

SUPPLEMENTARY DATA

**TABLE SI. The  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectroscopic data of isolated astilbin**

C	$^*\delta_{\text{C}}$	$\delta_{\text{C}}^{\text{a,c}}$	$\delta_{\text{H}}^{\text{a,d}}$ (mult., $J = \text{Hz}$ )
1	-	-	
2	82.8	82.6	5.11 (d, 10.0 Hz)
3	77.6	77.2	4.61 (d, 10.0 Hz)
4	195.2	194.8	-
5	164.3	164.1	-
6	97.2	95.9	5.94 (dd, 1.5, 13.0 Hz)
7	167.8	167.2	-
8	96.1	94.9	5.94 (dd, 1.5, 13.0 Hz)
9	163.2	162.7	-
10	101.9	101.1	-
1'	128.4	127.8	-
2'	116.4	114.9	6.98 (d, 1.5 Hz)
3'	145.6	145.2	-
4'	146.4	146.0	-
5'	115.4	113.9	6.84 (d, 8.0 Hz)
6'	120.2	119.1	6.87 (dd, 1.5, 8.0 Hz)
1''	101.2	100.7	4.07 (d, 1.5 Hz)
2''	70.8	70.4	3.55 (m)
3''	71.4	70.8	3.66 (m)
4''	72.8	72.4	3.32 (ddd, 3.0, 9.0 Hz)
5''	70.0	69.1	4.23 (dd, 3.0, 9.0 Hz)
6''	17.7	16.8	1.21 (d, 5.0 Hz)

<sup>a</sup>Measured in  $\text{CD}_3\text{OD}$ , <sup>c</sup>125 MHz, <sup>d</sup>500 MHz, <sup>\*</sup> $\delta_{\text{C}}$  (Acetone- $d_6$ - $\text{D}_2\text{O}$ ) followed by Kasai *et al* (32).

**TABLE SII. The  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectroscopic data of isolated 5-*O*-caffeoylshikimic acid**

C	$^*\delta_{\text{C}}^{\text{a}}$	$\delta_{\text{C}}^{\text{a,c}}$	$\delta_{\text{H}}^{\text{a,d}}$ (mult., $J = \text{Hz}$ )
1	132.8	130.4	-
2	136.8	138.8	6.87 (t, 3.5; 1.5 Hz)
3	67.5	67.3	4.42 (m)
4	71.6	71.4	5.26 (m)
5	70.5	70.0	3.93 (m)
6	30.0	29.2	2.32 (dd, 5.5; 18.5 Hz) 2.85 (dd, 5.5; 18.5 Hz)
COOH	169.9	169.7	-
1'	168.7	168.6	-
2'	115.4	115.0	6.31 (d, 16.0 Hz)
3'	147.2	146.8	7.59 (d, 16.0 Hz)
4'	127.9	127.7	-
5'	122.9	123.0	6.96 (d, 8.0 Hz)
6'	116.7	116.5	6.79 (d, 8.0 Hz)
7'	149.6	149.6	-
8'	146.7	147.2	-
9'	115.3	115.2	7.06 (d, 2.0 Hz)

<sup>a</sup>Measured in  $\text{CD}_3\text{OD}$ , <sup>c</sup>125 MHz, <sup>d</sup>500 MHz, <sup>\*</sup> $\delta_{\text{C}}^{\text{a}}$  5-*O*-caffeoylshikimic acid, followed by Fukuoka et al (33).