10-Hydroxyaloin A, B

Conversion of 10-hydroxyaloin by human intestinal flora

代謝実験

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単一化合物 10-hydroxyaloin A, B

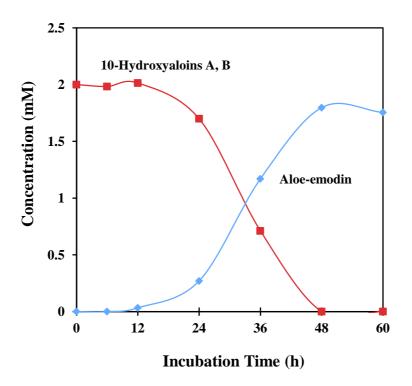


Fig. 1. Metabolic time course of 10-hydroxyaloins A, B by human intestinal bacteria

\blacksquare , 10-hydroxyaloins A and B; \blacklozenge , aloe-emodin

Metabolism of 10-hydroxyaloins A and B by human intestinal flora

A 0.5 ml portion of a bacterial suspension of *Eubacterium* sp. BAR cultured in GAM broth for 24 h at 37°C was inoculated into PYF broth (4.5 ml) containing 10-hydroxyaloin A or B (final concentration of 1 mM), and the mixture was anaerobically incubated at 37°C. The metabolite formation was monitored at intervals by TLC densitometry. Bacterial growth was monitored at 540 nm after 10-fold dilution of the culture.

Metabolism of 10-hydroxyaloins A and B 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 10-hydroxyaloin A or B, and the mixture was anaerobically incubated for 24 h at 37°C. 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 CHCl₃-MeOH-H₂O (7:3:0.5). The metabolite was detected at a wavelength of 360 nm.

10-Hydroxyaloin A

Yellow amorphous powder, FAB-MS: *m/z* 419 [M+H]⁺. ¹H-NMR (CD₃OD, 500 MHz) δ: 7.57 (1H, dd, *J*=7.6, 8.2 Hz, H-6), 7.47 (1H, dd, *J*=1.2, 7.6, Hz, H-5), 7.38 (1H, d, *J*=1.5 Hz, H-4), 6.95 (1H, d, *J*=1.5 Hz, H-2), 6.92 (1H, dd, *J*=1.2, 8.2 Hz, H-7), 4.71 (2H, d, *J*=14.7 Hz, 3-CH₂OH), 4.67 (1H, d, *J*=14.7 Hz, 3-CH₂OH), 3.58 (1H, dd, *J*=2.8, 11.9 Hz, H_a-6'), 3.37 (1H, dd, *J*=6.4, 11.9 Hz, H_b-6'), 3.27 (1H, d, *J*=9.8 Hz, H-1'), 3.24 (1H, t, *J*=8.9 Hz, H-3'), 2.95 (1H, dd, *J*=8.9, 9.8 Hz, H-2'), 2.94 (1H, m, H-5'), 2.82 (1H, dd, *J*=8.9, 9.6 Hz, H'-4). ¹³C-NMR (CD₃OD, 75 MHz) δ: 194.5 (C-9), 163.1 (C-1), 163.0 (C-8), 152.4 (C-3), 149.2 (C-10a), 146.7 (C-4a), 136.4 (C-6), 118.9 (C-5), 118.3 (C-7), 117.8 (C-8a), 116.3 (C-4), 115.9 (C-9a), 115.3 (C-2), 85.2 (C-1'), 81.7 (C-5'), 79.6 (C-3'), 76.9 (C-10), 73.0 (C-2'), 71.7 (C-4'), 64.7 (C-11), 63.3 (C-6').

10-Hydroxyaloin B

Yellow amorphous powder, FAB-MS: *m/z* 419 [M+H]⁺. ¹H-NMR (CD₃OD, 500 MHz) δ: 7.58 (1H, dd, *J*=7.6, 8.2 Hz, H-6), 7.48 (1H, d, *J*=1.5, Hz, H-4), 7.39 (1H, dd, *J*=1.2, 7.6 Hz, H-5), 6.93 (1H, d, *J*=1.5 Hz, H-2), 6.93 (1H, dd, *J*=1.2, 8.2 Hz, H-7), 4.69 (2H, d, *J*=14.5 Hz, 3-CH₂OH), 4.65 (1H, d, *J*=14.5 Hz, 3-CH₂OH), 3.56 (1H, dd, *J*=2.4, 11.6 Hz, H_a-6'), 3.36 (1H, dd, *J*=6.1, 11.6 Hz, H_b-6'), 3.26 (1H, d, *J*=9.2 Hz, H-1'), 3.25 (1H, t, *J*=8.9 Hz, H-3'), 2.99 (1H, dd, *J*=8.9, 9.2 Hz, H-2'), 2.92 (1H, m, H-5'), 2.83 (1H, dd, *J*=8.9, 9.8 Hz, H'-4). ¹³C-NMR (CD₃OD, 75 MHz) δ: 194.6 (C-9), 163.3 (C-1), 162.7 (C-8), 151.8 (C-3), 148.9 (C-10a), 147.0 (C-4a), 137.2 (C-6), 118.1 (C-5), 118.0 (C-7), 117.3 (C-8a), 117.0 (C-4), 116.6 (C-9a), 115.4 (C-2), 85.3 (C-1'), 81.8 (C-5'), 79.6 (C-3'), 76.8 (C-10), 73.0 (C-2'), 71.8 (C-4'), 64.7 (C-11), 63.4 (C-6').

参考文献

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