Supplementary Materials

Chemical Constituents of the Leaves of Butterbur (Petasites japonicus) and their Anti-Inflammatory Effects

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General Experimental Procedures

Optical rotations and UV spectra were obtained on a JASCO P-2000 polarimeter (JASCO, Tokyo, Japan) and Optizen pop instrument (Mecasys, Daejeon, Korea), respectively. ECD and VCD spectra were measured with a J-2200 circular dichroism spectrophotometer (JASCO) and a ChiralIR-2X TM FT-VCD spectrometer (BioTools, Jupiter, FL, USA), respectively. ECD and VCD spectra were calculated by Spartan’14 (Wavefunction, Inc., Irvine, CA, USA; 2014) and Gaussian 09 (Revision E.01; Gaussian, Inc., Wallingford, CT, USA; 2009). IR spectra were obtained on an Agilent Cary 630 FTIR spectrometer (Agilent Technologies, Santa Clara, CA, USA). NMR and HRESIMS spectra were obtained using a JEOL 500 MHz (JEOL, Tokyo, Japan) and a Q-TOF micro mass spectrometer (Waters, Milford, MA, USA), respectively. TLC analysis was performed on Silica gel 60 F254 (Merck, Kenilworth, NJ, USA) and RP-18 F254S (Merck) plates. Sephadex LH-20 (Amersham Pharmacia Biotech, Buckinghamshire, United Kingdom), Diaion HP-20 (Mitsubishi, Tokyo, Japan), and LiChroprep RP-18 (Merck, 40–63 μm) were used for column chromatography. MPLC and HPLC were performed using the flash purification system (Combi Flash Rf, Teledyne Isco, Lincoln, NE, USA) with Pre-packed cartridges, Redi Sep-C18 (13 g, 26 g, 43 g, 130 g, Teledyne Isco) and the Gilson purification system with a YMC Pack ODS-A column (250 × 20.0 mm i.d., 5.0 μm, YMC Co., Tokyo, Japan) and a Luna 10 μm C18(2) 100A column (250 × 21.2 mm i.d., 10.0 μm, Phenomenex, Torrance, CA, USA), respectively. All solvents used for the chromatographic separations were distilled before use.
Figure S1. HR-ESI-MS spectrum of compound 1.

Molecular formula: $\text{C}_{18}\text{H}_{14}\text{O}_6$
Figure S2. The $^1$H-NMR (500 MHz, CD$_3$OD) spectrum of compound 1.
Figure S3. The $^{13}$C-NMR (125 MHz, CD$_3$OD$_3$) spectrum of compound 1.
Figure S4. The HSQC spectrum of compound 1 in CD$_3$OD.
**Figure S5.** The COSY spectrum of compound 1 in CD$_3$OD.

X: parts per Million: Proton
Y: parts per Million: Proton

abundance

0 0.2 0.4 0.6 0.8 1.0

abundance

0 0.2 0.4 0.6 0.8 1.0
Figure S6. The HMBC spectrum of compound 1 in CD$_3$OD.
Figure S7. The NOESY spectrum of compound 1 in CD3OD.
**Molecular formula**: C_{18}H_{16}O_{7}

**Figure S8.** HR-ESI-MS spectrum of compound 2.
Figure S9. The $^1$H-NMR (500 MHz, CD$_3$OD) spectrum of compound 2.
Figure S10. The $^{13}$C-NMR (125 MHz, CD$_3$OD) spectrum of compound 2.
Figure S11. The HSQC spectrum of compound 2 in CD$_3$OD.
Figure S12. The COSY spectrum of compound 2 in CD$_3$OD.
Figure S13. The HMBC spectrum of compound 2 in CD3OD.
Figure S14. The NOESY spectrum of compound 2 in CD$_3$OD.
Figure 15. Cell viability of the isolates from *P. japonicus*. 