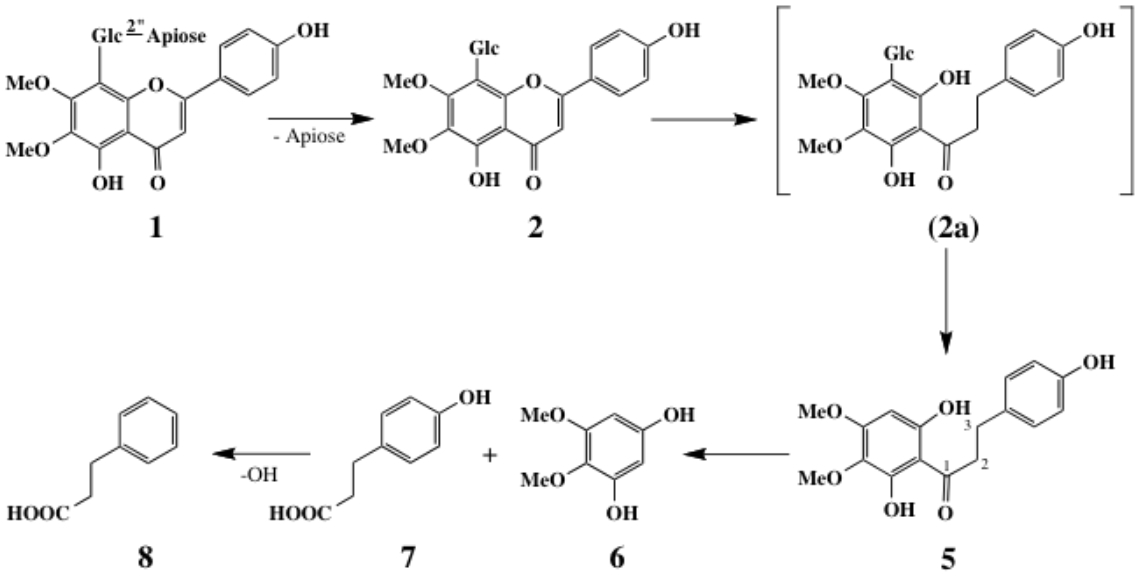
Abrusin 2″-O-β-D-apioside



Metabolic processes of abrusin 2″-*O*-*β*-D-apioside by a human intestinal bacterial mixture

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Transformation of abrusin 2″-*O*-*β*-D-apioside (1) by a human fecal suspension

Abrusin 2″-*O*-*β*-D-apioside (**1**, 200 mg in 2 ml H_2O) was incubated with human fecal suspension (5%, 200 ml) for 24 hr at 37°C in an anaerobic incubator. After acidification with 0.1% CH_3COOH, the reaction mixture was extracted with BuOH saturated with water (200 ml × 4) and the BuOH layer was evaporated *in vacuo* to give 910 mg of a dry residue. The residue was chromatographed over a column of RP-2 (MeOH-H_2O, 8:2) and then Sephadex LH-20 (elution with EtOH), which gave fractions A (84 mg) and B (35 mg). Fr. A was chromatographed on Silica gel ($CHCl_3$-MeOH, 8:2) and MPLC ($CHCl_3$-MeOH, 15:1, 6:1) to give compounds **2** (21 mg) and **5** (8 mg). Fr. B was further applied to a column of silica gel ($CHCl_3$, $CHCl_3$-MeOH, 15:1), and then preparative TLC ($CHCl_3$-MeOH, 20:1) to afford compounds **6** (11 mg), **7** (3 mg) and **8** (3 mg). [Li *et al*., *Chem. Pharm. Bull.,* **48**, 1239-1241 (2000)]

Abrusin (2)

Yellow amorphous powder. ESI-MS (negative mode) *m/z* 475 $[M-H]^-$.

1-(2′, 6′-Dihydroxyl-3′, 4′-dimethoxyphenyl)-3-(4″-hydroxyphenyl)propan-1-one (5)

Yellow amorphous powder. EI-MS *m/z* 318 $[M]^+$. IR (KBr) $\nu_{max}cm^{-1}$: 3300—3500 br (OH), 1738 (C=O), 1678, 1620, 1520, 1440 (C=C); ^{1}H-NMR (DMSO-d_6, 500 MHz): δ 2.96 (2H, t, *J*=7.4 Hz, H_2-3), 3.38 (2H, t, *J*=7.4 Hz, H_2-2), 3.83 (3H, s, -OCH_3), 3.88 (3H, s, -OCH_3), 6.06 (1H, s, H-5′), 6.76 (2H, d, *J*=8.3 Hz, H-3″ and H-5″), 7.13 (2H, d, *J*=8.3 Hz, H-2″ and H-6″); ^{13}C-NMR (DMSO-d_6, 125 MHz): δ 29.4 (C-3), 45.9 (C-2), 55.6, 60.3 (-O<u>C</u>H_3), 91.4 (C-5′), 104.4 (C-1′), 115.2 (C-3″, 5″), 121.4 (C-1″), 129.3 (C-2″, 6″), 131.6 (C-3′), 154.8 (C-2′ or C-6′), 155.5 (C-6′ or C-2′), 158.8 (C-4′), 159.8 (C-4″), 205.2 (C-1). [Li *et al*., *Chem. Pharm. Bull.,* **48**, 1239-1241 (2000)]

5, 6-Dimethoxybenzene-1, 3-diol (6)

Orange amorphous powder. EI-MS *m/z* 170 $[M]^+$. ^{1}H-NMR ($CDCl_3$, 500 MHz): δ 3.80 (3H, s, -OCH_3), 3.92 (3H, s, -OCH_3), 6.02 (1H, d, *J*=2.7 Hz, H-6), 6.10 (1H, d, *J*=2.7 Hz, H-2). ^{13}C-NMR ($CDCl_3$, 125 MHz): d 55.8, 61.2, 92.4, 95.0, 129.6, 149.6, 152.5, 153.0.

[Li *et al*., *Chem. Pharm. Bull.,* **48**, 1239-1241 (2000)]

3-(4′-Hydroxyphenyl)propionic Acid (7)

White amorphous powder. EI-MS *m/z* 166 $[M]^+$. The ^{1}H- and ^{13}C-NMR spectra were in good agreement with those of an authentic sample of 3-(4-hydroxyphenyl) propionic acid. [Li *et al*., *Chem. Pharm. Bull.,* **48**, 1239-1241 (2000)]

3-Phenylpropionic Acid (8)

White amorphous powder. EI-MS *m/z* 150 $[M]^+$. The ^{1}H- and ^{13}C-NMR spectra were in good agreement with those of an authentic sample of 3-phenylpropionic acid.

[Li *et al*., *Chem. Pharm. Bull.,* **48**, 1239-1241 (2000)]

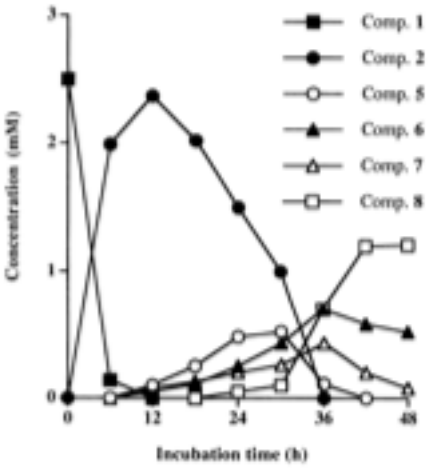

Fig. 1. Time course of conversion of abrusin 2"-*O*-β-D-apioside (**1**) by a human fecal suspension

Time course of the transformation of abrusin 2″-*O*-*β*-D-apioside (1)

Abrusin 2″-*O*-*β*-D-apioside (**1**, 10 mmol in 200 ml DMSO) was added to a human fecal suspension (5%, 3.8 ml) and incubated at 37°C in an anaerobic incubator. Samples were picked up at intervals and extracted with BuOH (saturated with water and acidified with CH_3COOH, 200 ml). After centrifugation at 8,800 × *g* for 5 min, 100 ml of the BuOH layer was evaporated *in vacuo* to give a residue. The residue was dissolved in MeOH (100 ml) and filtered through a Gelman filter (0.45 μm). The metabolites in the MeOH filtrate were analyzed by HPLC using calibration lines obtained with isolated compounds (**5** and **6**) or authentic samples (**1**, **2**, **7** and **8**). [Li *et al*., *Chem. Pharm. Bull.,* **48**, 1239-1241 (2000)]

参考文献

1) Li Y., Meselhy M. R., Wang L., Ma C., Nakamura N., and Hattori M.: Biotransformation of a *C*-glycosylflavone, abrusin 2″-*O*-*b*-D-apioside, by human intestinal bacteria. *Chem. Pharm. Bull.,* **48,** 1239-1241 (2000).