

AROMATIC COMPOUNDS FROM THREE BRAZILIAN LAURACEAE SPECIES

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NMR (¹H and ¹³C) data for the isolated compounds 1-10.

4-*O*-*E*-caffeoylquinic acid methyl ester (1): ¹H NMR (DMSO-*d*₆, 500 MHz) δ: 1.92 (1H, dd, *J* = 3.5 and 13.5 Hz, H-2ax.), 2.10 (2H, m, H-2eq. and H-6eq.), 3.57 (1H, m, H-3), 5.01 (1H, dd, *J* = 5.0 and 8.5 Hz, H-4), 3.88 (1H, m, H-5), 1.76 (dd, *J* = 9.5 and 12.5, H-6ax.), 3.55 (1H, s, H-8), 7.02 (1H, d, *J* = 2.0 Hz, H-2'), 6.76 (1H, d, *J* = 8.5 Hz, H-5'), 6.96 (1H, dd, *J* = 2.0 and 8.5 Hz, H-6'), 7.37 (1H, d, *J* = 16.0 Hz, H-7'), 6.10 (1H, d, *J* = 16.0 Hz, H-8'). ¹³C NMR (DMSO-*d*₆, 125 MHz) δ: 73.0 (C-1), 35.0 (C-2), 69.3 (C-3), 71.0 (C-4), 67.2 (C-5), 37.2 (C-6), 173.6 (C-7), 51.8 (C-8), 125.3 (C-1'), 114.6 (C-2'), 148.5 (C-3'), 145.6 (C-4'), 115.8 (C-5'), 121.3 (C-6'), 145.1 (C-7'), 113.8 (C-8'), 165.3 (C-9').

quercetin-3-*O*-β-D-glucoside (2): ¹H NMR (DMSO-*d*₆, 500 MHz) δ: 6.20 (1H, bs, H-6), 6.41 (1H, bs, H-8), 7.58 (1H, d, *J* = 2.0 Hz, H-2'), 6.84 (1H, d, *J* = 8.5 Hz, H-5'), 7.57 (1H, dd, *J* = 2.0 and 8.5 Hz, H-6'), 5.46 (1H, d, *J* = 7.0 Hz, H-1''), 3.58 - 3.24 (sugar H). ¹³C NMR (DMSO-*d*₆, 125 MHz) δ: 156.2 (C-2), 133.3 (C-3), 177.4 (C-4), 161.2 (C-5), 98.7 (C-6), 164.2 (C-7), 93.5 (C-8), 156.3 (C-9), 104.0 (C-10), 121.1 (C-1'), 115.2 (C-2'), 144.8 (C-3'), 148.4 (C-4'), 116.2 (C-5'), 121.6 (C-6'), 100.8 (C-1''), 74.1 (C-2''), 76.5 (C-3''), 69.9 (C-4''), 77.5 (C-5''), 60.9 (C-6'').

quercetin-3-*O*-β-D-galactoside (3): ¹H NMR (DMSO-*d*₆, 500 MHz) δ: 6.20 (1H, bs, H-6), 6.41 (1H, bs, H-8), 7.53 (1H, d, *J* = 2.0 Hz, H-2'), 6.81 (1H, d, *J* = 8.5 Hz, H-5'), 7.66 (1H, dd, *J* = 2.0 and 8.5 Hz, H-6'), 5.37 (1H, d, *J* = 7.0 Hz, H-1''), 3.56 - 3.28 (sugar H). ¹³C NMR (DMSO-*d*₆, 125 MHz) δ: 156.1 (C-2), 133.4 (C-3), 177.4 (C-4), 161.2 (C-5), 98.7 (C-6), 164.2 (C-7), 93.5 (C-8), 156.2 (C-9), 103.9 (C-10), 121.1 (C-1'), 115.2 (C-2'), 144.8 (C-3'), 148.5 (C-4'), 115.9 (C-5'), 121.9 (C-6'), 101.8 (C-1''), 71.2 (C-2''), 73.4 (C-3''), 67.9 (C-4''), 75.8 (C-5''), 60.1 (C-6'').

quercetin-3-*O*-β-D-xyloside (4): ¹H NMR (DMSO-*d*₆, 500 MHz) δ: 6.16 (1H, bs, H-6), 6.36 (1H, bs, H-8), 7.56 (1H, d, *J* = 2.0 Hz, H-2'), 6.84 (1H, d, *J* = 8.5 Hz, H-5'), 7.53 (1H, dd, *J* = 2.0 and 8.5 Hz, H-6'), 5.33 (1H, d, *J* = 7.0 Hz, H-1''), 3.31 - 2.96 (sugar H). ¹³C NMR (DMSO-*d*₆, 125 MHz) δ: 156.2 (C-2), 133.1 (C-3), 177.2 (C-4), 162.5 (C-5), 99.1 (C-6), 164.1 (C-7), 94.0 (C-8), 156.2 (C-9), 104.3 (C-10), 121.0 (C-1'), 116.2 (C-2'), 146.2 (C-3'), 150.1 (C-4'), 116.5 (C-5'), 121.9 (C-6'), 102.3 (C-1''), 74.5 (C-2''), 76.8 (C-3''), 70.2 (C-4''), 66.0 (C-5'').

rel-(1*R*, 4*S*)-7-hydroxycalamenene (5): ¹H NMR (CDCl₃, 500 MHz) δ: 2.64 (1H, m, H-1), 1.25 (1H, m, H-2a), 1.18 (1H, m, H-2b), 1.49 (1H, m, H-3a), 1.74 (1H, m, H-3b), 2.56 (1H, m, H-4), 6.86 (1H, s, H-5), 6.57 (1H, s, H-8), 2.12 (1H, m, H-11), 0.64 (3H, d, *J* = 6.5 Hz, H-12), 0.91 (3H, d, *J* = 6.5 Hz, H-13), 1.16 (3H, d, *J* = 7.0 Hz, H-14), 2.13 (3H, s, H-15). ¹³C NMR (CDCl₃, 125 MHz) δ: 32.6 (C-1), 30.8 (C-2), 21.6 (C-3), 43.1 (C-4), 130.5 (C-5), 120.6 (C-6), 151.4 (C-7), 113.0 (C-8), 142.1 (C-9), 132.2 (C-10), 31.9 (C-11), 17.3 (C-12), 21.2 (C-13), 22.2 (C-14), 15.5 (C-15).

rel-(2*R*, 3*R*)-astilbin (6): ¹H NMR (DMSO-*d*₆, 500 MHz) δ: 5.25 (1H, d, *J* = 10.0 Hz, H-2), 4.65 (1H, d, *J* = 10.0 Hz, H-3), 5.90 (1H, d, *J* = 2.0 Hz, H-6), 5.88 (1H, d, *J* = 2.0 Hz, H-8), 6.89 (1H, s, H-2'), 6.74 (2H, s, H-5' and H-6'), 4.04 (1H, d, *J* = 1.5 Hz, H-1''), 3.90 - 3.10 (sugar H), 1.05 (1H, d, *J* = 6.0 Hz, H-6''). ¹³C NMR (DMSO-*d*₆, 125 MHz) δ: 81.6 (C-2), 75.7 (C-3), 194.5 (C-4), 163.5 (C-5), 96.1 (C-6), 167.2 (C-7), 95.1 (C-8), 162.2 (C-9), 101.0 (C-10), 127.0 (C-1'), 114.8 (C-2'), 145.2 (C-3'), 145.9 (C-4'), 115.4 (C-5'), 119.0 (C-6'), 100.1 (C-1''), 70.1 (C-2''), 70.4 (C-3''), 71.7 (C-4''), 69.0 (C-5''), 17.8 (C-6'').

rel-(7*S*, 7'*S*, 8*R*, 8'*R*)-sesamin (7): ¹H NMR (CDCl₃, 500 MHz) δ: 6.77 (2H, d, *J* = 1.5 Hz, H-2 and H-2'), 6.71 (2H, d, *J* = 8.0 Hz, H-5 and H-5'), 6.70 (2H, dd, *J* = 1.5 and 8.0 Hz, H-6 and H-6'), 4.64 (2H, d, *J* = 4.0 Hz, H-7 and H-7'), 2.97 (2H, m, H-8 and H-8'), 4.15 (2H, dd, *J* = 7.0 and 9.0 Hz, H-9eq. and H-9'eq.), 3.78 (2H, dd, *J* = 4.0 and 9.0 Hz, H-9ax. and H-9'ax.), 5.87 (4H, s, O-CH₂-O). ¹³C NMR (CDCl₃, 125 MHz) δ: 135.0 (C-1 and C-1'), 106.4 (C-2 and C-2'), 147.0 (C-3 and C-3'), 147.9 (C-4 and C-4'), 108.1 (C-5 and C-5'), 119.2 (C-6 and C-6'), 85.7 (C-7 and C-7'), 54.3 (C-8 and C-8'), 71.6 (C-9 and C-9'), 101.0 (O-CH₂-O).

rel-(7*S*, 7'*S*, 8*R*, 8'*R*)-methylpiperitol (8): ¹H NMR (CDCl₃, 500 MHz) δ: 6.78 (1H, m, H-2), 6.70 (1H, dd, *J* = 0.5 and 8.0 Hz, H-5), 6.73 (1H, m, H-6), 4.66 (2H, m, H-7 and H-7'), 3.00 (2H, m, H-8 and H-8'), 4.17 (2H, m, H-9eq. and H-9'eq.), 3.81 (2H, m, H-9ax. and H-9'ax.), 6.83 (1H, d, *J* = 2.0 Hz, H-2'), 6.78 (2H, m, H-5' and H-6'), 5.87 (2H, s, O-CH₂-O), 3.80 (3H, s, OMe-3'), 3.82 (3H, s, OMe-4'). ¹³C NMR (CDCl₃, 125 MHz) δ: 135.1 (C-1), 106.4 (C-2), 147.1 (C-3), 147.9 (C-4), 108.1 (C-5), 119.3 (C-6), 85.7 (C-7 and C-7'), 54.1 (C-8 and C-8'), 71.7 (C-9 and C-9'), 133.5 (C-1'), 109.3 (C-2'), 148.7 (C-3'), 149.2 (C-4'), 111.3 (C-5'), 118.2 (C-6'), 101.0 (O-CH₂-O), 55.9 (OMe-3' and OMe-4').

rel-(7*S*, 7'*S*, 8*R*, 8'*R*)-eudesmin (9): ¹H NMR (CDCl₃, 500 MHz)

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δ : 6.83 (2H, d, $J = 1.5$ Hz, H-2 and H-2'), 6.77 (2H, d, $J = 8.0$ Hz, H-5 and H-5'), 6.79 (2H, dd, $J = 1.5$ and 8.0 Hz, H-6 and H-6'), 4.68 (2H, d, $J = 4.0$ Hz, H-7 and H-7'), 3.03 (2H, m, H-8 and H-8'), 4.18 (2H, dd, $J = 7.0$ and 9.0 Hz, H-9eq. and H-9'eq.), 3.81 (2H, m, H-9ax. and H-9'ax.), 3.80 (6H, s, OMe-3 and OMe-3'), 3.82 (6H, s, OMe-4 and OMe-4'). ^{13}C NMR (CDCl_3 , 125 MHz) δ : 133.6 (C-1 and C-1'), 109.3 (C-2 and C-2'), 148.7 (C-3 and C-3'), 149.2 (C-4 and C-4'), 111.1 (C-5 and C-5'), 118.2 (C-6 and C-6'), 85.8 (C-7 and C-7'), 54.2 (C-8 and C-8'), 71.7 (C-9 and C-9'), 55.9 (OMe-3, OMe-3', OMe-4 and OMe-4').

rel-(7*S*, 7'*S*, 8*R*, 8'*R*)-magnolin (**10**): ^1H NMR (CDCl_3 , 500 MHz)

δ : 6.83 (1H, d, $J = 2.0$ Hz, H-2), 6.77 (1H, d, $J = 8.0$ Hz, H-5), 6.80 (1H, dd, $J = 2.0$ and 8.0 Hz, H-6), 4.69 (1H, d, $J = 4.5$ Hz, H-7), 3.03 (1H, m, H-8), 4.21 (1H, dd, $J = 7.0$ and 9.0 Hz, H-9eq.), 3.82 (1H, m, H-9ax.), 6.50 (1H, s, H-2' and H-6'), 4.67 (1H, d, $J = 5.0$ Hz, H-7'), 3.03 (1H, m, H-8'), 4.20 (1H, m, H-9'eq.), 3.84 (1H, m, H-9'ax.), 3.80 (3H, s, OMe-3), 3.82 (3H, s, OMe-4), 3.79 (3H, s, OMe-3' and OMe-5'), 3.76 (3H, s, OMe-4'). ^{13}C NMR (CDCl_3 , 125 MHz) δ : 133.1 (C-1), 109.3 (C-2), 148.7 (C-3), 149.2 (C-4), 111.1 (C-5), 118.2 (C-6), 85.7 (C-7 and C-7'), 54.1 (C-8), 71.9 (C-9), 136.8 (C-1'), 102.9 (C-2' and C-6'), 153.4 (C-3' and C-5'), 137.6 (C-4'), 54.4 (C-8'), 71.7 (C-9'), 55.9 (OMe-3 and OMe-4), 56.2 (OMe-3' and OMe-5'), 60.8 (OMe-4').