

New naphthoquinone derivatives from *Fusarium napiforme* of a mangrove plant

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ABSTRACT: Two new naphthoquinone derivatives, 8-hydroxy-astropaquinone B (**1**) and astropaquinone D (**2**) was isolated from *Fusarium napiforme*, endophyte fungus isolated from a mangrove plant, *Rhizophora mucronata* together with a known compound, 3-*O*-methyl-9-*O*-methylfusarubin (**3**). The structures of **1** and **2** were determined by spectroscopic methods, mainly by 2D NMR spectroscopic analyses. Compounds **1**, **2** and **3** exhibited antimicrobial activities and phytotoxicities.

Keywords: Endophyte; naphthoquinone; *Fusarium napiforme*; astropaquinone; antimicrobial activity, phytotoxicity.

List of supporting information

Experimental

3.1. General experimental procedures

Optical rotations were measured with a Horiba SEPA-300 polarimeter, and UV and IR spectra were recorded with Shimadzu UV-1800 and Jasco J-20A (JASCO Co., Tokyo, Japan) spectrophotometers, respectively. Mass spectra were obtained with a Synapt G2. NMR spectra were recorded on a JEOL ECZ-600 at 600 MHz for ^1H and 150 MHz for ^{13}C . Chemical shifts are given on a δ (ppm) scale with TMS as an internal standard. ^1H , ^{13}C , COSY, HMQC and HMBC spectra were recorded using JEOL standard pulse sequences. Column chromatography was conducted on silica gel 60. TLC was carried out on Merck precoated silica gel 60 F₂₅₄ plates.

3.2 Fungal material and fermentation

The fungal strain of IP-28 was isolated from a surface sterilized branch of *Rhizophora mucronata*, collected in a cost in Takalar Regency, South Sulawesi Province, Indonesia (southern latitude: 5°36'27.65"; east longitude: 119°28'22.12"). Fungal strains IP-28 was identified as *Fusarium napiforme* by the using a DNA analysis of the 18S rDNA regions. They have been deposited at our laboratory in the Faculty of Agriculture of Yamagata. IP-28 strain was cultured on slants with PDA at 28 °C for 5 days. Fermentation was carried out in

Erlenmeyer flasks (1000 mL) containing 50 g of rice and water (70 mL per flask; total of 2000 g). After autoclaving, each flask was inoculated with hyphae inoculum and incubated at 25 °C for one month. The mycelia and solid rice medium were extracted with MeOH and then was concentrated under reduced pressure to give a crude extract (6.0 g).

Figure S1. ^1H - ^1H COSY, HMBC and NOE correlations for **1** and **2**.

Figure S2. Key NOE correlation for **1**.

Figure S3. The ^1H -NMR spectrum of **1** (600 MHz, CDCl_3).

Figure S4. The ^{13}C -NMR spectrum of **1** (150 MHz, CDCl_3).

Figure S5. The ^1H - ^1H COSY spectrum of **1** (600 MHz, CDCl_3).

Figure S6. The HMQC spectrum of **1** (600 MHz, CDCl_3).

Figure S7. The HMBC spectrum of **1** (600 MHz, CDCl_3).

Figure S8. The NOE spectrum of **1** (600 MHz, CDCl_3).

Figure S9. The NOE spectrum of **1** (600 MHz, CDCl_3).

Figure S10. The ^1H -NMR spectrum of **2** (600 MHz, CD_3OD).

Figure S11. The ^{13}C -NMR spectrum of **2** (150 MHz, CD_3OD).

Figure S12. The ^1H - ^1H COSY spectrum of **2** (600 MHz, CDCl_3).

Figure S13. The HMQC spectrum of **2** (600 MHz, CD_3OD).

Figure S14. The HMBC spectrum of **2** (600 MHz, CD_3OD).

Figure S15. The NOE spectrum of **1** (600 MHz, CDCl_3).

Figure S.16. Effect of compounds **1**, **2** and **3** on the Growth of Lettuce Seedlings.

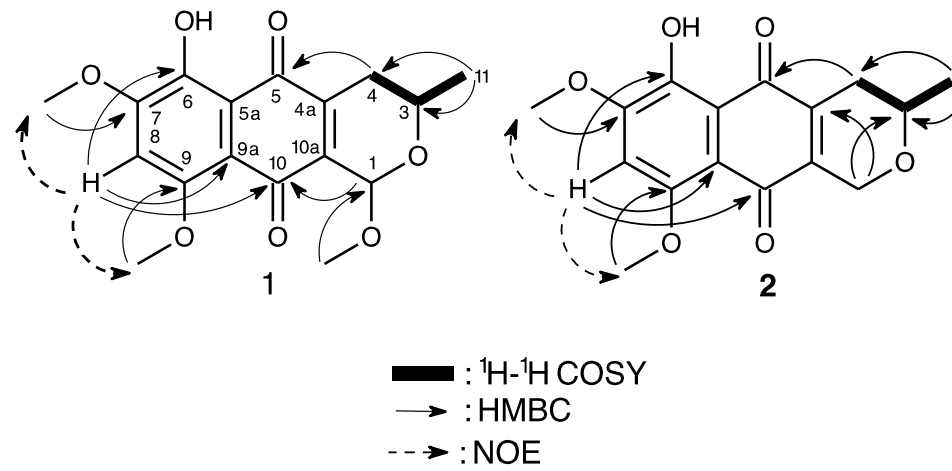


Figure S1. ^1H - ^1H COSY, HMBC and NOE correlations for **1** and **2**.

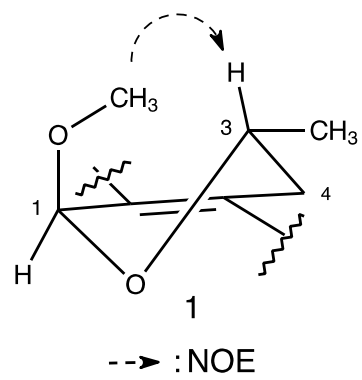


Figure S2. Key NOE correlation for **1**.

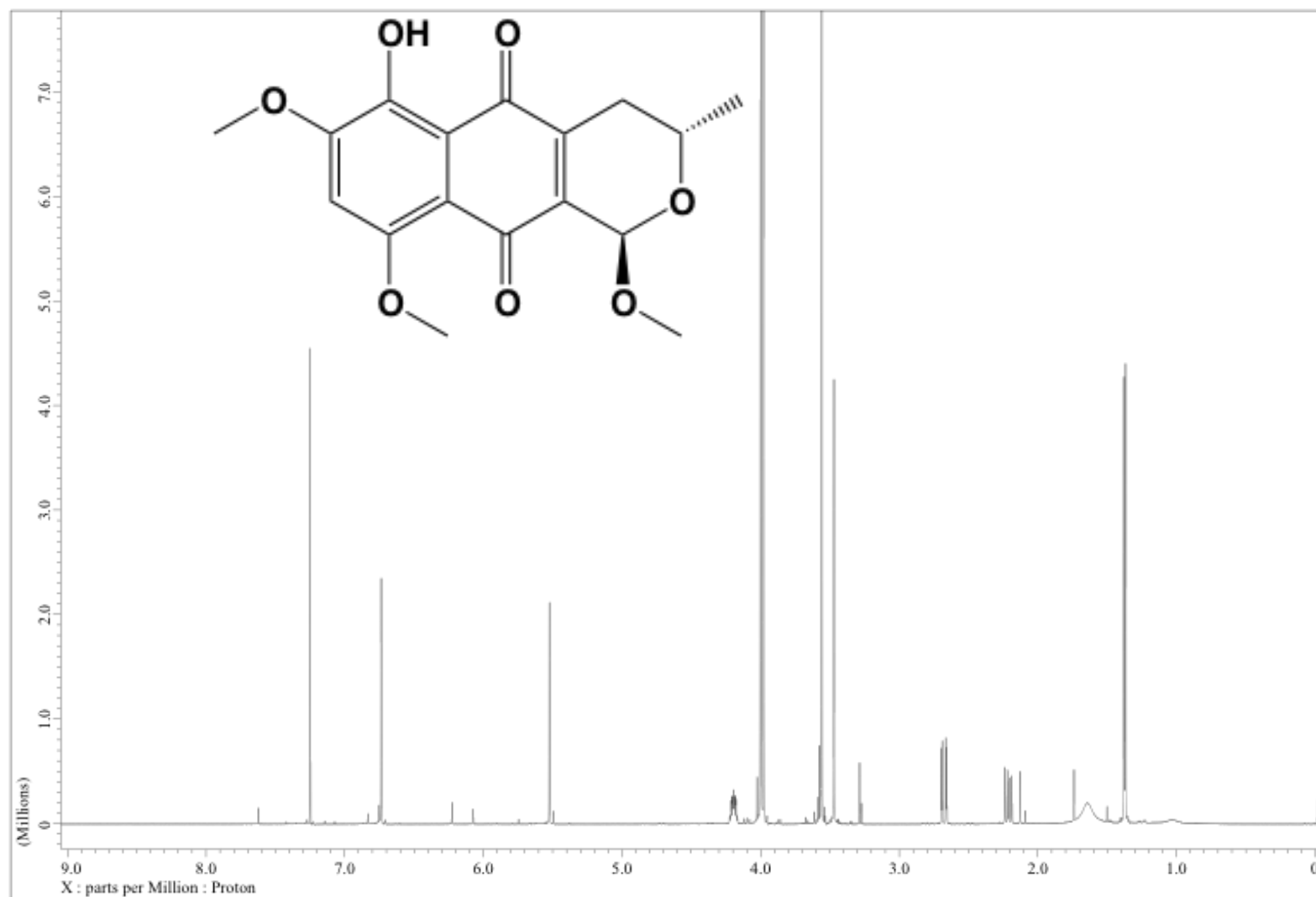


Figure S3. The $^1\text{H-NMR}$ spectrum of **1** (600 MHz, CDCl_3).

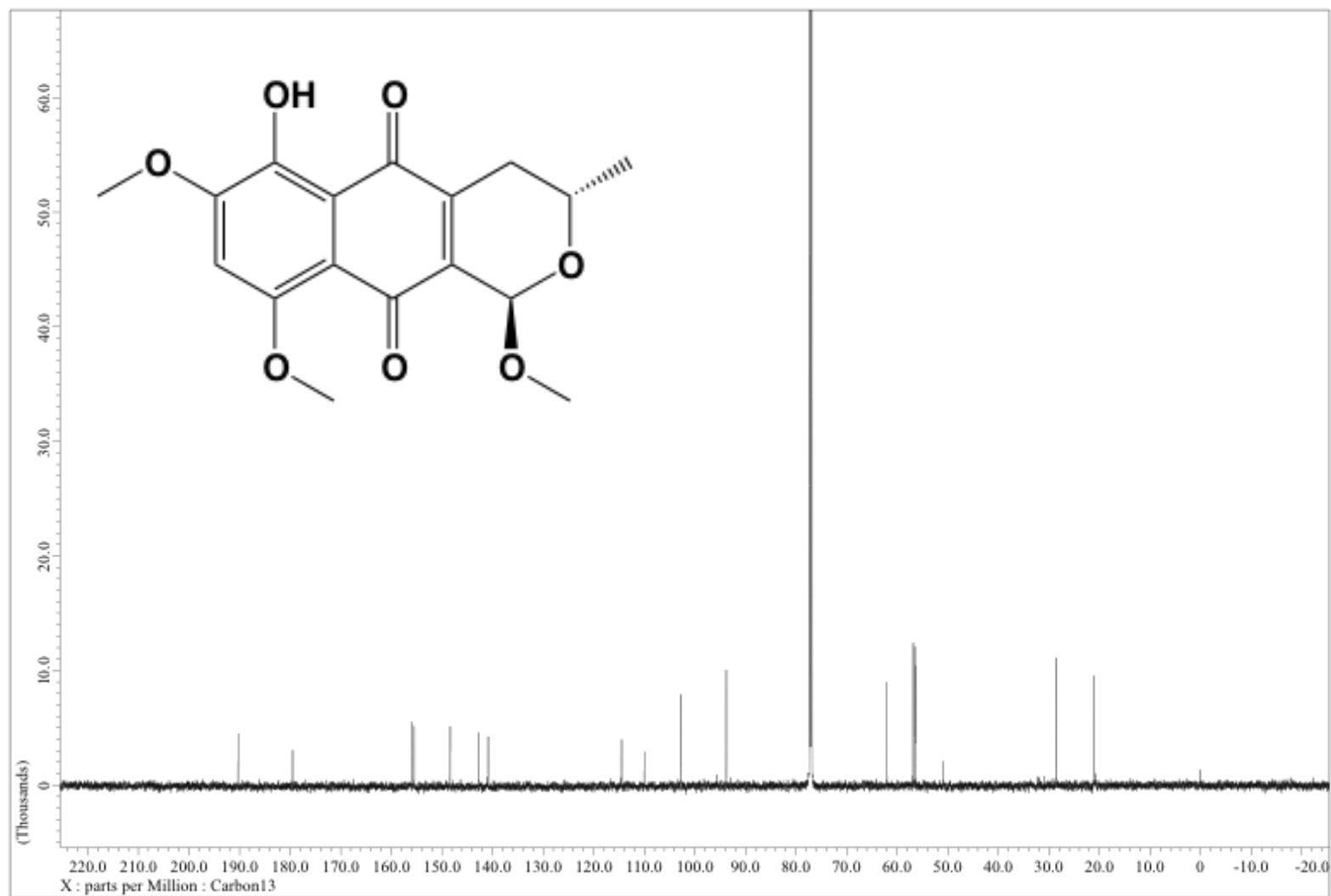


Figure S4. The ^{13}C -NMR spectrum of **1** (150 MHz, CDCl_3).

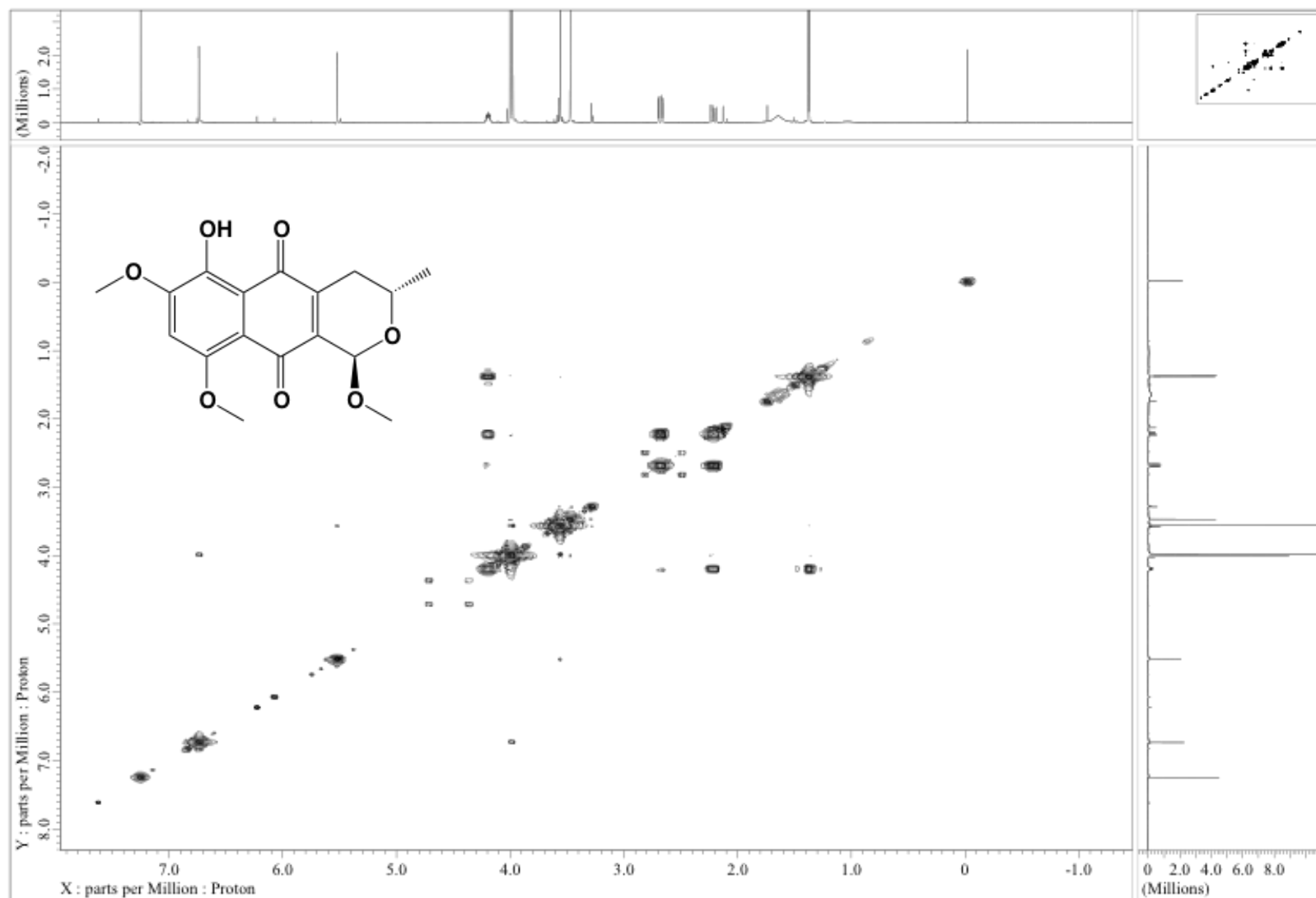


Figure S5. The ^1H - ^1H COSY spectrum of **1** (600 MHz, CDCl_3).

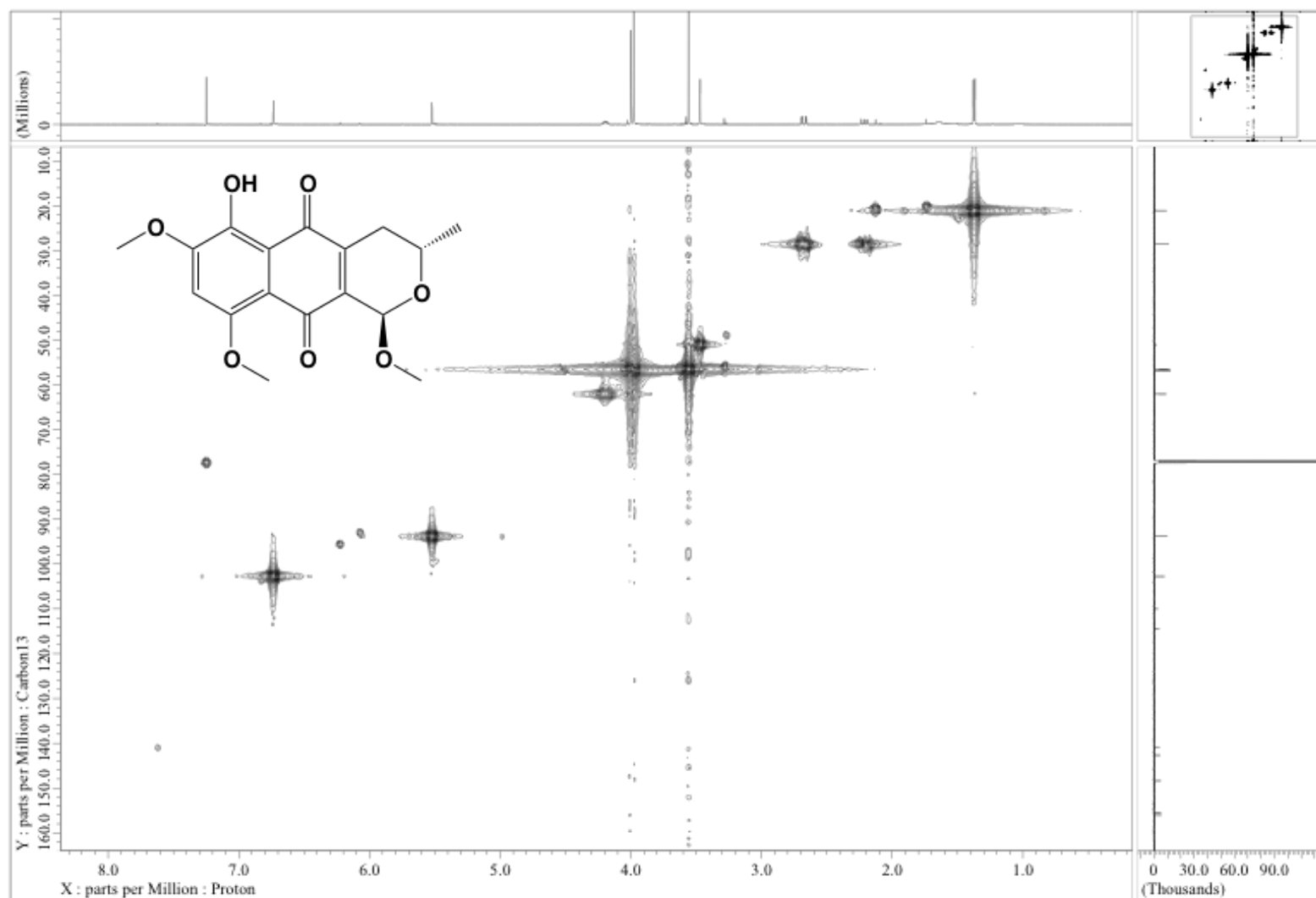


Figure S6. The HMQC spectrum of **1** (600 MHz, CDCl₃).

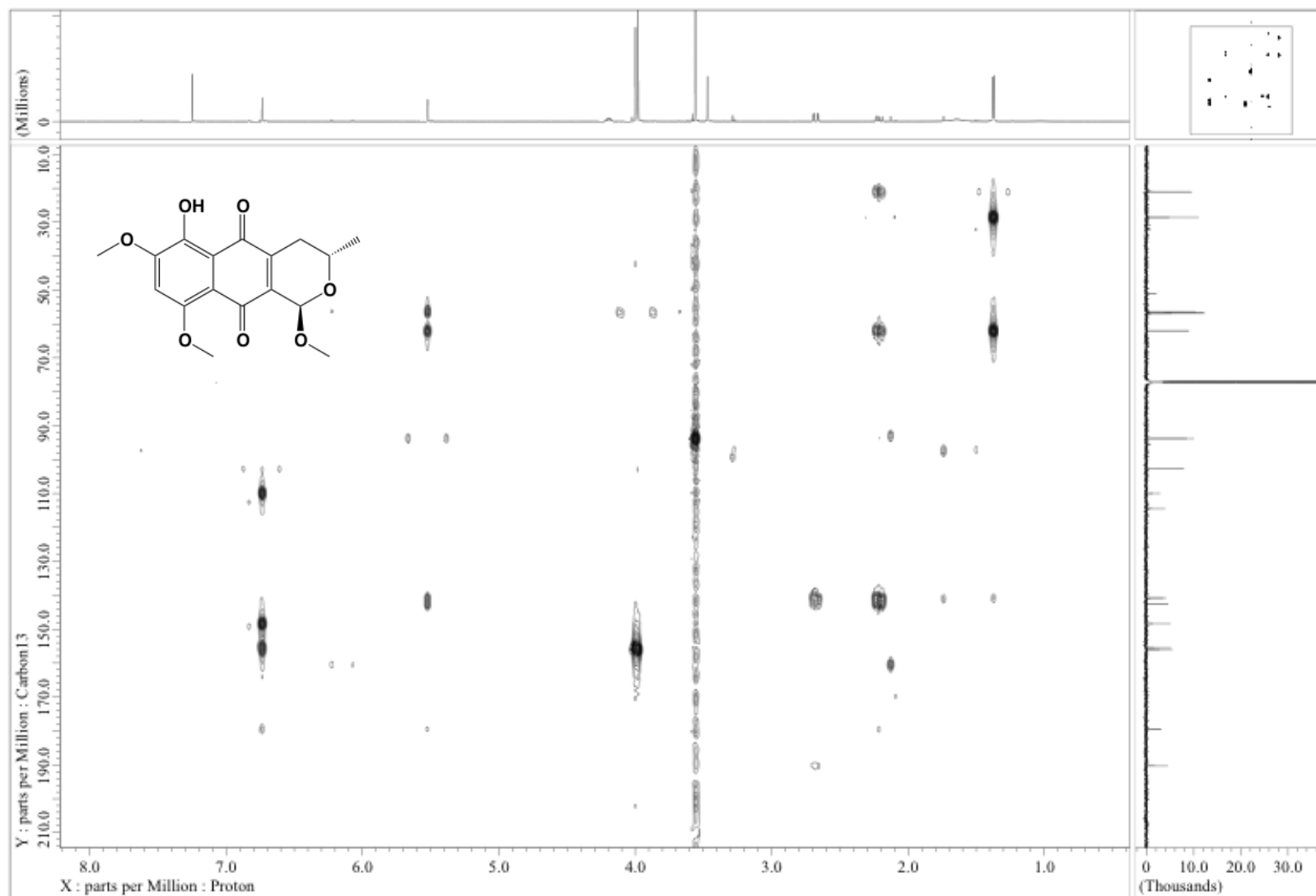


Figure S7. The HMBC spectrum of 1 (600 MHz, CDCl₃).

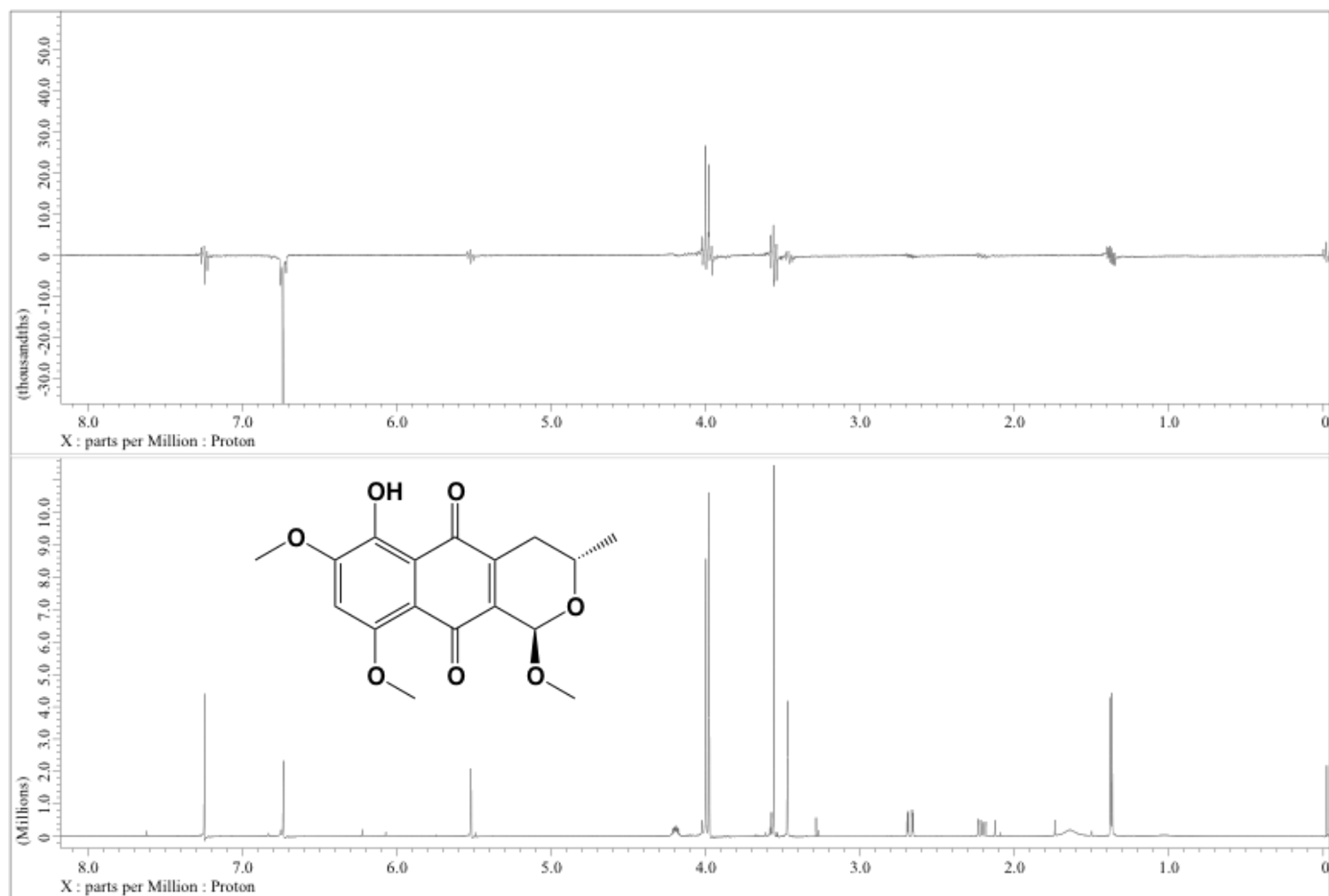


Figure S8. The NOE spectrum of **1** (600 MHz, CDCl₃).

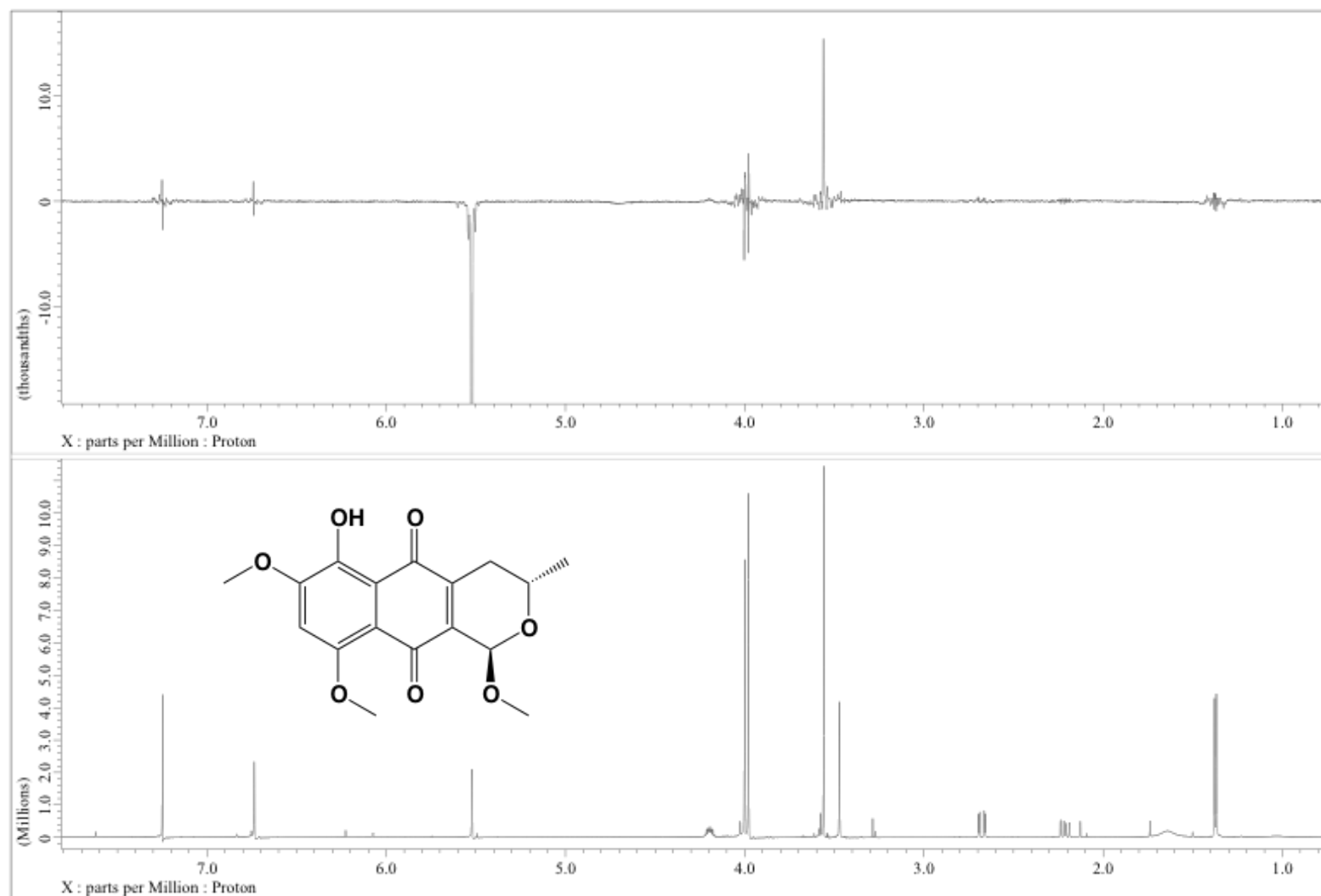


Figure S9. The NOE spectrum of **1** (600 MHz, CDCl₃).



Figure S10. The $^1\text{H-NMR}$ spectrum of **2** (600 MHz, CD_3OD).

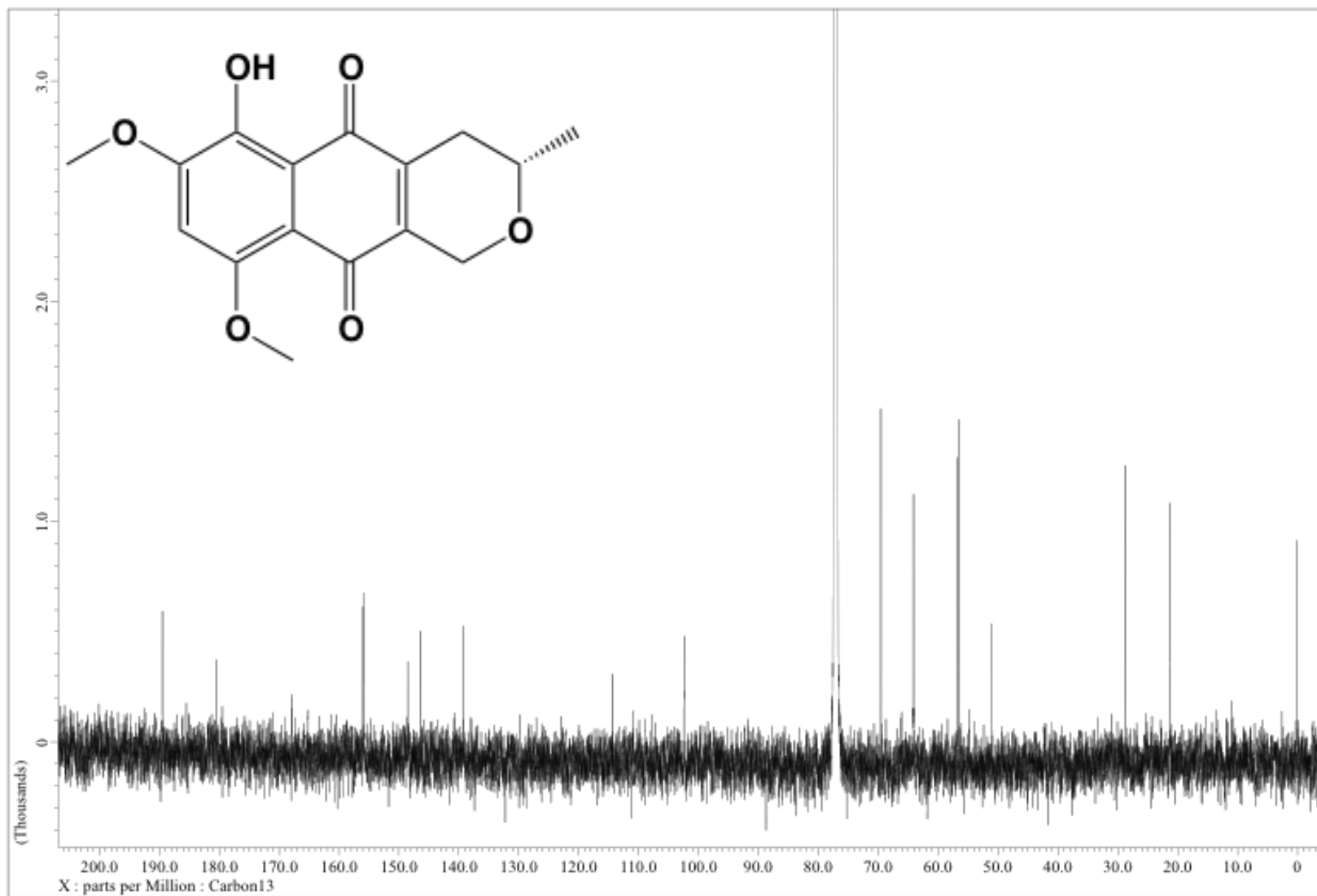


Figure S11. The ^{13}C -NMR spectrum of **2** (150 MHz, CD_3OD).

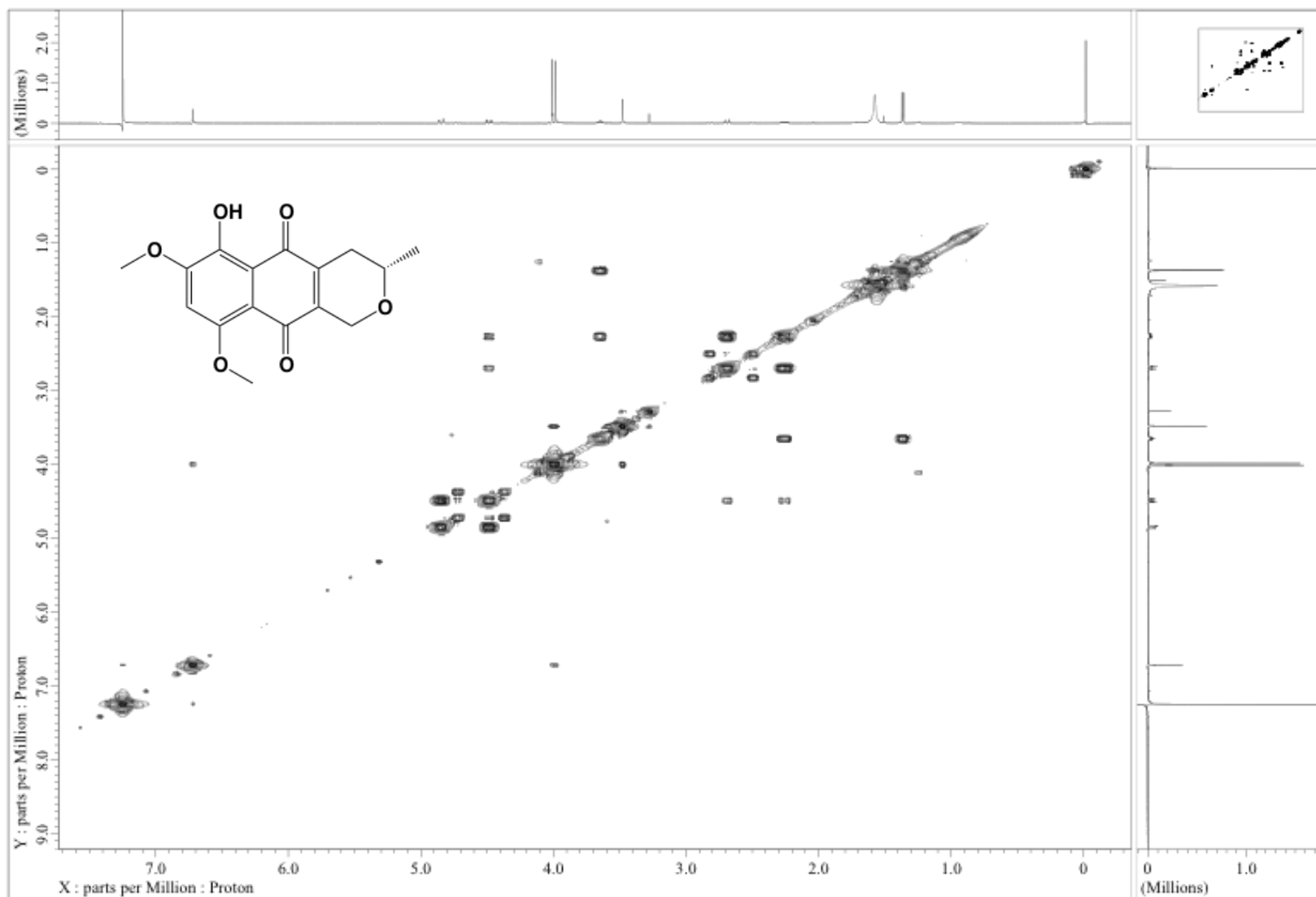


Figure S12. The ^1H - ^1H COSY spectrum of **2** (600 MHz, CDCl_3).

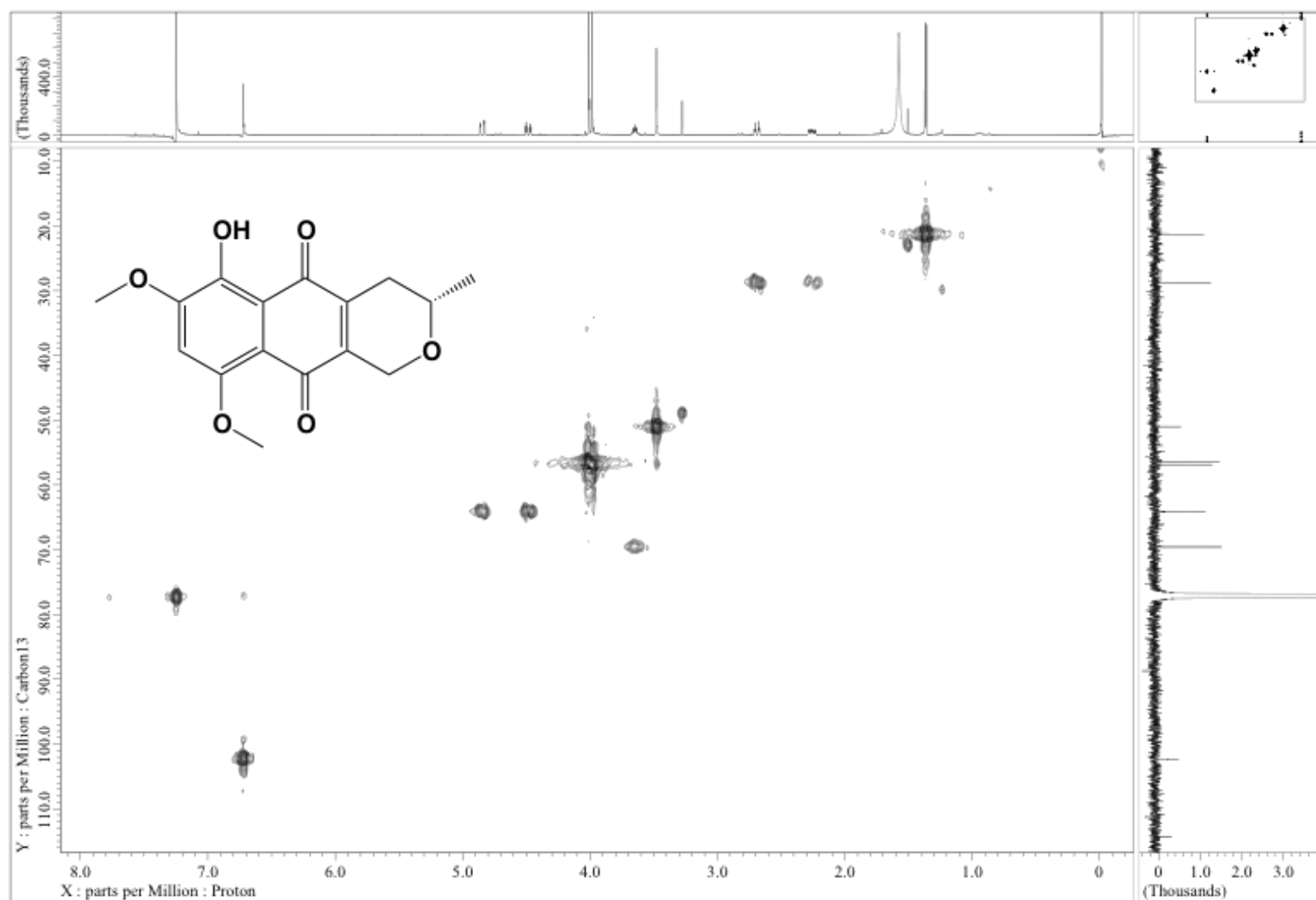


Figure S13. The HMQC spectrum of **2** (600 MHz, CD₃OD).

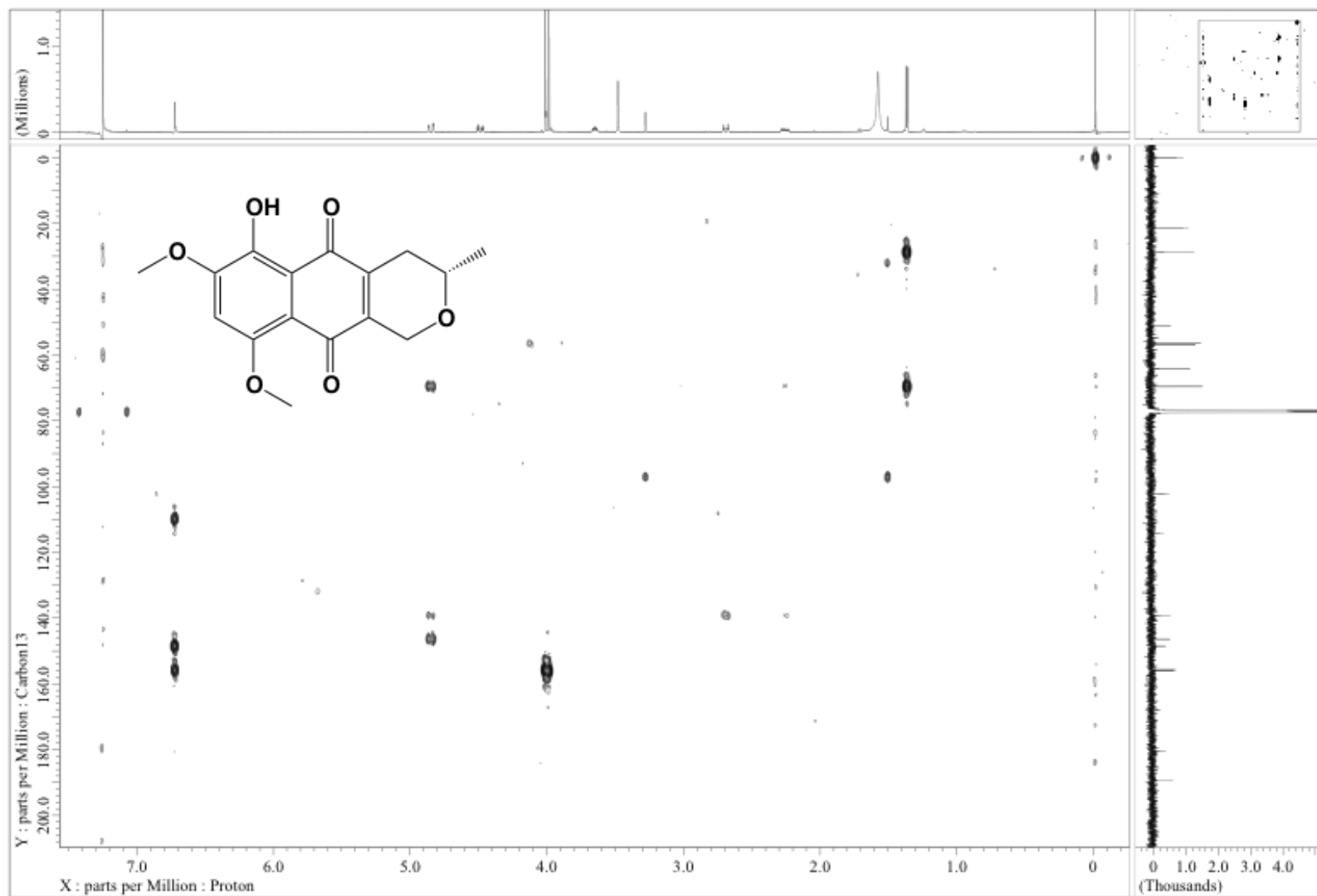
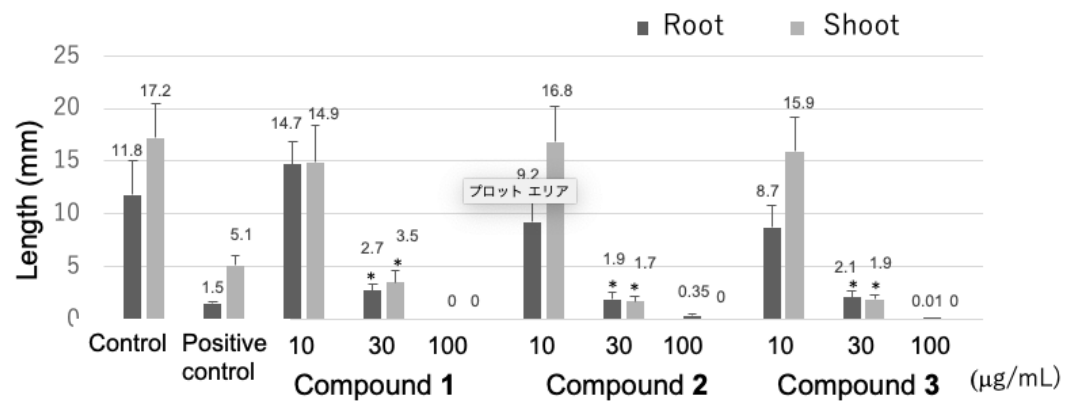


Figure S14. The HMBC spectrum of **2** (600 MHz, CD₃OD).



Figure S15. The NOE spectrum of **1** (600 MHz, CDCl₃).



Results are the mean \pm standard deviation (n=15). [*p < 0.01 (growth inhibition) versus control] and positive control: 2,4-dichlorophenoxyacetic acid (0.3 μ g/mL).

Figure S.16. Effect of compounds 1, 2 and 3 on the Growth of Lettuce Seedlings.