Anti-inflammatory and Anti-apoptotic Effects of Stybenpropol A

Isolated from Benzoinum on Human Umbilical Vein Endothelial Cells

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Extraction and isolation of 1

Benzoinum (5 kg) was extracted by maceration in EtOH/H₂O (95:5, 3 × 40 L) at room temperature, giving a crude extract (4.2 kg). The crude extract was suspended in water and extracted with petroleum ether and EtOAc, sequentially, and afforded an EtOAc-soluble extract (3.8 kg). The EtOAc-soluble fraction (2.0 kg) was subjected to a silica gel column using a petroleum ether/EtOAc gradient solvent system (50:1 to 0:100) to give seven fractions (B1-B7). Fraction B2 (598 g) was chromatographed over a silica gel column with petroleum ether/EtOAc mixtures (40:1 to 0:100) to yield fractions B2.1-B2.7. Fraction B2.2 (21.2 g) was fractionated into six parts (B2.2.1-B2.2.6) via MCI gel CHP 20P (MeOH/H₂O, 30:70 to100% MeOH). Fraction B2.2.4 (4.0 g) was separated by low and medium pressure ODS column eluted with MeOH/H₂O followed by semi-preparative HPLC (MeOH /H₂O, 80%) to yield 1 (6 mg).

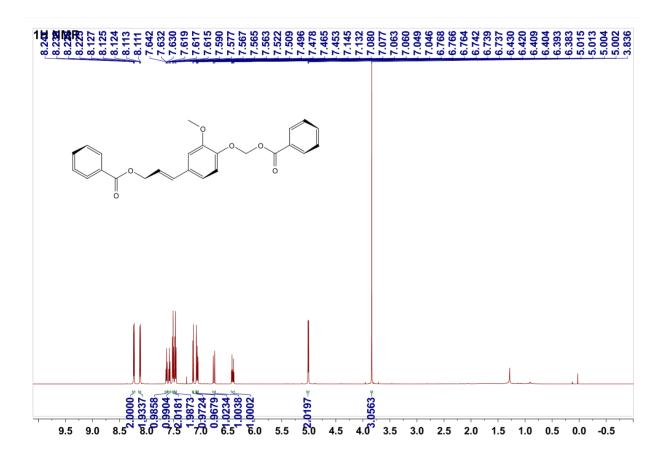


Figure S1. 1H NMR spectrum of 1

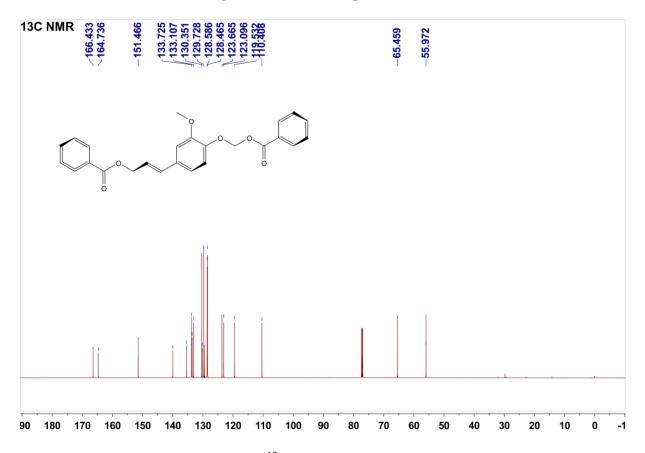


Figure S2. ¹³C NMR spectrum of 1

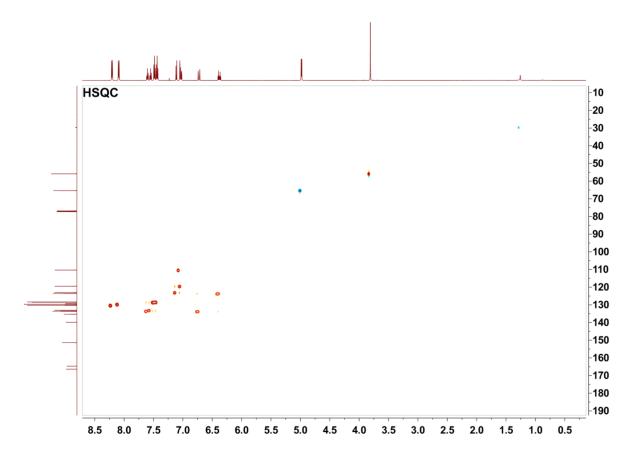


Figure S3. HSQC spectrum of 1 in MeOD.

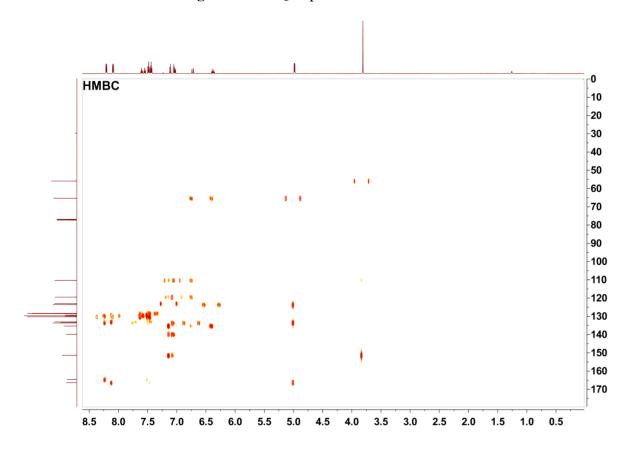


Figure S4. HMBC spectrum of 1 in MeOD.

Mass Analysis Report

Sample Name S2-3-2-2	Operator Q Exactive	Acquisition Date 11/22/2018	Method C:\Xcalibur\methods\fs_sim_ESI
Scan Mode	Scan polarity	Resolution	Isolation windown (m/z)
Full MS Targeted-SIM	Negative	70000	2

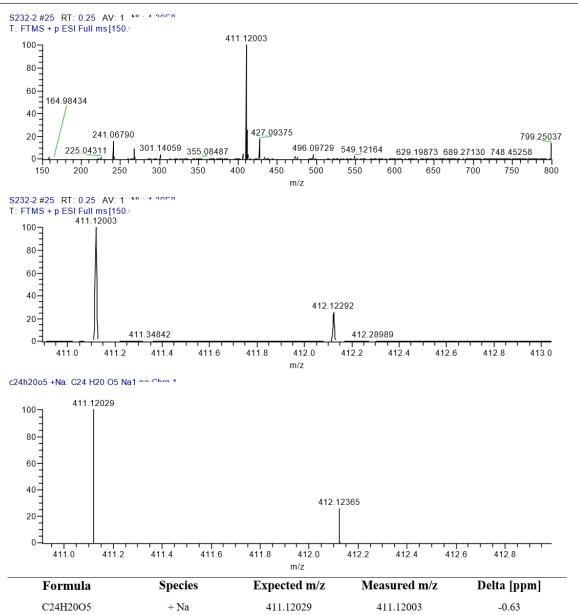


Figure S5. HRESIMS of 1.

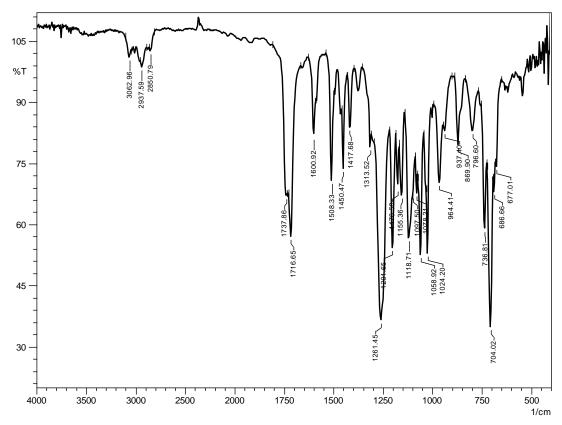


Figure S6. IR spectrum of 1.