

**Access to functionalized quinines via aromatic oxidation of phenols bearing
an alcohol or olefin function catalyzed by supported iron phthalocyanine.**

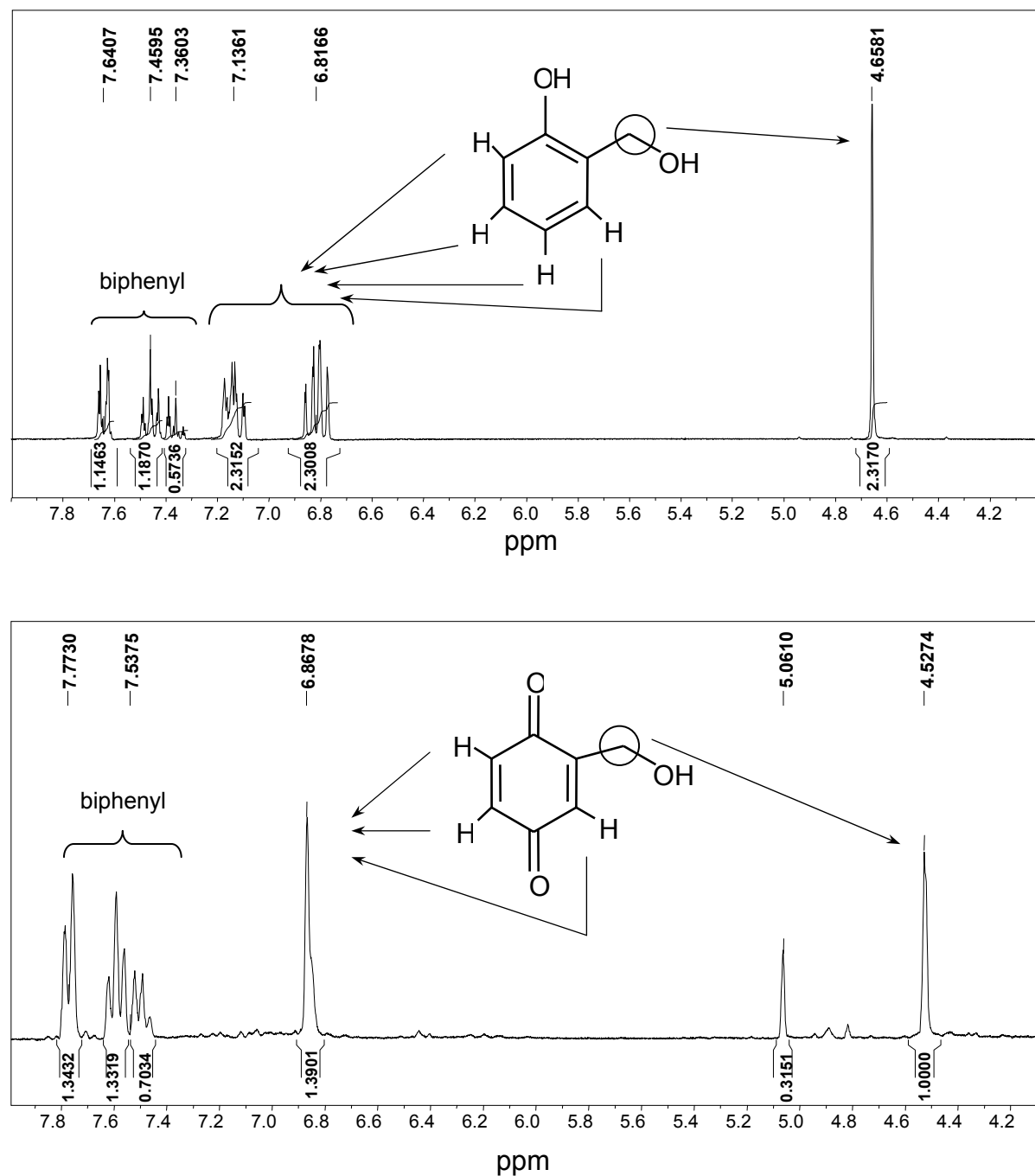
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Electronic Supporting Information

Figure S1. Oxidation of 2-hydroxybenzyl alcohol. Determination of the conversion and 2-hydroxymethyl-1,4-benzoquinone yield using the signals of benzylic protons and signals of biphenyl as an internal standard.



2-hydroxybenzyl alcohol

MS (EI) m/z (relative int.): 124 (45, [M]⁺), 106 (64, [M-H₂O]⁺), 78 (100, [M-H₂O-CO]⁺).

¹H NMR (CD₃COCD₃, 250 MHz): δ 4.70 (s, 2H, CH₂), 6.74-6.80 (m, 2H, CH aromatic), 7.05-7.25 (m, 2H, CH aromatic).

2-hydroxymethyl-1,4-benzoquinone

MS (EI) m/z (relative int.): 138 (20, [M]⁺), 122 (16, [M-O]⁺), 110 (100, [M-CO]⁺), 94 (10, [M-2O]⁺), 82 (28, [M-2CO]⁺).

¹H NMR (CD₃COCD₃, 250 MHz): δ 4.44 (s, 2H, CH₂), 6.74-6.78 (m, 3H, CH aromatic).

3-hydroxybenzyl alcohol

MS (EI) m/z (relative int.): 124 (100, [M]⁺), 123 (29, [M-H]⁺), 107 (18, [M-OH]⁺), 106 (16, [M-H₂O]⁺), 105 (23, [M-H₂O-H]⁺), 95 (60, [M-COH]⁺), 77 (60, [M-H₂O-COH]⁺).

¹H NMR (CD₃COCD₃, 250 MHz): δ 4.13 (t, 1H, OH, J=5.7 Hz), 4.54 (d, 2H, CH₂, J=5.7 Hz), 6.55 (d, 1H, CH aromatic, J=3.38 Hz), 6.77-6.85 (m, 2H, CH aromatic), 7.11 (t, 1H, CH aromatic, J=7.8 Hz).

3,5-dihydroxybenzyl alcohol

MS (EI) m/z (relative int.): 140 (100, [M]⁺), 139 (12, [M-H]⁺), 123 (14, [M-OH]⁺), 122 (15, [M-H₂O]⁺), 121 (18, [M-H₂O-H]⁺), 111 (54, [M-COH]⁺), 93 (22, [M-H₂O-COH]⁺).

¹H NMR (CD₃COCD₃, 250 MHz): δ 4.38 (s, 2H, CH₂), 6.14 (t, 1H, CH aromatic, J=2.3 Hz), 6.25-6.28 (m, 2H, CH aromatic).

2-hydroxy-6-hydroxymethyl-1,4-benzoquinone

MS (EI): unstable under analysis conditions

^1H NMR (CD_3COCD_3 , 250 MHz): δ 4.34 (s, 2H, CH_2), 5.8 (d, 1H, CH aromatic, $J=2.5$ Hz), 6.51 (d, 1H, CH aromatic, $J=2.5$ Hz).

3-hydroxyphenethyl alcohol

MS (EI) m/z (relative int.): 138 (61, $[\text{M}]^+$), 120 (6, $[\text{M}-\text{CO}]^+$), 108 (70, $[\text{M}-\text{CH}_2\text{O}]^+$), 107 (100, $[\text{M}-\text{CH}_2\text{OH}]^+$), 90 (12, $[\text{M}-\text{CH}_2\text{O}-\text{H}_2\text{O}]^+$), 77 (35, $[\text{M}-\text{CHCH}_2\text{O}-\text{H}_2\text{O}]^+$).

^1H NMR (CD_3COCD_3 , 250 MHz): δ 2.71 (t, 2H, $\underline{\text{CH}}_2\text{CH}_2\text{OH}$, $J=7.0$ Hz), 3.70 (t, 2H, $\underline{\text{CH}}_2\text{CH}_2\text{OH}$, $J=7.0$ Hz), 6.63-6.70 (m, 3H, CH aromatic), 7.07 (t, 1H, CH aromatic, $J=7.7$ Hz).

2-(2-hydroxyethyl)-1,4-benzoquinone

MS (EI): unstable under analysis conditions

^1H NMR (CD_3COCD_3 , 250 MHz): δ 2.54 (t, 2H, $\underline{\text{CH}}_2\text{OH}$, $J=6.3$ Hz), 3.65 (t, 2H, $\underline{\text{CH}}_2\text{CH}_2\text{OH}$, $J=6.3$ Hz), 6.57-6.72 (m, 3H, CH aromatic).

2-allylphenol

MS (EI) m/z (relative int.): 134 (100, $[\text{M}]^+$), 133 (38, $[\text{M}-\text{H}]^+$), 119 (33, $[\text{M}-\text{CH}_3]^+$), 115 (34, $[\text{M}-\text{H}_2\text{O}-\text{H}]^+$), 107 (19, $[\text{M}-\text{CH}_2\text{CH}]^+$), 105 (21, $[\text{M}-\text{COH}]^+$), 91 (41, $[\text{M}-\text{CH}_2-\text{COH}]^+$), 77 (30, $[\text{M}-\text{CH}_2\text{CH}_2-\text{COH}]^+$).

^1H NMR (CD_3CN , 250 MHz): δ 3.34 (d, 2H, $\underline{\text{CH}}_2\text{CH}=\text{CH}_2$, $J=6.5$ Hz), 5.00-5.08 (m, 2H, $\text{CH}_2\text{CH}=\underline{\text{CH}}_2$), 5.92-6.08 (m, 1H, $\text{CH}_2\underline{\text{CH}}=\text{CH}_2$), 6.78-6.81 (m, 2H, CH aromatic), 6.84 (s, 1H, OH), 7.03-7.10 (m, 2H, CH aromatic).

2-allyl-1,4-benzoquinone

MS (EI) m/z (relative int.): 148 (33, [M]⁺), 147 (42, [M-H]⁺), 131 (6, [M-OH]⁺), 120 (54, [M-CO]⁺), 105 (13, [M-CH₂-COH]⁺), 92 (13, [M-2CO]⁺), 91 (100, [M-2CO-H]⁺).

¹H NMR (CD₃CN, 250 MHz): δ 3.15 (dd, 2H, CH₂CH=CH₂, J₁=6.8 Hz, J₂=1.4), 4.98-5.12 (m, 2H, CH₂CH=CH₂), 5.80-6.10 (m, 1H, CH₂-CH=C), 6.54-6.77 (m, 3H aromatic).