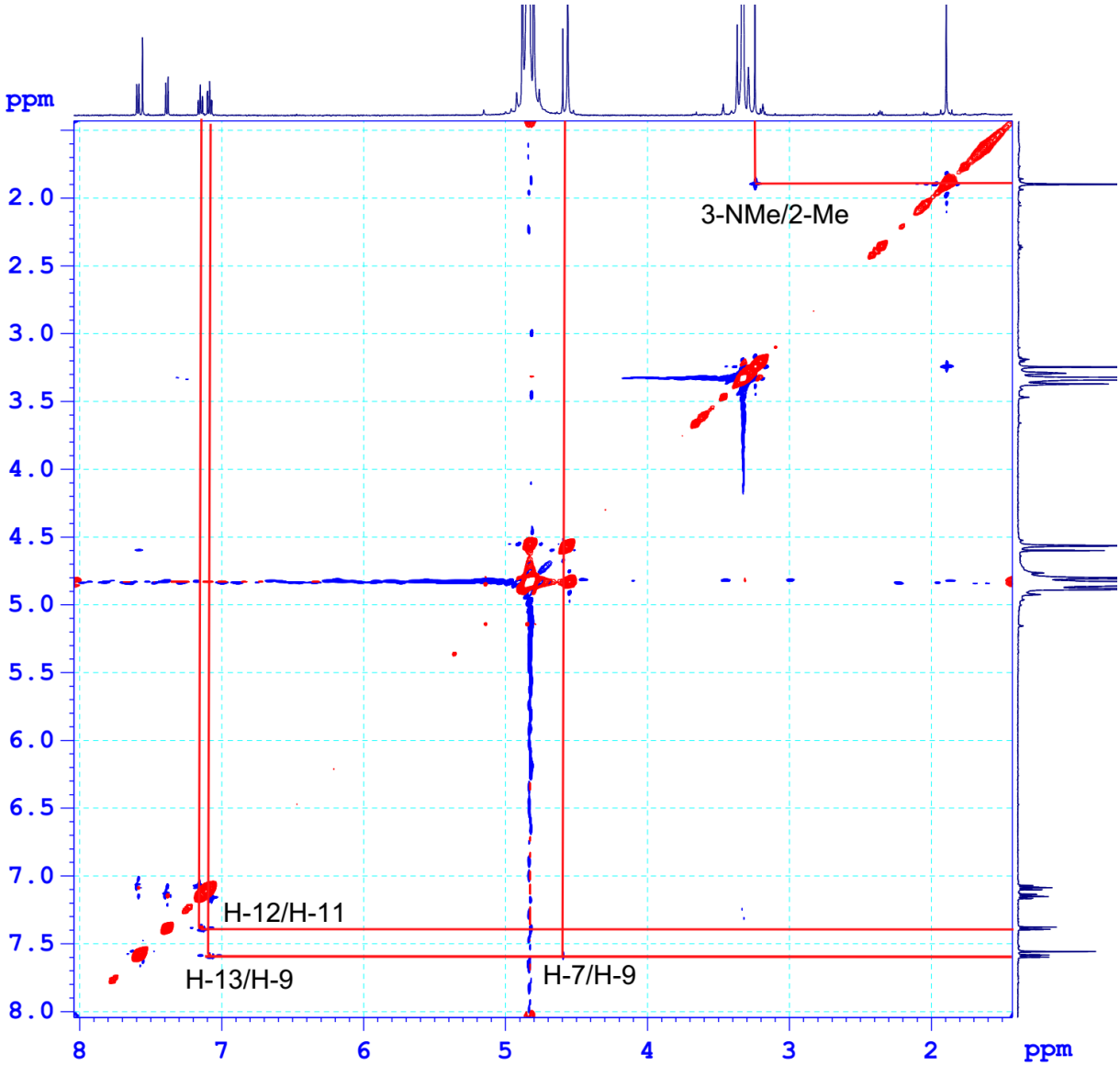


Figure S8:NOESY NMR spectrum of compound (**1**). Measured in CD_3OD

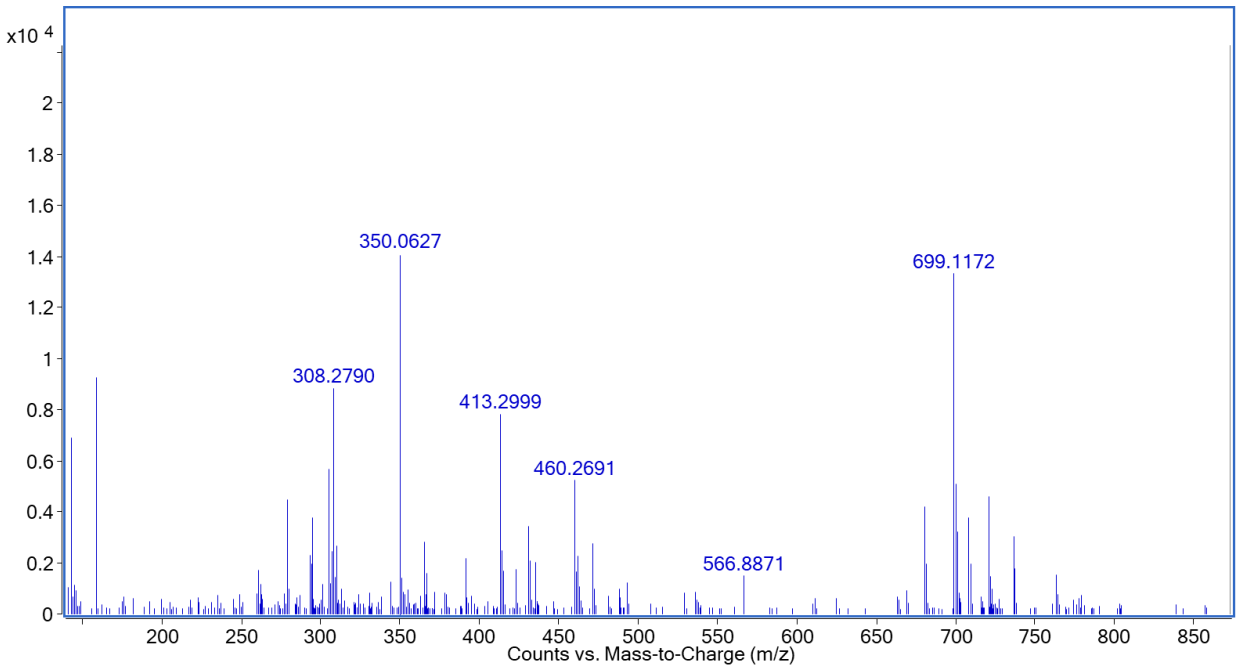


Figure S9:HRESIMS spectrum of compound **(2)**

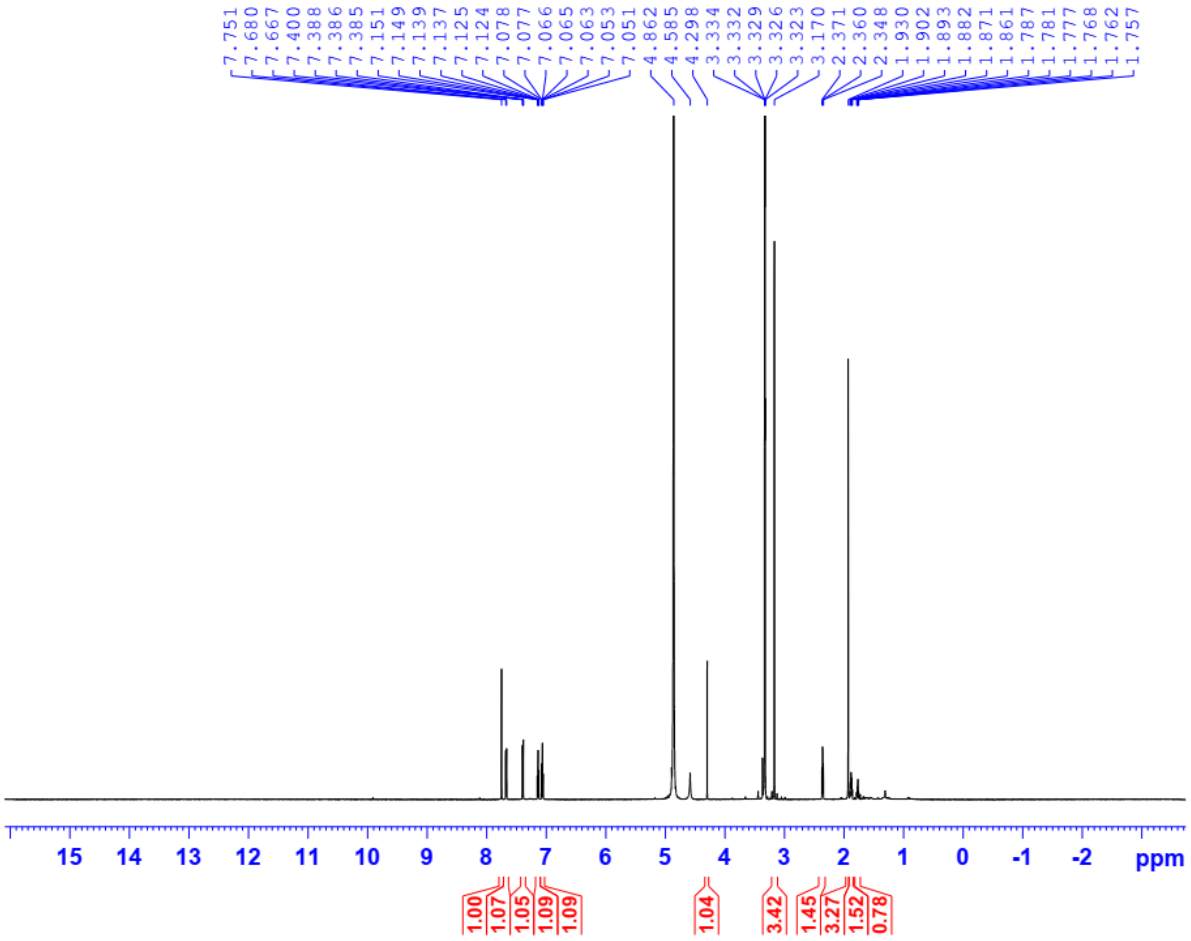


Figure S10:^{1}H NMR spectrum of compound **(2)**. Measured in CD_3OD, 600 MHz

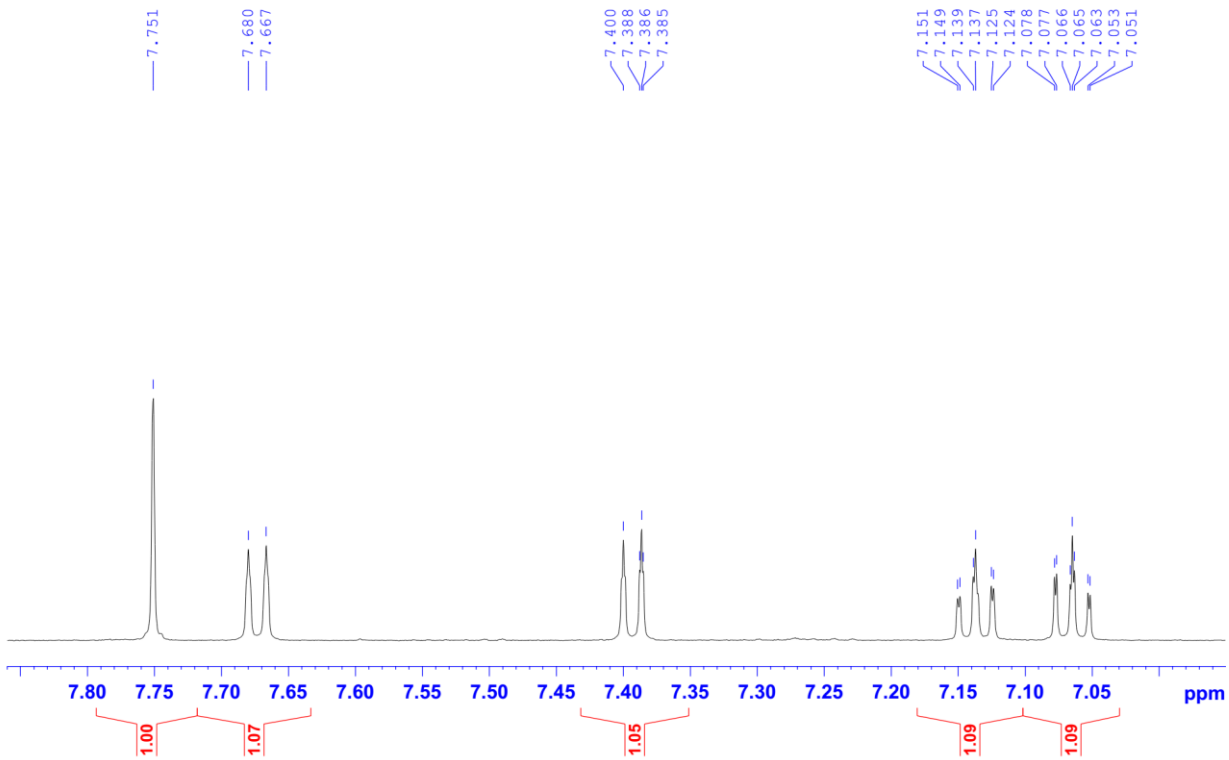


Figure S11: ^{1}H NMR spectrum (7.0-7.9 ppm) of compound **(2)**. Measured in CD_3OD, 600 MHz

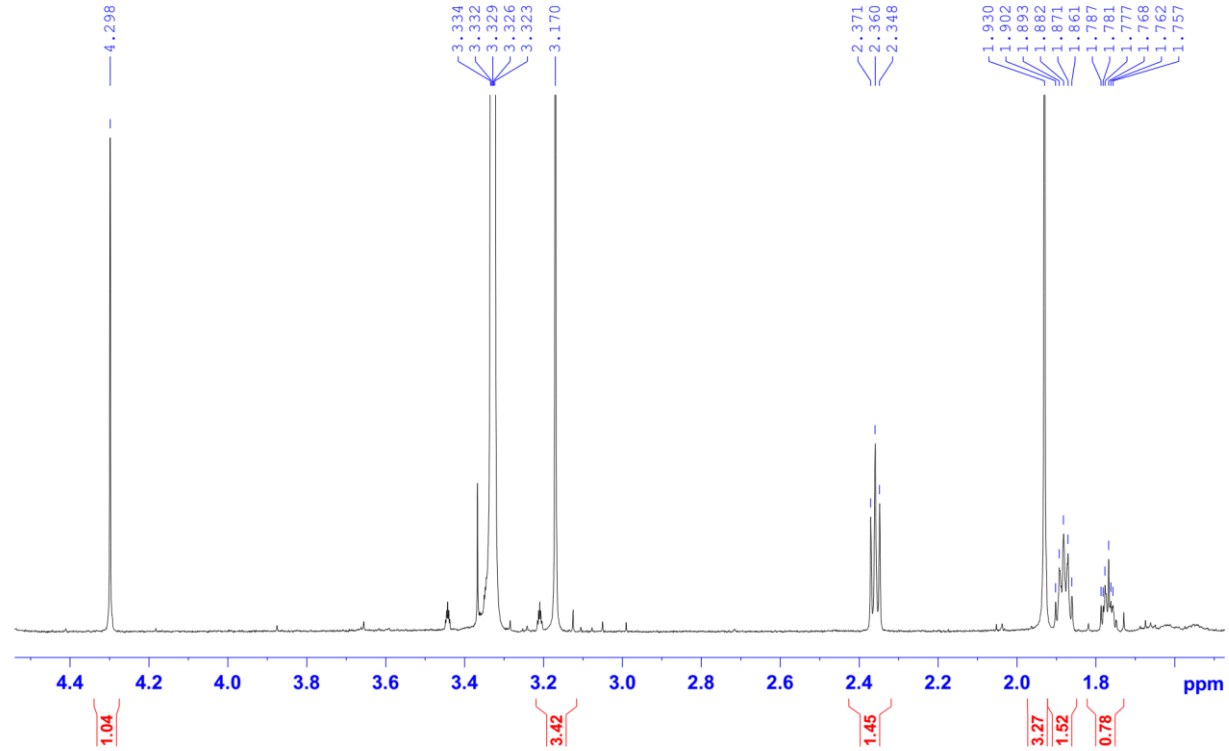


Figure S12: ^{1}H NMR spectrum (1.6 - 4.5 ppm) of compound **(2)**. Measured in CD_3OD, 600 MHz

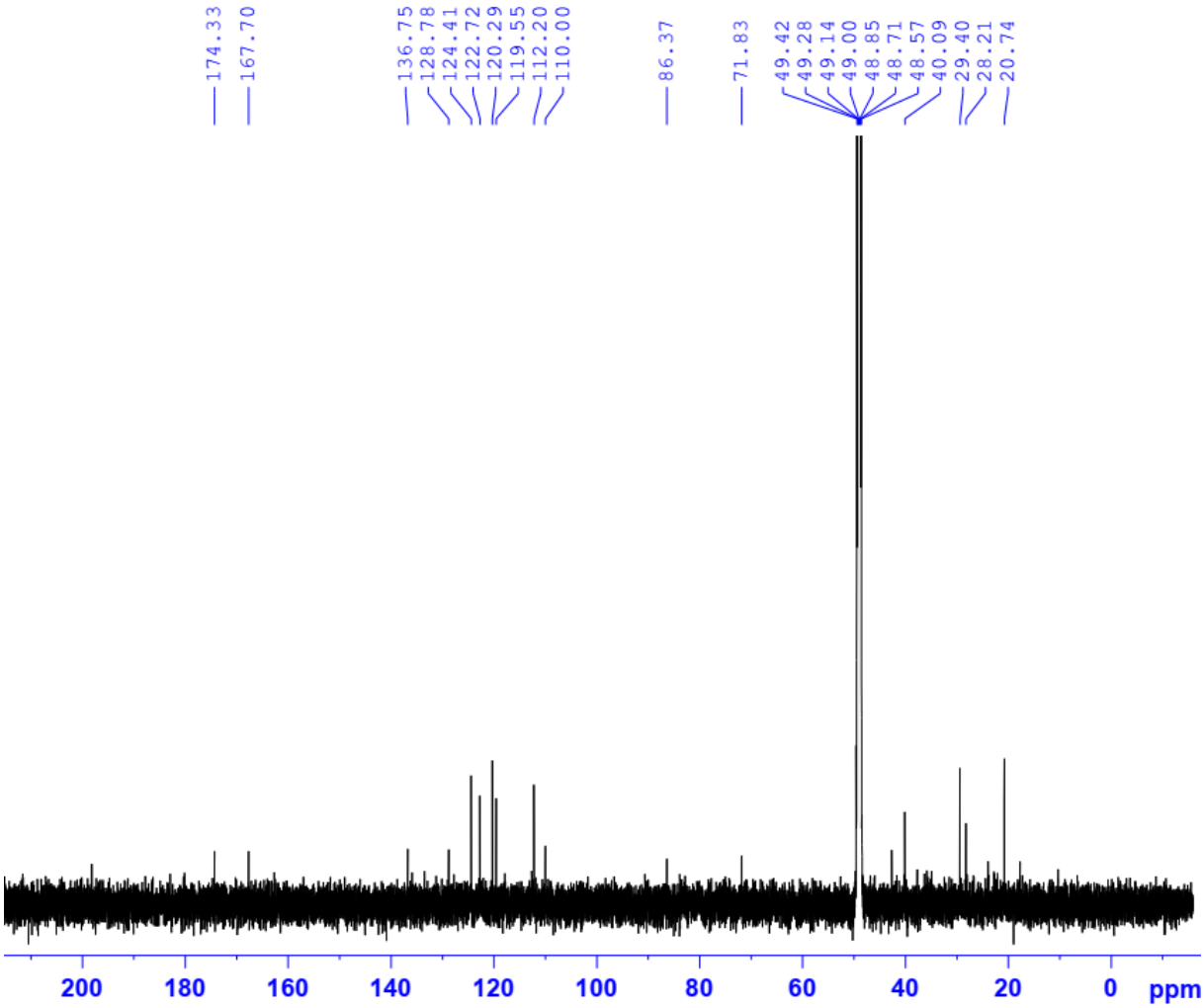


Figure S13: ^{13}C NMR spectrum of compound **(2)**. Measured in CD_3OD, 150 MHz

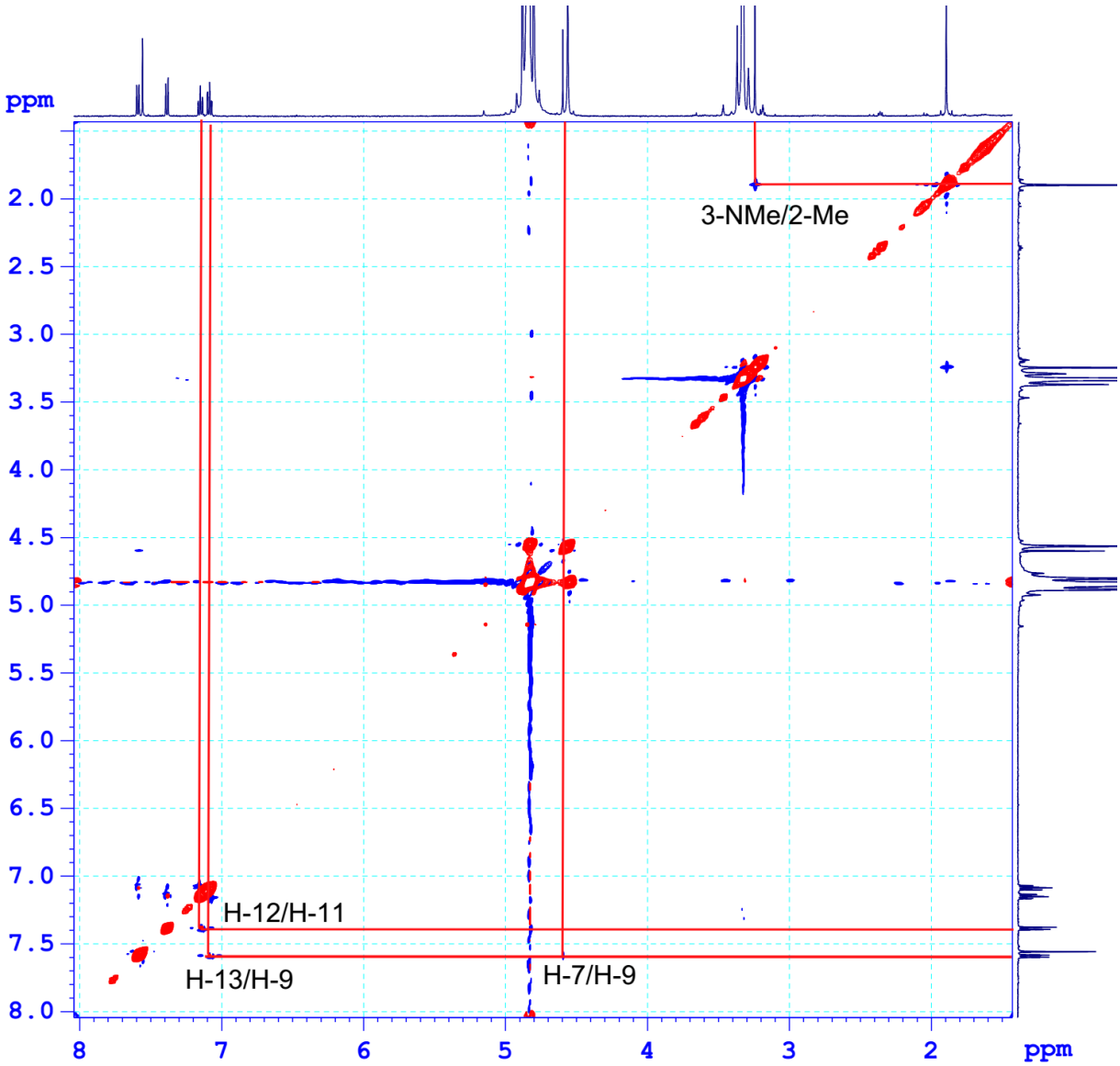
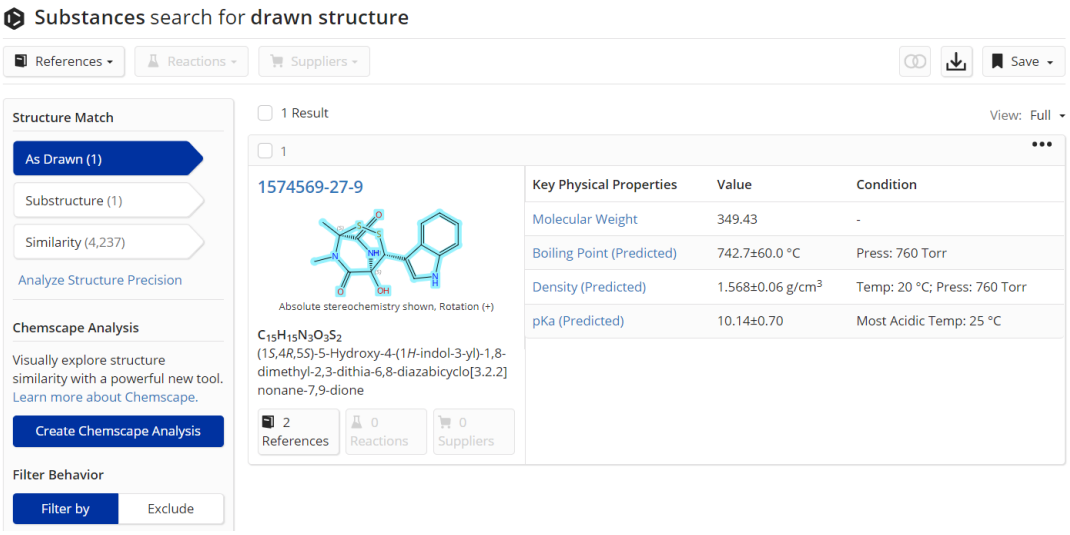


Figure S14:NOESY NMR spectrum of compound (**2**). Measured in CD_3OD

a)



b)

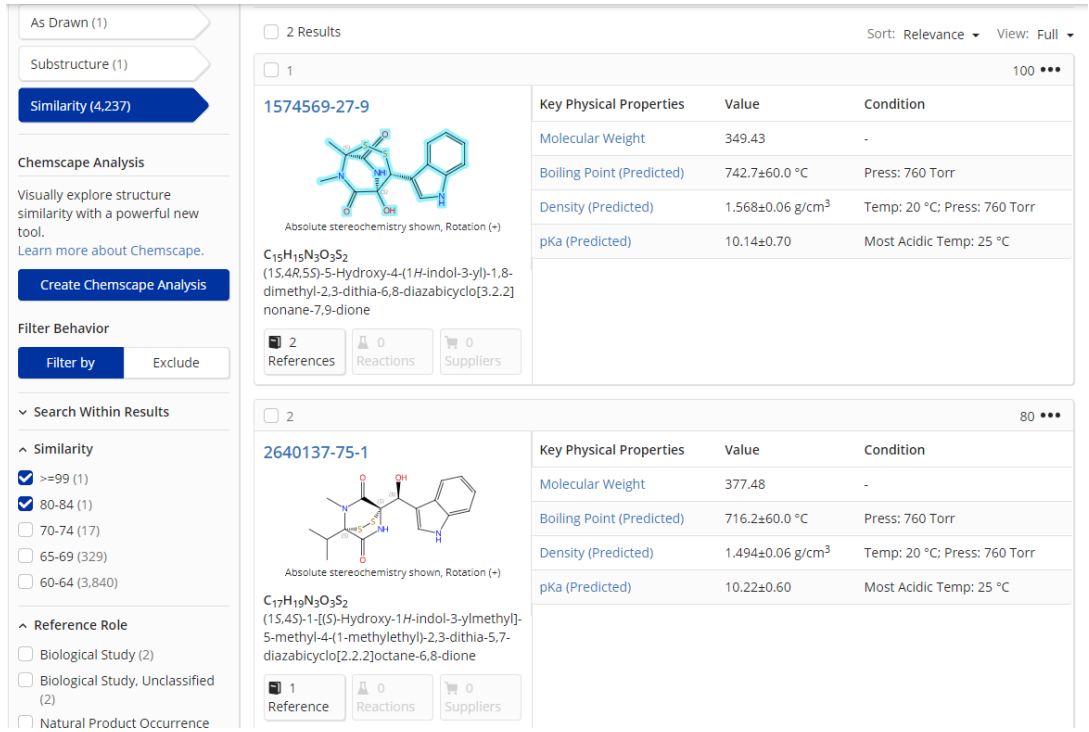
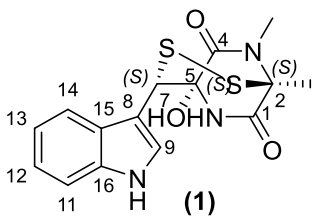
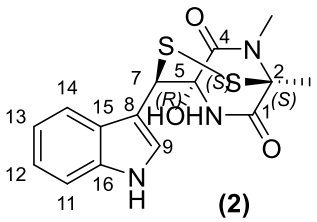


Figure S15: The SciFinder search for compounds **1** and **2**
a) Search for the structure: only compound **2** (2*S*,5*S*,7*R* configuration) was found, meanwhile, compound **1** (2*S*,5*S*,7*S* configuration) was not in the database; b) Search for the compound at the similarity over 80%.

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



7-epi lasiodipline D (1)



Lasiodipline D (2)

No.	δ_C [#,a]	δ_H [#,b]	δ_C [#,a]	δ_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 CD_3OD, [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 (μM)	NO production inhibition (%)	Cell viability (%)
1	10	15.36 ± 2.44	99.53 ± 3.15
	50	45.54 ± 3.87	96.41 ± 5.64
2	10	11.78 ± 1.67	95.77 ± 6.39
	50	42.79 ± 6.28	97.71 ± 7.11
3	10	28.64 ± 1.29	94.29 ± 1.27
	50	40.38 ± 7.98	88.42 ± 1.55
Cardamonin	2.5	46.31 ± 3.30	99.95 ± 4.20
	10	83.87 ± 3.42	97.83 ± 3.83