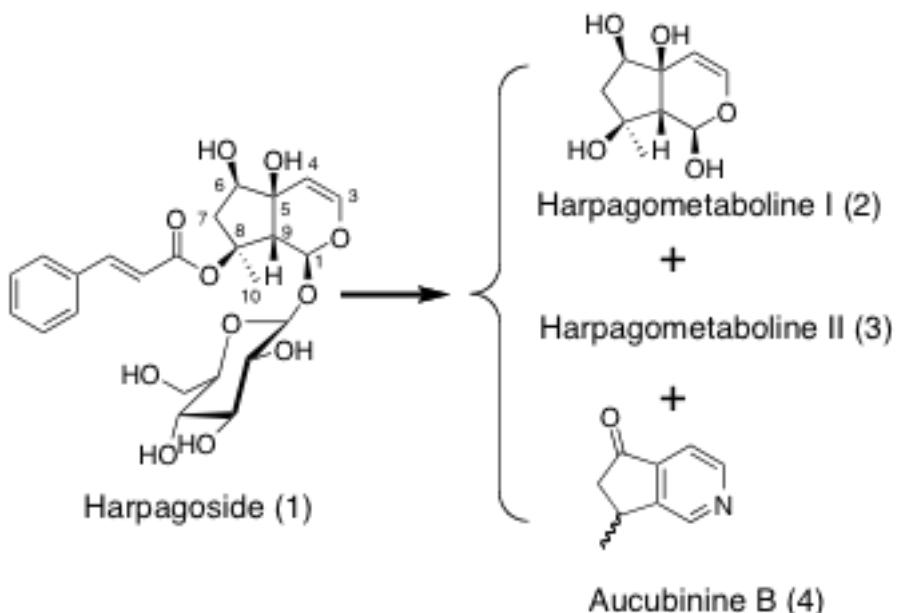


Harpagoside



Metabolic conversion of harpagoside by human intestinal bacteria

代謝実験

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单一化合物 harpagoside

Metabolite A (Harpagometabolin I)

Yellowish oil. IR ν_{max} : 3425, 1715, 1605 cm^{-1} . FABMS (positive): m/z 206 [$\text{M}+\text{Na}$]⁺, 184 [$\text{M} + 1$]⁺. HR-FAB-MS m/z 184.0989 [$\text{M} + 1$]⁺ (calcd for $\text{C}_9\text{H}_{14}\text{NO}_3$ 184.0973). ¹H NMR: δ 5.154, 2.79 (each dd, $J=12.5, 18.9$ Hz and $7.3, 18.9$ Hz), 8.5.30 (dd, $J=4.5, 7.3$ Hz), 2.84 (s), 8.1.25 (s), 8.8.74, 8.53, 8.45 (H-1, H-3, H-4). [Yang et al., *Chinese Chemical Letters*, **11**, 779-782 (2000)]

Metabolite B (Harpagometabolin II)

Yellowish oil. El-MS: m/z 147 [M]⁺, 132 [$\text{M}-\text{Me}$]⁺, 118 [$\text{M}-\text{C}_2\text{H}_5$]⁺, 104 [$\text{M}-\text{C}_3\text{H}_7$]⁺, 91 [$\text{M}-\text{C}_3\text{H}_7-\text{N}$]⁺. IR ν_{max} : 3435, 1725, 1660 cm^{-1} for the OH, C=N and C=C. HR-EI-MS m/z 147.0696 [M]⁺ (calcd for $\text{C}_9\text{H}_9\text{NO}$ 147.0684). [Yang et al., *Chinese Chemical*

Letters, **11**, 779-782 (2000)]

Metabolite C (AucubinineB)

Yellowish oil. IR ν_{max} : 3420, 1725, 1600 cm^{-1} . EI-MS: m/z 147 [M]⁺, 132 [M-Me]⁺, 118 [M-C₂H₅]⁺, 104 [MC₃H₇]⁺, 91 [M-C₃H₇-N]⁺. HREI-MS m/z 147.0699 [M]⁺ (calcd for C₉H₉NO 147.0684). [Yang et al., *Chinese Chemical Letters*, **11**, 779-782 (2000)]

参考文献

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