Electronic Supplementary Information

An efficient approach to the ammoxidation of alcohols to nitriles and the aerobic oxidation of alcohols to aldehydes in water using Cu(II)/pypzacac complexes as catalysts

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Contents

benzonitrile. ^{1}H NMR ($CDCl_3$, ppm, 400 Hz): δ 7.62 (s, 1H, aromatic CH), 7.61-7.56 (m, 2H, aromatic CH), 7.46(t, J = 8 Hz, 2H, aromatic CH).

2-methylbenzonitrile. ^{1}H NMR ($CDCl_3$, ppm, 400 Hz): δ 7.61 (d, J = 7.6 Hz, 1H, aromatic CH), 7.51 (t, J = 7.6 Hz, 1H, aromatic CH), 7.34-7.28 (m, 3H, aromatic CH), 2.56 (s, 3H).

3-methylbenzonitrile. ^{1}H NMR ($CDCl_3$, ppm, 400 Hz): δ 7.43-7.38 (m, 3H, aromatic CH), 7.35 (t, J = 7.6Hz, 1H, aromatic CH), 2.37 (s, 3H).

4-methylbenzonitrile. ^{1}H NMR ($CDCl_3$, ppm, 400 Hz): δ 7.55 (d, J = 8Hz, 2H, aromatic CH), 7.28 (d, J = 8Hz, 2H, aromatic CH), 2.42 (s, 3H).

2-methoxybenzonitrile. ^{1}H NMR ($CDCl_3$, ppm, 400 Hz): δ 7.51-7.46 (m, 2H, aromatic CH), 6.96 (t, J = 8Hz, 2H, aromatic CH), 3.86 (s, 3H).

3-methoxybenzonitrile. ^{1}H NMR ($CDCl_3$, ppm, 400 Hz): δ 7.36 (d, J = 8Hz, 1H, aromatic CH), 7.20 (d, J = 7.6Hz, 1H, aromatic CH), 7.11 (d, J = 6.4Hz, 2H, aromatic CH), 3.79 (s, 3H).

4-methoxybenzonitrile. ^{1}H NMR ($CDCl_3$, ppm, 400 Hz): δ 7.58 (d, J = 8.8Hz, 2H, aromatic CH), 6.95 (d, J = 8.8Hz, 2H, aromatic CH), 3.85 (s, 3H).

4-chlorobenzonitrile. ^{1}H NMR ($CDCl_3$, ppm, 400 Hz): δ 7.60 (d, J = 8.4Hz, 2H, aromatic CH), 7.46 (d, J = 8Hz, 2H, aromatic CH).

4-nitrobenzonitrile. ^{1}H NMR ($CDCl_3$, ppm, 400 Hz): δ 8.36 (d, J = 8.4Hz, 2H, aromatic CH), 7.90 (d, J = 8.8Hz, 2H, aromatic CH).

3,4-(methylenedioxy)benzonitrile. ^{1}H NMR ($CDCl_3$, ppm, 400 Hz): δ 7.18 (d, J = 8.4Hz, 1H, aromatic CH), 6.99 (s, 1H), 6.84 (d, J = 8Hz, 2H, aromatic CH), 6.04 (s, 2H).

3-cyanopyridine. ^{1}H NMR ($CDCl_3$, ppm, 400 Hz): δ 8.90 (s,1H), 8.83 (d, J = 4Hz, 1H), 7.99 (d, J = 8Hz, 1H), 7.47 (dd, J_1 = 5.2Hz, J_2 = 7.6Hz, 1H).

2-thiophenecarbonitrile. ^{1}H NMR ($CDCl_3$, ppm, 400 Hz): δ 7.63 (t, J = 4.4 Hz, 2H), 7.14(t, J = 4.4 Hz, 1H).

benzaldehyde. ^{1}H NMR ($CDCl_3$, ppm, 400 Hz): δ 9.96 (s, 1H) , 7.83 (d, J = 1.2 Hz, 1H, aromatic CH), 7.81 (d, J = 1.2 Hz, 1H, aromatic CH), 7.58-7.54 (m, 1H, aromatic CH), 7.48 (t, J = 7.6 Hz, 2H, aromatic CH).

2-methylbenzaldehyde. ^{1}H NMR ($CDCl_3$, ppm, 400 Hz): δ 10.26 (s, 1H), 7.80 (d, J= 7.6 Hz, aromatic CH), 7.49 (t, J= 7.6 Hz, 1H, aromatic CH), 7.37 (t, J= 7.6 Hz, 1H, aromatic CH),

7.26 (d, *J*= 7.6 Hz, 1H, aromatic CH), 2.66 (s, 3H).

3-methylbenzaldehyde. ^{1}H NMR ($CDCl_3$, ppm, 400 Hz): δ 9.94 (s, 1H), 7.64 (d, J = 5.2 Hz, 2H, aromatic CH), 7.39 (t, J = 7.6 Hz, 2H, aromatic CH), 2.38 (s, 3H).

4-methylbenzaldehyde. ^{1}H NMR ($CDCl_3$, ppm, 400 Hz): δ 9.97 (s, 1H), 7.79 (d, J = 7.6 Hz, 2H, aromatic CH), 7.35 (d, J = 7.6 Hz, 2H, aromatic CH), 2.45 (s, 3H).

2-methoxybenzaldehyde. ^{1}H NMR ($CDCl_3$, ppm, 400 Hz): δ 10.41 (s, 1H), 7.77 (dd, J_1 = 1.6 Hz, J_2 = 7.6 Hz, 1H, aromatic CH), 7.51-7.47 (m, 1H, aromatic CH), 6.98 (m, 2H, aromatic CH), 3.85 (s, 3H).

3-methoxybenzaldehyde. ^{1}H NMR ($CDCl_3$, ppm, 400 Hz): δ 9.87 (s, 1H), 7.36-7.29 (m, 3H, aromatic CH), 7.09-7.06 (m, 1H, aromatic CH), 3.75 (s, 3H).

4-methoxybenzaldehyde. ^{1}H NMR ($CDCl_3$, ppm, 400 Hz): δ 9.77 (s, 1H), 7.74 (d, J = 8.4 Hz, 2H, aromatic CH), 6.91 (d, J = 8.4 Hz, 2H, aromatic CH), 3,77 (s, 3H).

4-chlorobenzaldehyde. ^{1}H NMR ($CDCl_3$, ppm, 400 Hz): δ 9.99 (s, 1H), 7.84 (d, J = 7.6 Hz, 2H, aromatic CH), 7.54 (d, J = 8.4 Hz, 2H, aromatic CH).

4-nitrobenzaldehyde. ^{1}H NMR ($CDCl_3$, ppm, 400 Hz): δ 10.16 (s,1H), 8.40 (d, J = 7.6 Hz, 2H, aromatic CH), 8.09 (d, J = 7.6 Hz, 2H, aromatic CH).

3,4-(methylenedioxy)benzaldehyde. ^{1}H NMR ($CDCl_3$, ppm, 400 Hz): δ 9.81 (s,1H), 7.42 (d, J = 7.6 Hz, 1H, aromatic CH), 7.33 (s, 1H, aromatic CH), 6.94 (d, J = 8 Hz, 1H, aromatic CH), 6.07 (s,2H).

3-pyridinecarboxaldehyde. ^{1}H NMR ($CDCl_3$, ppm, 400 Hz): δ 9.99 (s, 1H), 8.95 (d, J = 1.2 Hz, 1H), 8.72 (dd, J_1 = 1.6 Hz, J_2 = 4.8 Hz, 1H), 8.06-8.03 (m, 1H), 7.38 (m, 1H).

2-thenaldehyde. ^{1}H NMR ($CDCl_3$, ppm, 400 Hz): δ 9.95 (d, J = 1.2 Hz, 1H), 7.80-7.76 (m, 3H), 7.23-7.21 (m, 1H).

Fig. S1 The ^{1}H NMR spectrum of benzonitrile

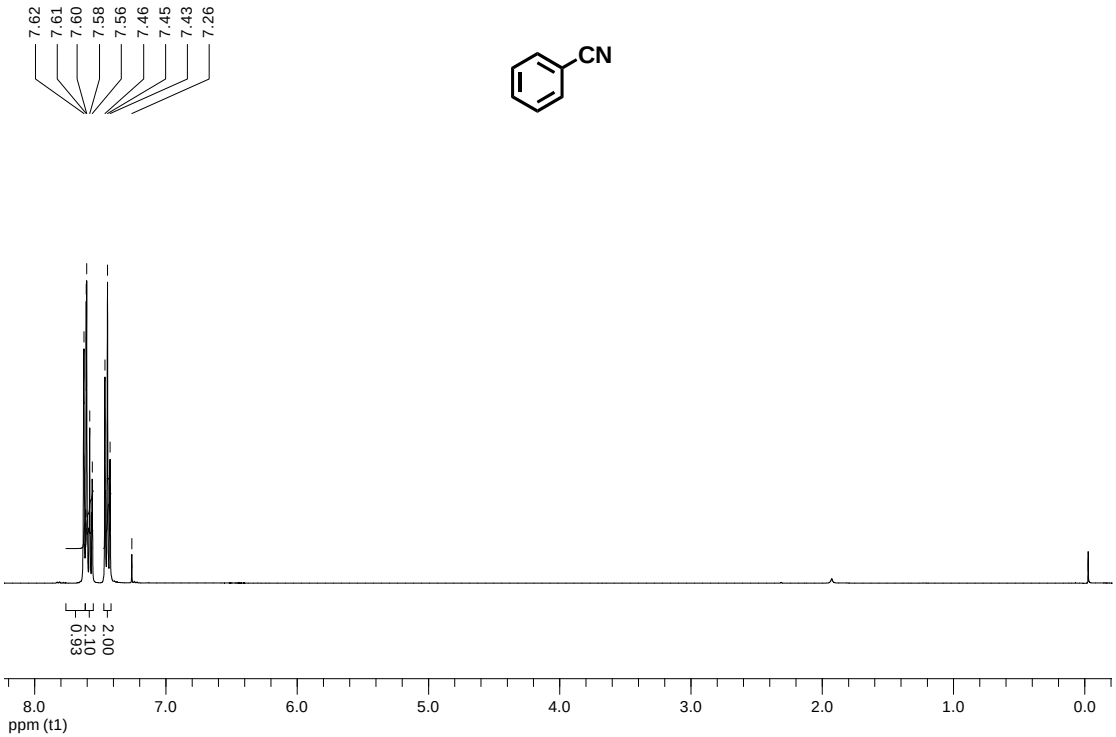

Fig. S2 The ^{1}H NMR spectrum of 2-methylbenzonitrile

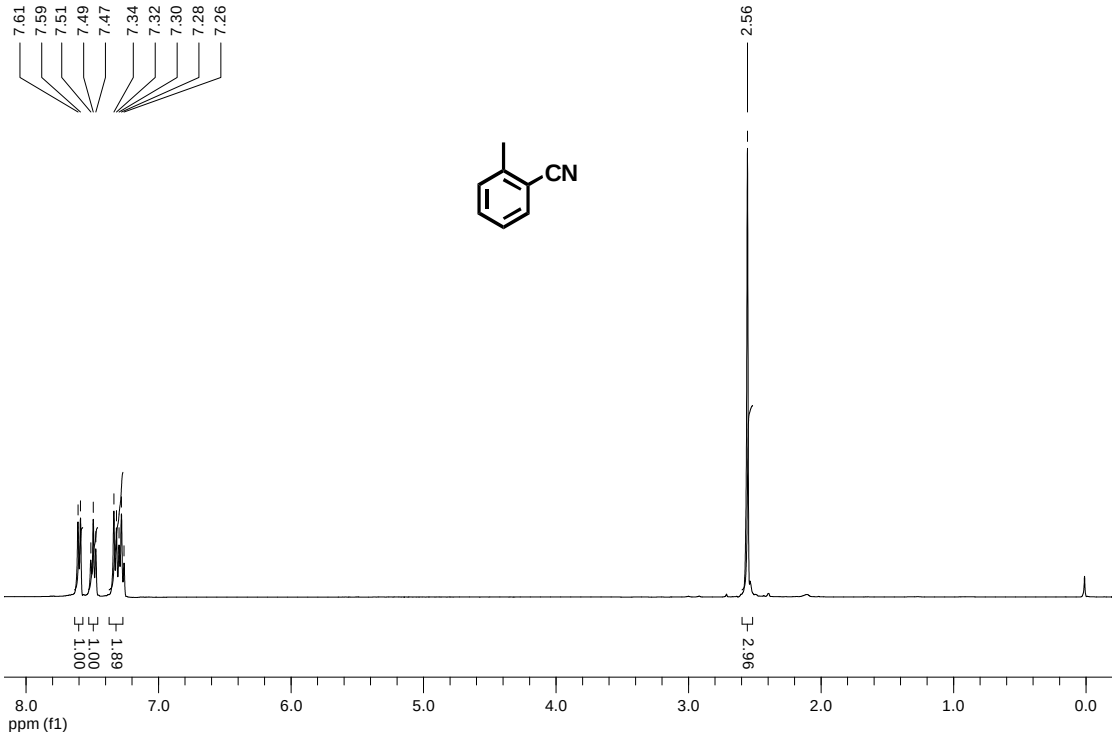

Fig. S3 The ^{1}H NMR spectrum of 3-methylbenzonitrile

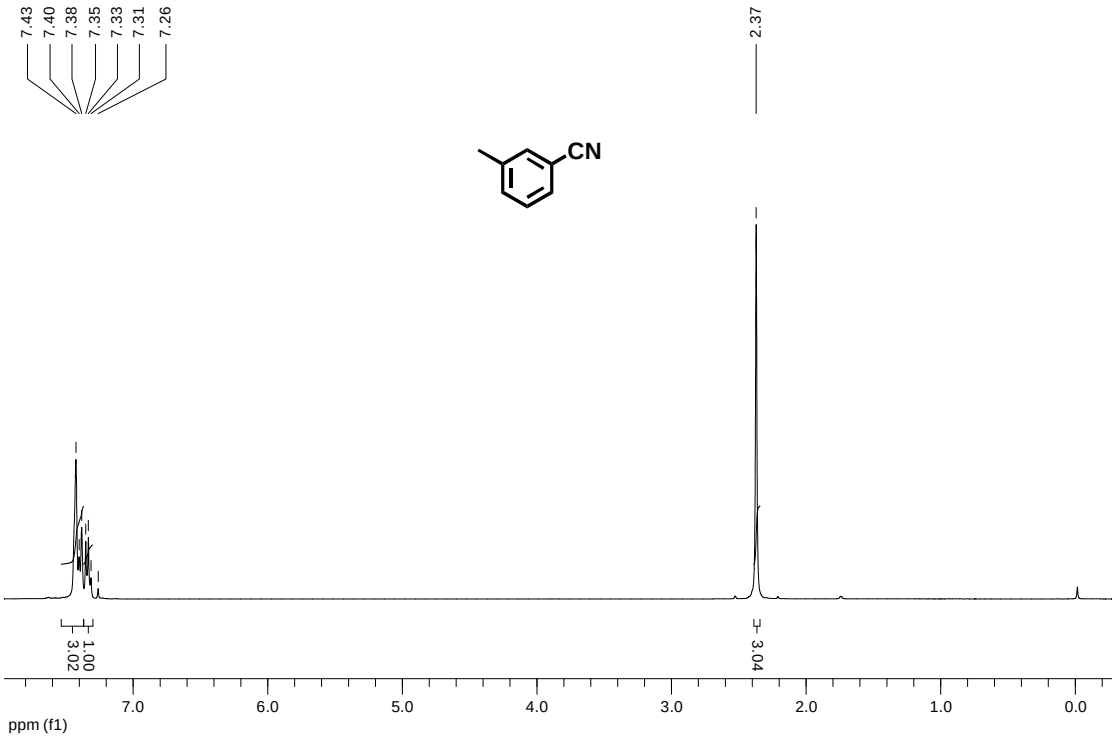

Fig. S4 The ^{1}H NMR spectrum of 4-methylbenzonitrile

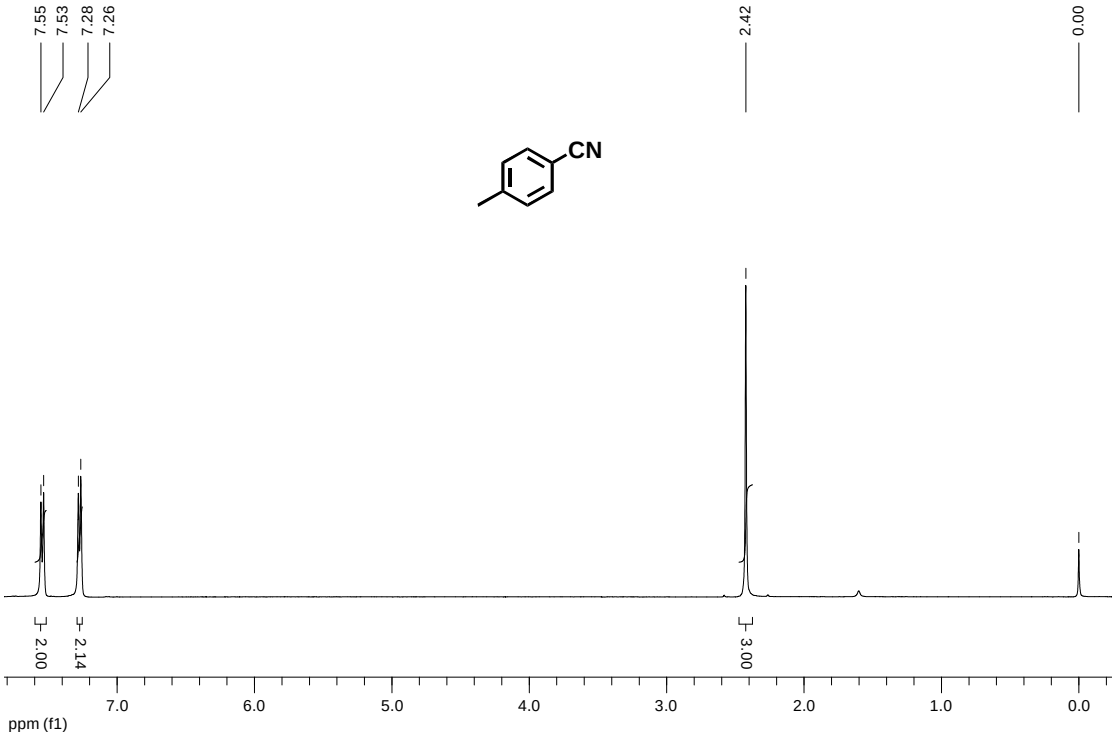

Fig. S5 The ^{1}H NMR spectrum of 2-methoxybenzonitrile

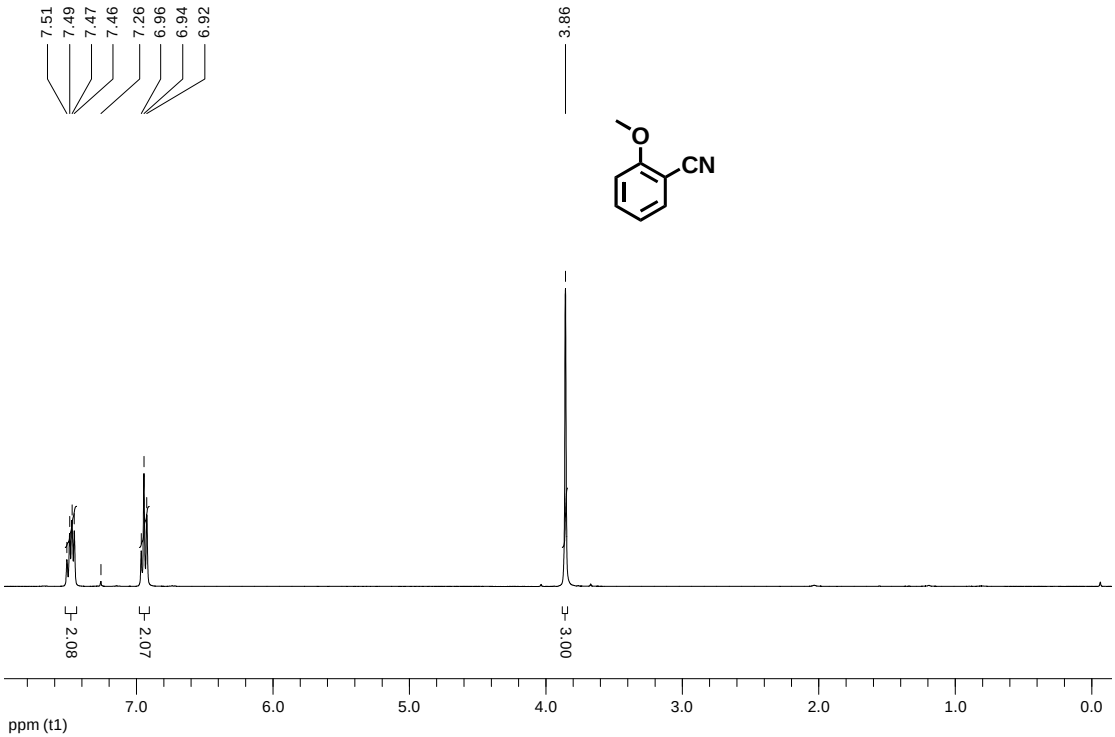

Fig. S6 The ^{1}H NMR spectrum of 3-methoxybenzonitrile

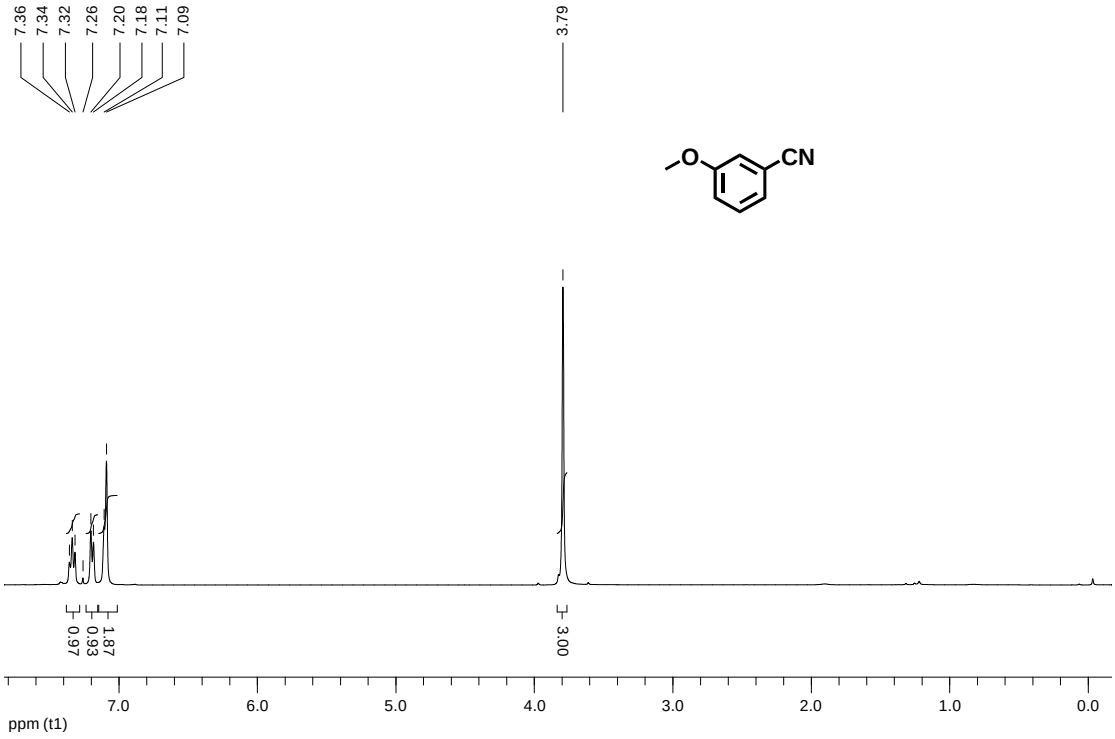

Fig. S7 The ^{1}H NMR spectrum of 4-methoxybenzonitrile

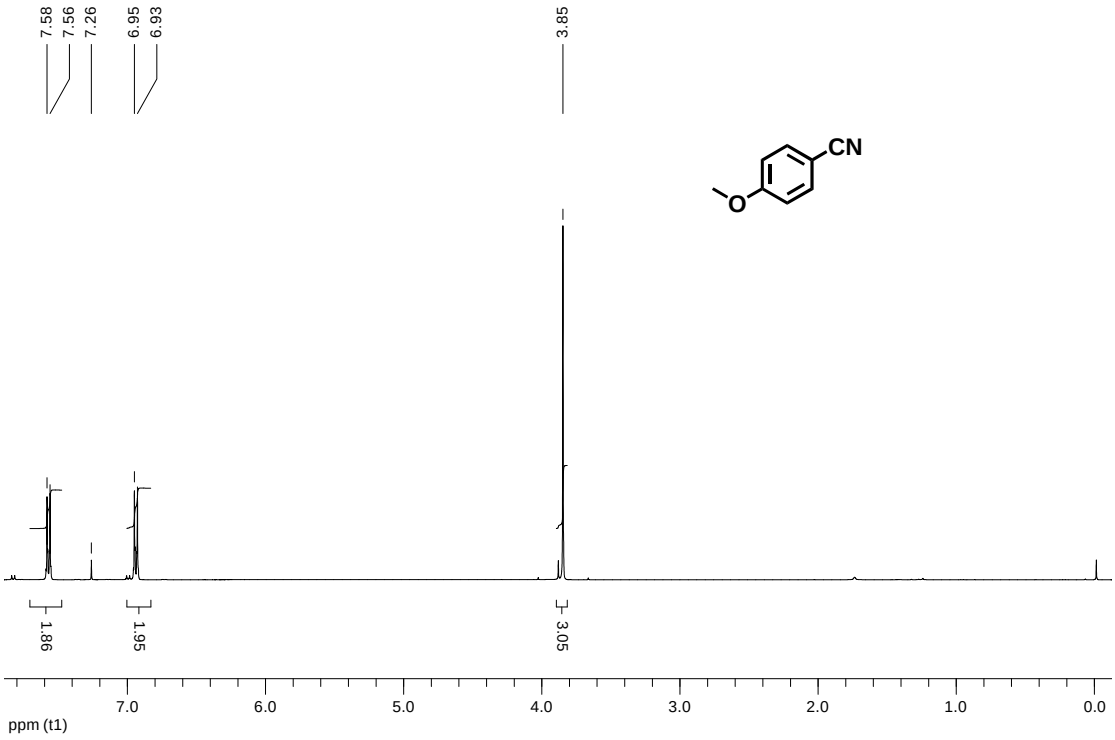

Fig. S8 The ^{1}H NMR spectrum of 4-chlorobenzonitrile

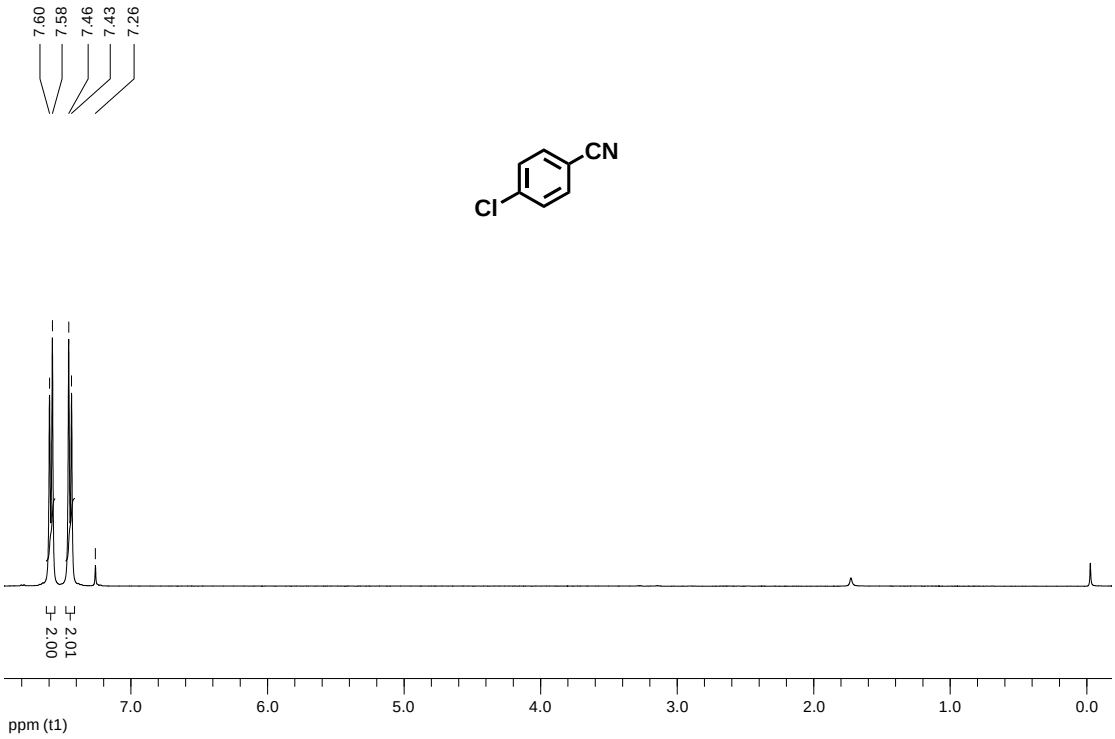

Fig. S9 The ^{1}H NMR spectrum of 4-nitrobenzonitrile

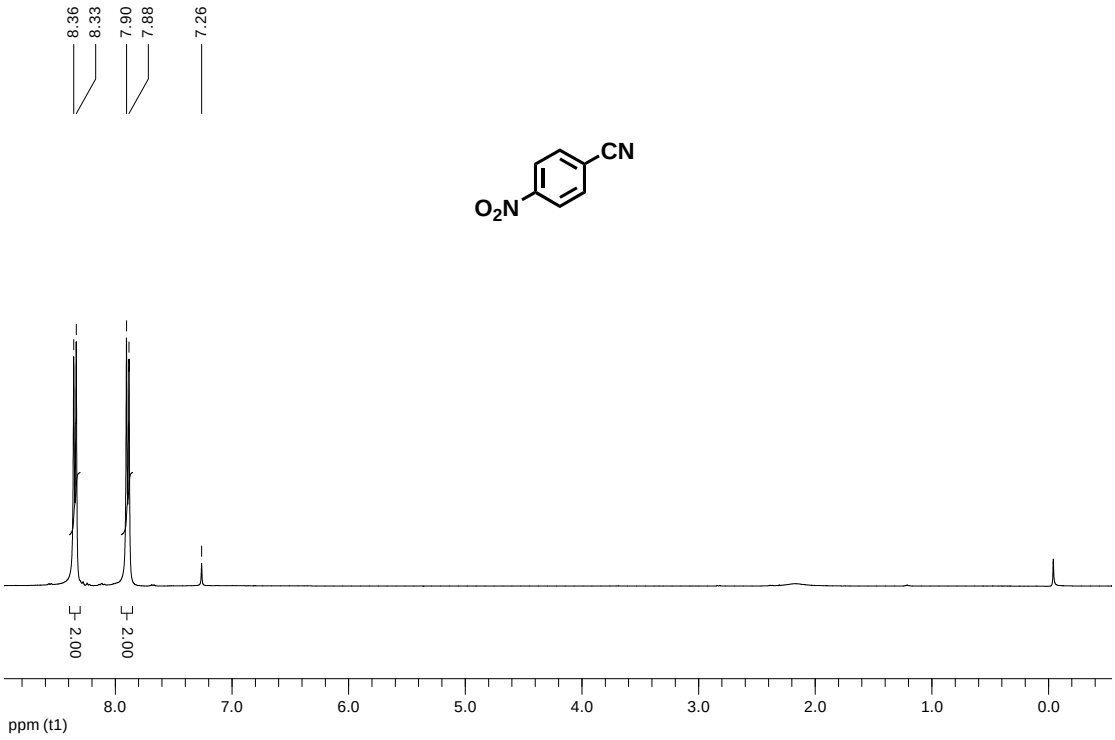

Fig. S10 The ^{1}H NMR spectrum of 3,4-(methylenedioxy)benzonitrile

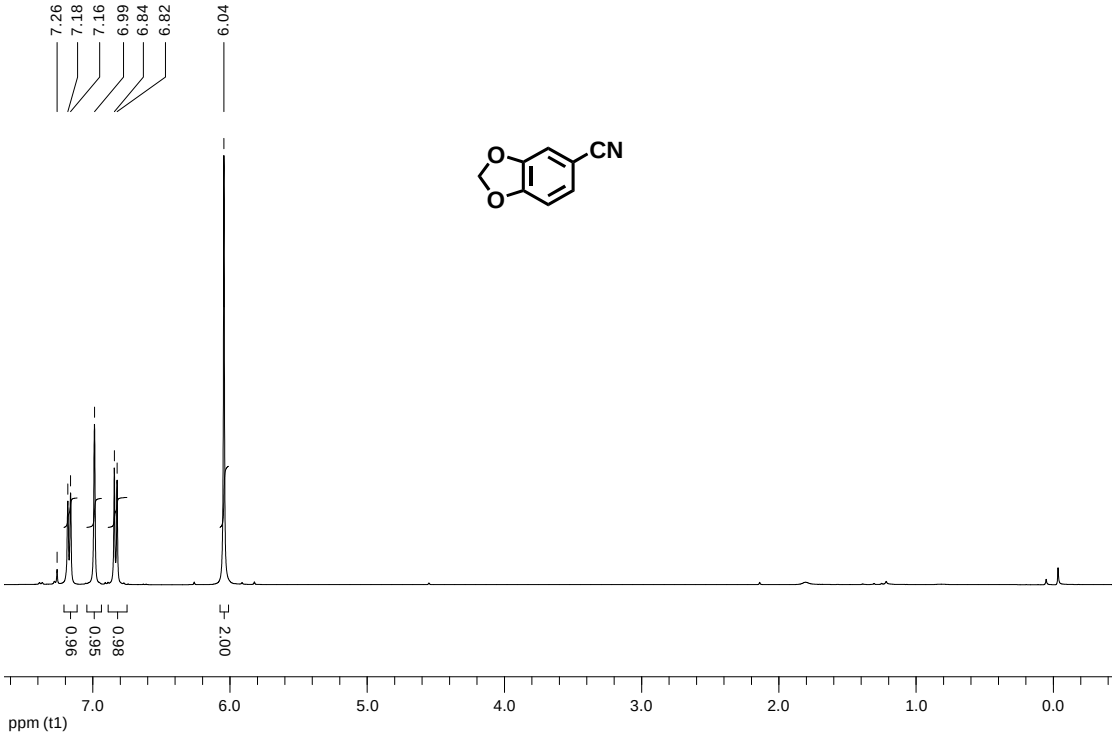

Fig. S11 The ^{1}H NMR spectrum of 3-cyanopyridine

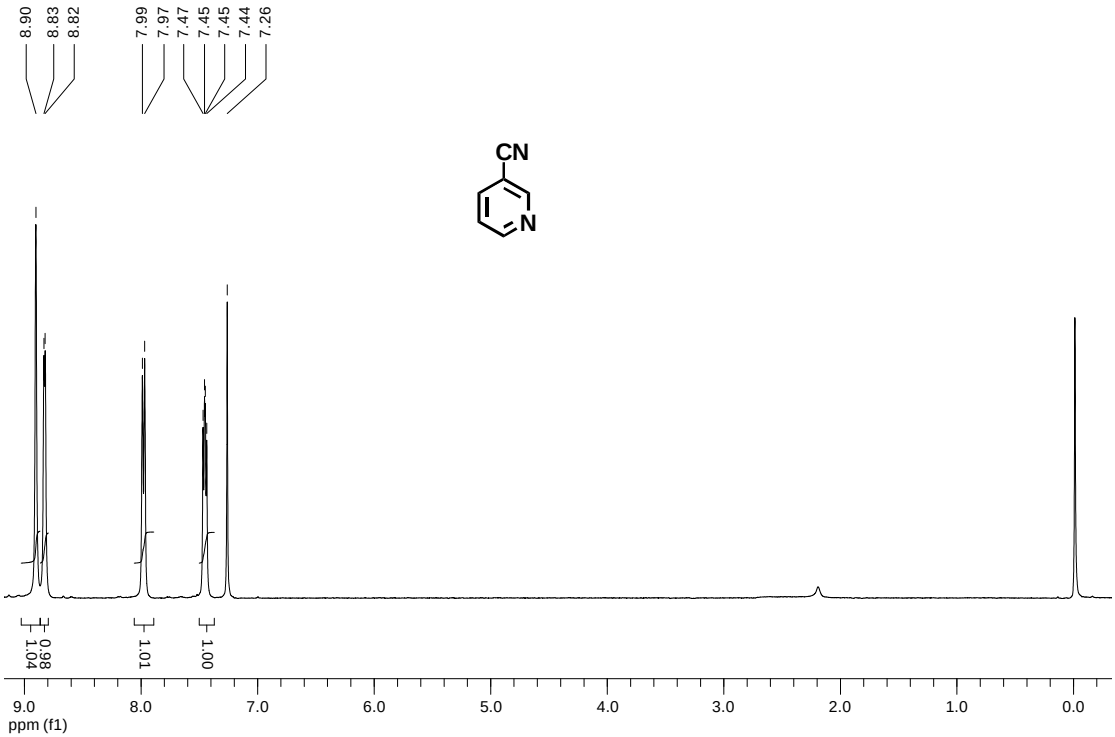

Fig. S12 The ^{1}H NMR spectrum of 2-thiophenecarbonitrile

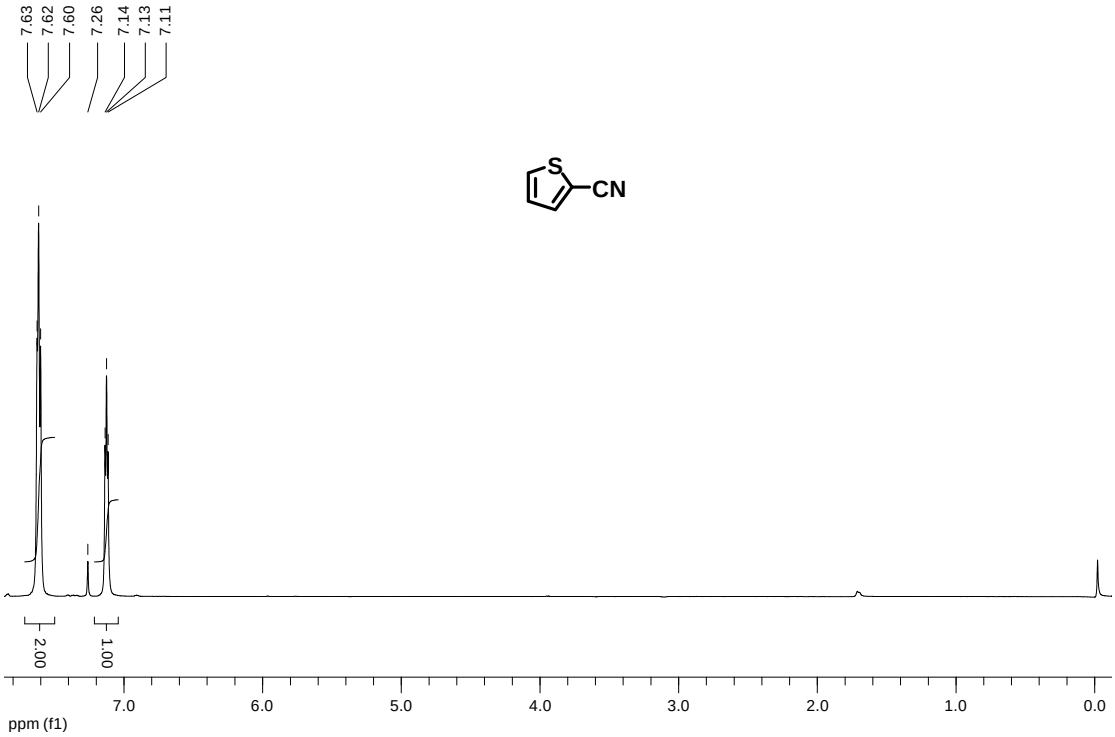

Fig. S13 The ^{1}H NMR spectrum of benzaldehyde

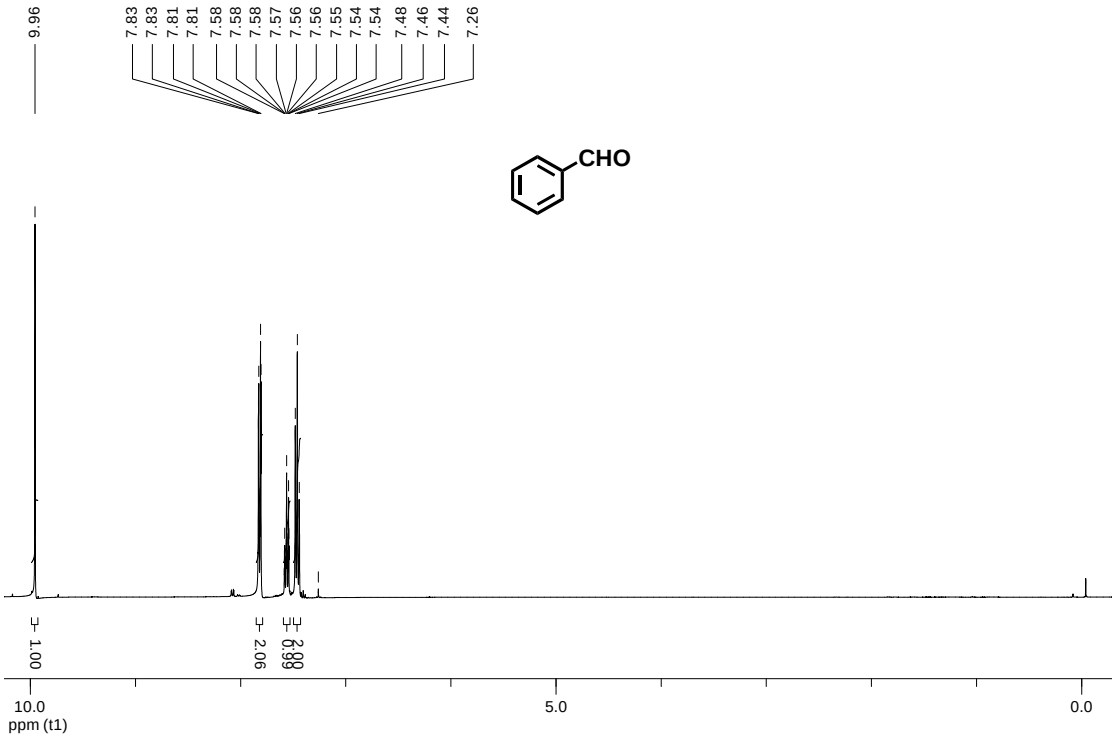

Fig. S14 The ^{1}H NMR spectrum of 2-methylbenzaldehyde

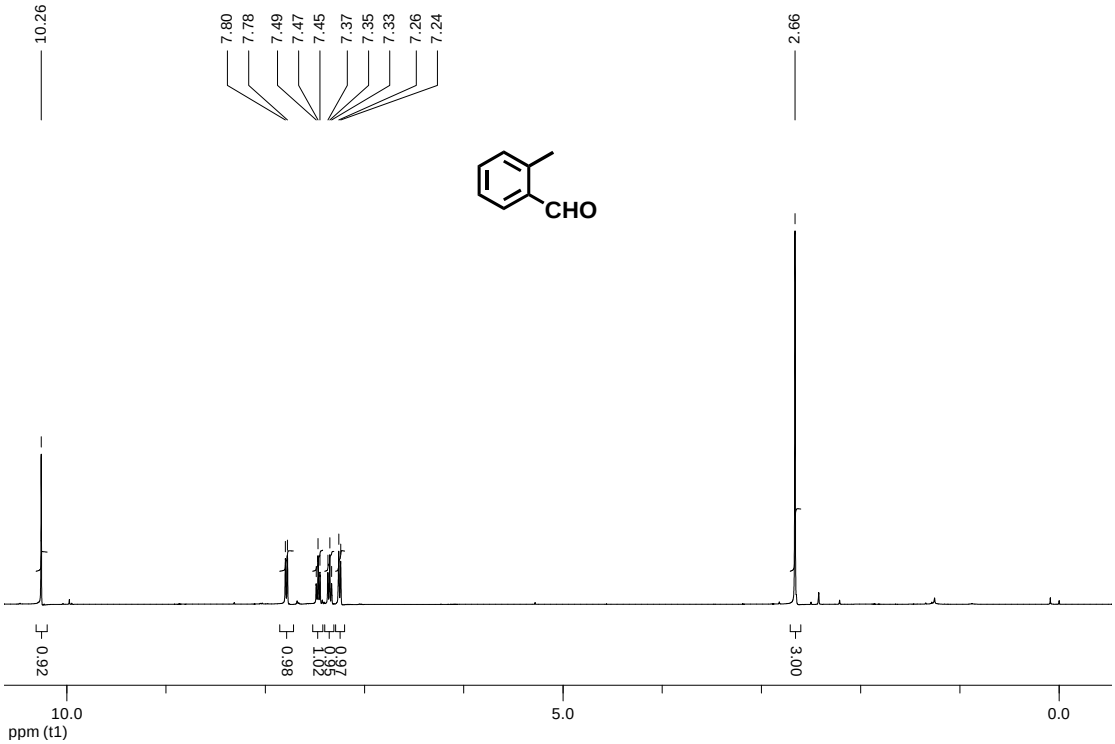

Fig. S15 The ^{1}H NMR spectrum of 3-methylbenzaldehyde

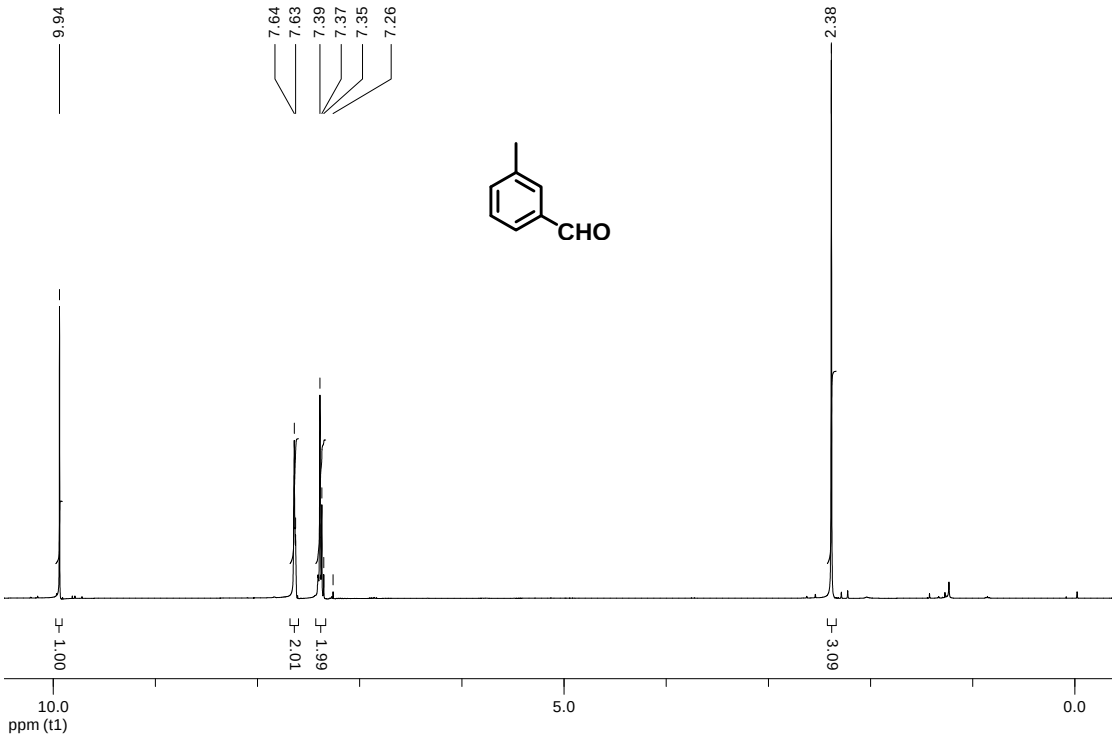

Fig. S16 The ^{1}H NMR spectrum of 4-methylbenzaldehyde

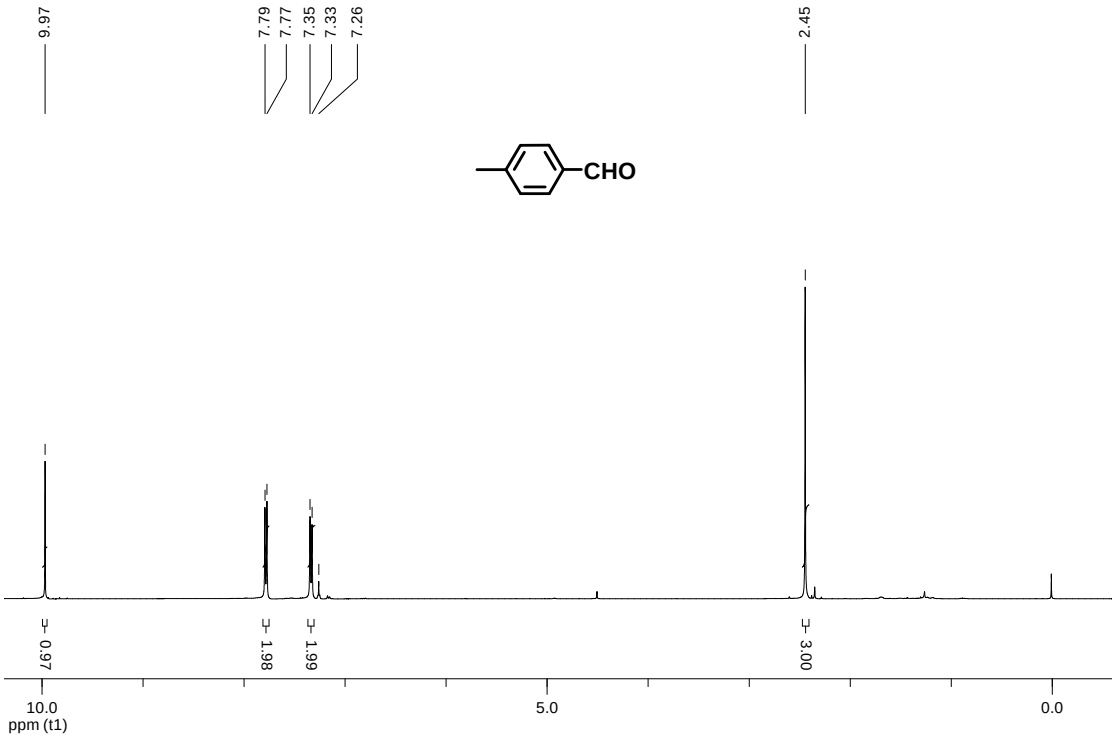

Fig. S17 The ^{1}H NMR spectrum of 2-methoxybenzaldehyde

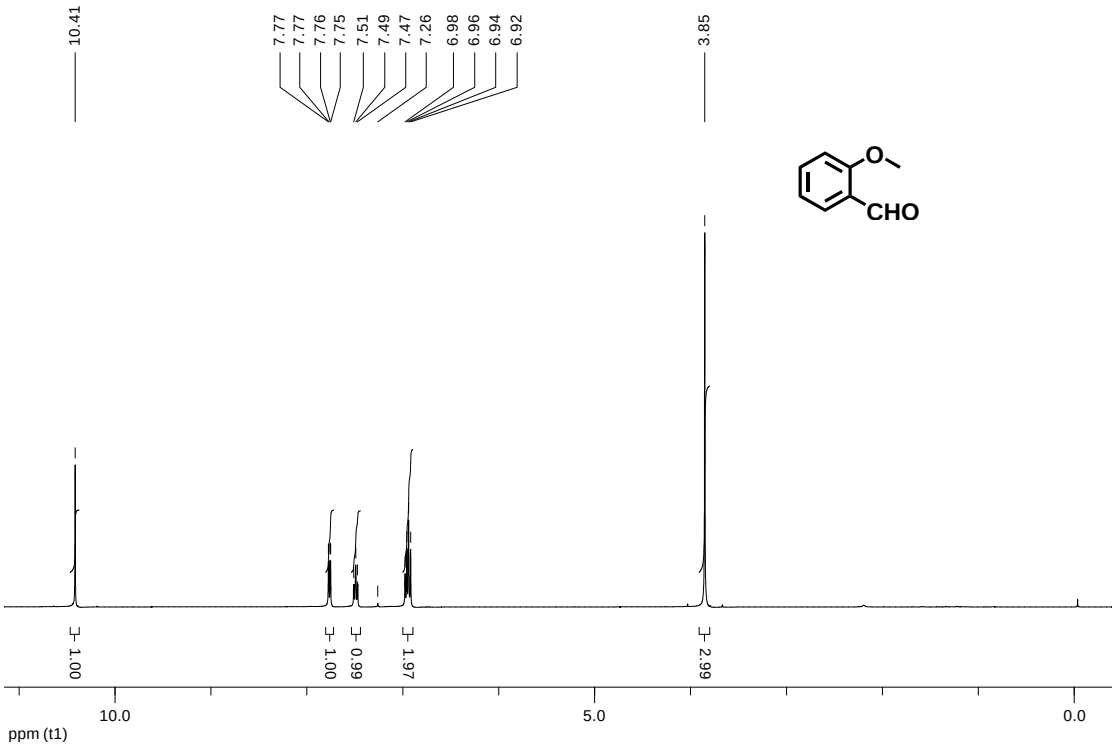

Fig. S18 The ^{1}H NMR spectrum of 3-methoxybenzaldehyde

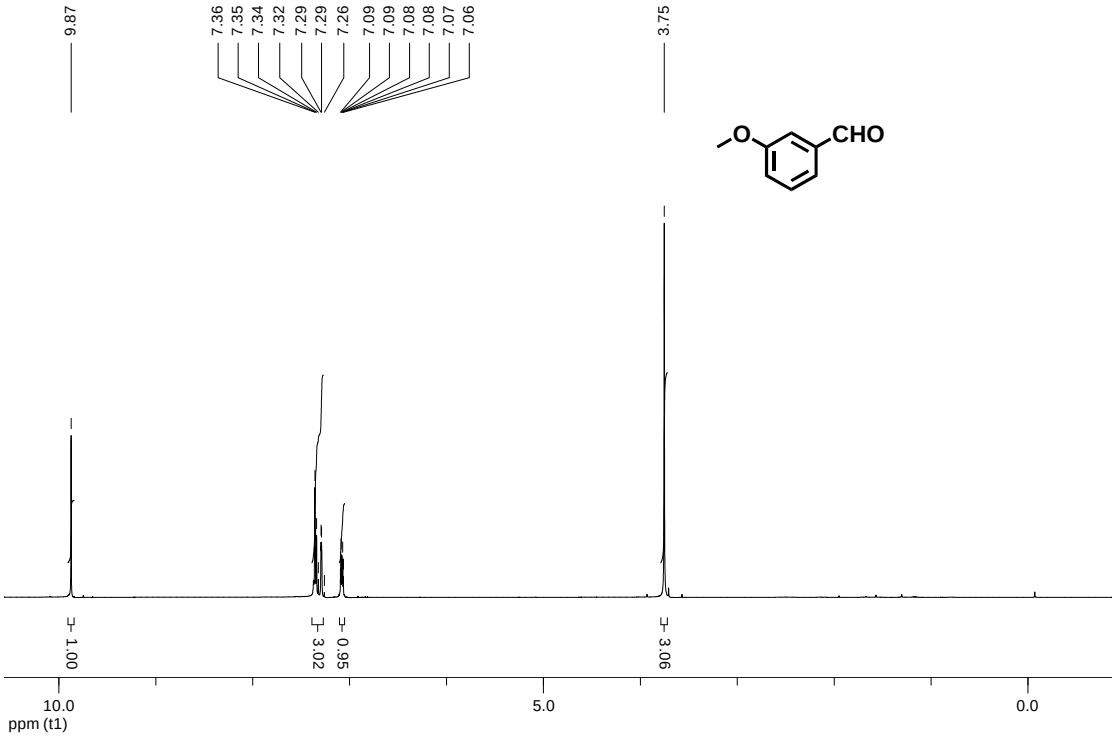

Fig. S19 The ^{1}H NMR spectrum of 4-methoxybenzaldehyde

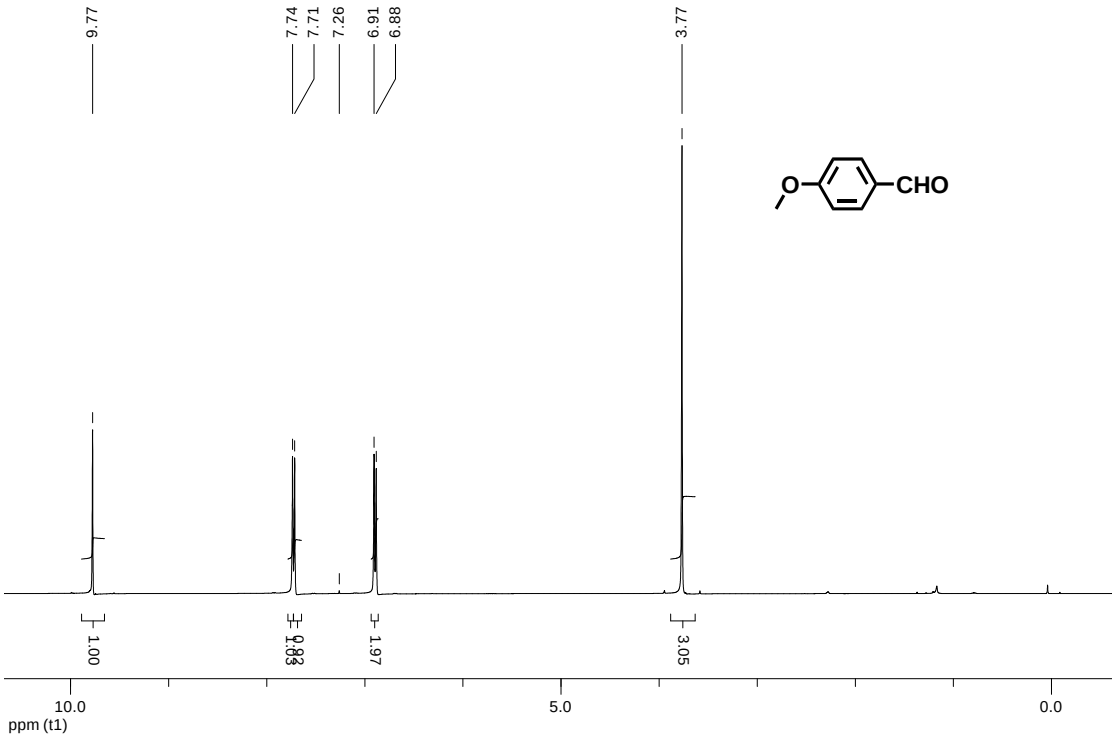

Fig. S20 The ^{1}H NMR spectrum of 4-chlorobenzoic aldehyde

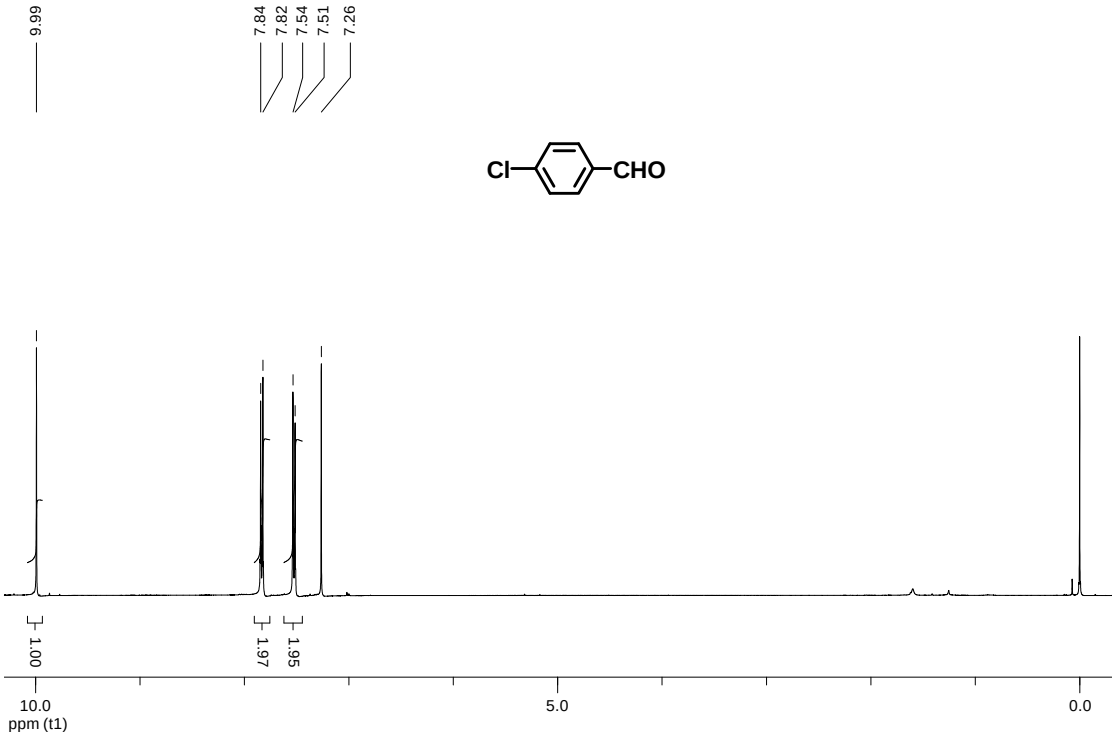

Fig. S21 The ^{1}H NMR spectrum of 4-nitrobenzaldehyde

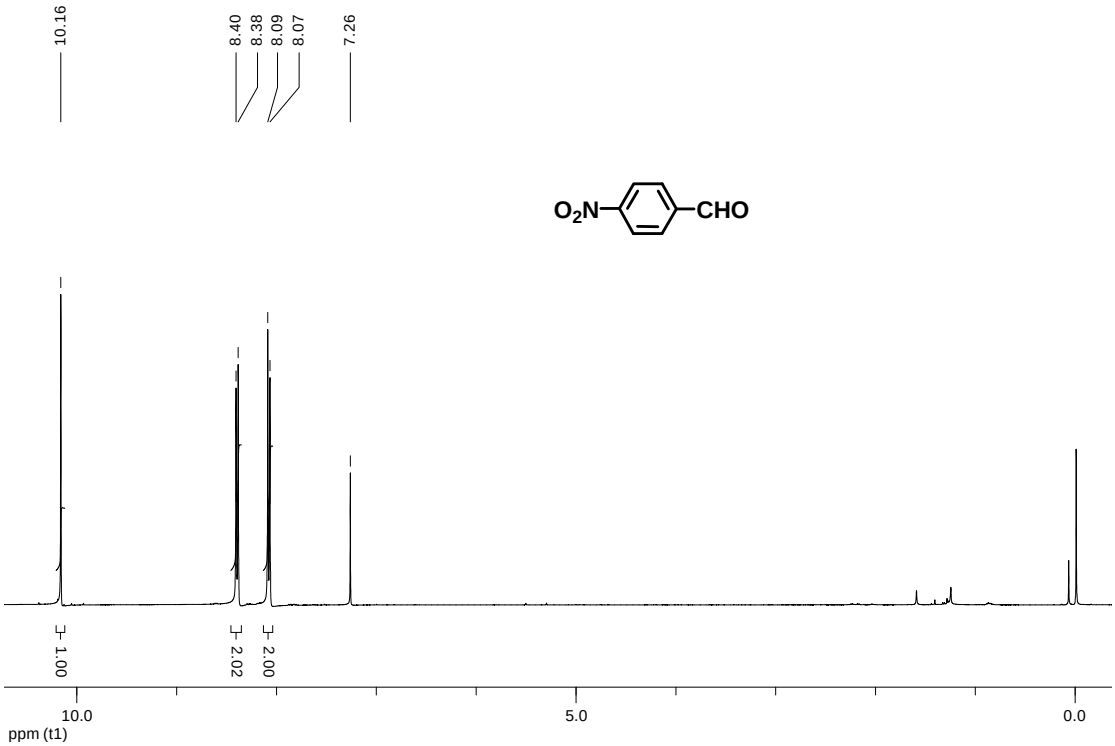

Fig. S22 The ^{1}H NMR spectrum of 3,4-(methylenedioxy)benzaldehyde

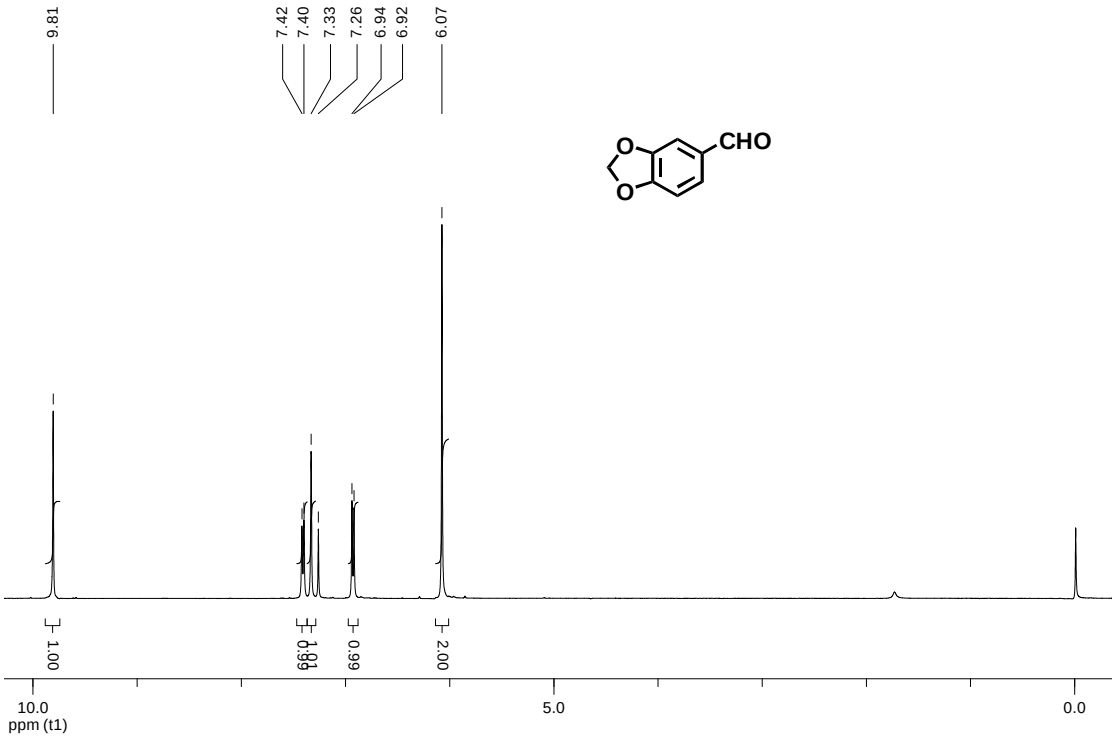

Fig. S23 The ^{1}H NMR spectrum of 3-pyridinecarboxaldehyde

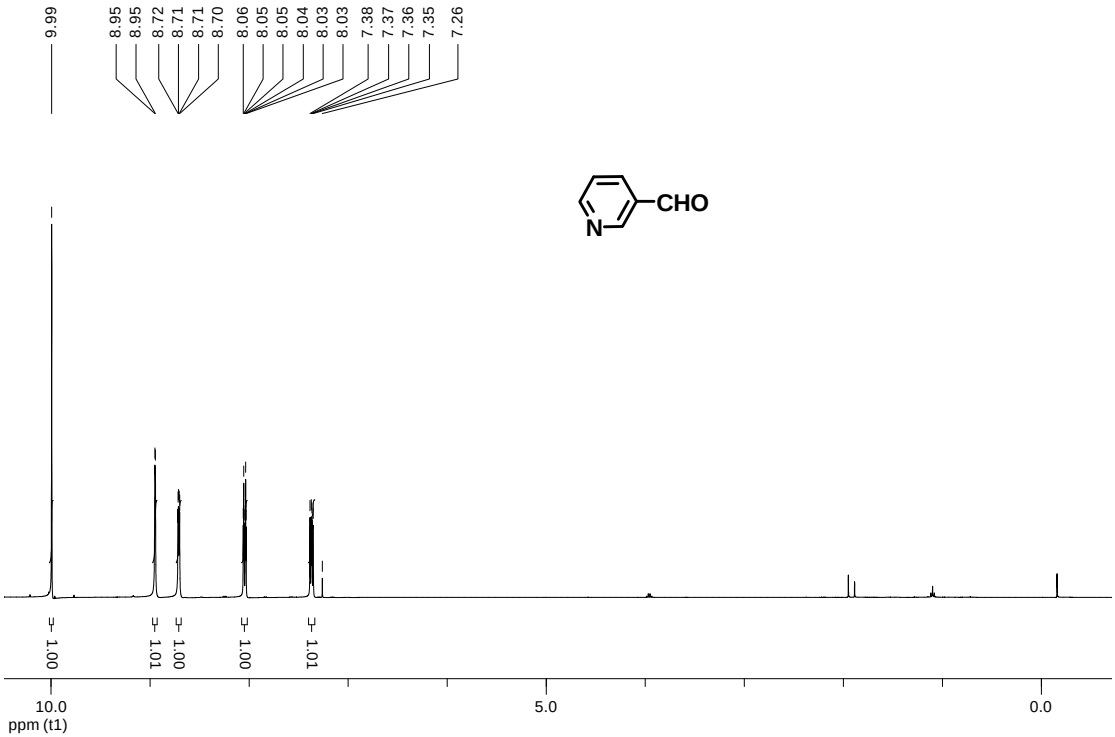

Fig. S24 The ^{1}H NMR spectrum of 2-thenaldehyde