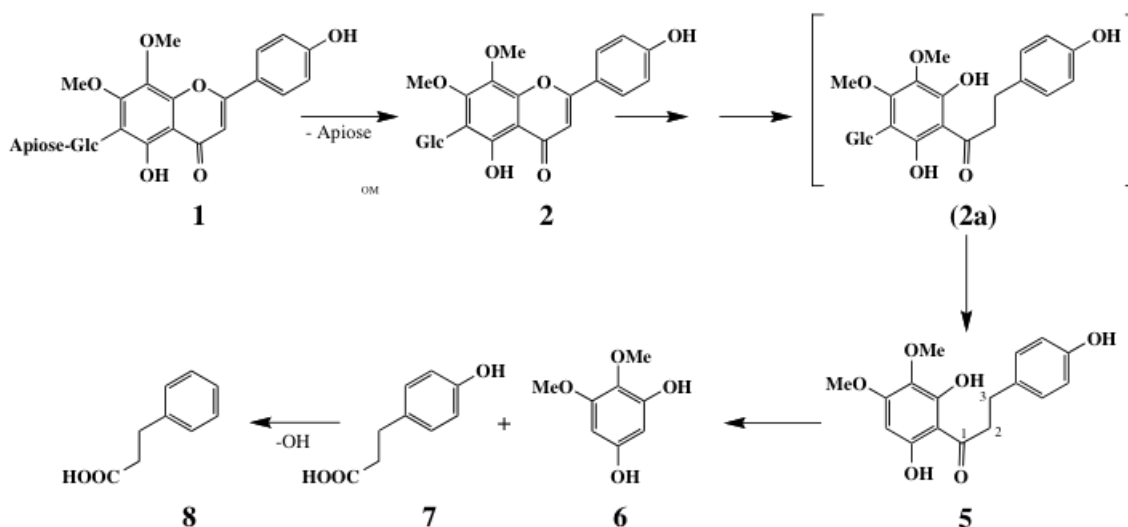


## Precatorin II



Metabolic processes of precatorin II by a human intestinal microflora

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### Preparation of an intestinal bacterial mixture

Fresh feces obtained from a healthy subject were thoroughly suspended in 100-fold of 50 mM K-phosphate buffer (pH 7.3) to give a human fecal suspension, which was use in this experiment. [Li *et al.*, *Chem. Pharm. Bull.*, **48**, 1239-1241 (2000)]

### Precatorin II (1)

Yellow amorphous powder,  $[\alpha]_D^{27} -50.6^\circ$  ( $c = 0.40$ , MeOH). IR  $\nu$   $\text{cm}^{-1}$  (KBr): 3600—3100 br, 1650, 1610, 1570, 1480, 1450, 1350, 1220, 1100, 1040. UV  $\lambda_{\text{max}}$  nm ( $\epsilon$ ): 275 (18500), 295 (16700), 327 (22200). FAB-MS (positive)  $m/z$ : 609  $[\text{M} + \text{H}]^+$ , 477  $[\text{M} - \text{api} + \text{H}]^+$ , 357, 343, 327, 313. Anal. Calcd for  $\text{C}_{28}\text{H}_{32}\text{O}_{15} \cdot 2\text{H}_2\text{O}$ : C, 52.18; H, 5.63. Found: C, 52.00; H, 5.29.  $^1\text{H}$ -NMR and  $^{13}\text{C}$ -NMR: see the following reference: Ma *et al.*, *Chem. Pharm. Bull.* **46**, 982-987 (1998)

### Precatorin I (2)

Yellow needles (EtOH), mp 278—280°C.  $[\alpha]_D^{27} +4.3^\circ$  ( $c = 0.44$ , MeOH). IR  $\nu$  cm<sup>-1</sup> (KBr): 3450—3200 br, 1650, 1610, 1580, 1480, 1440, 1350, 1220, 1100, 1040. UV /C°H nm (e): 275 (19000), 295 (17500), 327 (21900). FAB-MS (positive)  $m/z$ : [M+H]<sup>+</sup>, 357, 343, 327, 313. <sup>1</sup>H-NMR and <sup>13</sup>C-NMR: see the following reference: Ma *et al.*, *Chem. Pharm. Bull.* **46**, 982-987 (1998)

**1-(2', 6'-Dihydroxyl-3', 4'-dimethoxyphenyl)-3-(4''-hydroxyphenyl) propan-1-one (5)**

Yellow amorphous powder. EI-MS  $m/z$  318 [M]<sup>+</sup>. IR (KBr)  $\nu_{\max}$  cm<sup>-1</sup>: 3300—3500 br (OH), 1738 (C=O), 1678, 1620, 1520, 1440 (C=C); <sup>1</sup>H-NMR (DMSO-*d*<sub>6</sub>, 500 MHz):  $\delta$  2.96 (2H, t,  $J=7.4$  Hz, H<sub>2</sub>-3), 3.38 (2H, t,  $J=7.4$  Hz, H<sub>2</sub>-2), 3.83 (3H, s, -OCH<sub>3</sub>), 3.88 (3H, s, -OCH<sub>3</sub>), 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''); <sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>, 125 MHz):  $\delta$  29.4 (C-3), 45.9 (C-2), 55.6, 60.3 (-OCH<sub>3</sub>), 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)]

**4, 5-Dimethoxybenzene-1, 3-diol (6)**

Orange amorphous powder. EI-MS  $m/z$  170 [M]<sup>+</sup>. <sup>1</sup>H-NMR (CDCl<sub>3</sub>, 500 MHz):  $\delta$  3.80 (3H, s, -OCH<sub>3</sub>), 3.92 (3H, s, -OCH<sub>3</sub>), 6.02 (1H, d,  $J=2.7$  Hz, H-2), 6.10 (1H, d,  $J=2.7$  Hz, H-6). <sup>13</sup>C-NMR (CDCl<sub>3</sub>, 125 MHz):  $\delta$  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]<sup>+</sup>. The <sup>1</sup>H- and <sup>13</sup>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]<sup>+</sup>. The <sup>1</sup>H- and <sup>13</sup>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)]

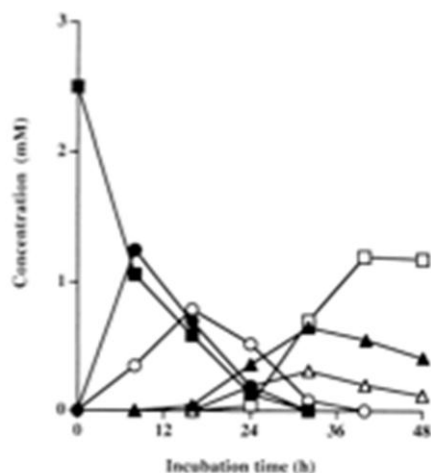


Fig. 1. Time course of conversion of precatorin II by a human fecal suspension

(■), compound 1 (precatorin II); (●), compound 2 (precatorin); (○), compound 5; (▲), compound 6; (△), compound 7; (□), compound 8

### Time course of the transformation of precatorin II

Precatorin II (3, 10 mmol in 200 ml of 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 treated as mentioned above. Metabolites were quantitatively determined by HPLC. [Li *et al.*, *Chem. Pharm. Bull.*, **48**, 1239-1241 (2000)]

### 参考文献

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- 2) Ma C. M., Nakamura N., and Hattori M.: Saponins and C-glucosyl flavones from the seeds of *Abrus precatorius*. *Chem. Pharm. Bull.* **46**, 982-987 (1998).

