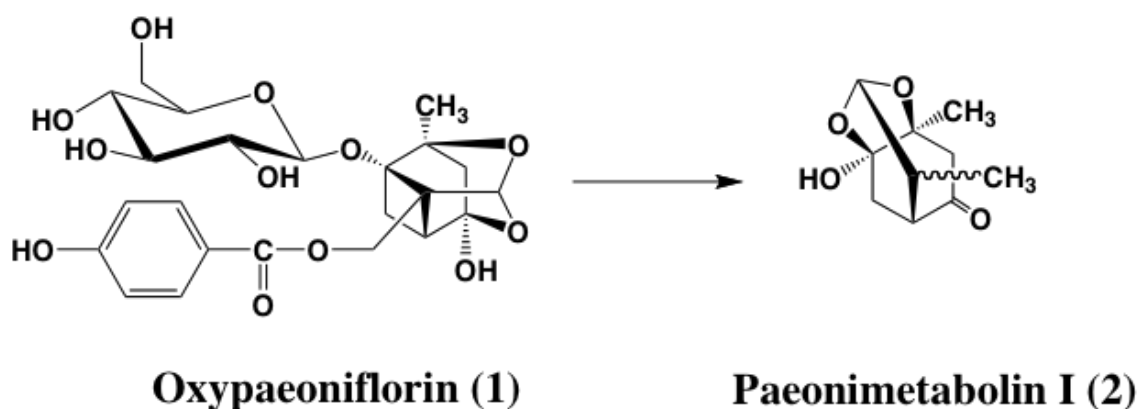


Oxypaeoniflorin



Metabolism of oxypaeoniflorin by human intestinal bacteria

代謝実験

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単一化合物 oxypaeoniflorin

Incubation of oxypaeoniflorin (1) with an intestinal bacterial mixture

Oxypaeoniflorin (**1**, 600 mg) dissolved in EtOH (4 ml) was added to a human intestinal bacterial mixture (600 ml). The mixture was anaerobically incubated at 37 °C for 24 h and extracted three times with AcOEt (600 ml each). The AcOEt phase was concentrated to a small volume *in vacuo*. The mixture thus obtained was applied to a silica gel column (68 g, 2.4 cm i.d. x 27cm). The column was washed with benzene and then eluted with CHCl₃. Fractions of 50 ml/flask were collected and monitored by silica gel TLC. Fractions 15—24 were pooled and evaporated to dryness *in vacuo*. The residue (68 mg) was purified by re-chromatography (silica gel, 30 g; column size, 1.9 cm i.d. x 16 cm). A pure oily compound was eluted with CH₂Cl₂–AcOEt (100:3); yield, 32 mg (13%). This compound was identical with paeonimetabolin I (**2**) obtained from paeoniflorin based on a comparison of the *R_f* values in various solvent systems and the IR spectra. [Hattori *et al.*, *Chem. Pharm. Bull.*, **33**, 3838-3846 (1985).]

7*S*-Paeonimetabolin I (2a)

The physical properties were reported in the following paper: Hattori *et al.*, *Chem. Pharm. Bull.*, **33**, 3838-3846 (1985).

7R-Paeonimetabolin I (2b)

Colorless prisms, mp 146-148 °C. High resolution MS: Found, 198.0853; Calcd for M^+ , $C_{10}H_{14}O_4$, 198.0892. IR ν_{\max} cm^{-1} : 3420 (OH), 1705 (C=O). 1H -NMR ($CDCl_3$, 400 MHz) δ : 0.90 (3H, d, $J=7.3$ Hz, 8- H_3), 1.29 (3H, s, 10- H_3), 2.07 (1H, dq, $J=7.5$, 7.3 Hz, 7-H), 2.15 and 2.35 (each 1H, dd, $J=13.4$, 2.3 Hz; $J=13.4$, 3.4 Hz, 5- H_2), 2.60 and 2.64 (2H, ABq, $J=17.7$ Hz, 2- H_2), 2.65 (1H, m, 4-H), 5.14 (1H, brs, 9-H). MS m/z : 198 (M^+), 180 (M^+-H_2O), 152, 124, 109, 98, 83, 69 (base peak), 55. ^{13}C -NMR: see Table I in the reference: [Shu *et al.*, *Chem. Pharm. Bull.*, **35**, 3726-3733 (1987)]

参考文献

- 1) Hattori M., Shu Y. Z., Shimizu M., Hayashi T., Morita N., Kobashi K., Xu G. J. and Namba T.: Metabolism of paeoniflorin and related compounds by human intestinal bacteria. *Chem. Pharm. Bull.*, **33**, 3838-3846 (1985).
- 2) Shu Y. Z., Hattori M., Akao T., Kobashi K., Kakei K., Fukuyama K., Tsukihara T. and Namba T.: Metabolism of paeoniflorin and related compounds by human intestinal bacteria. II. Structures of 7S- and 7R-paeonimetabolins I and II formed by *Bacteroides fragilis* and *Lactobacillus brevis*. *Chem. Pharm. Bull.*, **35**, 3726-3733 (1987).