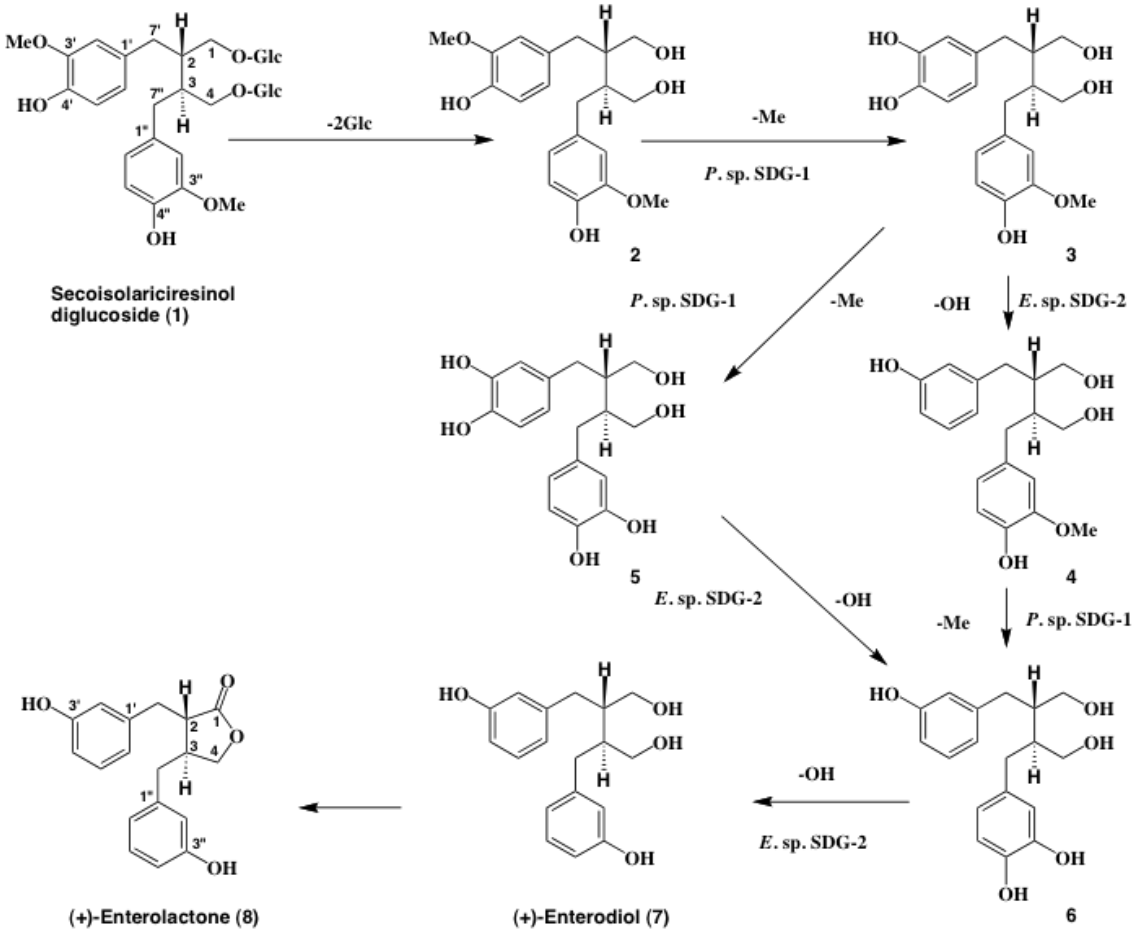
Secoisolariciresinol Diglucoside



Metabolic processes of secoisolariciresinol by human intestinal bacteria
[Wang *et al*., *Chem. Pharm. Bull.,* **48**, 1606-1610 (2000) 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、ヒト腸内細菌株 *Peptostreptococcus* sp. SDG-1、*Eubacterium* sp. SDG-2
単一化合物　secoisolariciresinol

Incubation of secoisolariciresinol diglucoside (1) with a human fecal suspension

Secoisolariciresinol diglucoside (**1**, 300 mg) dissolved in PYF broth (250 ml) was

incubated with a human fecal suspension (50 ml) at 37°C in an anaerobic incubator for 15 h. [Wang *et al*., *Chem. Pharm. Bull.,* **48**, 1606-1610 (2000)]

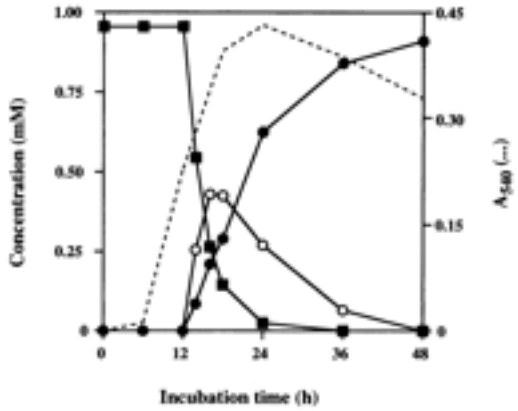


Fig. 1 Time course of transformation of secoisolariciresinol (**2**) by *Peptostreptococcus* sp. SDG-1

GAM broth (4 ml) containing **2** (a final concentration of 1 mM) was incubated at 37°C with a bacterial suspension of *P*. sp. SDG-1 (100 μl) in an anaerobic incubator. A 150 μl portion was taken out at intervals and extracted with BuOH saturated with H_2O (150 μl). The BuOH extract was evaporated in *vacuo* to give a residue. The residue was dissolved in MeOH (150 μl) and the MeOH extract was analyzed by HPLC. Bacterial growth in GAM broth was monitored by measuring turbidity at 540 nm. [Wang *et al*., *Chem. Pharm. Bull.,* **48**, 1606-1610 (2000)]

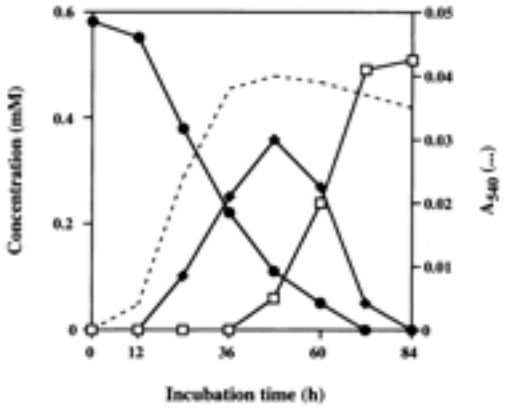


Fig. 2 Time course of transformation of compound 5 by *Eubacterium* sp. SDG-2

GAM broth (6 ml) containing **5** (a final concentration of 0.8 mM) was incubated at 37°C with a bacterial suspension of *E.* sp. SDG-2 (100 μl) under anaerobic conditions. Samples were taken at intervals and analyzed by HPLC. [Wang *et al*., *Chem. Pharm. Bull.,* **48**, 1606-1610 (2000)]

Secoisolariciresinol (2)

Amorphous powder. EI-MS *m/z*: 362 $[M]^+$. ^{1}H-NMR (400 MHz, $CDCl_3$) δ: 1.84 (2H, m, H-2, 3), 2.66 (H, m, H-7′, 7″), 3.46 (4H, m, H-1, 4), 3.80 (6H, s, OC$\underline{H}_3$), 6.60 (4H, overlapped, H-2′, 2″, 5′, 5″), 6.75 (2H, dd, *J*=8.4, 3.0 Hz, H-6′, 6″). [Wang *et al*., *Chem. Pharm. Bull.,* **48**, 1606-1610 (2000)]

Compound 3

Amorphous powder. EI-MS *m/z*: 348 $[M]^+$. ^{1}H-NMR (400 MHz, MeOH-d_4) δ: 1.91 (2H, m, H-2, 3), 2.60 (4H, m, H-7′, 7″), 3.53 (2H, dd, *J*=11.1, 5.1 Hz, H_a-1, H_a-4), 3.59 (2H, dd, *J*=11.1, 4.8 Hz, H_b-1, H_b-4), 3.76 (3H, s, -OC$\underline{H}_3$), 6.43 (1H, dd, *J*=8.0, 1.9 Hz, H-6′), 6.56 (1H, dd, *J*=8.0, 1.9 Hz, H-6″), 6.57 (1H, d, *J*=1.9 Hz, H-2′); 6.63 (1H, d, *J*=1.9 Hz, H-2″), 6.63 (1H, d, *J*=8.0 Hz, H-5″), 6.66 (1H, d, *J*=8.0 Hz, H-5′). [Wang *et al*., *Chem. Pharm. Bull.,* **48**, 1606-1610 (2000)]

Compound 4

Amorphous powder. $[\alpha]_D$ 24.4 ^{o} (*c*=0.16, MeOH). UV (MeOH) nm: 227, 280. EI-MS

m/z: 332 $[M]^+$. ^{1}H-NMR (400 MHz, MeOH-d_4) δ: 1.95 (2H, m, H-2, 3), 2.63 (4H, m, H-7′, 7″), 3.55 (2H, ddd, *J*=11.1, 5.7, 2.7 Hz, H_a-1, H_a-4), 3.62 (2H, ddd, *J*=11.1, 6.8, 2.4 Hz, H_b-1, H_b-4), 3.78 (3H, s, -OC$\underline{H}_3$) 6.57 (1H, dd, *J*=8.0, 1.9 Hz, H-6″), 6.60 (3H, overlapped, H-2′, 4′, 6′), 6.65 (1H, d, *J*=1.9 Hz, H-2″), 6.68 (1H, d, *J*=8.0 Hz, H-5″), 7.04 (1H, t, *J*=8.0 Hz, H-5′). [Wang *et al*., *Chem. Pharm. Bull.,* **48**, 1606-1610 (2000)]

Compound 5

Amorphous powder. EI-MS *m/z*: 334 $[M]^+$. ^{1}H-NMR (400 MHz, MeOH-d_4) δ: 1.86 (2H, m, H-2, 3), 2.51 (4H, m, H-7′, 7″), 3.45 (2H, dd, *J*=11.1, 5.3 Hz, H_a-1, H_a-4), 3.56 (2H, dd, *J*=11.1, 3.8 Hz, H_b-1, H_b-4), 6.41 (2H, dd, *J*=8.0, 2.2 Hz, H-6′, 6″), 6.55 (2H, dd, *J*=2.2 Hz, H-2′, 2″), 6.60 (2H, d, *J*=8.0 Hz, H-5′, 5″). [Wang *et al*., *Chem. Pharm. Bull.,* **48**, 1606-1610 (2000)]

Compound 6

Amorphous powder. EI-MS *m/z*: 318 $[M]^+$. ^{1}H-NMR (400 MHz, MeOH-d_4) δ: 1.94 (2H, m, H-2, 3), 2.56 (2H, m, H-7′ or H-7″), 2.62 (2H, m, H-7″ or H-7′), 3.50 (2H, ddd, *J*=11.1, 6.0, 3.6 Hz, H_a-1, H_a-4), 3.61 (2H, ddd, *J*=11.1, 7.0, 4.1 Hz, H_b-1, H_b-4), 6.45 (1H, dd, *J*=8.0, 2.1 Hz, H-4′), 6.58 (1H, ddd, *J*=8.0, 2.1, 2.1 Hz, H-6′), 6.59 (1H, s, H-2″), 6.59 (1H, t, *J*=2.1 Hz, H-2′), 6.61 (1H, d, *J*=8.0 Hz, H-6″), 6.64 (1H, d, *J*=8.0 Hz, H-5″), 7.03 (1H, t, *J*=8.0 Hz, H-5′). [Wang *et al*., *Chem. Pharm. Bull.,* **48**, 1606-1610 (2000)]

Compound 7

Amorphous powder. EI-MS *m/z*: 302 $[M]^+$. ^{1}H-NMR (400 MHz, MeOH-d_4) δ: 1.98 (2H, m, H-2, 3), 2.64 (4H, m, H-7′, 7″), 3.53 (2H, dd, *J*=11.1, 5.3 Hz, H_a-1, H_a-4), 3.63 (2H, dd, *J*=11.1, 3.8 Hz, H_b-1, H_b-4), 6.60 (2H, ddd, *J*=7.8, 2.2, 1.2 Hz, H-4′, 4″), 6.62 (4H, overlapped, H-2′, 2″, 6′, 6″), 7.05 (2H, t, *J*=7.8 Hz, H-5′, 5″). [Wang *et al*., *Chem. Pharm. Bull.,* **48**, 1606-1610 (2000)]

(+)-Enterolactone (8)

Amorphous powder. $[\alpha]_D$ 34.8 (*c*=0.12, MeOH). EI-MS *m/z*: 298 $[M]^+$. ^{1}H-NMR (400 MHz, MeOH-d_4) δ: 2.50 (2H, m, H_a-7″, 3), 2.59 (1H, m, H-2), 2.61 (1H, m, H_b-7″), 2.91 (1H, m, H_a-7′), 3.00 (1H, m, H_b-7′), 3.87 (1H, dd, *J*=9.1, 7.6 Hz, H_a-4), 4.14 (1H,

dd, *J*=9.1, 7.0 Hz, H_b-4), 6.47 (1H, t, *J*=1.6 Hz, H-2″), 6.59 (1H, t, *J*=1.6 Hz, H-2′), 6.60 (1H, ddd, *J*=7.9, 1.6, 1.6 Hz, H-6″), 6.70 (1H, m, H-4′), 6.73 (1H, dt, *J*=7.9, 1.6, 1.6 Hz, H-6′), 6.74 (1H, m, H-4″), 7.15 (1H, t, *J*=7.9 Hz, H-5″), 7.18 (1H, t, *J*=7.9 Hz, H-5′). [Wang *et al*., *Chem. Pharm. Bull.,* **48**, 1606-1610 (2000)]

参考論文

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2) Gao J. J. and Hattori M.: Metabolic activation of lignans to estrogenic and anti-eatrogenic substances by human intestinal bacteria. *J. Trad. Med*., **22**, 213-221 (2005).