SUPPORTING INFORMATION

Model Studies on the Effect of Aldehyde Structure on Their Selective Trapping by Phenolic Compounds

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NMR and MS Data of Compounds 19–32

4-(1-Methoxypropyl)benzene-1,3-diol (**19**). ^{1}H NMR (CD_3OD): δ (ppm) 0.88 (t, 3, *J* = 7.5 Hz, H-3'), 1.67 and 1.77 (m, 2, H-2'), 3.22 (s, 3, CH_3O), 4.42 (t, 1, *J* = 6.7 Hz, H-1'), 6.29 (d, 1, *J* = 2.3 Hz, H-2), 6.31 (dd, 1, *J* = 2.3 Hz, *J* = 8.2 Hz, H-6), and 6.96 (d, 1, *J* = 8.2 Hz, H-5). ^{13}C NMR (CD_3OD): δ (ppm) 9.15 (C-3'), 28.98 (C-2'), 55.24 (CH_3O), 80.31 (C-1'), 102.07 (C-2), 106.39 (C-6), 118.25 (C-4), 127.61 (C-5), 156.17 (C-3), and 157.21 (C-1). MS, *m/z* (%, ion structure): 150 (100, $M^+ - CH_3OH$), 133 (19, 150 – OH), and 123 (36, $C_7H_7O_2$).

4-(1-Methoxypentyl)benzene-1,3-diol (**20**). ^{1}H NMR (CD_3OD): δ (ppm) 0.90 (t, 3, *J* = 7.2 Hz, H-5'), 1.35 (m, 4, H-3' and H-4'), 1.65 and 1.75 (m, 2, H-2'), 3.21 (s, 3, CH_3O), 4.50 (t, 1, *J* = 6.6 Hz, H-1'), 6.28 (d, 1, *J* = 2.4 Hz, H-2), 6.31 (dd, 1, *J* = 2.4 Hz, *J* = 8.2 Hz, H-6), and 6.96 (d, 1, *J* = 8.2 Hz, H-5). ^{13}C NMR (CD_3OD): δ (ppm) 13.02 (C-5'), 22.26 (C-4'), 27.73 (C-3'), 35.92 (C-2'), 55.14 (CH_3O), 78.31 (C-1'), 102.03 (C-2), 106.40 (C-6), 118.55 (C-4), 127.52 (C-5), 156.14 (C-3), and 157.20 (C-1). MS, *m/z* (%, ion structure): 178 (38, $M^+ - CH_3OH$), and 149 (100, 178 – CH_3CH_2).

2-(1-Hydroxypentyl)benzene-1,3-diol (**21**). ^{1}H NMR (CD_3OD): δ (ppm) 0.92 (t, 3, *J* = 7.2 Hz, H-5'), 1.36 (m, 2, H-4'), 1.36 and 1.49 (m, 2, H-3'), 1.78 and 1.81 (m, 2, H-2'), 5.22 (dd, 1, *J* = 5.4 Hz, *J* = 7.7 Hz, H-1'), 6.27 (d, 2, *J* = 8.1 Hz, H-4 and H-6), and 6.87 (t, 1, *J* = 8.1 Hz, H-5). ^{13}C NMR (CD_3OD): δ (ppm) 13.03 (C-5'), 22.27 (C-4'), 27.48 (C-3'), 36.17 (C-2'), 68.95 (C-1'), 106.76 (C-4 and C-6), 115.54 (C-2), 127.54 (C-5), and 155.72 (C-1 and C-3). MS of the dehydrated product formed from compound **21**, *m/z* (%, ion structure): 178 (48, M^+), 149 (100, $M^+ - H_2O - CH_3CH_2$), and 123 (56, $C_7H_7O_2$).

4-(1-Methoxy-2-methylbutyl)benzene-1,3-diol (**22a**). ^{1}H NMR (CD_3OD): δ (ppm) 0.73 (d, 3, *J* = 6.9 Hz, CH_3C2'), 0.92 (t, 3, *J* = 7.5 Hz, H-4'), 1.21 and 1.76 (m, 2, H-3'),

1.73 (m, 2, H-2'), 3.19 (s, 3, CH_3O), 4.24 (d, 1, *J* = 7.8 Hz, H-1'), 6.28 (d, 1, *J* = 2.4 Hz, H-2), 6.32 (dd, 1, *J* = 2.4 Hz, *J* = 8.2 Hz, H-6), and 6.92 (d, 1, *J* = 8.2 Hz, H-5). ^{13}C NMR (CD_3OD): δ (ppm) 10.19 (C-4'), 14.26 (CH_3C2'), 24.98 (C-3'), 40.21 (C-2'), 55.44 (CH_3O), 83.13 (C-1'), 101.93 (C-2), 106.16 (C-6), 117.37 (C-4), 128.46 (C-5), 156.60 (C-3), and 157.09 (C-1). MS, *m/z* (%, ion structure): 178 (100, $M^+ - CH_3OH$), 163 (71, 178 – CH_3), 149 (84, 178 – CH_3CH_2), and 123 (75, $C_7H_7O_2$).

4-(1-Methoxy-2-methylbutyl)benzene-1,3-diol (**22b**). ^{1}H NMR (CD_3OD): δ (ppm) 0.86 (t, 3, *J* = 7.5 Hz, H-4'), 0.95 (d, 3, *J* = 6.7 Hz, CH_3C2'), 1.10 and 1.37 (m, 2, H-3'), 1.73 (m, 2, H-2'), 3.20 (s, 3, CH_3O), 4.28 (d, 1, *J* = 6.9 Hz, H-1'), 6.28 (d, 1, *J* = 2.4 Hz, H-2), 6.32 (dd, 1, *J* = 2.4 Hz, *J* = 8.2 Hz, H-6), and 6.93 (d, 1, *J* = 8.2 Hz, H-5). ^{13}C NMR (CD_3OD): δ (ppm) 10.51 (C-4'), 13.90 (CH_3C2'), 25.53 (C-3'), 40.18 (C-2'), 55.60 (CH_3O), 82.98 (C-1'), 101.96 (C-2), 106.26 (C-6), 117.54 (C-4), 128.26 (C-5), 156.40 (C-3), and 157.17 (C-1). MS, *m/z* (%, ion structure): 178 (100, $M^+ - CH_3OH$), 163 (80, 178 – CH_3), 149 (95, 178 – CH_3CH_2), and 123 (81, $C_7H_7O_2$).

4-(1-Methoxyhexyl)benzene-1,3-diol (**23**). ^{1}H NMR (CD_3OD): δ (ppm) 0.88 (t, 3, *J* = 6.9 Hz, H-6'), 1.27 (m, 6, H-3', H-4', and H-5'), 1.66 (m, 2, H-2'), 3.21 (s, 3, CH_3O), 4.48 (t, 1, *J* = 6.7 Hz, H-1'), 6.26 (dd, 1, *J* = 2.5 Hz, *J* = 8.1 Hz, H-6), 6.30 (d, 1, *J* = 2.5 Hz, H-2), and 6.94 (d, 1, *J* = 8.1 Hz, H-5). ^{13}C NMR (CD_3OD): δ (ppm) 14.40 (C-6'), 23.70 (C-5'), 26.58 (C-4'), 32.94 (C-3'), 37.62 (C-2'), 56.51 (CH_3O), 79.93 (C-1'), 103.33 (C-6), 107.74 (C-2), 119.93 (C-4), 128.82 (C-5), 157.55 (C-3), and 158.60 (C-1). MS, *m/z* (%, ion structure): 192 (34, $M^+ - CH_3OH$), 163 (2, 192 – CH_3CH_2), and 149 (100, 192 – $CH_3CH_2CH_2$).

4-(1-Methoxypropyl)-2-methylbenzene-1,3-diol (**24**). ^{1}H NMR (CD_3OD): δ (ppm) 0.88 (t, 3, *J* = 7.5 Hz, H-3'), 1.68 and 1.83 (m, 2, H-2'), 2.07 (s, 3, CH_3C2), 3.29 (s, 3,

CH_3O), 4.23 (t, 1, *J* = 6.9 Hz, H-1'), 6.33 (d, 1, *J* = 8.2 Hz, H-6), and 6.96 (d, 1, *J* = 8.2 Hz, H-5). ^{13}C NMR (CD_3OD): δ (ppm) 7.08 ($\underline{C}H_3C2$), 9.32 (C-3'), 28.84 (C-2'), 55.60 (CH_3O), 80.81 (C-1'), 106.04 (C-6), 111.36 (C-2), 116.85 (C-4), 125.02 (C-5), 153.92 (C-3), and 155.41 (C-1). MS, *m/z* (%, ion structure): 164 (100, $M^+ - CH_3OH$), 149 (42, 164 – CH_3), 147 (17, 164 – OH), and 137 (20, $C_8H_9O_2$).

4-(1-Methoxypentyl)-2-methylbenzene-1,3-diol (**25**). ^1H NMR (CD_3OD): δ (ppm) 0.89 (t, 3, *J* = 7.2 Hz, H-5'), 1.23 and 1.38 (m, 2, H-3'), 1.31 (m, 2, H-4'), 1.65 and 1.82 (m, 2, H-2'), 2.08 (s, 3, CH_3C2), 3.28 (s, 3, CH_3O), 4.31 (t, 1, *J* = 6.9 Hz, H-1'), 6.33 (d, 1, *J* = 8.2 Hz, H-6), and 6.69 (d, 1, *J* = 8.2 Hz, H-5). ^{13}C NMR (CD_3OD): δ (ppm) 7.09 (CH_3C2), 13.04 (C-5'), 22.23 (C-4'), 27.84 (C-3'), 35.72 (C-2'), 55.52 (CH_3O), 83.31 (C-1'), 106.05 (C-6), 111.36 (C-2), 117.15 (C-4), 124.89 (C-5), 153.89 (C-3), and 155.41 (C-1). MS, *m/z* (%, ion structure): 192 (36, $M^+ - CH_3OH$), and 163 (100, 192 – CH_3CH_2).

2-Methyl-4-(pent-1-en-1-yl)benzene-1,3-diol (**26**). ^1H NMR (CD_3OD): δ (ppm) 0.95 (t, 3, *J* = 7.4 Hz, H-5'), 1.50 (sx, 2, *J* = 7.4 Hz, H-4'), 2.08 (s, 3, CH_3C2), 2.18 (qd, 2, *J* = 1.4 Hz, *J* = 7.2 Hz, H-3'), 5.98 (dt, 1, *J* = 7.2 Hz, *J* = 15.7 Hz, H-2'), 6.33 (d, 1, *J* = 8.4 Hz, H-6), 6.63 (d, 1, *J* = 15.7 Hz, H-1'), and 7.03 (d, 1, *J* = 8.4 Hz, H-5). ^{13}C NMR (CD_3OD): δ (ppm) 7.48 (CH_3C2), 12.74 (C-5'), 22.62 (C-4'), 35.27 (C-3'), 106.98 (C-6), 111.33 (C-2), 117.90 (C-4), 123.04 (C-5), 125.02 (C-1'), 127.45 (C-2'), 152.39 (C-3), and 154.86 (C-1). MS, *m/z* (%, ion structure): 192 (35, M^+), and 163 (100, $M^+ - CH_3CH_2$).

4-(1-Methoxy-2-methylbutyl)-2-methylbenzene-1,3-diol (**27a**). ^1H NMR (CD_3OD): δ (ppm) 0.71 (d, 3, *J* = 6.9 Hz, CH_3C2'), 0.84 (t, 3, *J* = 7.4 Hz, H-4'), 1.20 and 1.80 (m, 2, H-3'), 1.79 (m, 1, H-2'), 2.07 (s, 3, CH_3C2), 3.28 (s, 3, CH_3O), 4.01 (d, 1, *J* = 8.1 Hz, H-1'), 6.32 (d, 1, *J* = 8.2 Hz, H-6), and 6.65 (d, 1, *J* = 8.2 Hz, H-5). ^{13}C NMR (CD_3OD): δ (ppm) 7.09 (CH_3C2), 10.52 (C-4'), 14.60 (CH_3C2'), 25.10 (C-3'), 39.78 (C-2'), 55.99

(CH_3O), 88.17 (C-1'), 105.79 (C-6), 111.23 (C-2), 115.60 (C-4), 126.11 (C-5), 154.22 (C-3), and 154.33 (C-1). MS, *m/z* (%, ion structure): 192 (82, $M^+ - CH_3OH$), 177 (48, 192 – CH_3), 163 (100, 192 – CH_3CH_2), and 137 (49, $C_8H_9O_2$).

4-(1-Methoxy-2-methylbutyl)-2-methylbenzene-1,3-diol (**27b**). ^{1}H NMR (CD_3OD): δ (ppm) 0.92 (t, 3, *J* = 6.9 Hz, H-4'), 0.99 (d, 3, *J* = 6.7 Hz, CH_3C2'), 1.05 and 1.30 (m, 2, H-3'), 1.72 (m, 1, H-2'), 2.07 (s, 3, CH_3C2), 3.29 (s, 3, CH_3O), 4.07 (d, 1, *J* = 7.5 Hz, H-1'), 6.33 (d, 1, *J* = 8.2 Hz, H-6), and 6.66 (d, 1, *J* = 8.2 Hz, H-5). ^{13}C NMR (CD_3OD): δ (ppm) 7.09 (CH_3C2), 10.16 (C-4'), 14.15 (CH_3C2'), 25.65 (C-3'), 40.39 (C-2'), 56.12 (CH_3O), 87.98 (C-1'), 105.87 (C-6), 111.23 (C-6), 115.83 (C-4), 125.88 (C-5), 154.17 (C-3), and 155.41 (C-1). MS, *m/z* (%, ion structure): 192 (90, $M^+ - CH_3OH$), 177 (45, 192 – CH_3), 163 (100, 192 – CH_3CH_2), and 137 (49, $C_8H_9O_2$).

4-(1-Methoxy-3-methylbutyl)-2-methylbenzene-1,3-diol (**28**). ^{1}H NMR (CD_3OD): δ (ppm) 0.92 (d, 3, *J* = 6.6 Hz, H-4'), 0.94 (d, 3, *J* = 6.6 Hz, CH_3C3'), 1.46 and 1.76 (m, 2, H-3'), 1.67 (hp, 1, *J* = 6.6 Hz, H-3'), 2.08 (s, 3, CH_3C2), 3.27 (s, 3, CH_3O), 4.42 (dd, 1, *J* = 6.0 Hz, *J* = 8.2 Hz, H-1'), 6.34 (d, 1, *J* = 8.2 Hz, H-6), and 6.71 (d, 1, *J* = 8.2 Hz, H-5). ^{13}C NMR (CD_3OD): δ (ppm) 7.09 (CH_3C2), 21.42 (CH_3C3'), 22.07 (C-4'), 24.53 (C-3'), 45.26 (C-2'), 55.43 (CH_3O), 81.33 (C-1'), 106.14 (C-6), 111.40 (C-2), 117.45 (C-4), 124.70 (C-5), 153.92 (C-3), and 155.41 (C-1). MS, *m/z* (%, ion structure): 192 (67, $M^+ - CH_3OH$), 177 (83, 192 – CH_3), 175 (19, 192 – OH), and 137 (100, $C_8H_9O_2$).

4-(Hex-1-en-1-yl)-2-methylbenzene-1,3-diol (**29**). ^{1}H NMR (CD_3OD): δ (ppm) 0.93 (t, 3, *J* = 7.3 Hz, H-6'), 1.40 (m, 4, H-4' and H-5'), 2.06 (s, 3, CH_3C2), 2.18 (qd, 2, *J* = 1.5 Hz, *J* = 7.1 Hz, H-3'), 5.96 (dt, 1, *J* = 7.1 Hz, *J* = 15.7 Hz, H-2'), 6.32 (d, 1, *J* = 8.3 Hz, H-6), 6.60 (dt, 1, *J* = 1.5 Hz, 15.7 Hz, H-1'), and 7.01 (d, 1, *J* = 8.3 Hz, H-5). ^{13}C NMR (CD_3OD): δ (ppm) 8.87 (CH_3C2), 14.39 (C-6'), 23.36 (C-5'), 33.16 (C-4'), 34.21

(C-3'), 108.29 (C-6), 112.61 (C-2), 119.26 (C-4), 124.36 (C-5), 126.15 (C-1'), 128.93 (C-2'), 153.72 (C-3), and 156.19 (C-1). MS, *m/z* (%, ion structure): 206 (39, M^+), 191 (1, $M^+ - CH_3$), 177 (100, $M^+ - CH_3CH_2$), 163 (100, $M^+ - CH_3CH_2CH_2$), and 137 (19, $C_8H_9O_2$).

1-(2,4-Dihydroxyphenyl)-2-hydroxyethan-1-one (**30**). ^{1}H NMR (CD_3OD): δ (ppm) 4.80 (s, 2, CH_2OH), 6.28 (d, 1, *J* = 2.3 Hz, H-2), 6.35 (dd, 1, *J* = 2.3 Hz, *J* = 8.7 Hz, H-6), and 7.59 (d, 1, *J* = 8.7 Hz, H-5). ^{13}C NMR (CD_3OD): δ (ppm) 65.21 (CH_2OH), 103.70 (C-2), 109.39 (C-6), 111.84 (C-4), 132.15 (C-5), 165.80 (C-3), 166.53 (C-1), and 202.57 (CO). MS, *m/z* (%, ion structure): 168 (15, M^+), and 137 (100, $M^+ - CH_2OH$).

1-(2,4-Dihydroxy-3-methylphenyl)-2-hydroxyethan-1-one (**31**). ^{1}H NMR (CD_3OD): δ (ppm) 2.01 (s, 3, CH_3C2), 4.78 (s, 2, CH_2OH), 6.35 (d, 1, *J* = 8.8 Hz, H-6), and 7.36 (d, 1, *J* = 8.8 Hz, H-5). ^{13}C NMR (CD_3OD): δ (ppm) 7.54 ($\underline{C}H_3$C2), 64.72 (CH_2OH), 108.24 (C-6), 111.15 (C-4), 112.43 (C-2), 128.56 (C-5), 163.59 (C-3), 166.98 (C-1), and 202.70 (CO). MS, *m/z* (%, ion structure): 182 (15, M^+), and 151 (100, $M^+ - CH_2OH$).

2-Ethyl-3-methyl-2*H*-chromen-7-ol (**32**). ^{1}H NMR (CD_3OD): δ (ppm) 0.99 (t, 3, *J* = 7.3 Hz, $C\underline{H}_3CH_2$), 1.65 (m, 2, CH_2C2), 1.78 (s, 3, CH_3C3), 4.49 (dd, 1, *J* = 3.8 Hz, *J* = 7.7 Hz, H-2), 6.07 (s, 1, H-4), 6.19 (d, 1, *J* = 2.7 Hz, H-8), 6.24 (dd, 1, *J* = 2.7 Hz, *J* = 8.0 Hz, H-6), and 6.70 (d, 1, *J* = 8.5 Hz, H-5). ^{13}C NMR (CD_3OD): δ (ppm) 9.92 ($\underline{C}H_3CH_2$), 19.55 (CH_3C3), 26.73 (CH_2C2), 81.19 (C-2), 103.87 (C-8), 108.68 (C-6), 116.42 (C-4a), 119.99 (C-4), 127.19 (C-5), 131.61 (C-3), 154.12 (C-8a), and 158.78 (C-7). MS, *m/z* (%, ion structure): 190 (12, M^+), and 161 (100, $M^+ - CH_3CH_2$).