Isoxanthohumol (1): white amorphous powder, $[\alpha]_D +0.0^\circ$ (c 0.2, MeOH); UV $\lambda_{\text{max}}$ (MeOH) (log $\varepsilon$) 286 (4.34), 397 (3.56); IR (KBr) $\nu_{\text{max}}$: 3393, 1597, 1519, 1450, 1349, 1274, 1148, 1092, 834 cm$^{-1}$; $^1$H NMR (CD$_3$OD, 500 MHz) $\delta$ 7.30 (2H, d, $J = 8.5$ Hz, H-2', 6'), 6.82 (2H, d, $J = 8.5$ Hz, H-3', 5'), 6.12 (1H, s, 1H), 5.26 (1H, dd, $J = 12.8$, 2.8 Hz, H-2), 5.13 (1H, brt, $J = 7.2$ Hz, H-2''), 3.79 (3H, s, 5-OCH$_3$), 3.20 (2H, m, H-1''), 2.96 (1H, dd, $J = 16.8$, 13.0 Hz, H-3a), 2.66 (1H, dd, $J = 16.8$, 3.0 Hz, H-3b), 1.61 (3H, s, H-5''), 1.55 (3H, s, H-4''); $^{13}$C NMR (CD$_3$OD, 125 MHz) $\delta$ 193.2 (C-4), 164.5 (C-8a) 164.0 (C-7), 162.0 (C-5), 158.9 (C-4'), 131.9 (C-3''), 131.7 (C-1'), 129.0 (C-2',6'), 124.0 (C-2''), 116.0 (C-3',5'), 110.1 (C-8), 105.9 (C-4a), 93.6 (C-6), 80.1 (C-2), 56.1 (5-OCH$_3$), 46.3 (C-3), 26.1 (C-5''), 22.8 (C-1''), 18.1 (C-4''); EIMS 70eV $m/z$ 354 [M]$^+$, 339, 311, 299, 234, 219, 191, 179, 120 (calcd. for C$_{21}$H$_{22}$O$_5$).

Figure S1. $^1$H NMR spectrum of 1

Figure S2. $^{13}$C NMR spectrum of 1
Scheme S1. HPLC profiles of oxygenated metabolites (2-7) of isoxanthohumol (1)
HPLC was performed on a Hewlett Packard 1100 series composed of a degasser, a binary mixing pump, a column oven and a DAD detector using Waters SunFire™ (4.6 × 150 mm, 5 μm) with acetonitrile (solvent A) and water containing 0.1% formic acid (solvent B) at 1 mL/min under the wavelength 280 nm.
Figure S3. $^1$H NMR spectrum of the new compound 2
Figure S4. $^{13}$C NMR spectrum of 2
Figure S5. \(^1\)H NMR spectrum of the new compound 3
Figure S6. $^{13}$C NMR spectrum of the new compound 3
Figure S7. HSQC NMR spectrum of a mixture of 2 and 3
Figure S8. HMBC NMR Spectrum of a mixture of 2 and 3
Figure S9. $^1$H NMR spectrum of the new compound 4
Figure S10. $^{13}$C NMR spectrum of the new compound 4

* C-7 carbon signal was identified from HMBC NMR spectrum.
Figure S11. $^1$H NMR spectrum of the new compound 5
Figure S12. $^{13}$C NMR spectrum of the new compound 5

* C-7 carbon signal was identified from HMBC NMR spectrum.
Figure S13. HSQC NMR spectrum of a mixture of 4 and 5
Figure S14. HMBC NMR spectrum of a mixture 4 and 5
Figure S15. $^1$H NMR spectrum of 6
Figure S16. $^{13}$C NMR spectrum of 6
Figure S17. $^1$H NMR spectrum of 7
Figure S18. $^{13}$C NMR spectrum of 7
Figure S19. High resolution ESIMS data of metabolites 2–7

a) Metabolite 2

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<th>Mass</th>
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<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>i-FIT (Norm)</th>
<th>Formula</th>
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Minimum: 3.0  Maximum: 10.0  Drop: -1.5

b) Metabolite 3

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<th>PPM</th>
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<th>i-FIT</th>
<th>i-FIT (Norm)</th>
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Minimum: 3.0  Maximum: 10.0  Drop: -1.5

c) Metabolite 4

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Minimum: 3.0  Maximum: 10.0  Drop: -1.5
d) Metabolite 5

Minimum: 3.0
Maximum: 10.0
Mass Calc. Mass mDa PPM DBE i-FIT i-FIT (Norm) Formula
389.1600 389.1600 0.0 0.0 9.5 247.2 0.0 C21 H25 O7

e) Metabolite 6

Minimum: 5.0
Maximum: 10.0
Mass Calc. Mass mDa PPM DBE i-FIT i-FIT (Norm) Formula
393.1307 393.1314 -0.7 -1.8 10.5 344.2 0.0 C21 H22 O6 Na

f) Metabolite 7

Minimum: 10.0
Maximum: 10.0
Mass Calc. Mass mDa PPM DBE i-FIT i-FIT (Norm) Formula
393.1316 393.1314 0.2 0.5 10.5 195.6 0.0 C21 H22 O6 Na
Figure S20. Circular dichroism (CD) profiles of metabolites 2–7
Isoxanthohumol

Rhizopus oryzae
KCTC6399

4: 2S

5: 2R

\[ \text{CD (mdeg)} \]

\[ \lambda \text{ (nm)} \]
*Fusarium oxysporum* f. sp. *lini*  
*KCTC16325*

**Isoxanthohumol**

**CD (mdeg)**

![CD spectrum](image)

- **2S**
- **2R**

**λ (nm)**

- 240
- 280
- 320
- 360
- 400