

NMR data for [6]-, [8]-, and [10]-gingerol, [6]-, [8]-, and [10]-shogaol, [6]-paradol, and [1]-dehydrogingerdione

[6]-gingerol: pale yellow oil; ESI-MS m/z : 295 $[M + H]^+$; ^1H NMR (400 MHz) δ : 0.88 (3H, t, $J=6.8$ Hz, H-10), 1.23-1.68 (8H, m, H-6~H-9), 2.52 (1H, d, $J=8.4$ Hz, H-4a), 2.54 (1H, d, $J=3.6$ Hz, H-4b), 2.73 (2H, brd, $J=6.8$ Hz, H-2), 2.81 (2H, brd, $J=6.8$ Hz, H-1), 3.84 (3H, s, OCH_3), 4.03 (1H, m, H-5), 6.64 (1H, dd, $J=8, 2$ Hz, H-6'), 6.67 (1H, s, H-2'), 6.81 (1H, d, $J=8$ Hz, H-5'); ^{13}C NMR (100 MHz) δ : 13.8 (C-10, q), 22.3 (C-9, t), 24.9 (C-7, t), 29.0 (C-8, t), 31.1 (C-1, t), 36.2 (C-6, t), 45.2 (C-2, t), 49.1 (C-4, t), 55.6 (OCH_3 , q), 67.5 (C-5, d), 110.9 (C-2', d), 114.3 (C-5', d), 120.4 (C-6', d), 132.4 (C-1', s), 143.7 (C-4', s), 146.3 (C-3', s), 211.3 (C-3, s).

[8]-gingerol: pale yellow oil; ESI-MS m/z : 323 $[M + H]^+$; ^1H NMR (400 MHz) δ : 0.90 (3H, t, $J=6.4$ Hz, H-12), 1.27-1.46 (10H, m, H-7~H-11), 1.49 (2H, m, H-6), 2.48 (1H, d, $J=8.8$ Hz, H-4b), 2.55 (1H, m, H-4ba), 2.74 (2H, dd, $J=7.6$ Hz and 6.8 Hz, H-2), 2.85 (2H, dd, $J=7.2, 6.8$ Hz, H-1), 3.89 (3H, s, OCH_3), 4.05 (1H, m, H-5), 6.68 (1H, brd, $J=8$ Hz, H-6'), 6.7 (1H, s, H-2'), 6.84 (1H, d, $J=7.6$ Hz, H-5'); ^{13}C NMR (100 Hz) δ : 13.8 (C-12, q), 22.4 (C-11, t), 25.2 (C-7, t), 29.0 (C-9, t; C-8, t), 29.3 (C-10, t), 31.6 (C-1, t), 36.2 (C-6, t), 45.2 (C-2, t), 49.1 (C-4, t), 55.6 (OCH_3 , q), 67.4 (C-5, d), 110.7 (C-2', d), 114.1 (C-5', d), 132.4 (C-1', s), 143.7 (C-4', s), 146.2 (C-3'), 211.3 (C-3, s).

[10]-gingerol: pale yellow oil; ESI-MS m/z : 351 $[M + H]^+$; ^1H NMR (400 MHz) δ : 0.87 (3H, t, $J=6.4$ Hz, H-14), 1.31-1.46 (14H, m, H-7~H-14), 1.49 (2H, m, H-6), 2.42-2.65 (2H, m, H-4), 2.75 (2H, dd, $J=10$ Hz and 7.8 Hz, H-2), 2.85 (2H, dd, $J=20, 7.8$ Hz, H-1),

3.88 (3H, s, OCH₃), 4.07 (1H, m, H-5), 6.67 (1H, dd, J=9.6, 2 Hz, H-6'), 6.71 (1H, s, H-2'), 6.84 (1H, d, 8, H-5'); ¹³C NMR (100 MHz) δ: 13.9 (C-14, q), 22.5 (C-13, t), 25.2 (C-7, t), 29.0, 29.1 (C-11, t; C-10, t), 29.3 (C-9, t), 29.3 (C-8, t), 31.7 (C-1, t), 36.2 (C-6, t), 45.2 (C-2, t), 49.1 (C-4, t), 55.6 (OCH₃, q), 67.4 (C-5, d), 110.7 (C-2', d), 114.1 (C-5', d), 132.4 (C-1', s), 143.7 (C-4', s), 146.2 (C-3'), 211.3 (C-3, s).

[6]-shogaol: pale yellow oil; ESI-MS *m/z*: 277 [M + H]⁺; ¹H NMR (400 MHz) δ: 0.88 (3H, t, J=6.8 Hz, H-10), 1.26-1.31 (4H, m, H-8 and H-9), 1.42 (2H, m, H-7), 2.17 (2H, m, H-6), 2.84 (4H, m, H-1 and H-2), 3.82 (3H, s, OCH₃), 6.09 (1H, dt, J=16, 1.6 Hz, H-4), 6.66 (1H, dd, J=8, 2Hz, H-6'), 6.70 (1H, d, J= 1.6 Hz, H-2'), 6.81 (1H, d, J= 7.6 Hz, H-5') 6.83 (1H, d, J=16.0 Hz, H-5); ¹³C NMR (100 MHz) δ: 13.7 (C-10, q), 22.2 (C-9, t), 27.5 (C-7, t), 29.6 (C-8, t), 31.1 (C-1, t), 32.2 (C-6, t), 41.6 (C-2, t), 55.5 (OCH₃, q), 111.0 (C-2', d), 114.2 (C-5',d), 120.5 (C-6', d), 130.8 (C-4, d) 132.8 (C-1', s), 143.7 (C-4',s), 146.3 (C-3', s), 147.4 (C-5, d), 199.9 (C-3, s).

[8]-shogaol: pale yellow oil; ESI-MS *m/z*: 305 [M + H]⁺; ¹H NMR (400 MHz) δ: 0.90 (3H, t, J= 6.0 Hz, H-12), 1.29-1.44 (8H, m, H-8 ~ H-11), 1.45 (2H, m, H-7), 2.21 (2H, m, H-6), 2.87 (4H, m, H-1 and H-2), 3.90 (3H, s, OCH₃), 6.11 (1H, dt, J= 16, 1.6 Hz, H-4), 6.70 (1H, dd, J=8, 2 Hz, H-6'), 6.73 (1H, d, J= 1.6 Hz, H-2'), 6.83 (1H, brd, J= 7.6 Hz, H-5') 6.86 (1H, H-5); ¹³C NMR (100 MHz) δ: 13.9 (C-12, q), 22.4 (C-11, t), 27.8 (C-9, t), 28.1 (C-7, t), 28.9 (C-8, t), 29.6(C-10, t), 31.5 (C-1, t) 32.2 (C-6, t), 41.7 (C-2, t), 55.6 (OCH₃, q), 110.8 (C-2', d), 114.0 (C-5', d), 120.5 (C-6', d), 130.0 (C-4, d) 133.0 (C-1', s), 143.6 (C-4', s), 146.1 (C-3', s), 147.4 (C-5, d), 199.9 (C-3, s).

[10]-shogaol: pale yellow oil; ESI-MS m/z : 333 $[M + H]^+$; ^1H NMR (400 MHz) δ : 0.89 (3H, t, 8.4, H-14), 1.27-1.31 (12H, m, H-8~H-13), 1.45 (2H, m, H-7), 2.21 (2H, m, H-1), 2.86 (4H, m, H-1 and H-2), 3.85 (3H, s, OCH₃), 6.11(1H, brd, J=16 Hz, H-4), 6.68 (1H, dd, J= 8, 2 Hz, H-6'), 6.72 (1H, d, J= 1.6 Hz, H-2'), 6.83 (1H, d, J= 8 Hz, H-5'), 6.86 (1H, d, J= 7.2 Hz, H-5); ^{13}C NMR (100 MHz) δ : 13.9 (C-14, q), 22.4 (C-13, t), 27.8 (C-11, t), 28.9, 29.1, 29.2 29.6 (C-7, t; C-8, t; C-9, t; C-10, t), 31.6 (C-1, t) 32.3 (C-6, t), 41.7 (C-2, t), 55.6 (OCH₃, q), 110.9 (C-2', d), 114.2 (C-5',d), 120.5 (C-6', d), 130.0 (C-4, d) 132.9 (C-1', s), 143.7 (C-4',s), 146.2 (C-3', s), 147.8 (C-5, d), 199.7 (C-3, s).

[6]-paradol: pale yellow oil; ESI-MS m/z : 279 $[M + H]^+$; ^1H NMR (400 MHz) δ : 0.89 (3H, t, J= 6.8 Hz, H-10), 1.27-1.32 (8H, m, H-6, H-7, H-8, H-9), 1.56 (2H, brt, J= 6.4Hz, H-5), 2.39 (2H, t, J=7.6 Hz, H-4), 2.71 (2H, t, J= 7.6 Hz, H-2), 2.84 (2H, t, 7.6, H-1), 3.88 (3H, s, OCH₃), 6.67 (1H, brd, J= 8 Hz, H-6'), 6.71 (1H, brs, H-2'), 6.83 (1H, d, 8, H-5'); ^{13}C NMR (100 MHz) δ : 13.8 (C-10, q), 22.4 (C-9, t), 23.6 (C-5, t), 28.8 (C-7, t), 28.9 (C-6, t), 29.3 (C-8, t), 31.4 (C-1, t) 42.9 (C-2, t), 44.4 (C-4, t), 55.6 (OCH₃, q), 110.8 (C-2', d), 114.1 (C-5',d), 120.5 (C-6', d), 132.9 (C-1', s), 143.6 (C-4',s), 146.1(C-3', s), 211.3 (C-3, s).

[1]-dehydrogingerdione: pale yellow oil; ESI-MS m/z : 291 $[M + H]^+$; ^1H NMR (400 MHz) δ : 0.92 (3H, t, J= 6.4 Hz, H-10), 1.34 (4H, m, H-8, H-9), 1.66 (2H, m, H-7), 2.40 (2H, m, H-6), 3.93 (3H, s, OCH₃), 5.64 (2H, s, H-4), 6.36 (1H, dd, J= 15.6, 6 Hz, H-2), 6.94 (1H, dd, J= 8, 4.8 Hz, H-5'), 7.03 (1H, d, J=1.6 Hz, H-2'), 7.09 (1H, dd, J= 8, 2 Hz,

H-6'), 7.55 (1H, dd, J= 15.2, 4.8 Hz, H-1); ¹³C NMR (100 MHz) δ: 13.7 (C-10, q), 22.2 (C-9, t), 25.1 (C-8, t), 31.2 (C-7, t), 39.9 (C-6, t), 55.7 (OCH₃, q), 99.9 (C-4, t), 109.2 (C-2', d), 116.6 (C-5', d), 120.2 (C-2, d) 122.4 (C-6', d) 127.4 (C-1', s), 139.7 (C-1, d), 146.6 (C-4',s), 147.5 (C-3', s), 177.5 (C-3, s), 200.0 (C-5, s).