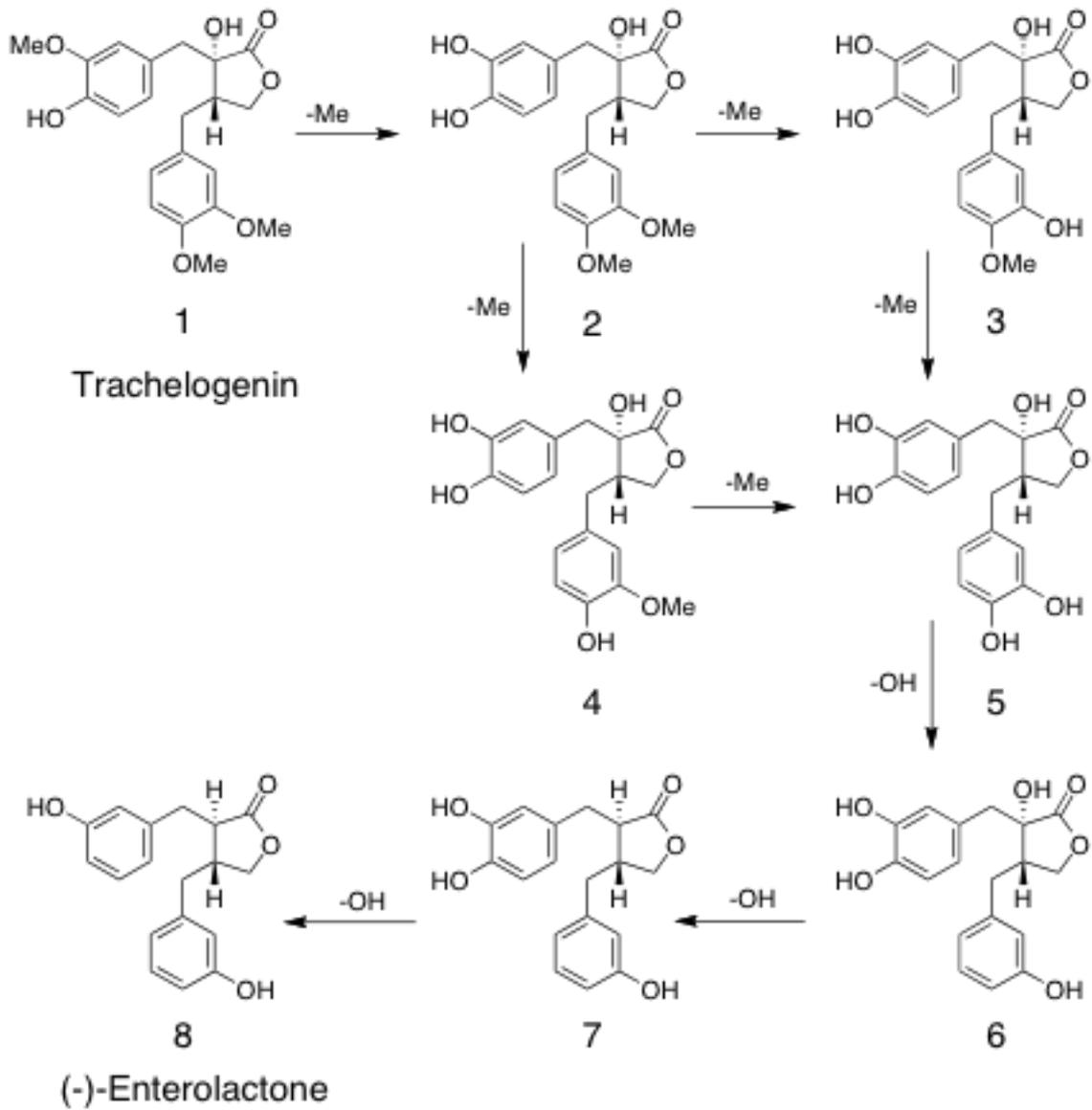


Trachelogenin

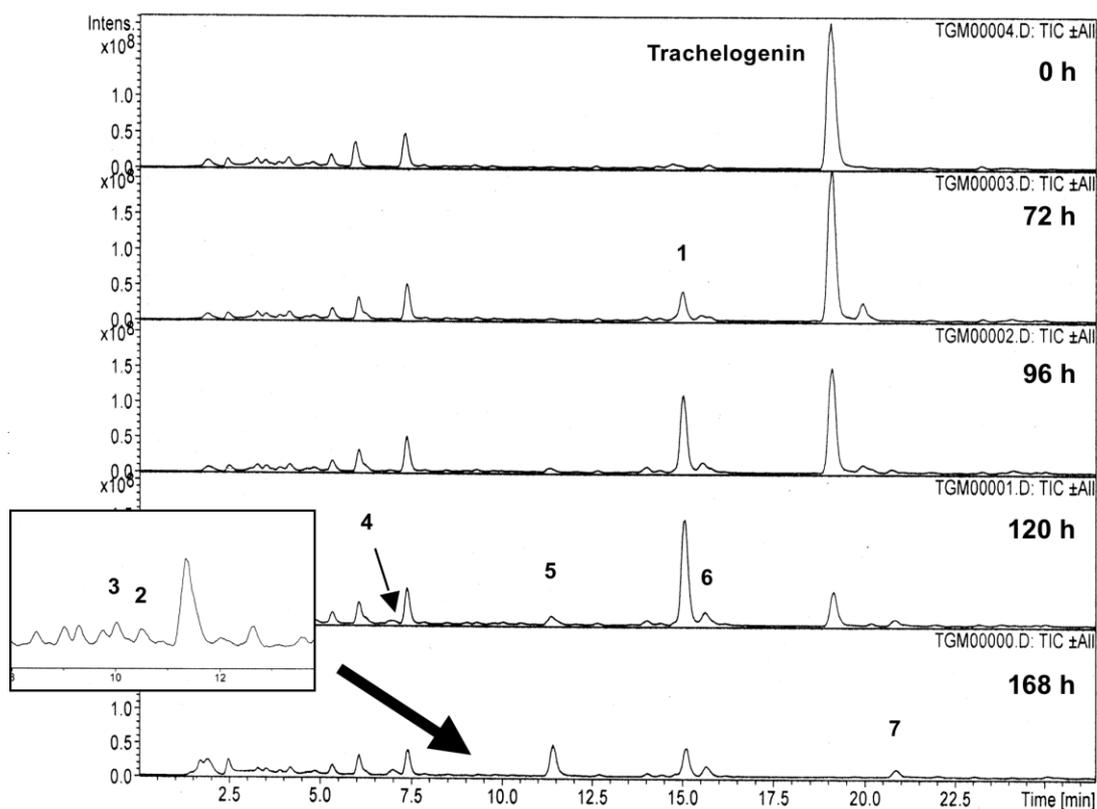


Metabolic processes of trachelogenin by human intestinal bacteria

代謝実験

腸内細菌代謝 ヒト腸内細菌フローラ

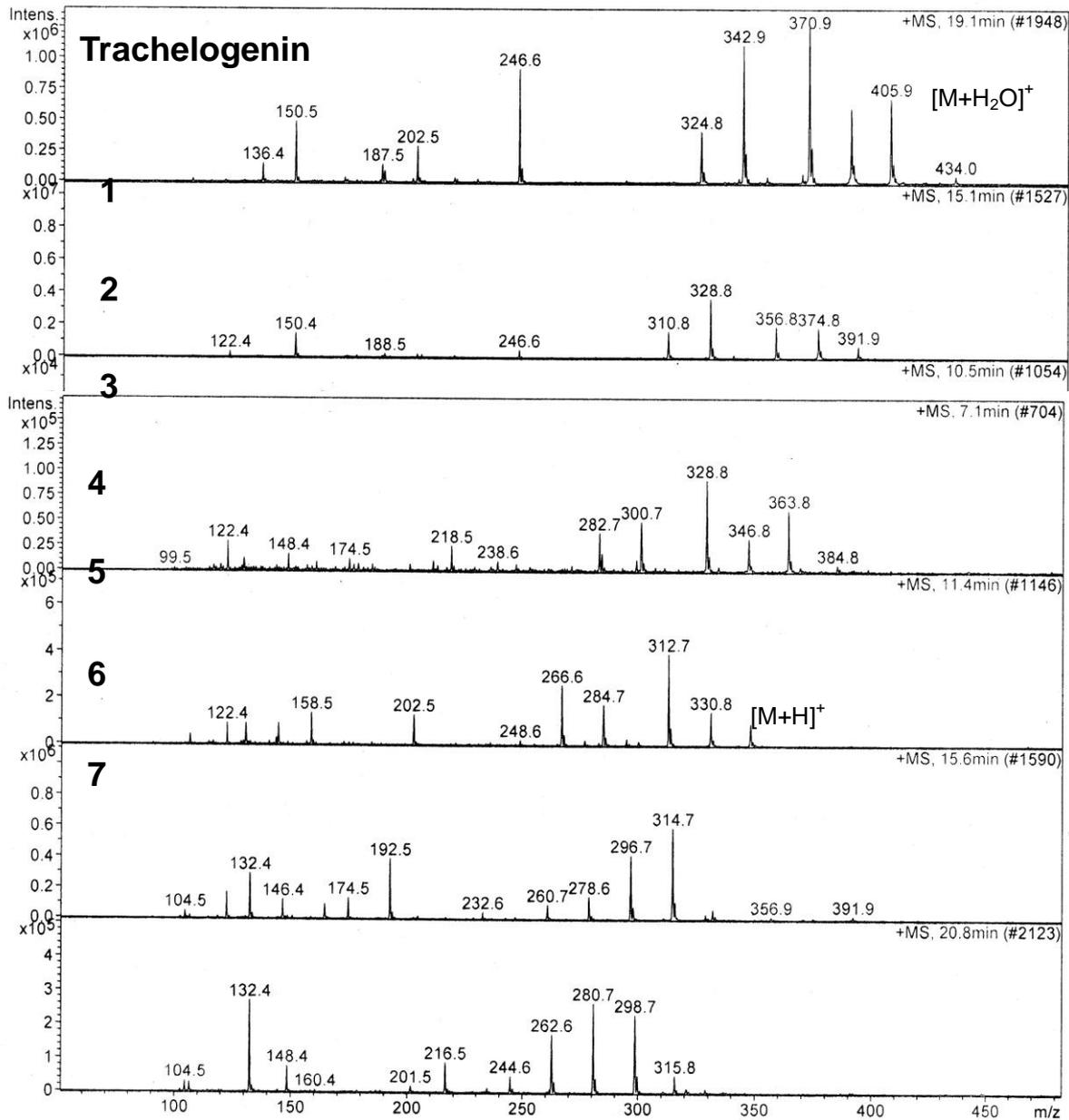
単一化合物 trachelogenin



HPLC elution profiles of transformation of trachelogenin by human intestinal bacteria (HIB)

Incubation of trachelogenin with a mixture of human intestinal bacteria

A 6 ml portion of a 5% HIB mixture was inoculated to 60 ml of GAM broth containing 0.5 mM trachelogenin and anaerobically incubated at 37°C. A 750 µl aliquot was then taken out at 12 h intervals and extracted three times with 300 µl of ethyl acetate. After evaporation of the ethyl acetate under reduced pressure, the residue was dissolved in 50 µl of MeOH. The MeOH solution was filtered through a 0.2 µm membrane filter, and a 10 µl portion was injected to a column for HPLC analysis. [submitted to *J. Food Sci.*]



Analysis of transformation products was performed under the following conditions: column, TSK-gel ODS-80Ts (Tosoh Co., Tokyo, Japan, 4.6 mm × 150 mm); mobile phase, 0.1 % acetic acid (solvent system A) and CH₃CN (solvent system B) in a linear gradient mode (B from 20 to 50% in 30 min); flow rate, 1.0 ml/min; detection, UV 254 nm; temperature, 30°C. Analysis of (+)- and (-)-ENL was performed under the following conditions: column, chiral CD-Ph (Shiseido, Tokyo, Japan, 4.6 mm × 250 mm); mobile phase, 0.1 % acetic acid (solvent system A) and CH₃CN (solvent system B) in a linear gradient mode (B from 30 to 48 % for 36 min); flow rate, 0.5 ml/min; detection, UV at 280 nm; temperature, 30°C. High-purity nitrogen was used as dry gas

at a flow rate at 10 L/min, dry temperature at 360°C. Helium was used as nebulizer at 50 psi. The ESI interface and mass spectrometric parameters were optimized to obtain maximum sensitivity. [submitted to *J. Food Sci.*]

(3*S*,4*S*)-3-(3,4-Dihydroxybenzyl)-4-(3,4-dimethoxybenzyl)-3-hydroxydihydrofuran-2(3*H*)-one (1)

Colorless oil. ESI-MS m/z : 375 [M+H]⁺, 392 [M+H₂O]⁺. [submitted to *J. Food Sci.*]

(3*S*,4*S*)-3-(3,4-Dihydroxybenzyl)-3-hydroxy-4-(3-hydroxy-4-methoxybenzyl)-dihydrofuran-2(3*H*)-one (2)

Colorless oil. ESI-MS m/z : 361 [M+H]⁺, 378 [M+H₂O]⁺. ¹H-NMR (CD₃OD, 500 MHz) δ : 2.50-2.85 (3H, m, H-4, H-7''), 2.90 (1H, dd, $J=7.0, 14.5$ Hz, H_a-7'), 3.03 (1H, dd, $J=5.5, 14.5$ Hz, H_b-7'), 3.80 (3H, s, -OCH₃), 3.84 (1H, dd, $J=7.5, 8.5$ Hz, H_a-5), 4.01 (1H, dd, $J=7.5, 8.5$ Hz, H_b-5), 6.57 (2H, dd, $J=2.0, 8.0$ Hz, H-6', 6''), 6.66 (1H, d, $J=2.0$ Hz, H-2''), 6.70 (1H, d, $J=2.5$ Hz, H-2'), 6.74 (1H, d, $J=8.0$ Hz, H-5'), 6.80 (1H, d, $J=8.0$ Hz, H-5''). [submitted to *J. Food Sci.*]

(3*S*,4*S*)-3-(3,4-Dihydroxybenzyl)-3-hydroxy-4-(4-hydroxy-3-methoxybenzyl)-dihydrofuran-2(3*H*)-one (3)

Colorless oil. ESI-MS m/z : 361 [M+H]⁺, 378 [M+H₂O]⁺. ¹H-NMR (CD₃OD, 500 MHz) δ : 2.57-2.84 (3H, m, H-3, 7''), 2.98 (2H, d, $J=6.5$ Hz, H-7'), 3.81 (3H, s, -OCH₃), 3.86 (1H, dd, $J=8, 8.5$ Hz, H_a-5), 4.03 (1H, dd, $J=7, 9$ Hz, H_b-5), 6.52-6.62 (3H, m, H-6', 2'', 6''), 6.66 (1H, d, $J=2.5$ Hz, H-2'), 6.76 (1H, d, $J=7.5$ Hz, H-5'), 6.81 (1H, d, $J=8.0$ Hz, H-5''). [submitted to *J. Food Sci.*]

(3*S*,4*S*)-3,4-Bis(3,4-dihydroxybenzyl)-3-hydroxydihydrofuran-2(3*H*)-one (4)

Colorless oil. ESI-MS m/z : 347 [M+H]⁺, 364 [M+H₂O]⁺. ¹H-NMR (CD₃OD, 500 MHz) δ : 2.43-2.71 (3H, m, H-4, H-7''), 2.95 (2H, d, $J=6.5$ Hz, H-7'), 3.87 (1H, t, $J=8.5$ Hz, H_a-5), 4.02 (1H, t, $J=7.5$ Hz, H_b-5), 6.45 (1H, dd, $J=2,8$ Hz, H-6''), 6.47 (1H, dd, $J=2,8$ Hz, H-6'), 6.56 (1H, d, $J=2.5$ Hz, H-2''), 6.64 (1H, d, $J=2.0$ Hz, H-2'), 6.66 (1H, d, $J=8.5$ Hz, H-5''), 6.68 (1H, d, $J=8.0$ Hz, H-5'). [submitted to *J. Food Sci.*]

(3*S*,4*S*)-3-(3,4-Dihydroxybenzyl)-3-hydroxy-4-(3-hydroxybenzyl)dihydrofuran-2(3*H*)-one (5)

Colorless oil. ESI-MS m/z : 331 [M+H]⁺, 348 [M+H₂O]⁺. ¹H-NMR (CD₃OD, 500 MHz) δ : 2.50-2.78 (3H, m, H-4, 7''), 2.97(2H, m, H-7'), 3.85 (1H, t, $J=8.0, 8.5$ Hz, H_a-5), 4.03 (1H, d, $J=7.5$ Hz, H_b-5), 6.48 (1H, dd, $J=2,8$ Hz, H-6'), 6.58 (1H, s, H-2''), 6.61 (1H, d,

$J=8.0$ Hz, H-6''), 6.63 (1H, d, $J=8.0$ Hz, H-5'), 6.66 (1H, d, $J=2.0$ Hz, H-2'), 6.70 (1H, dd, $J=2.0, 8.0$ Hz, H-4''), 7.08 (1H, t, $J=8.0$ Hz, H-5''). [submitted to *J. Food Sci.*]

**(3*R*,4*R*)-3-(3,4-Dihydroxybenzyl)-4-(3-hydroxybenzyl)dihydrofuran-2(3H)-one
[(-)-4'-Hydroxyenterolactone] (6)**

Colorless oil. $[\alpha]_D -44^\circ$ ($c = 0.1$). ESI-MS m/z : 315 $[M+H]^+$. [submitted to *J. Food Sci.*]

(3*R*,4*R*)-3,4-Bis(3-hydroxybenzyl)dihydrofuran-2(3H)-one [(-)-Enterolactone] (7)

Amorphous powder. $[\alpha]_D -42^\circ$ ($c = 0.1$). ESI-MS m/z : 299 $[M+H]^+$, 316 $[M+H_2O]^+$. [submitted to *J. Food Sci.*]