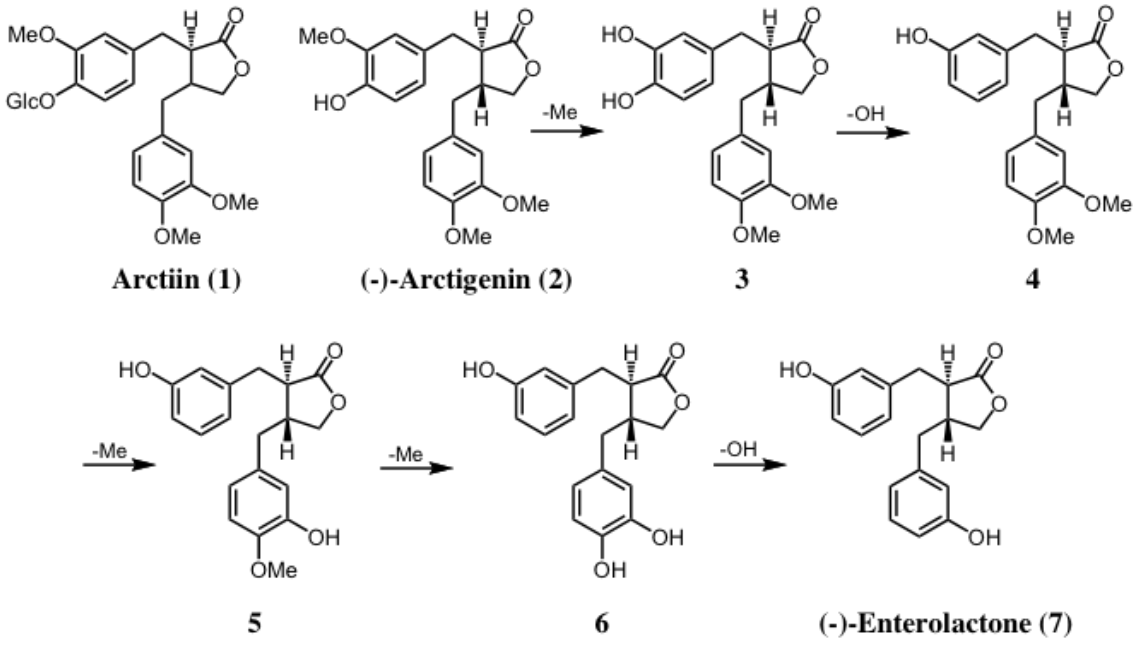
Arctiin



Metabolic processes of arctiin (**1**) by human intestinal microflora

[Xie *et al*., *Chem. Pharm. Bull.*, **51**, 378-384 (2003) and Gao *et al., J. Trad. Med*., **22**, 213-221 (2005)].

代謝実験

腸内細菌代謝　ヒト腸内細菌フローラ

単一化合物化合物　arctiin

(-)-Arctigenin (2)

Colorless prisms. $[\alpha]_D$ –25.8° (*c*=0.20, MeOH). UV λ_{max} (MeOH): 231, 281 nm. IR (KBr) ν_{max}: 3424 (OH), 1762 (γ-lactone CO), 1608, 1515, 1458, 1268, 1242, 1142, 1062 cm^{-1}. EI-MS *m/z*: 372 $[M]^+$. ^{1}H-NMR ($CDCl_3$, 400 MHz): δ 2.45-2.66 (4H, m, H-2, 3, 7''), 2.92 (2H, m, H-7'), 3.81 (3H, s, -OC$\underline{H}_3$), 3.82 (3H, s, -OC$\underline{H}_3$), 3.85 (3H, s, -OC$\underline{H}_3$), 3.88 (1H, dd, *J*=9.18, 7.28 Hz, H_a-4), 4.13 (1H, dd, *J*=9.18, 7.24 Hz, H_b-4), 6.46 (1H, d, *J*=1.94 Hz, H-2''), 6.55 (1H, dd, *J*=8.23, 2.18 Hz, H-6''), 6.61 (1H, dd, *J*=7.95, 1.94Hz, H-6'), 6.64 (1H, d, *J*=1.94 Hz, H-2'), 6.75 (1H, d, *J*=8.19 Hz, H-5''), 6.83 (1H, d, *J*=7.99 Hz, H-5'). CD (MeOH): λ_{ext} 281.5 nm (Δε-0.102), 232.9 nm (-3.06). ^{13}C-NMR: see the

reference [Xie *et al*., *Chem. Pharm. Bull.*, **51**, 378-384 (2003)].

(2*R*,3*R*)-2-(3',4'-Dihydroxybenzyl)-3-(3",4"-dimethoxybenzyl) butyrolactone (3)
Amorphous powder. $[\alpha]_D$ –42.8° (*c*=0.13, MeOH). UV λ_{max} (MeOH): 228, 281 nm. IR (KBr) ν_{max}: 3421 (-OH), 1751 (γ-lactone CO), 1604, 1516, 1458, 1261, 1238, 1153, 1022 cm^{-1}. EI-MS *m/z*: 358 $[M]^+$. ^{1}H-NMR ($CDCl_3$, 400 MHz): δ 2.48-2.64 (4H, m, H-2, 3, 7"), 2.85 (2H, d, J=5.88 Hz, H-7'), 3.81 (3H, s, -OC$\underline{H}_3$), 3.85 (3H, s, -OC$\underline{H}_3$), 3.88 (1H, dd, *J*=8.94, 7.24 Hz, H_a-4), 4.14 (1H, dd, *J*=8.94, 7.00 Hz, H_b-4), 6.48 (1H, d, *J*=1.94 Hz, H-2"), 6.51 (1H, dd, *J*=7.99, 1.94Hz, H-6'), 6.57 (1H, dd, *J*=8.19, 1.94 Hz, H-6"), 6.63 (1H, d, *J*=1.94 Hz, H-2'), 6.75 (1H, d, *J*=8.19 Hz, H-5'), 6.76 (1H, d, *J*=8.19Hz, H-5'). CD (MeOH): λ_{ext} 281.5 nm (Δε-0.65), 233.3 nm (-3.08). ^{13}C-NMR: see the reference [Xie *et al*., *Chem. Pharm. Bull.*, **51**, 378-384 (2003)].

(2*R*,3*R*)-2-(3'-Hydroxybenzyl)-3-(3",4"-dimethoxybenzyl) butyrolactone (4)
Amorphous powder. $[\alpha]_D$ –51.1° (*c*=0.12, MeOH). UV λ_{max} (MeOH): 224, 276 nm. IR (KBr) ν_{max}: 3309 (-OH), 1747 (γ-lactone CO), 1589, 1512, 1462, 1269, 1246, 1157, 1026 cm^{-1}. EI-MS *m/z*: 342 $[M]^+$. ^{1}H-NMR ($CDCl_3$, 400 MHz): δ 2.47-2.51 (2H, m, H-3, H_a-7"), 2.59-2.62 (2H, m, H-2, H_b-7"), 2.89 (1H, dd, *J*=14.01, 6.77 Hz, H_a-7'), 2.98 (1H, dd, *J*=14.01, 5.30 Hz, H_b-7'), 3.82 (3H, s, -OC$\underline{H}_3$), 3.85 (3H, s, -OC$\underline{H}_3$), 3.88 (1H, dd, *J*=9.18, 7.72 Hz, H_a-4), 4.14 (1H, dd, *J*=9.18, 7.24 Hz, H_b-4), 6.48 (1H, d, *J*=2.18 Hz, H-2"), 6.56 (1H, dd, *J*=8.19, 1.94Hz, H-6"), 6.61 (1H, t, *J*=2.18 Hz, H-2'), 6.69 (1H, m, H-6'), 6.70 (1H, m, H-4'), 6.76 (1H, d, *J*=7.99 Hz, H-5"), 7.14 (1H, t, *J*=7.72 Hz, H-5'). CD (MeOH): λ_{ext} 280.3 nm (Δε-0.46), 230.5 nm (-3.11). ^{13}C-NMR: see the reference [Xie *et al*., *Chem. Pharm. Bull.*, **51**, 378-384 (2003)].

(2*R*,3*R*)-2-(3'-hydroxybenzyl)-3-(3"-hydroxy-4"-methoxybenzyl) butyrolactone (5)
Amorphous powder. $[\alpha]_D$ –30.7° (*c*=0.10, MeOH). UV λ_{max} (MeOH): 220, 279 nm. IR (KBr) ν_{max}: 3568 (-OH), 1747 (γ-lactone CO), 1512, 1458, 1272, 1246, 1018 cm^{-1}. EI-MS *m/z*: 328 $[M]^+$. ^{1}H-NMR ($CDCl_3$, 400 MHz): δ 2.43-2.48 (2H, m, H-3, H_a-7"), 2.56-2.59 (2H, m, H-2, H_b-7"), 2.90 (1H, dd, *J*=13.77, 6.77 Hz, H_a-7'), 2.97 (1H, dd, *J*=13.77, 5.30 Hz, H_b-7'), 3.87 (3H, s, -OC$\underline{H}_3$), 3.85 (1H, dd, *J*=8.94, 7.72 Hz, H_a-4), 4.10 (1H, dd, *J*=8.94, 7.24 Hz, H_b-4), 6.59 (1H, d, *J*=2.18 Hz, H-2"), 6.50 (1H, dd, *J*=7.95, 2.18 Hz, H-6"), 6.61 (1H, t, *J*=2.0, H-2'), 6.73 (1H, m, H-6'), 6.73 (1H, m, H-4'),

6.74 (1H, d, *J*=7.95 Hz, H-5''), 7.17 (1H, t, *J*=7.72 Hz, H-5'). CD (MeOH): λ_{ext} 279.1 nm (Δε-0.46), 229.3 nm (-3.10). ^{13}C-NMR: see the reference [Xie *et al*., *Chem. Pharm. Bull.*, **51**, 378-384 (2003)].

(2*R*,3*R*)-2-(3'-Hydroxybenzyl)-3-(3'',4''-dihydroxybenzyl) butyrolactone (6)

Amorphous powder. $[\alpha]_D$ –36.7^o (*c*=0.12, MeOH). UV λ_{max} (MeOH): 223, 281 nm. IR (KBr) ν_{max}: 3332 (-OH), 1751 (γ-lactone CO), 1589, 1520, 1485, 1362, 1284, 1253, 1157, 1010 cm^{-1}. EI-MS *m*/*z*: 314 $[M]^+$. ^{1}H-NMR ($CDCl_3$, 400 MHz): δ 2.35 (1H, m, H_a-7''), 2.47 (H, m, H-3), 2.51 (1H, m, H_b-7''), 2.65 (1H, m, H-2), 2.83 (1H, dd, *J*=14.01, 7.0 Hz, H_a-7'), 2.92 (1H, dd, *J*=14.01, 5.30 Hz, H_b-7'), 3.85 (1H, m, H_a-4), 4.05 (1H, dd, *J*=8.94, 7.24 Hz, H_b-4), 6.37 (1H, dd, *J*=7.95, 2.18 Hz, H-6''), 6.50 (1H, d, *J*=2.18 Hz, H-2''), 6.63-6.66 (3H, m, H-2', H-4', H-6', H-5''), 7.10 (1H, t, *J*=7.95 Hz, H-5'). CD (MeOH): λ_{ext} 280.5 nm (Δε-0.51), 230.1nm (-3.13). ^{13}C-NMR: see the reference [Xie *et al*., *Chem. Pharm. Bull.*, **51**, 378-384 (2003)].

(-)-Enterolactone (7)

Amorphous powder. $[\alpha]_D$ –46.0^o (*c*=0.15, MeOH). UV λ_{max} (MeOH): 219, 277nm. IR (KBr) ν_{max}: 3394 (-OH), 1747 (γ-lactone CO), 1593, 1458, 1273, 1161, 1018 cm^{-1}. EI-MS *m*/*z*: 298 $[M]^+$. ^{1}H-NMR ($CDCl_3$, 400 MHz): δ 2.50 (1H, m, H_a-7''), 2.48 (H, m, H-3), 2.61 (1H, m, H_b-7''), 2.59 (1H, m, H-2), 2.88 (1H, dd, *J*=14.01, 6.77 Hz, H_a-7'), 2.96 (1H, dd, *J*=14.01, 5.30 Hz, H_b-7'), 3.90 (1H, dd, *J*=9.18, 7.52 Hz, H_a-4), 4.12 (1H, dd, *J*=9.18, 7.00 Hz, H_b-4), 6.47 (1H, t, *J*=1.90 Hz, H-2''), 6.59 (1H, dt, *J*=7.90, 1.90,1.90 Hz, H-6''), 6.61 (1H, t, *J*=1.9, H-2'), 6.72 (1H, m, H-6'), 6.74 (1H, m, H-4'), 6.71 (1H, m, H-4''), 7.13 (1H, t, *J*=7.90 Hz, H-5'), 7.16 (1H, t, *J*=7.90 Hz, H-5''). CD (MeOH): λ_{ext} 280.1 nm (Δε-0.26), 220.0 nm (-3.60). ^{13}C-NMR: see the reference [Xie *et al*., *Chem. Pharm. Bull.*, **51**, 378-384 (2003)].

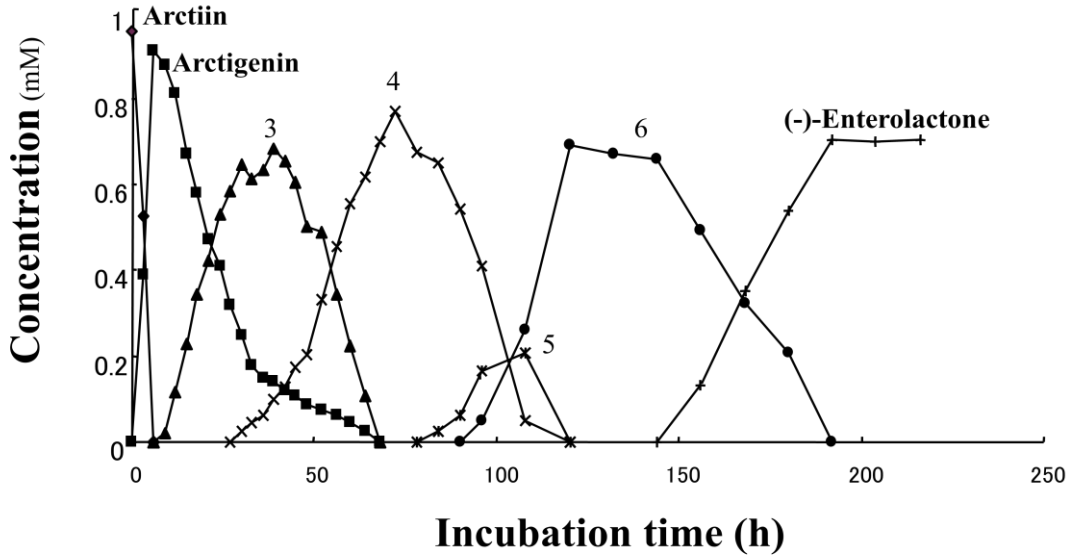


Fig. 1. Time course for metabolism of arctiin by a intestinal bacterial mixture of humans. [Xie *et al*., *Chem. Pharm. Bull.*, **51**, 378-384 (2003)]

参考論文

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