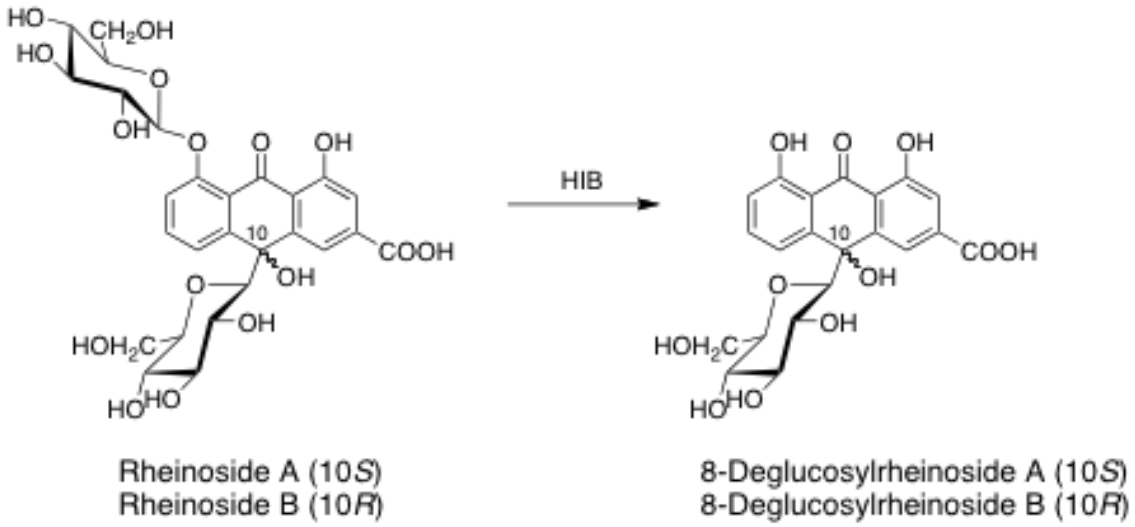
Rheinoside A, B



Metabolic processes of rheinosides A and B by human intestinal bacteria

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　rheinoside A, B

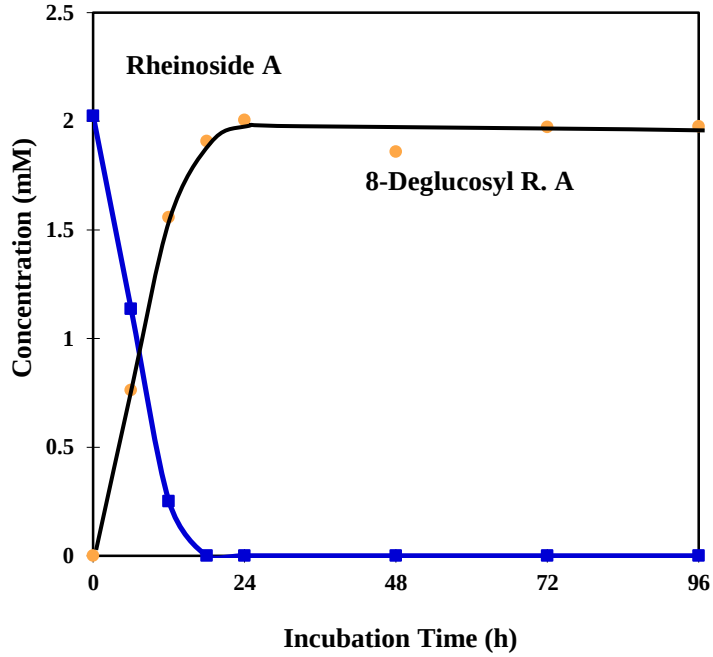


Fig. 1. Metabolic time course of rheinoside A by human intestinal bacterial flora

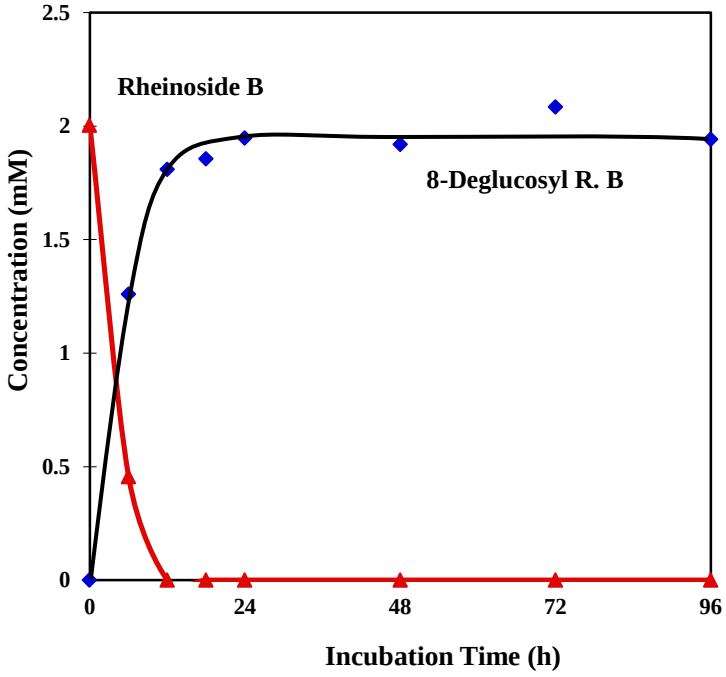


Fig. 2. Metabolic time course of rheinoside B by human intestinal bacterial

flora

Metabolism of rheinosides by human intestinal flora

A fecal bacterial suspension (0.5 ml) precultured for 24 h was inoculated into PYF broth (4.5 ml) containing 2 mM rheinoside A or B, and the mixture was anaerobically incubated for 24 h.

Detection for metabolites of rheinosides A and B

A 50 ml portion was taken out, and mixed with 50 ml of MeOH containing 0.1% AcOH, followed by centrifugation at 8800 x g for 1 min to separate a supernatant and precipitates. A portion of the supernatant was applied to a normal phase TLC plate of silica gel and developed with a mixed solvent $CHCl_3$-MeOH-H_2O (6 : 4 : 1). The metabolite was quantitatively determined by TLC-densitomstry at a wavelength of 350 nm.

Rheinoside A

Pale yellow amorphous powder, FAB-MS: *m/z* 611 $[M+H]^+$. ^{1}H-NMR (D_2O, 500 MHz)δ: 7.76 (1H, brs, H-4), 7.69 (1H, dd, *J*=7.2, 7.6 Hz, H-6), 7.60 (1H, brd, *J*=7.6 Hz, H-5), 7.28 (1H, d, *J*=7.2 Hz, H-7), 7.27 (1H, brs, H-2), 5.14 (1H, d, *J*=7.7 Hz, H-1″), 3.93 (1H, dd, *J*=2.1, 12.4 Hz, H_a-6″), 3.74－3.80 (2H, m, H-2″, H_b-6″), 3.51－3.66 (4H, m, H_a-6′, H-3″, H-4″, H-5″), 3.37 (1H, dd, *J*=5.8, 12.2 Hz, H_b-6′), 3.24－3.29 (2H, m, H-1′, H-3′), 2.86－2.96 (3H, m, H-2′, H-4′, H-5′). ^{13}C-NMR (D_2O, 75 MHz)δ: 188.9 (C-9), 168.8 (COOH), 158.1 (C-1), 156.6 (C-8), 145.1 (C-10a), 145.0 (C-4a), 135.2 (C-3, C-6), 121.0 (C-8a), 120.9 (C-9a), 120.7 (C-5), 117.8 (C-2), 117.2 (C-4), 115.8 (C-7), 100.6 (C-1″), 82.2(C-1′), 79.5 (C-5′), 77.4 (C-3′), 76.3 (C-5″), 75.8 (C-3″), 75.0 (C-10), 73.0 (C-2’, C-2″), 71.5 (C-4″), 69.3 (C-4′), 61.1 (C-6′), 60.6 (C-6″).

Rheinoside B

Pale yellow amorphous powder, FAB-MS: *m/z* 611 $[M+H]^+$. ^{1}H-NMR (D_2O, 500 MHz)δ: 7.89 (1H, d, *J*=1.2 Hz, H-4), 7.72－7.79 (2H, m, H-5, H-6), 7.50 (1H, d, *J*=1.2 Hz, H-2), 7.38 (1H, d, *J*=8.1 Hz, H-7), 5.24 (1H, d, *J*=7.7 Hz, H-1″), 3.91 (1H, dd, *J*=2.1, 12.4 Hz, H_a-6″), 3.72－3.76 (2H, m, H-2″, H_b-6″), 3.61－3.67 (2H, m, H-3″,

H-5″), 3.51－3.59 (2H, m, H_a-6′, H-4″), 3.40－3.45 (2H, m, H-1′, H_b-6′), 3.32 (1H, t, *J*=9.0 Hz, H-3′), 3.04 (1H, m, H-5′), 2.87－2.94 (2H, m, H-2′, H-4′). ^{13}C-NMR (D_2O, 75 MHz) δ: 189.4 (C-9), 169.2 (COOH), 158.9 (C-1), 156.5 (C-8), 147.1 (C-4a), 143.6 (C-10a), 135.9 (C-3), 135.3 (C-6), 121.8 (C-8a or C-9a), 121.3 (C-8a or C-9a), 120.7(C-5), 118.2 (C-4), 118.0 (C-2), 117.7 (C-7), 102.0 (C-1″), 82.2 (C-1′), 79.7 (C-5′), 77.6 (C-3′ or C-5″), 76.7 (C-3’ or C-5″), 75.5 (C-3″), 75.3 (C-10), 73.3 (C-2″), 71.7 (C-2′), 69.7 (C-4″), 69.4 (C-4′), 61.3 (C-6′), 61.0 (C-6″).

8-Deglucosylrheinoside A

Pale yellow amorphous powder, FAB-MS: *m/z* 449 $[M+H]^+$. ^{1}H-NMR (D_2O, 300 MHz) δ: 7.79 (1H, brs, H-4), 7.61 (1H, dd, *J*=7.4, 8.2 Hz, H-6), 7.41 (1H, brs, H-2), 7.35 (1H, d, *J*=7.4 Hz, H-5), 6.95 (1H, d, *J*=8.2 Hz, H-7), 3.65 (1H, brd, *J*=12.2 Hz, H_a-6′), 3.45 (1H, dd, *J*=6.6, 12.2 Hz, H_b-6′), 3.39 (1H, d, *J*=9.5 Hz, H-1′), 3.19 (1H, t, *J*=9.5 Hz, H-3′), 3.08 (1H, m, H-5′), 2.87 (1H, t, *J*=9.5 Hz, H-4′), 2.63 (1H, t, *J*=9.5 Hz, H-2′). ^{13}C-NMR (D_2O, 75 MHz) δ: 192.2 (C-9, C=O), 169.2 (COOH), 160.6, 159.9, 145.6, 144.8, 137.1, 136.9, 118.9 (2C), 118.1, 118.0, 117.6, 115.7, 83.9, 79.8, 77.6, 74.4, 71.4, 69.5, 61.4.

8-Deglucosylrheinoside B

Pale yellow amorphous powder, FAB-MS: *m/z* 449 $[M+H]^+$. ^{1}H-NMR (D_2O, 300 MHz) δ: 7.65 (1H, brs, H-4), 7.57 (1H, dd, *J*=8.2, 9.1 Hz, H-6), 7.36 (1H, d, *J*=9.1 Hz, H-5), 7.34 (1H, brs, H-2), 6.94 (1H, d, *J*=8.2 Hz, H-7), 3.67 (1H, brd, *J*=12.2 Hz, H_a-6′), 3.48 (1H, dd, *J*=6.2, 12.2 Hz, H_b-6′), 3.37 (1H, d, *J*=9.4 Hz, H-1′), 3.16 (1H, t, *J*=9.4 Hz, H-3′), 3.10 (1H, m, H-5′), 2.87 (1H, t, *J*=9.4 Hz, H-4′), 2.56 (1H, t, *J*=9.4 Hz, H-2′). ^{13}C-NMR (D_2O, 75 MHz)δ: 192.3 (C-9, C=O), 169.5 (COOH), 160.5, 160.0, 145.4, 145.1, 137.3 (2C), 118.9, 118.8, 118.4, 118.2, 117.5, 115.2, 84.0, 79.9, 77.6, 74.3, 71.5, 69.7, 61.5.

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