Electronic Supplementary Material (ESI) for Green Chemistry

Supporting Information

A comparative study of different metal acetylacetonates covalently anchored onto amine functionalized silica: A study of the oxidation of aldehydes and alcohols to corresponding acids in water

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Spectral data of the compounds

Benzoic acid (Table 3, Entry 1): ^{1}H NMR (DMSO-d_6): δ 7.45–7.64 (*m*, 3H, H_{arom}), 8.13 (*d*, 2H, H_{arom}); ^{13}C NMR (DMSO-d_6): δ 172.5, 133.8, 130.2, 128.4; IR (ν_{max} in cm^{-1}): 1670 (C=O stretch), 2950 (O-H stretch); ms (m/z): 122 (M^+).

4-Methoxybenzoic acid (Table 3, Entry 2): ^{1}H NMR (DMSO-d_6): δ 3.79 (*s*, 3H, OCH_3), 6.85 (*d*, 2H, H_{arom}), 7.94 (*d*, 2H, H_{arom}); ^{13}C NMR (DMSO-d_6): δ 168.7, 163.3, 131.8, 114.6, 55.2; IR (ν_{max} in cm^{-1}): 1690 (C=O stretch), 2995 (O-H stretch); ms (m/z): 152 (M^+).

4-Chlorobenzoic acid (Table 3, Entry 3): ^{1}H NMR (DMSO-d_6): δ 7.56 (*d*, 2H, H_{arom}), 7.93 (*d*, 2H, H_{arom}); ^{13}C NMR (DMSO-d_6): δ 166.4, 137.8, 131.1, 129.6, 128.7; IR (ν_{max} in cm^{-1}): 1687 (C=O stretch), 2985 (O-H stretch); ms (m/z): 156 (M^+), 158 (M+2).

4-Bromobenzoic acid (Table 3, Entry 4): ^{1}H NMR (DMSO-d_6): δ 7.66 (*d*, 2H, H_{arom}), 7.95 (*d*, 2H, H_{arom}); ^{13}C NMR (DMSO-d_6): δ 165.4, 133.8, 131.1, 127.6, 128.7; IR (ν_{max} in cm^{-1}): 1685 (C=O stretch), 3010 (O-H stretch); ms (m/z): 200 (M^+), 202 (M+2).

Cinnamic acid (Table 3, Entry 5): ^{1}H NMR ($CDCl_3$): δ 6.47 (*d*, 1H, =CH), 7.42-7.56 (*m*, 5H, H_{arom}), 7.81 (*d*, 1H, =CH); ^{13}C NMR (DMSO-d_6): δ 170.6, 148.0, 135.2, 126.4, 115.6; IR (ν_{max} in cm^{-1}): 1667 (C=O stretch), 2885 (O-H stretch); ms (m/z): 148 (M^+).

Furan-2-carboxylic acid (Table 3, Entry 6)*:* ^{1}H NMR (DMSO-d_6): δ 6.49-6.99 (*m*, 2H, H_{arom}), 7.58 (*dd*, 1H, H_{arom}); ^{13}C NMR (DMSO-d_6): δ 161.7,148.2, 146.8, 120.7, 113.2; IR (ν_{max} in cm^{-1}): 1708 (C=O stretch), 3016 (O-H stretch); ms (m/z): 112 (M^+).

(*Z*)-3-Chloro-3-(4-methoxyphenyl)acrylic acid (Table 5, Entry 1): ^{1}H NMR ($CDCl_3$): δ 3.85 (*s*, 3H, OCH_3), 6.50 (*s*, 1H, =CH), 6.98 (*d*, 2H, H_{arom}), 7.73 (*d*, 2H, H_{arom}); ^{13}C NMR ($CDCl_3$): δ 165.6, 162.1, 145.2, 129.3, 129.1, 113.1, 55.7; IR (ν_{max} in cm^{-1}): 1674 (C=O stretch), 2905 (O-H stretch); ms (m/z): 214 (M^+), 216 (M+2).

(*Z*)-3-Chloro-3-(4-chlorophenyl)acrylic acid (Table 5, Entry 2): ^{1}H NMR ($CDCl_3$): δ 6.62 (*s*, 1H, =CH), 7.44 (*d*, 2H, H_{arom}), 7.65 (*d*, 2H, H_{arom}); ^{13}C NMR ($CDCl_3$): δ 165.9, 146.5, 135.1, 129.2, 127.5, 115.3; IR (ν_{max} in cm^{-1}): 1672 (C=O stretch), 2890 (O-H stretch); ms (m/z): 216 (M^+), 218 (M+2).

(*Z*)-3-Chloro-3-(4-nitrophenyl)acrylic acid (Table 5, Entry 3): ^{1}H NMR ($CDCl_3$): δ 6.85 (*s*, 1H, =CH), 7.78 (*d*, 2H, H_{arom}), 7.98 (*d*, 2H, H_{arom}); ^{13}C NMR (DMSO-d_6): δ 165.1, 146.2, 143.5, 126.5, 121.5, 110.6; IR (ν_{max} in cm^{-1}): 1680 (C=O stretch), 2877 (O-H stretch); ms (m/z): 227 (M^+), 229 (M+2).

2-Chloroquinoline-3-carboxylic acid (Table 5, Entry 4): ^{1}H NMR (DMSO-d_6): δ 7.43-7.68 (*m*, 3H, H_{arom}), 8.05-8.71 (*d*, 2H, H_{arom}); ^{13}C NMR (DMSO-d_6): δ 169.4, 151.7,149.1, 140,

133.4, 129.4,127.6, 125.3; IR (ν_{max} in cm^{-1}): 1720 (C=O stretch), 2925 (O-H stretch); ms (m/z): 207 (M^+), 209 (M+2).

4-Nitrobenzoic acid (Table 5, Entry 5): ^{1}H NMR (DMSO-d_6): δ 8.15-8.30 (*m*, 4H, H_{arom}); ^{13}C NMR (DMSO-d_6): δ 165.8, 150.0, 136.4, 130.7, 123.7; IR (ν_{max} in cm^{-1}): 1695 (C=O stretch), 3116 (O-H stretch); ms (m/z): 166 (M^+).

2-Nitobenzoic acid (Table 5, Entry 6): ^{1}H-NMR (DMSO-d_6): δ 7.74-7.97 (*m*, 4H, H_{arom}); ^{13}C NMR (DMSO-d_6): δ 165.9, 148.4, 133.1, 132.4) 129.9, 127.3, 123.7; IR (ν_{max} in cm^{-1}): 1683 (C=O stretch), 2888 (O-H stretch; ms (m/z): 166 (M^+).

4-Hydroxybenzoic acid (Table 5, Entry 7): ^{1}H NMR (DMSO-d_6): δ 6.83 (*d*, 2H, H_{arom}), 7.80 (*d*, 2H, H_{arom}); ^{13}C NMR (DMSO-d_6): δ 169.4, 163.7, 131.7, 122.9, 115.8; IR (ν_{max} in cm^{-1}): 1688 (C=O stretch), 2921 (O-H stretch); ms (m/z): 138 (M^+).

2-Hydroxybenzoic acid (Table 5, Entry 8): ^{1}H NMR (DMSO-d_6): δ 6.80–6.95 (*m*, 2H, H_{arom}), 7.45–7.82 (*m*, 2H, H_{arom}); ^{13}C NMR (DMSO-d_6): δ 172.1, 161.5, 135.2, 130.2, 118.7, 116.9, 112.7; IR (ν_{max} in cm^{-1}): 1678 (C=O stretch), 2905 (O-H stretch); ms (m/z): 138 (M^+).

2,4-Dichlorobenzoic acid (Table 5, Entry 9): ^{1}H NMR (DMSO-d_6): δ 6.58 (*d*, 1H, H_{arom}), 7.01-7.44 (*m*, 2H, H_{arom}); ^{13}C NMR (DMSO-d_6): δ 169.7, 139.4, 136.2, 133.6, 131.5, 127.0, 126.8; IR (ν_{max} in cm^{-1}): 1688 (C=O stretch), 2895 (O-H stretch); ms (m/z): 191 (M^+), 193 (M+2).

3-Nitrobenzoic acid (Table 5, Entry 10): ^{1}H NMR (DMSO-d_6): δ 7.77-8.45 (*m*, 4H, H_{arom}); ^{13}C NMR (DMSO-d_6): δ 165.9, 148.4, 133.1, 132.4, 129.9, 127.3, 123.7; IR (ν_{max} in cm^{-1}): 1710 (C=O stretch), 2925 (O-H stretch); ms (m/z): 167 (M^+).

3,4,5-Trimethoxybenzoic acid (Table 5, Entry 11): ^{1}H NMR (DMSO-d_6): δ 3.79 (*s*, 3H, OCH_3), 3.94 (*s*, 6H, 2 × OCH_3), 7.18 (*s*, 2H, H_{arom}); ^{13}C NMR (DMSO-d_6): δ 169.4, 150.7, 144.4, 56.5, 56.2; IR (ν_{max} in cm^{-1}): 1680 (C=O stretch), 3005 (O-H stretch; ms (m/z): 212 (M^+).

Butyric acid (Table 5, Entry 12): ^{1}H NMR (DMSO-d_6): δ 0.92 (*t*, 3H, CH_3), 1.60 (*m*, 2H, CH_2), 2.25 (*t*, 2H, CH_2); ^{13}C NMR (DMSO-d_6): δ 177, 37.5, 18.1, 13.2; IR (ν_{max} in cm^{-1}): 1705 (C=O stretch), 2995 (O-H stretch; ms (m/z): 88 (M^+).

Glutaric acid (Table 5, Entry 13): ^{1}H NMR (DMSO-d_6): δ 1.65 (*m*, 2H, CH_2), 2.25-2.42 (*t*, 4H, -CH_2); ^{13}C NMR (DMSO-d_6): δ 177, 37.5, 18.1, 13.2; IR (ν_{max} in cm^{-1}): 1715 (C=O stretch), 3010 (O-H stretch); ms (m/z): 132 (M^+).

2-Methoxybenzoic acid (Table 5, Entry 14): ^{1}H NMR ($CDCl_3$): δ 3.98 (*s*, 3H, OCH_3), 6.73-7.11 (*m*, 2H, H_{arom}), 7.49-8.02 (*m,* 2H, H_{arom}); ^{13}C NMR (DMSO-d_6): δ 166, 158.3, 135.1, 133.4, 121.8, 117.5, 111.8, 56.6; IR (ν_{max} in cm^{-1}): 1690 (C=O stretch), 2995 (O-H stretch); ms (m/z): 152 (M^+).