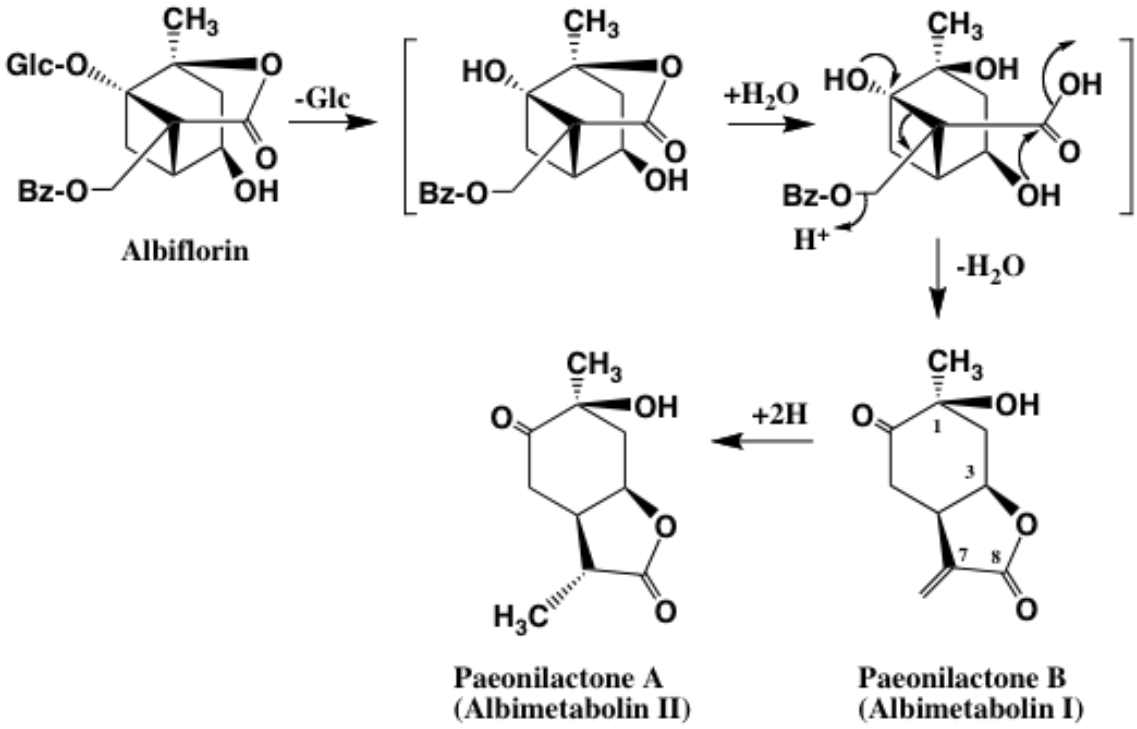
Arbiflorin



Metabolic processes of albiflorin by human intestinal bacteria

代謝実験

腸内細菌代謝　ヒト腸内細菌フローラ

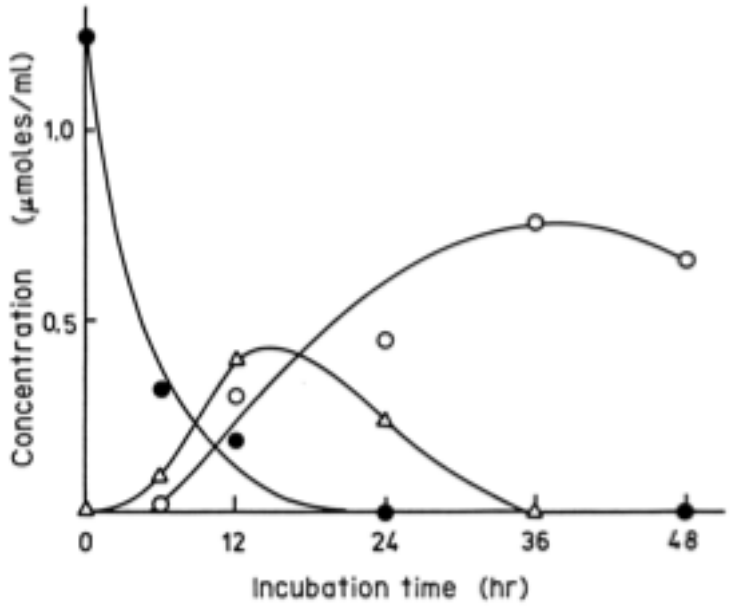


Fig. 1 Time course of the metabolism of albiflorin.

(●), albiflorin ; (○), Al (paeonilactone-A) ; (△), A2 (paeonilactone-B)

PIncubation of albiflorin with a fecal suspension

Albiflorin (85 mg) was added to a fecal suspension (100 ml). The mixture was incubated for 30 hrs at 37°C in an anaerobic jar, in which the air had been replaced with oxygen-free carbon dioxide in the presence of activated steel wool (steel wool method), and then extracted four times with ethylacetate (AcOEt, 100 ml each). The solution was evaporated *in vacuo* to give an oily residue (*ca*. 600 mg). The residue was applied to a column of silica gel (40 g, 1.9 cm i.d. x 24 cm). The column was washed with benzene (500 ml) and benzene-$CHCl_3$ (1 : 1, 500 ml), and then eluted with $CHC1_3$. The fractions (50 ml each) containing metabolites were pooled and evaporated to dryness *in vacuo*. The crude metabolites were further purified by repeated crystallization and preparative TLC. Al and A2 were obtained in yields of 11 mg (29 %) and 1 mg (2 %), respectively. [Hattori *et al*., *J. Med. Pharm. Soc. Wakan-Yaku*, **2**, 398-404 (1985)]

Metabolite Al

Colorless needles, mp 106°C from acetone-cyclohexane, high resolution MS : Calcd. for $C_{10}H_{14}O_4$, M^+ 198.0891, Found : 198.0861 ; IR ν cm^{-1} : 3400 (OH), 1760 (γ-lactone), 1720 (ketone), 1170 (C-O-C) ^{1}H-NMR ($CDCl_3$, 400 MHz): δ 1.26 (3H, d, *J* = 7Hz, CH_3-6CH-), 1.46 (3H, s,CH_3-C-), 1.87 and 2.61 (each 1H, dd, *J* = 14 and 11Hz and *J* = 14 and 6Hz, -C-CH_2-CH-O), 2.38 (1H, dq, *J* = 12 and 7Hz, CH_3-CH-CH-), 2.64 and 2.94 (each 1H, dd, *J* = 15 and 2Hz and *J* = 15 and 8Hz, -CH-CH_2-CO-), 2.75 (1H, m, -CH- CH-CH_2-), 4.90 (1H, sext, *J* = 11, 6 and 6Hz, -CH-O-CO-). low resolution MS (*m/z*) : 198(M^+), 180, 170, 152, 124, 110, 87, 56, 43 (base peak). [Hattori *et al*., *J. Med. Pharm. Soc. Wakan-Yaku*, **2**, 398-404 (1985)]

Metabolite A2 (6)

$C_{10}H_{12}O_4$, ^{1}H - NMR ($CDCl_3$, 400 MHz) : δ 1.40 (3H, s, CH_3-C-), 1.96 and 2.53 (each 1H, dd, *J* = 14 and 9 Hz, and *J* = 14 and 6Hz, -C-CH_2-CH-O), 2.79 and 2.96 (each 1H, dd, *J* = 16 and 4Hz, and *J* = 16 and 8Hz, -CH_2-CO-), 3.68 (1H, m, -CH-C=), 4.99 (1H, sext, *J* = 9,9 and 6Hz, -CH-O-CO-), 5.68 and 6.37 (each 1H, d, *J* = 3 Hz and *J* = 3Hz, CH_2=). [Hattori *et al*., *J. Med. Pharm. Soc. Wakan-Yaku*, **2**, 398-404 (1985)]

参考文献

1) Hattori M., Shu Y. Z., Kobashi K. and Namba T.: Metabolism of albiflorin by human intestinal bacteria. *J. Med. Pharm. Soc. Wakan-Yaku*, **2**, 398-404 (1985).
and analyzed by TLC-densitometry.