Supporting Information

Pharmacokinetics, Tissue Distribution and Protein Binding Studies of Chrysocauloflavone I in Rats

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The ESI-MS, $^1$H NMR, and $^{13}$C NMR data of compound SSB-4

(−) ESI-MS $m/z$ 539.1 [M − H$^-$], (+) ESI-MS $m/z$ 541.2 [M + H$^+$]. $^1$H NMR (DMSO-$d_6$, TMS) δ ppm: 7.79 (2H, d, $J = 8.4$ Hz, 2$'$-H, 6$'$-H), 7.49 (2H, d, $J = 8.4$ Hz, 2$'$-H, 6$'$-H), 7.09 (2H, d, $J = 8.8$ Hz, 3$''$-H, 5$''$-H), 6.88 (2H, d, $J = 8.8$ Hz, 3$'$-H, 5$'$-H), 6.85 (1H, s, 3$''$-H), 6.50 (1H, d, $J = 1.2$ Hz, 8-H), 6.21 (1H, d, $J = 1.2$ Hz, 6-H), 5.88 (1H, d, $J = 1.6$ Hz, 8-H$''$), 5.46 (1H, s, 6-H$''$), 6.19 (1H, d, $J = 1.6$ Hz, 6-H$'''$). $^{13}$C NMR (DMSO-$d_6$, TMS) δ ppm: 195.9 (C-4$''$), 182 (C-4), 175.8 (C-7$''$), 166.9 (C-7), 165.3 (C-5$''$), 164.3 (C-8a$''$), 162.9 (C-5$''$), 161.9 (C-4), 161.2 (C-8a), 160.6 (C-4$'''$), 156.6 (C-2), 132.7 (C-1$'''$), 131.7 (C-3), 130.0 (C-2$'$, C-6$'$), 128.3 (C-2$''$, C-6$'''$), 119.8 (C-1$'$), 121.9 (C-1$'''$), 116.4 (C-3$'$, C-5$'$), 115.0 (C-3$'''$, C-5$'''$), 105.0 (C-4a), 101.7 (C-4a$''$), 98.7 (C-6), 96.7 (C-6$''$), 95.7 (C-8$'''$), 94.4 (C-8), 78.8 (C-2$''$), 42.4 (C-3$''$).

Cytotoxicity assay

Human lung cancer cell lines (NCI-H1975 and A549) and the human hepatoma cell line (HepG-2) were obtained from the Department of Pharmacology of Fujian Medical University. The cytotoxicity assay was performed with our previous procedures with little modification [4]. Briefly, all cell lines were grown and maintained in a humidified incubator at 37°C and in a 5% CO$_2$ atmosphere. DMEM supplemented with 10% fetal bovine serum (FBS), 100 units/mL penicillin, and 100
μg/mL streptomycin was used for the cell cultures of A549, NCI-H1975, and HepG-2. Chrysocauloflavone I was dissolved in DMSO and the final concentration of DMSO in culture medium did not exceed 0.1%.

Cytotoxicity was assessed with the MTT method [4]. Briefly, after being harvested from culture flasks, the cells were counted using a hemocytometer and the cell viability was determined by trypan blue exclusion. For all of the cell lines, 4 × 10³ cells were seeded in 96-well plates containing 180 μL of the growth medium per well. The cells were permitted to incubate for 24 h, and then were treated with various concentrations of the compounds for 48 h. After that, the growth medium was changed for the new, followed by adding 20 μL of 5 mg/mL MTT in PBS to each well. The plate was then incubated at 37°C for 4 h. The medium was removed and 150 μL of DMSO was added to each well. After incubation at 37°C for 10 min, the absorbance of the dissolved solutions at 490 nm was detected by a microplate reader (Bio-Tek ELX800). The absorbance of the control cells (treated with 0.1% DMSO) was considered 100%. A chemotherapeutic anticancer drug, adriamycin hydrochloride (purity ≥ 98%, Sigma-aldrich Co.), was used as the positive control.