

Ent*-homocyclopiamine B, a prenylated indole alkaloid of biogenetic interest from the endophytic fungus *Penicillium concentricum

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LC-MS

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Figure S11. Growth inhibition by 50 nmoles of kanamycin (Km) or *ent*-homocyclopiamine B (**1**) against bacterial strains on agar plates. Solvent controls did not result in zones of inhibition.

IND-ALK-2 #7 RT: 0.17 AV: 1 NL: 5.52E6
T: FTMS + p ESI sid=35.00 Full ms [400.00-600.00]

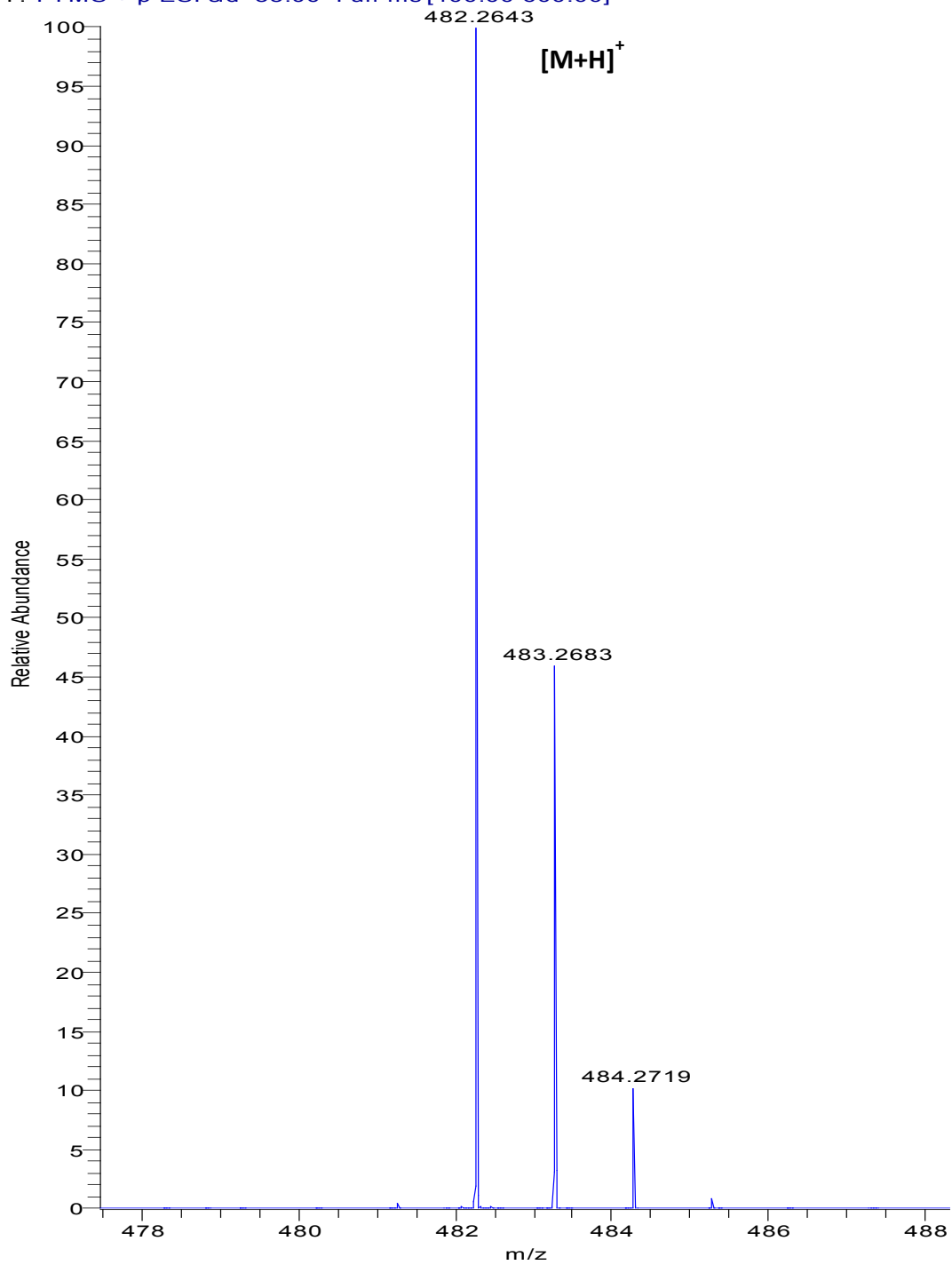


Figure S1. HRESIMS spectrum of compound **1**

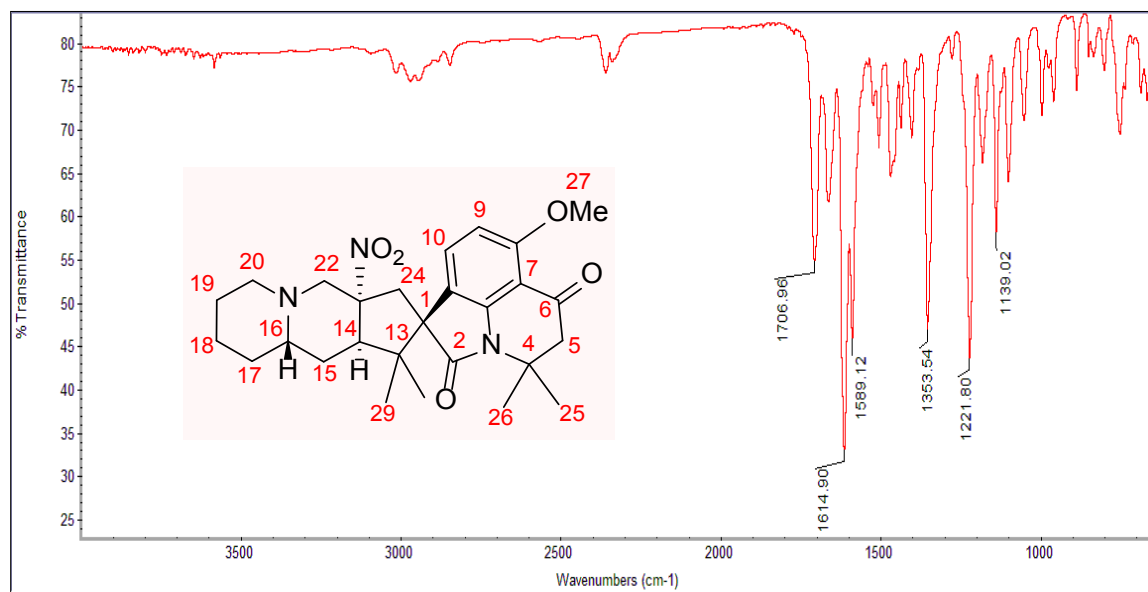


Figure S2. IR spectrum of compound **1**.

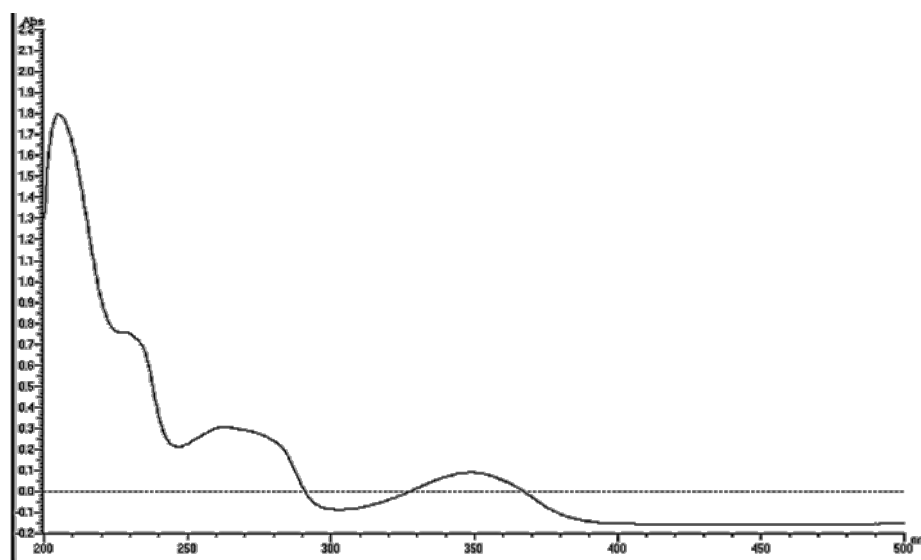


Figure S3. UV/vis spectrum of compound **1**.

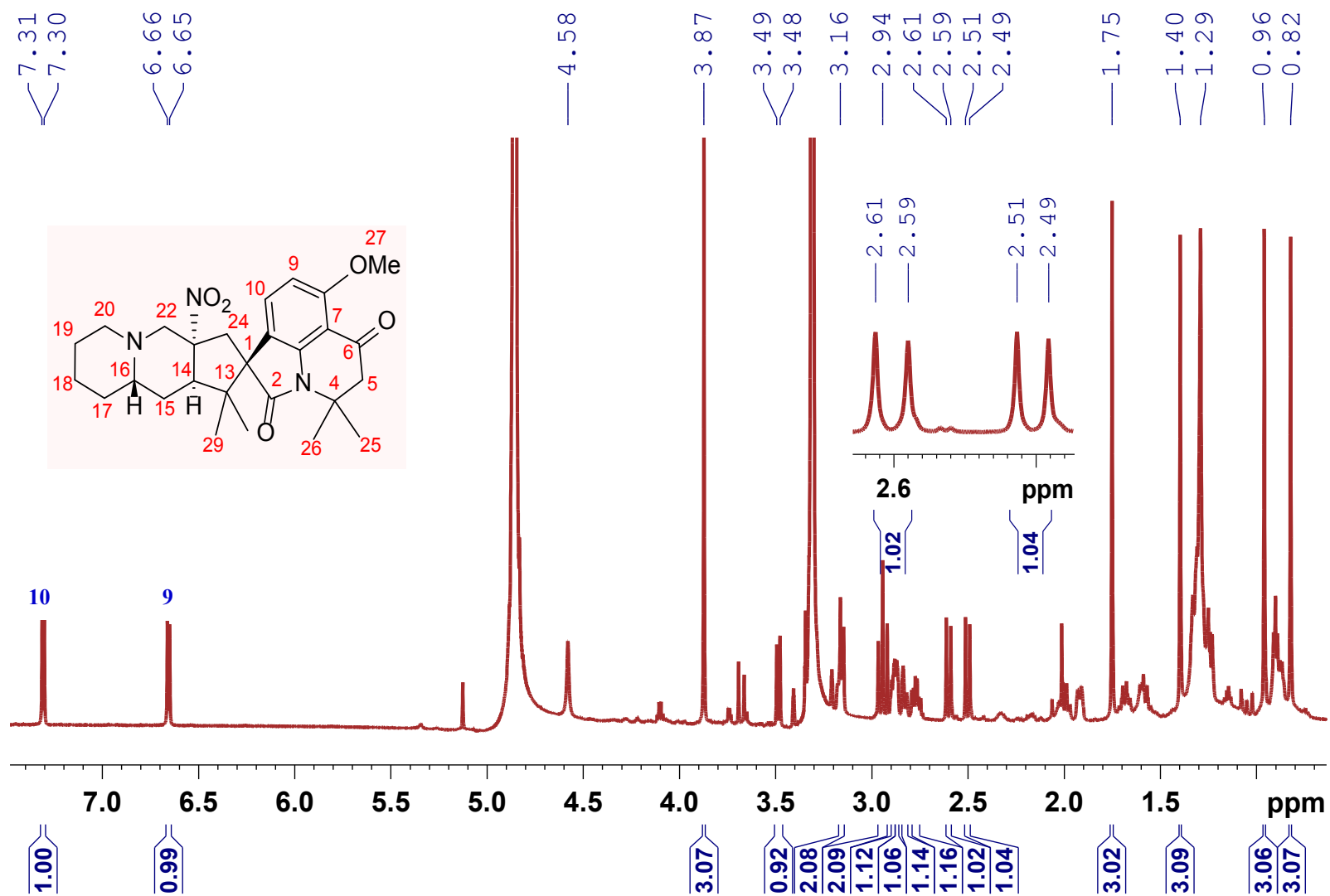


Figure S4. ¹H NMR spectrum of compound **1** in CD₃OD-*d*₄ (700 MHz)

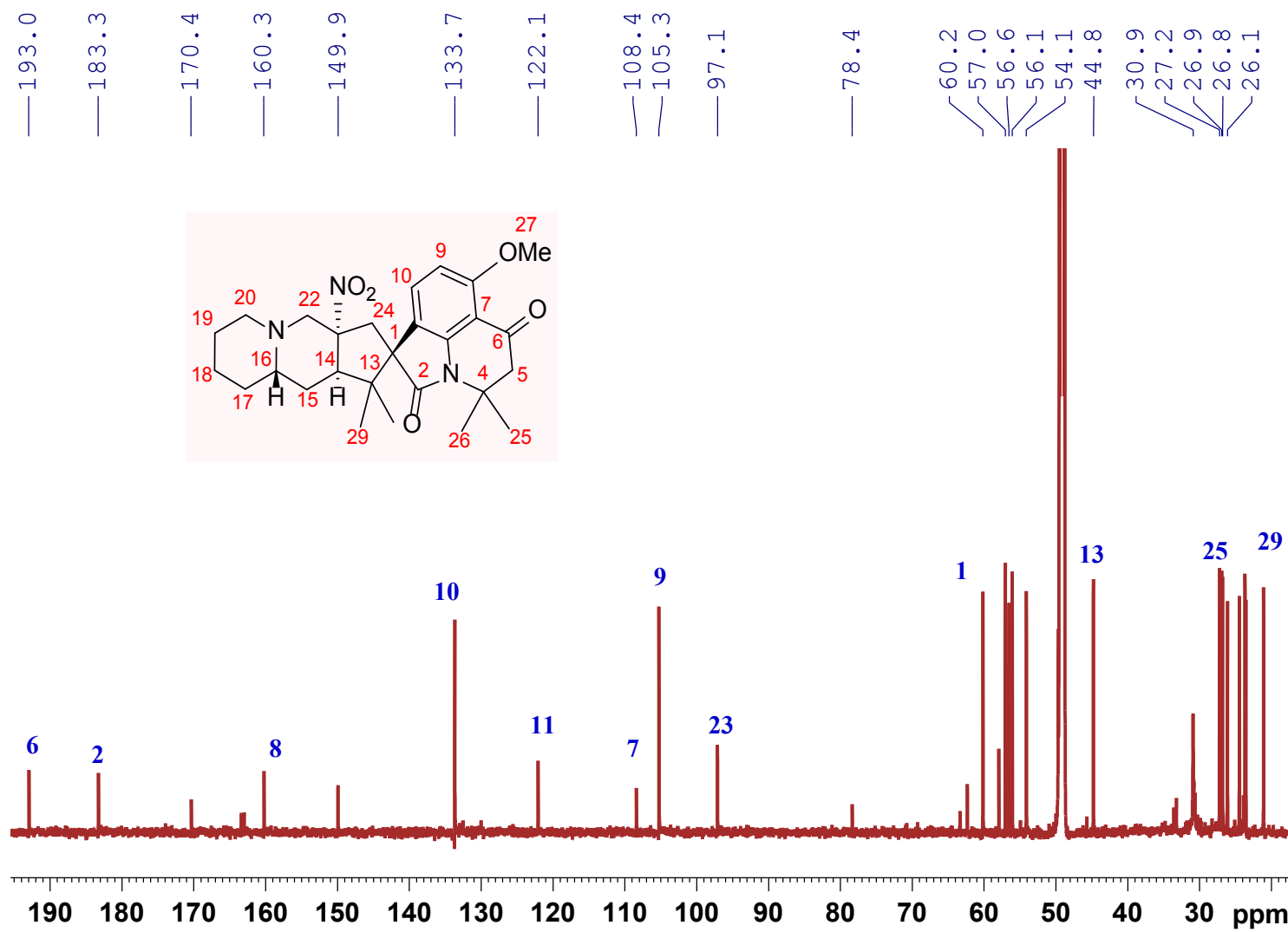


Figure S5. ¹³C NMR spectrum of compound **1** in CD₃OD-*d*₄ (175 MHz)

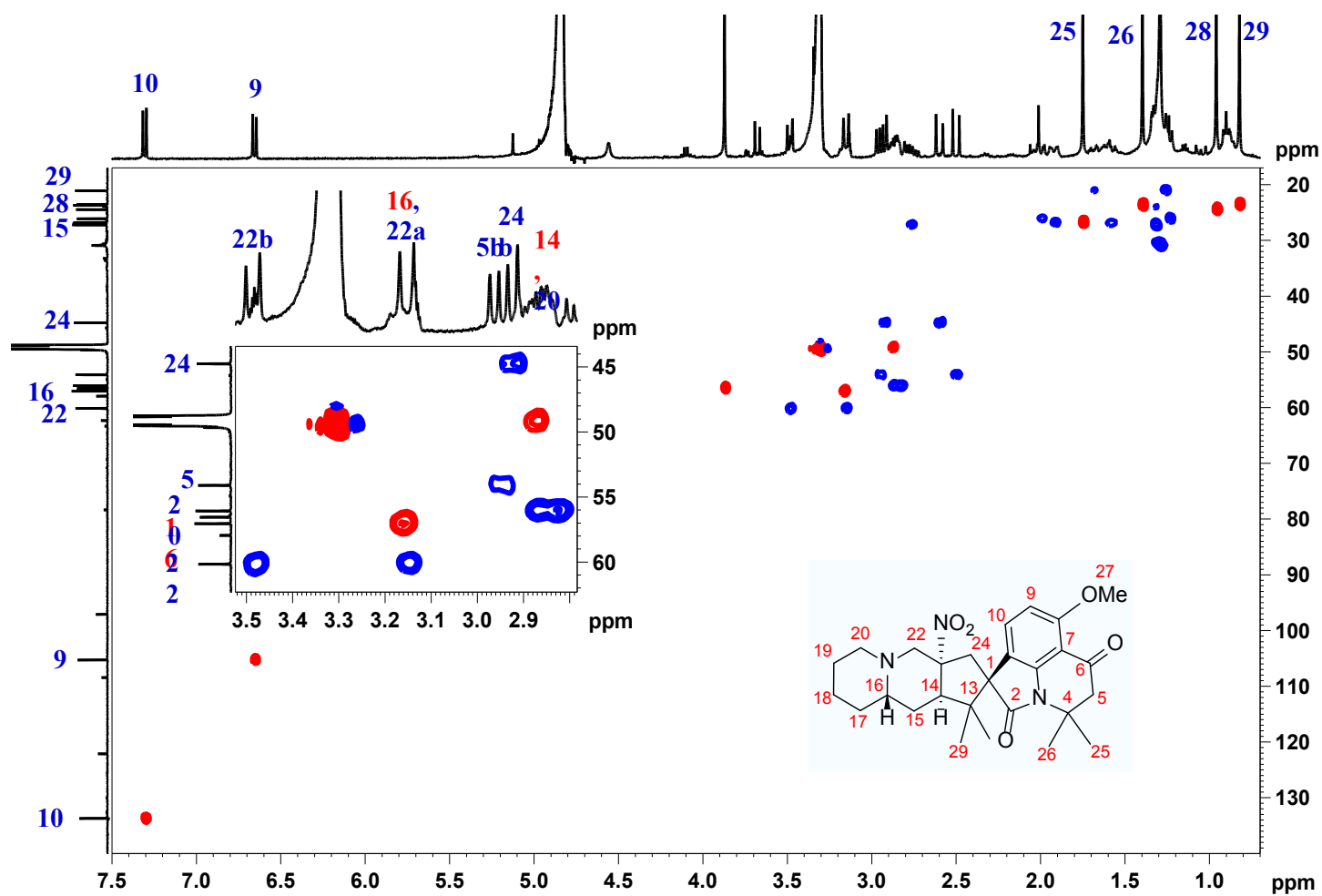


Figure S6. HSQC spectrum of compound 1 CD₃OD-*d*₄ (700 MHz)

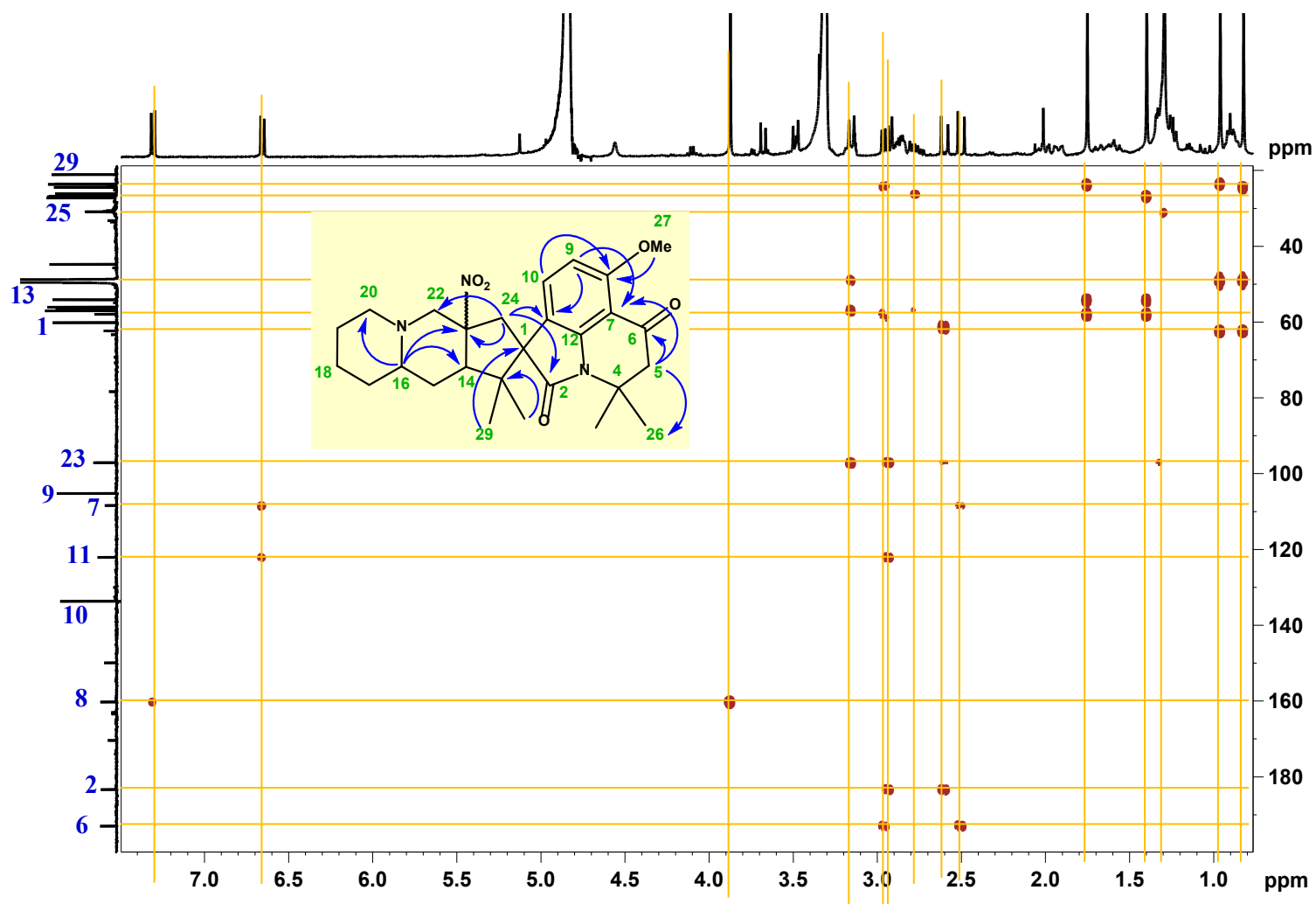


Figure S7a. HMBC NMR spectrum of **1**. Recorded in $\text{CD}_3\text{OD}-d_4$ at 700 MHz (^1H) and 175 MHz (^{13}C)

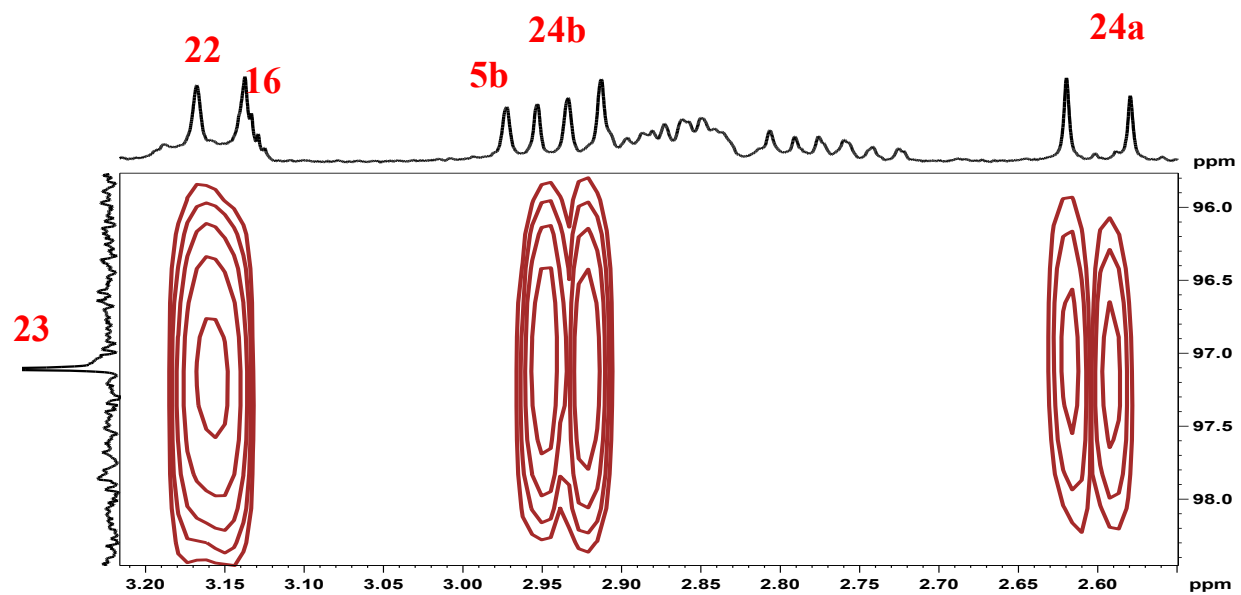


Figure S7b. Expanded HMBC NMR spectrum of **1**. Recorded in $\text{CD}_3\text{OD}-d_4$ at 700 MHz (^1H) and 175 MHz (^{13}C)

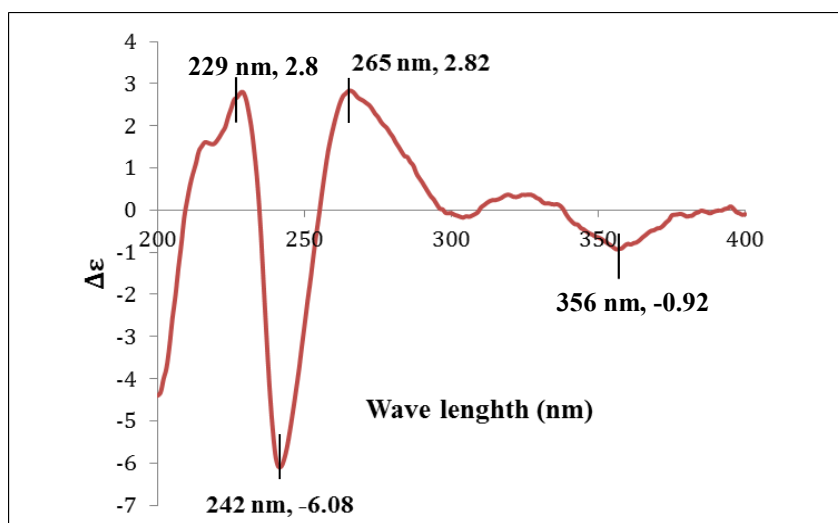


Figure S9. Experimental CD spectrum of **1**.

LC-MS

The ethyl acetate extract of *P. concentricum* grown on brown rice medium only for 11 days and the ethyl acetate extract of the fungus fermented on brown rice with supplementation of CH₂FCOONa were each evaporated to dryness under vacuum. Few milligrams aliquot of each of these extract residue was dissolved in methanol and 1.5 mL of the extract was filtered using a 0.45 µm syringe filter prior to placing it into an autosampler vial.

The samples were analysed using the parameters below:

LC/MS/MS	Liquid Chromatograph: Agilent 1100				
	Mass Spectrometer: Thermo LTQ Orbitrap				
LC Column	Beckman ODS, 5µm, 4.6 mm, 25 cm				
	Part#: 235329				
Injection Vol	100 µL				
Oven Temp	25 °C				
Mobile Phase A	0.1% Formate in Water				
Mobile Phase B	0.1% Formate in Methanol				
Gradient (min)	0.0	3.0	20.0	23.0	26.0
%B	5.0	5.0	95.0	95.0	5.0
Flow Rate (mL/min)	1.0	1.0	1.0	1.0	1.0
Ion Source Parameters	Sheath Gas Flow Rate (arb) 35				
	Aux Gas Flow Rate (arb) 25				
	Sweep Gas Flow Rate (arb) 0				
	Spray Voltage (kV) 3.50				
	Temperature (°C) 275.0				
	Capillary Voltage (V) 45.0				
	Tube Lens (V) 180.0				
MS/MS Parameters	Collision Gas: Helium				
	Sheath/Aux/Ion Sweep Gas: Helium				
	Ionization Mode: Electron Spray Ionization (ESI)				
	Ion Mode: Positive				

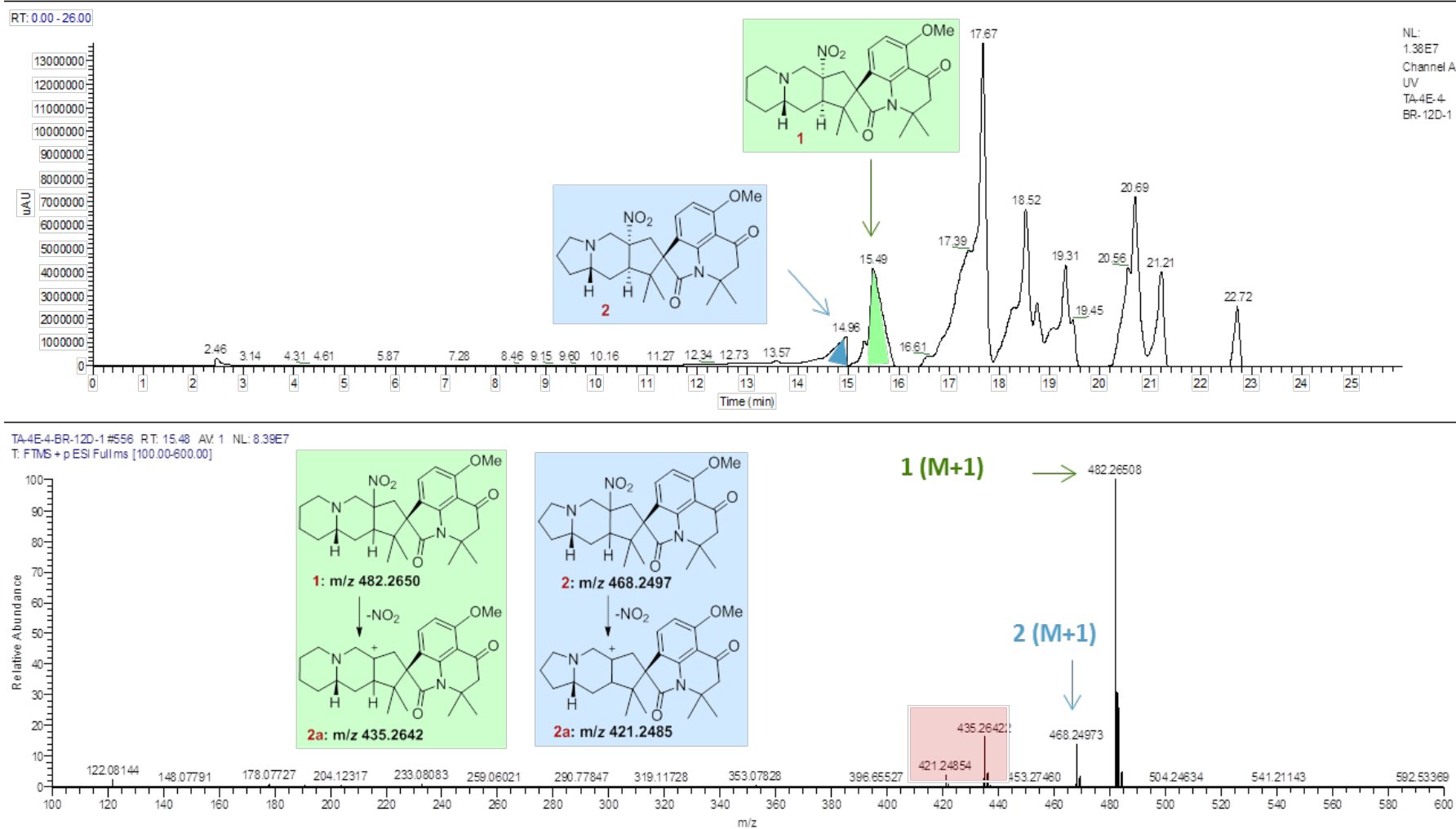


Figure S10. Positive ion LC-MS total ion chromatogram with detection of the protonated ions of 1 and 3 in the ethyl acetate extract of *P. concentricum* cultured on rice medium. Compounds corresponding to the loss of the nitro-radical from 1 and 3 are labeled as **1a** and **3a**, respectively.

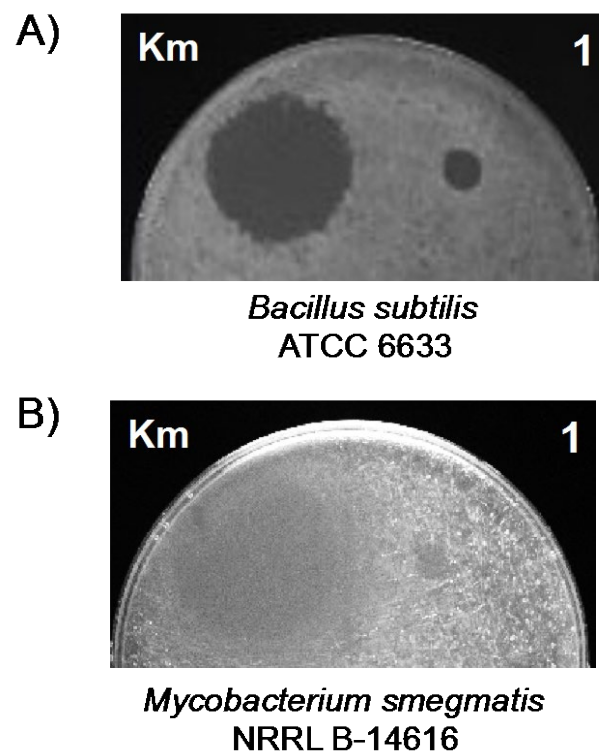


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