Supplementary Data

Phytochemical Investigation of Bioactive Compounds from White Kidney Beans (Fruits of *Phaseolus multiflorus* var. *albus*): Identification of Denatonium with Osteogenesis-Inducing Effect

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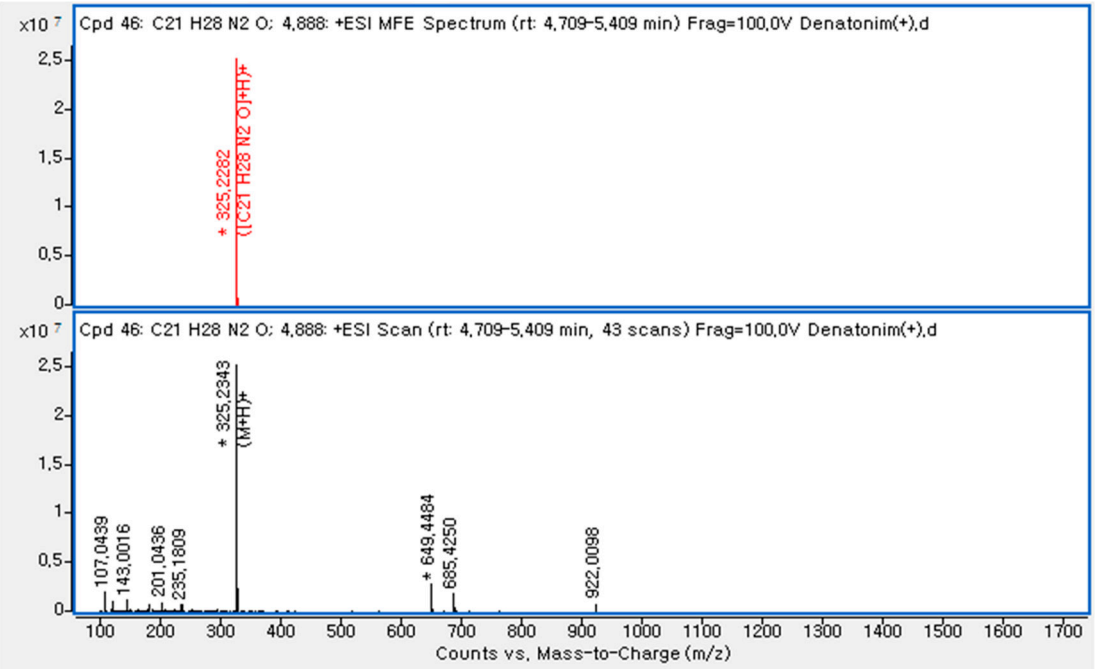

Figure S1 : HR-ESIMS data of **1**

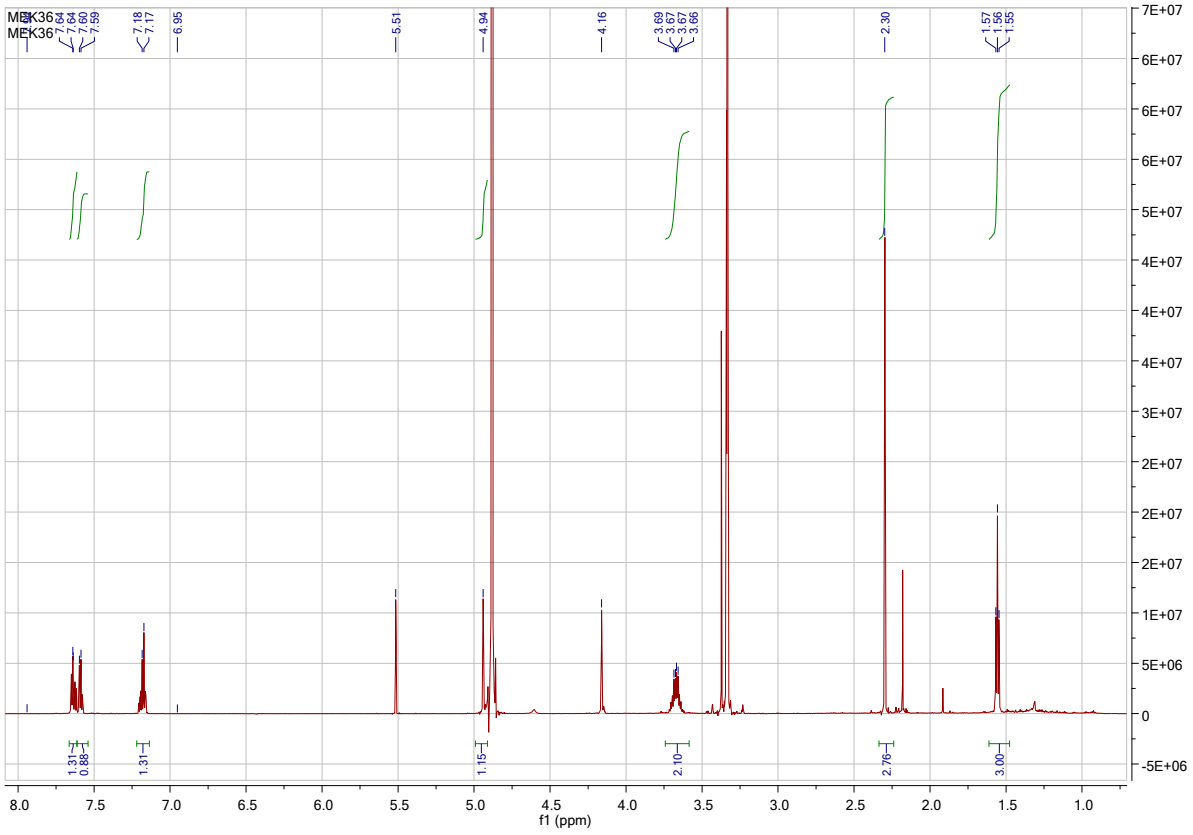

Figure S2 : ^{1}H NMR spectrum of **1** (CD_3OD, 850 MHz)

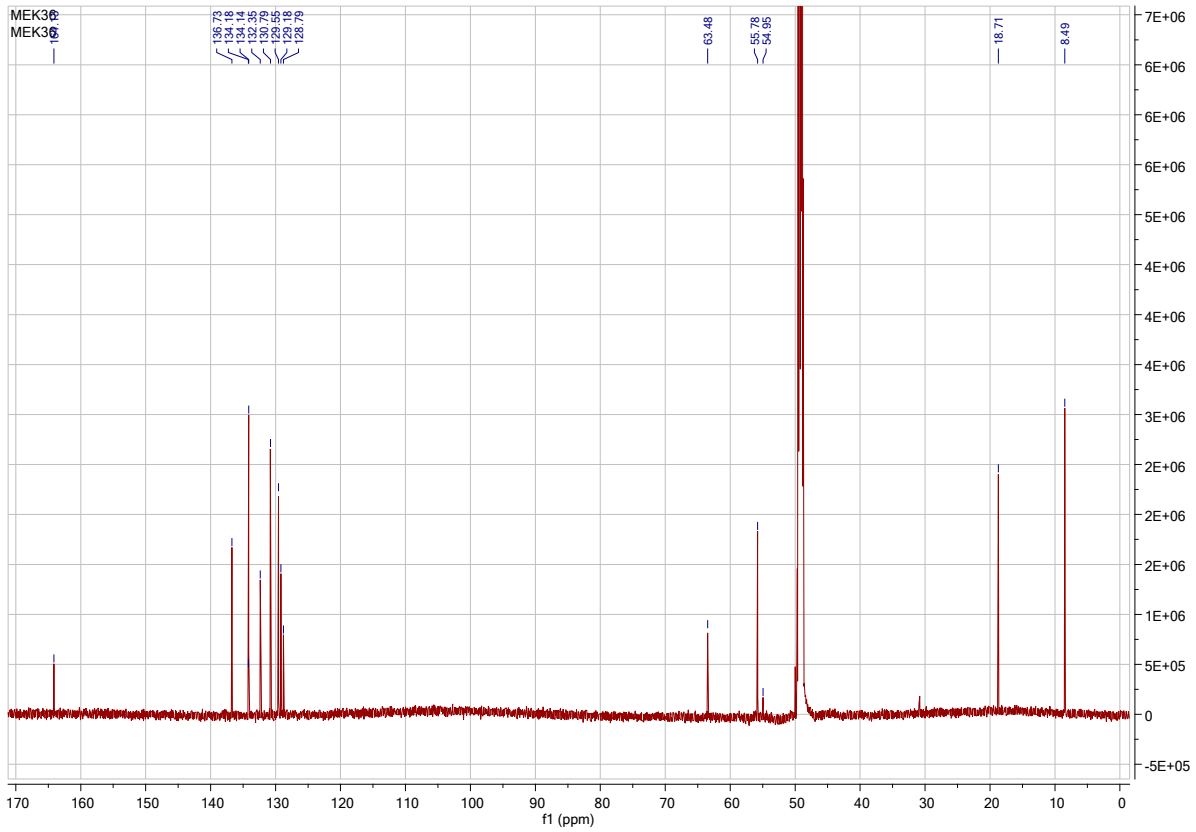

Figure S3 : ^{13}C NMR spectrum of **1** (CD_3OD, 212.5 MHz)

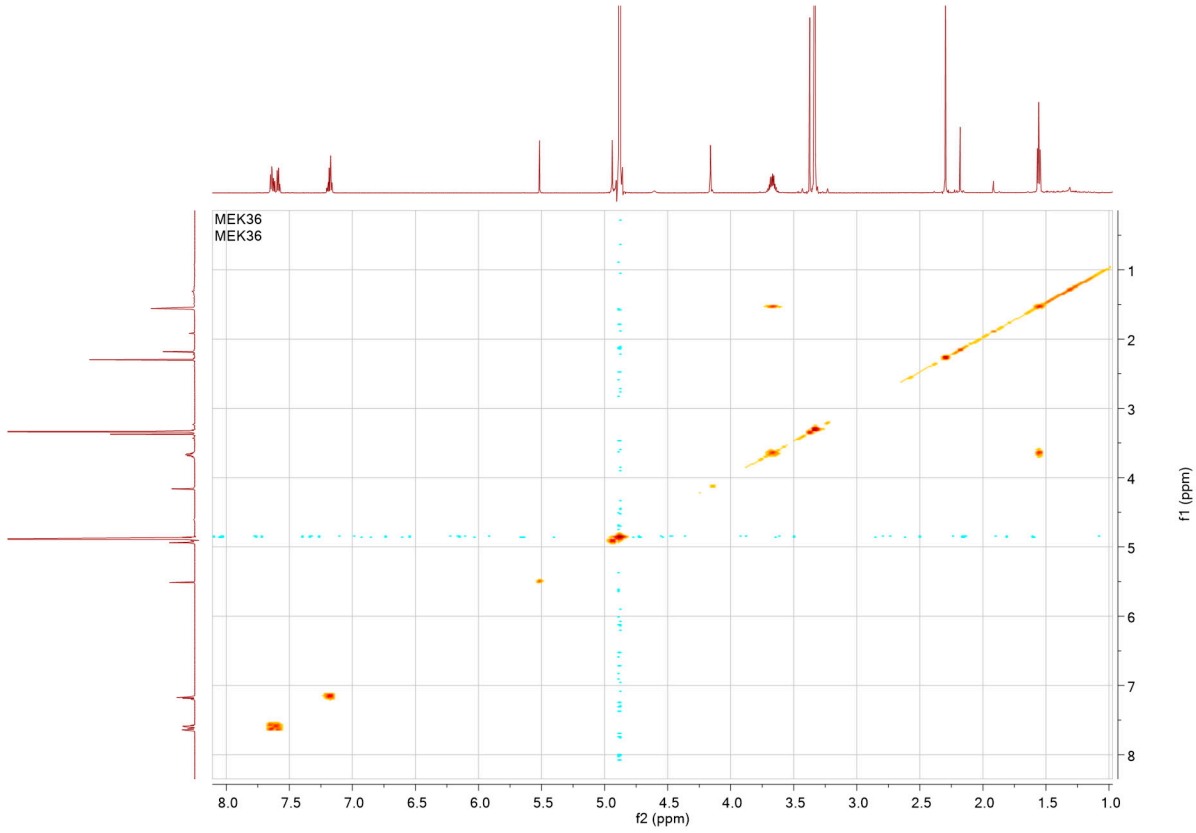

Figure S4 : ^{1}H-^{1}H COSY spectrum of **1** (CD_3OD)

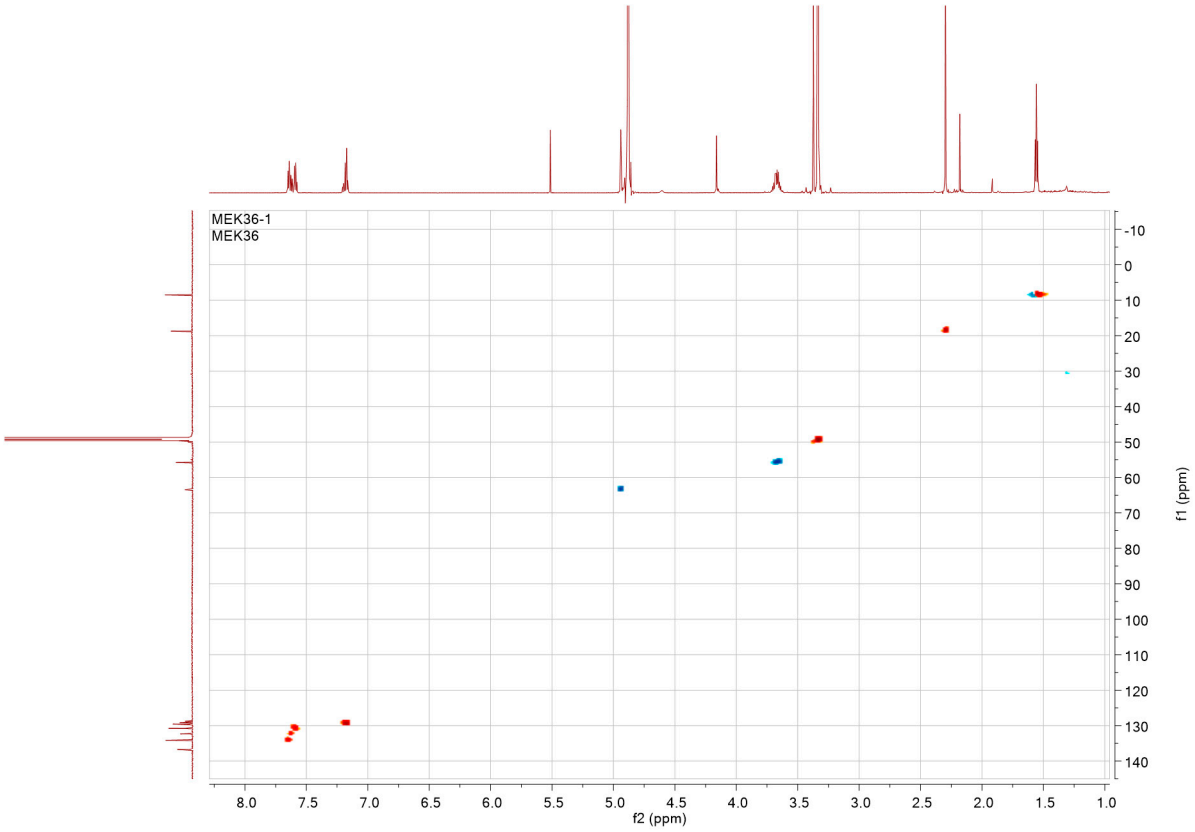

Figure S5 : HSQC spectrum of **1** (CD_3OD)

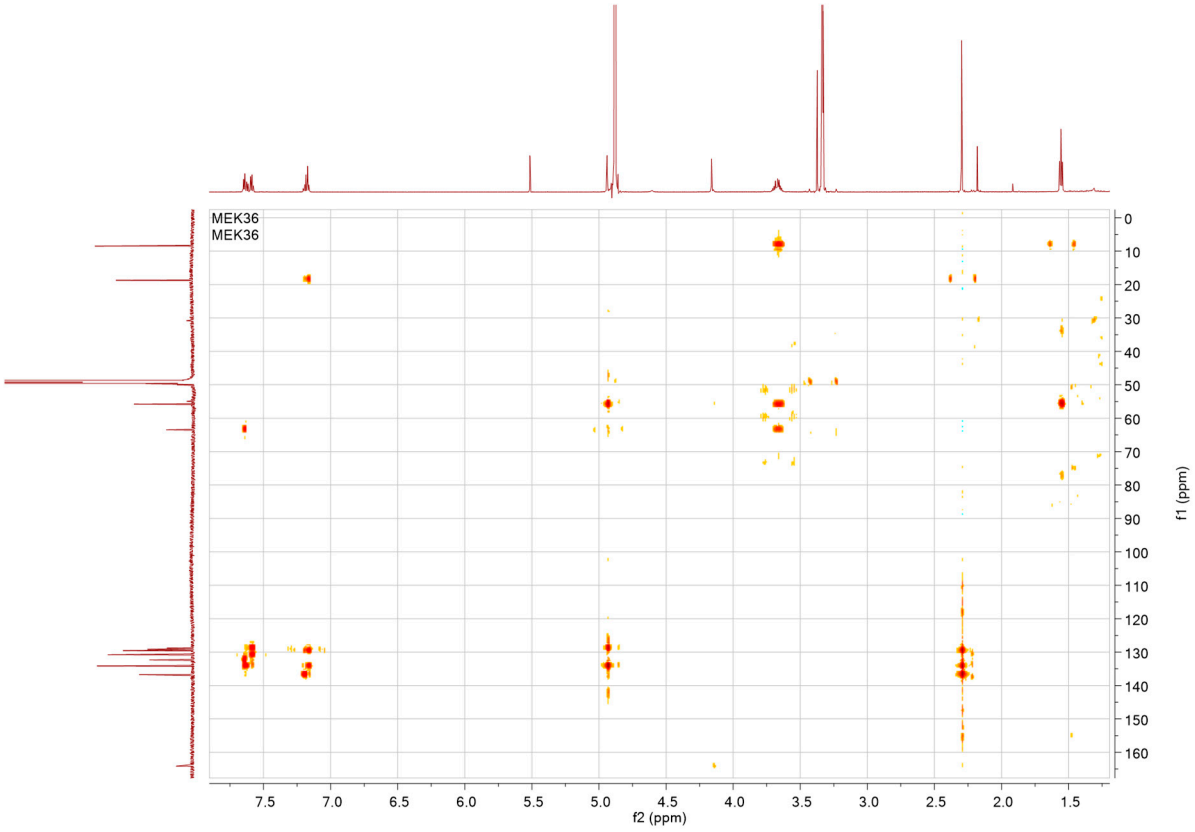

Figure S6 : HMBC spectrum of **1** (CD_3OD)

General experimental procedures

Optical rotations were acquired using a JASCO P-2000 polarimeter (JASCO, Easton, MD, USA). Ultraviolet (UV) spectra were recorded on an Agilent 8453 UV-visible spectrophotometer (Agilent Technologies, Santa Clara, CA, USA). NMR spectra were recorded using a Bruker AVANCE III HD 850 NMR spectrometer with a 5-mm TCI CryoProbe, operated at 850 MHz (^{1}H) and 212.5 MHz (^{13}C). The chemical shifts are represented in ppm (δ) for the ^{1}H and ^{13}C NMR analyses. HRESIMS spectra were recorded on an Agilent 1290 Infinity II series with a 6545 LC/Q-TOF mass spectrometer (Agilent Technologies) with an Agilent EclipsePlus C_{18} column (2.1 mm × 50 mm i.d., 1.8 µm; flow rate: 0.3 mL/min) maintained at 20 °C. Medium-pressure liquid chromatography (MPLC) was performed on a Smart Flash AKROS (Yamazen, Osaka, Japan) using an analytical Universal ODS-SM 120 Å column (3.0 × 20.0 cm, 50 µm) (Yamazen) and Universal Premium Silica gel 60 Å column (2.3 × 12.3 cm, 30 µm) (Yamazen). Semi-preparative HPLC was performed on a Waters 1525 binary HPLC pump with a Waters 996 photodiode array detector (Waters Corporation, Milford, CT, USA) using a Phenomenex Luna Phenyl-hexyl 100 Å column (250 × 10 mm, 10 µm; flow rate: 2 mL/min). The LC/MS analysis was performed on an Agilent 1200 series HPLC system with a diode array detector and a 6130 Series ESI mass spectrometer using an analytical Kinetex C_{18} 100 Å column (100 mm × 2.1 mm i.d., 5 µm; flow rate: 0.3 mL/min) (Phenomenex). Silica gel 60 (230–400 mesh; Merck, Darmstadt, Germany), RP-C_{18} silica gel (230–400 mesh; Merck), and silica Sep-Pak Vac 6 cc cartridges (Waters) were used for column chromatography. Sephadex LH-20 (Pharmacia, Uppsala, Sweden) was used as the packing material for molecular sieve column chromatography. TLC was performed using precoated silica gel F_{254} plates and RP-C_{18} F_{254s} plates (Merck), and spots were detected under UV light or by heating after spraying with anisaldehyde-sulfuric acid.

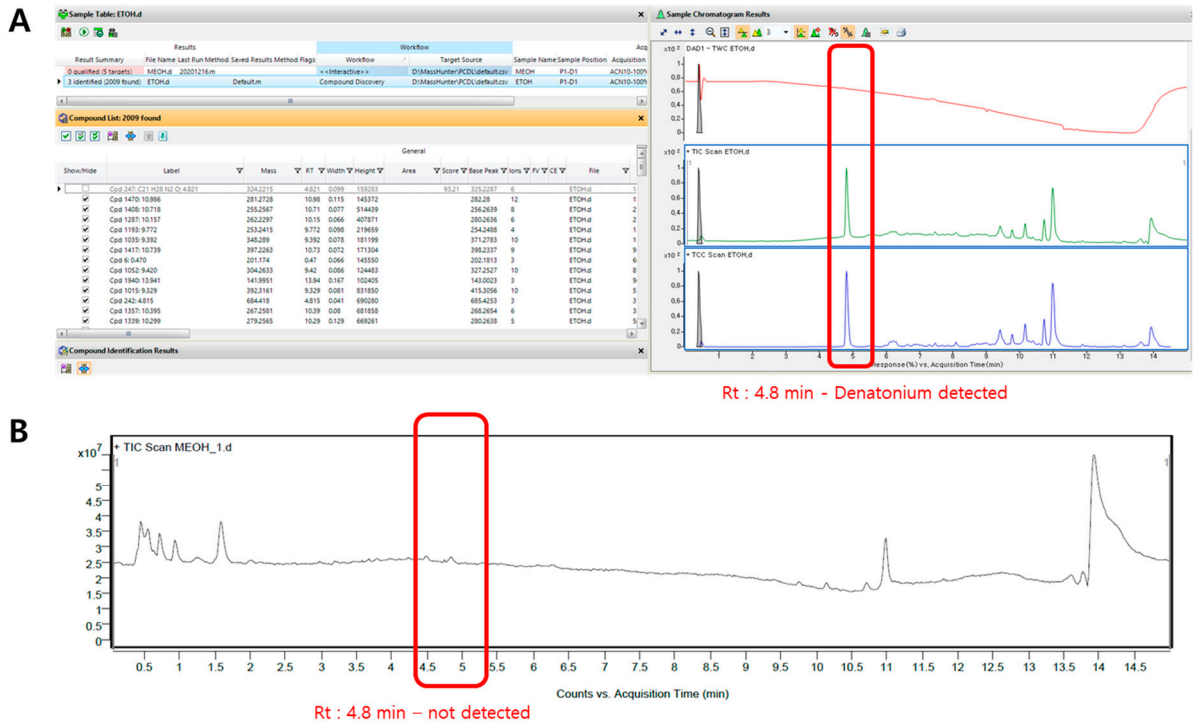

Figure S7 : The total ion chromatogram of ethanol (A) and methanol (B) that we used for extraction in positive ion mode by UPLC-QTOF MS.

Method: The analysis was performed on an Agilent 1290 Infinity II HPLC instrument (Agilent Technologies, Foster City, CA, USA) coupled to a G6545B quadrupole time-of-flight (Q-TOF) mass spectrometer (Agilent Technologies). The analysis was carried out on an Agilent EclipsePlus C18 column (2.1 mm × 50 mm, 1.8 µm) maintained at 20 °C with flow rate of 0.3 mL/min. The mobile phrase consisted of solvent A (water + 0.1% formic acid) and solvent B (100% acetonitrile). The gradient elution system was eluted with 90% A → 100% B (0-10 min), 100% B (11–16 min), and 90% A (16–20 min) for equilibration before the next injection. The samples were monitored at 254 and 210 nm for chromatographic run. Mass spectral analysis was carried out on a MassHunter software (Agilent).