

SUPPLEMENTARY INFORMATION

Dimethylglyoxime as an Efficient Ligand for Copper-Catalyzed Hydroxylation of Aryl Halides

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Spectral data of compounds

- 1) **Phenol (Table 2, entry 1):** m/z : 94 (M⁺). ¹H NMR (400 MHz, CDCl₃/TMS (ppm): 4.73 (s, 1H), 6.783 (d, 2H, $J = 7.5$ Hz), 6.83 (t, 1H, $J = 7.5$ Hz), 7.23-7.36 (m, 2H). ¹³C NMR (100 MHz, CDCl₃/TMS (ppm): 115.3, 120.6, 131.9, 156.5.
- 2) **4-Chlorophenol (Table 2, entry 2):** m/z : 128 (M⁺) ¹H NMR (400 MHz, CDCl₃): $\delta = 7.18$ (d, $J = 8.8$ Hz, 2H), 6.79 (d, $J = 8.8$ Hz, 2H). ¹³C NMR (100 MHz, CDCl₃): $\delta = 154.23, 129.65, 125.67, 116.87$.
- 3) **4-Hydroxy acetophenone (Table 2, entry 3):** m/z : 136 (M⁺) ¹H NMR (400 MHz, CDCl₃): $\delta = 7.85$ (d, $J = 8.8$ Hz, 2H), 6.86 (d, $J = 8.8$ Hz, 2H), 2.63 (s, 3H), 2.0 (s, 1H). ¹³C NMR (100 MHz, CDCl₃) $\delta = 185.81, 162.06, 132.64, 130.99, 115.30$
- 4) **4-nitrophenol (Table 2, entry 4):** ¹H NMR (400 MHz, CDCl₃ (3:1)): $\delta = 8.00$ (dd, $J = 9.2, 2$ H), 6.79 (dd, $J = 9.2$ 2H), 2.72 (br s, 1H). ¹³C NMR (100 MHz, CDCl₃): $\delta = 163.74, 141.36, 127.03, 116.69$.
- 5) **4-Methyl phenol (Table 2, entry 5):** m/z : 108 (M⁺) ¹H NMR (400 MHz, CDCl₃): $\delta = 7.02$ (d, $J = 8.4$ Hz, 2H), 6.78 (d, $J = 8.4$ Hz, 2H), 5.57 (s, 1H), 2.3 (s, 3H). ¹³C NMR (100 MHz, CDCl₃): $\delta = 154.39, 131.26, 133.12, 114.5$
- 6) **4-methoxyphenol (Table 2, entry 6):** m/z : 124 (M⁺) ¹H NMR (400 MHz, CDCl₃): $\delta = 6.89-6.68$ (m, 4H), 5.26 (s, 1H), 3.85 (s, 1H). ¹³C NMR (100 MHz, CDCl₃): $\delta = 154.88, 148.72, 115.28, 116.09, 55.04$.
- 7) **4-tertiary butylphenol (Table 2, entry 7):**
 m/z : 159 (M⁺) ¹H NMR (400 MHz, CDCl₃): $\delta 1.25$ (9H, s), 6.70 (2H, dd, $J = 8.3$ Hz), 7.28 (2H, dd, $J = 8.3$ Hz). ¹³C NMR δ (ppm) : 116.8, 115.8, 127.4, 15.7, 34.65, 31.25, 31.25, 143.5
- 8) **4-chloro 2-methylphenol (Table 2, entry 8):**
 m/z : 142 (M⁺) ¹H NMR (400 MHz, CDCl₃) : $\delta 2.19$ (3H, s), 6.72 (1H, dd, $J = 8.5$ Hz), 6.89-7.03 (2H, 7.00 (dd, $J = 8.5$ Hz), 7.03 (dd, $J = 2.2, 0.5$ Hz)). ¹³C NMR δ (ppm) 116.1, 126.3, 128.26, 152.2, 15.7, 129.2, 125.8
- 9) **2,6 dimethyl phenol (Table 2, entry 9):** m/z : 122 (M⁺) ¹H NMR (400 MHz, CDCl₃): $\delta = 6.81$ (d, $J = 7.6$ Hz, 2H), 6.68 (t, $J = 7.6$ Hz, 1H), 4.6 (s, 1H) 2.27 (s, 6H). ¹³C NMR (100 MHz, CDCl₃): $\delta = 152.36, 128.79, 123.18, 120.39, 16.04$.
- 10) **4-butoxyphenol (Table 2, entry 10):**

m/z : 166 (M⁺) ¹H NMR(400 MHz, CDCl₃): δ 0.100 (3H, t, J = 7.1 Hz), 1.46 (2H, tq, J = 7.4, 7.1 Hz), 1.78 (2H, quint, J = 7.4 Hz), 4.02 (2H, t, J = 7.4 Hz), 6.79-6.87 (4H, 6.84 (ddd, J = 8.7, 2.7, 0.5 Hz), 6.83 (ddd, J = 8.7, 2.7, 0.5 Hz)). ¹³C NMR (100 MHz, CDCl₃): δ (ppm) 68.92, 116.10, 154.66, 19.25, 116.02, 151.9, 13.83, 31.10

11) 2-Naphthol (Table 2, entry 11):

m/z : 144 (M⁺) ¹H NMR(400 MHz, CDCl₃): δ 7.08 (1H, ddd, J = 8.9, 5 Hz), 7.30-7.40 (2H, 7.33 (ddq, J = 2.4, 1.3, 0.4 Hz), 7.35 (dddd, J = 7.8, 7.4, 1.6, 0.5 Hz)), 7.51 (1H, dddd, J = 7.9, 7.4, 1.4, 0.4 Hz), 7.60 (1H, ddq, J = 8.9, 1.5, 0.4 Hz), 7.73-7.87 (2H, 7.84 (dddd, J = 7.8, 2.4, 1.4, 0.5, 0.4 Hz), 7.77 (dddtd, J = 7.9, 1.6, 1.5, 0.5, 0.4 Hz)). ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 154.71 34.60, 126.5, 109.5, 126.3, 127.72, 129.8, 126.56, 128.89, 117.50

Mass spectra, ^1HMR and ^{13}C NMR spectra of compounds

Figure S1. (Table 2, entry 1). Mass spectra of phenol

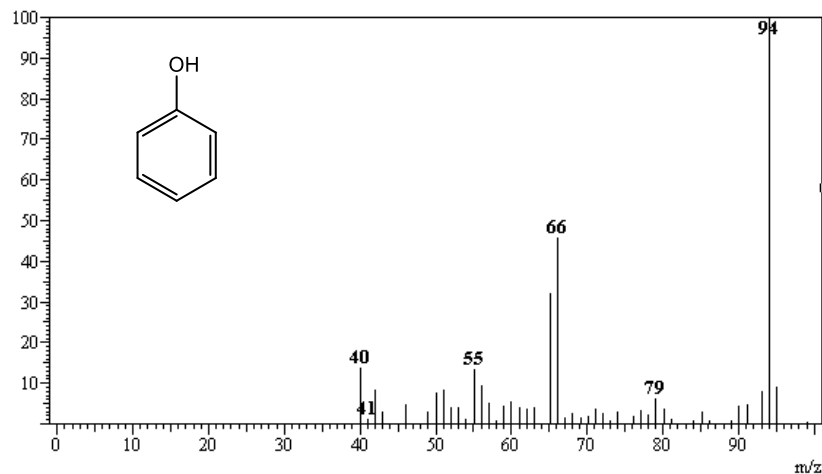


Figure S2. (Table 2, entry 1). ^1HMR spectra of phenol

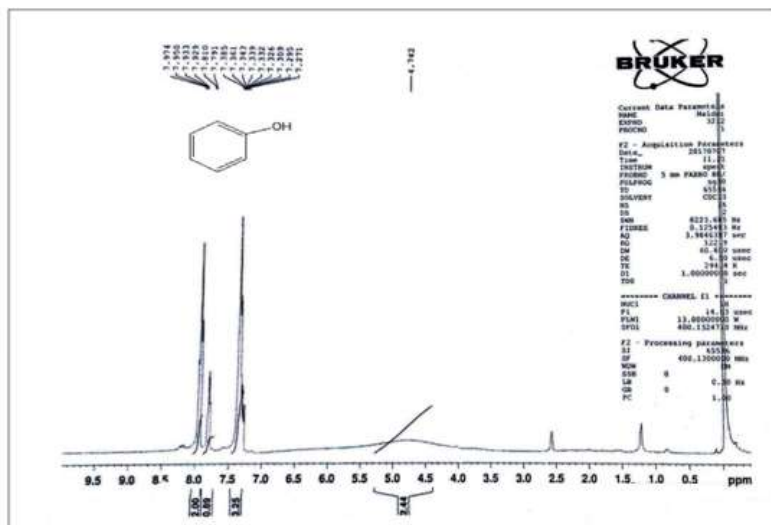


Figure S3. (Table 2, entry 1). ^{13}C NMR spectra of phenol

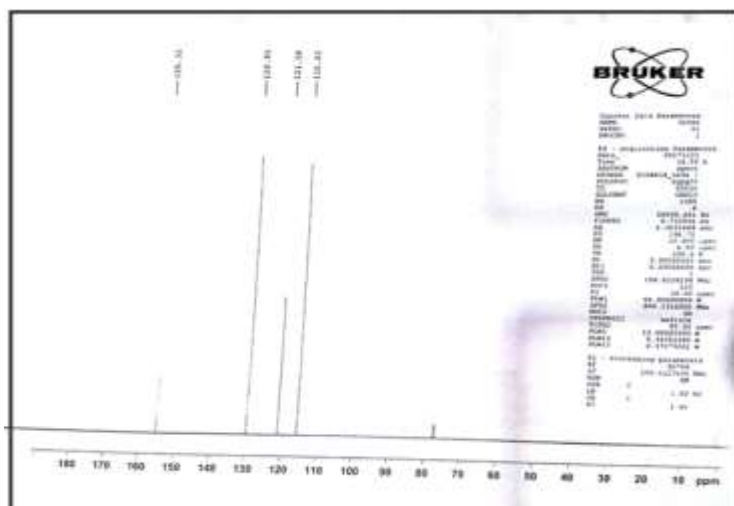


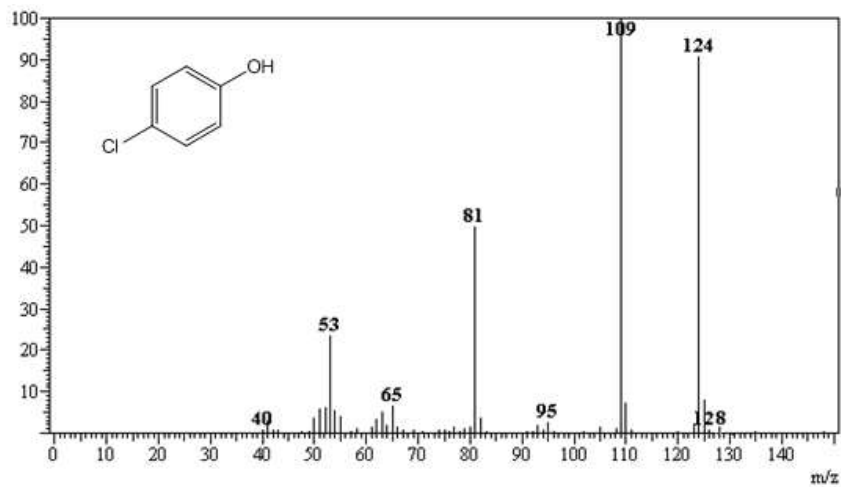
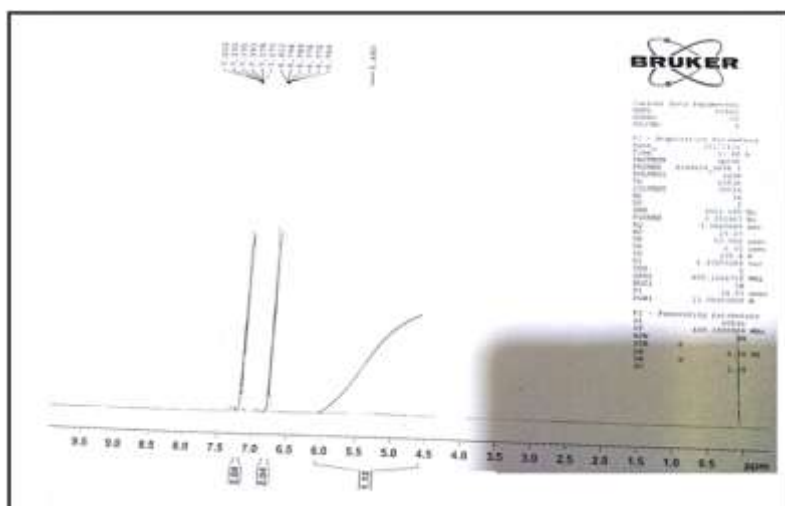
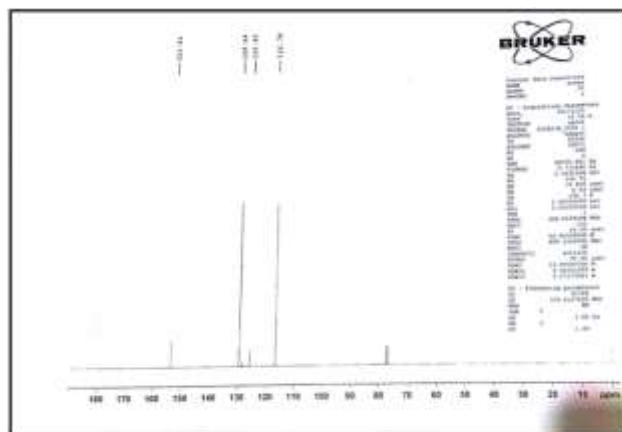
Figure S4. (Table 2, entry 2) Mass spectra 4-Chlorophenol.**Figure S5.** (Table 2, entry 2) ^1H NMR spectra 4-Chlorophenol.**Figure S6.** (Table 2, entry 2) ^{13}C NMR spectra 4-Chlorophenol

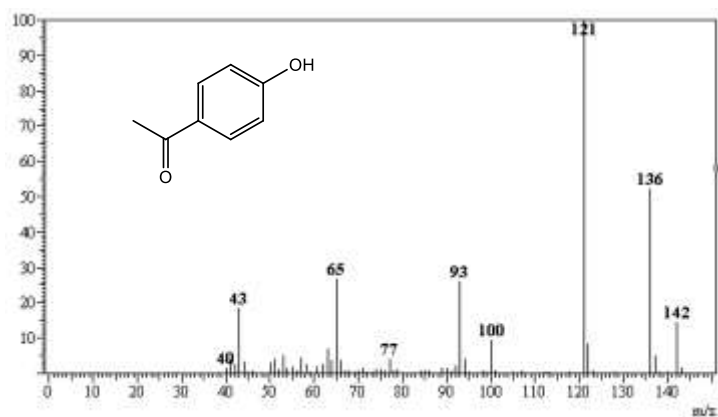
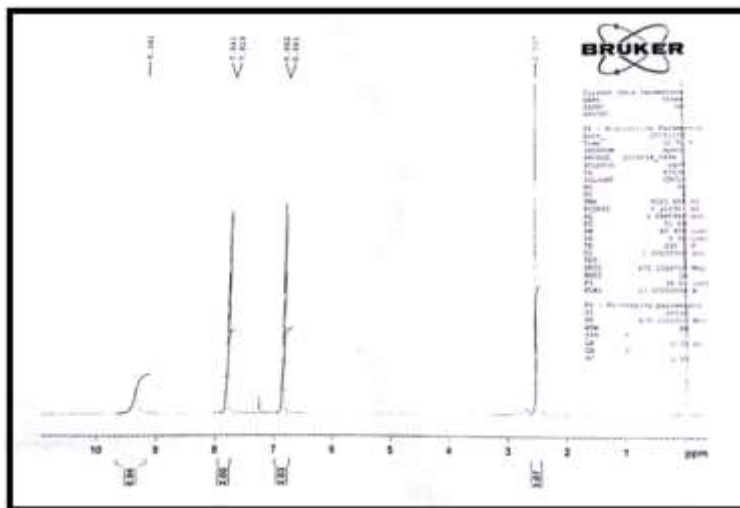
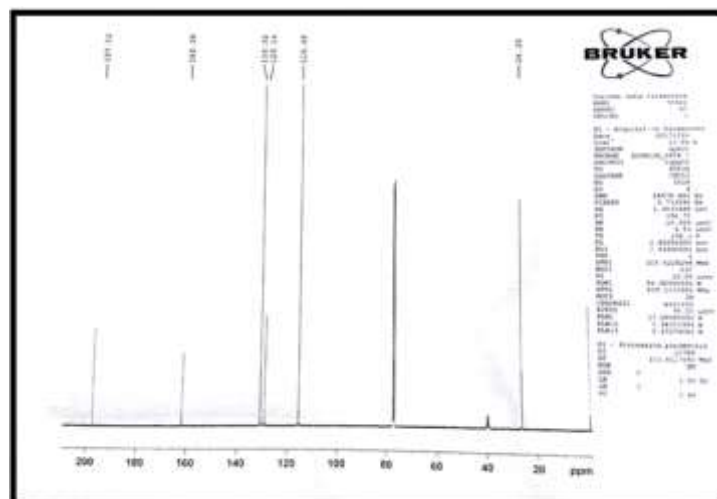
Figure S7. (Table 2, entry 3) Mass spectra 4-Hydroxy acetophenone**Figure S8.** (Table 2, entry 3) ¹H NMR spectra 4-Hydroxy acetophenone**Figure S9.** (Table 2, entry 3) ¹³C NMR spectra 4-Hydroxy acetophenone

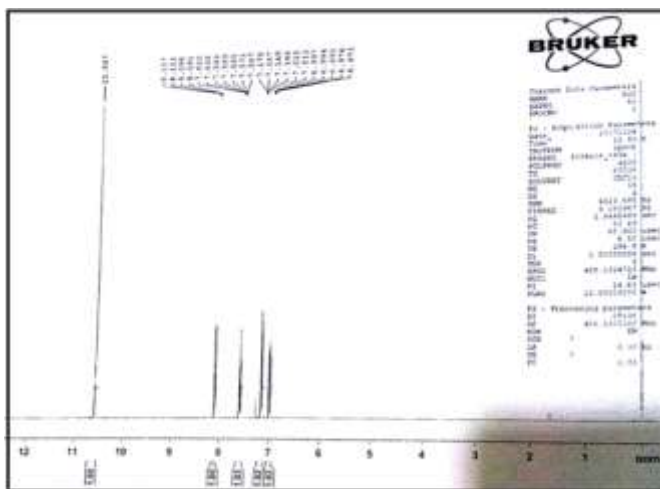
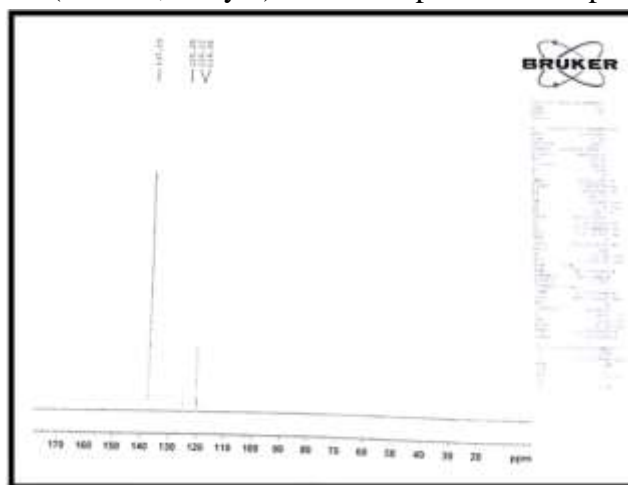
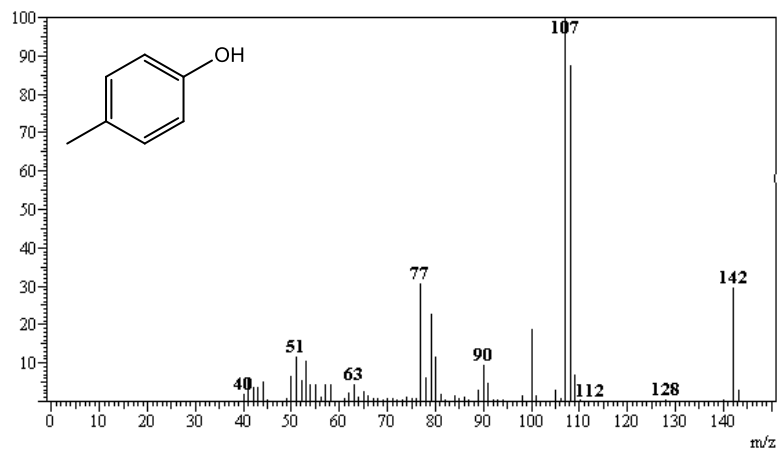
Figure S10. (Table 2, entry 4) ^1H NMR spectra 4-nitrophenol**Figure S11.** (Table 2, entry 4) ^{13}C NMR spectra 4-nitrophenol**Figure S12.** (Table 2, entry 5) Mass spectra 4-methylphenol

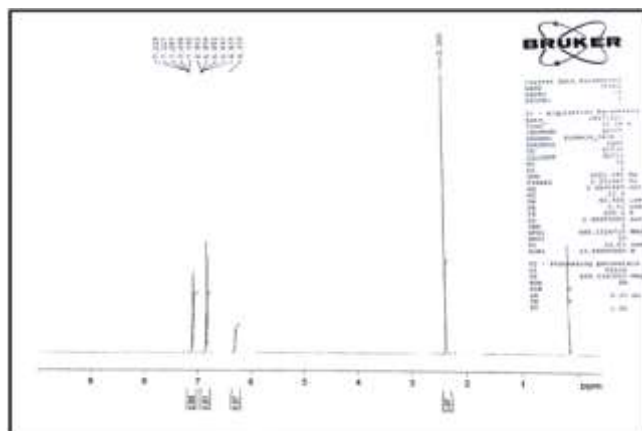
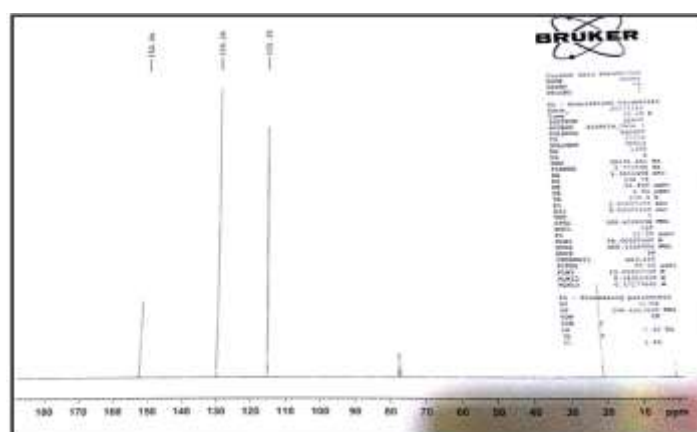
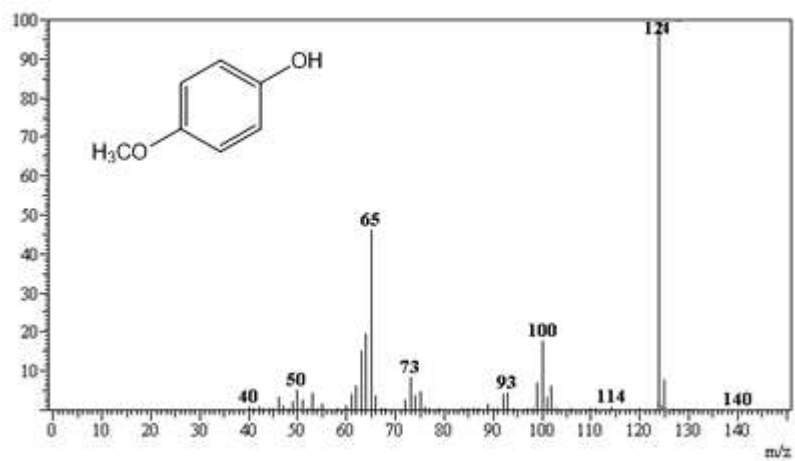
Figure S13. (Table 2, entry 5) ^1H NMR spectra 4-methylphenol**Figure S14.** (Table 2, entry 5) ^{13}C NMR spectra 4-methylphenol**Figure S15.** (Table 2, entry 6) mass spectra 4-methoxyphenol

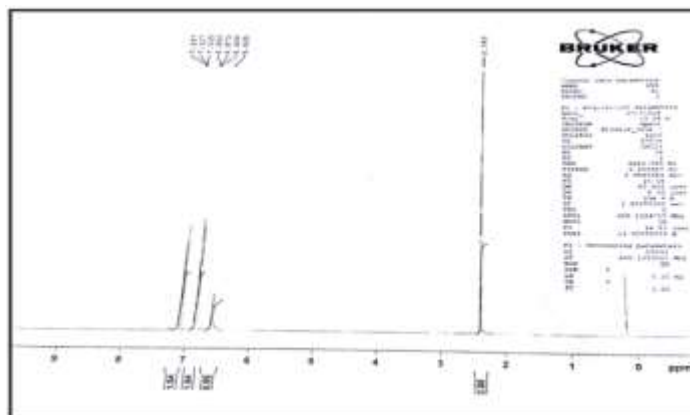
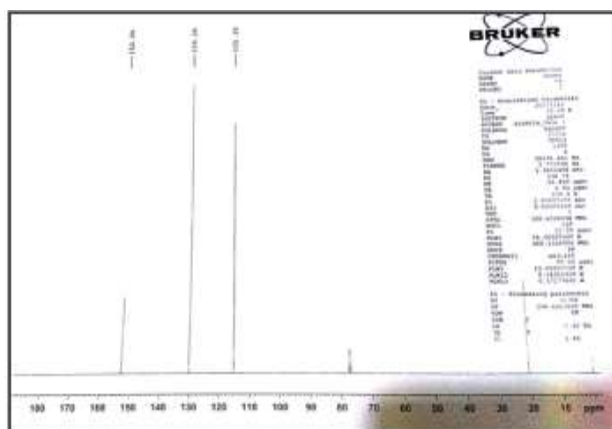
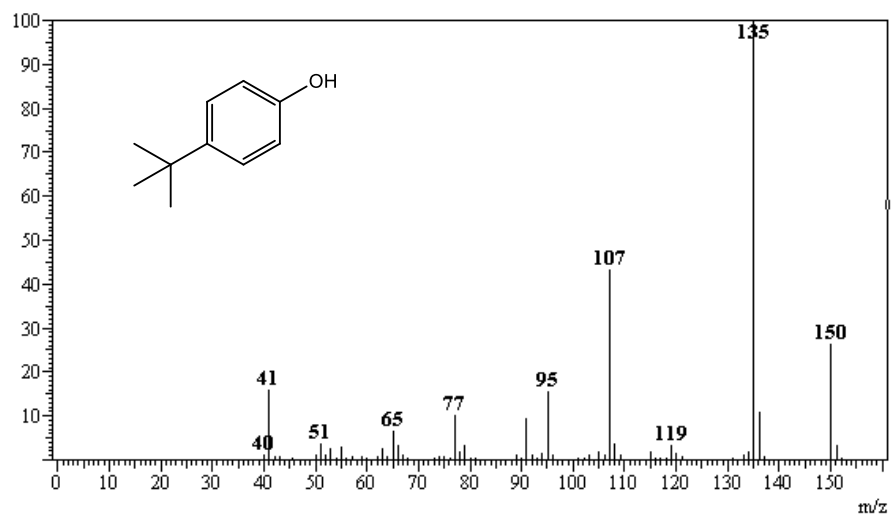
Figure S16. (Table 2, entry 6) ^1H NMR spectra 4-methoxyphenol**Figure S17.** (Table 2, entry 6) ^{13}C NMR spectra 4-methoxyphenol**Figure S18.** (Table 2, entry 7) Mass spectra 4-tertiary butylphenol

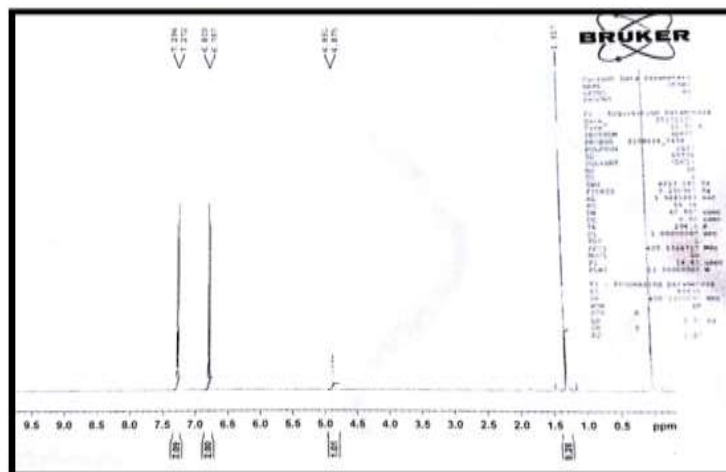
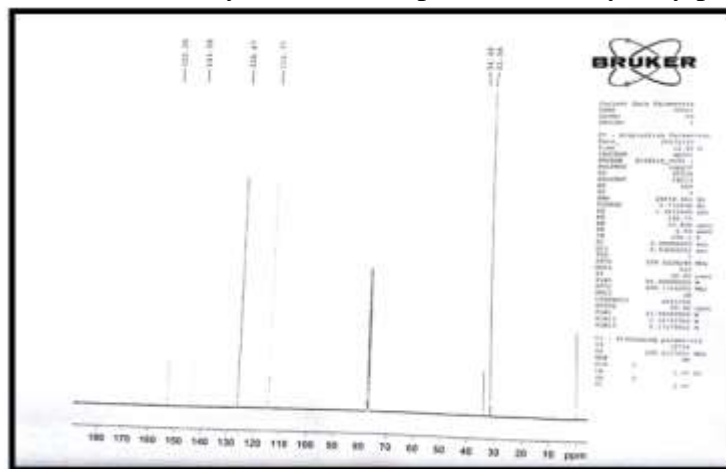
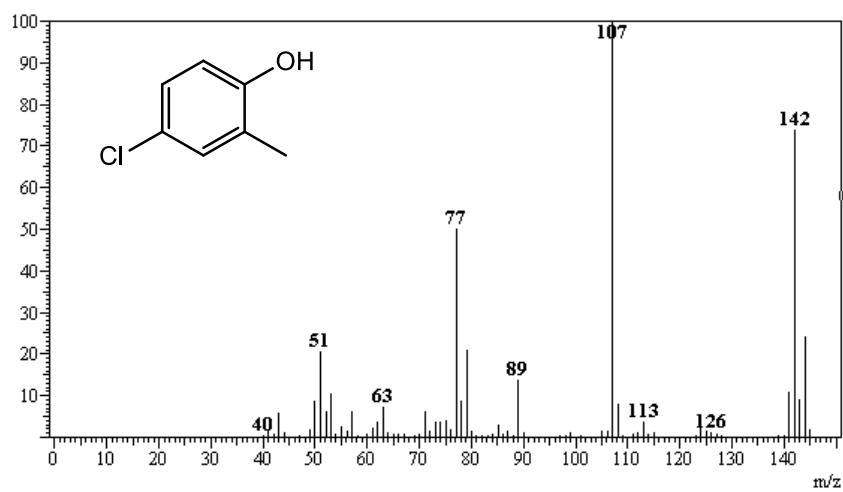
Figure S19. (Table 2, entry 7) ^1H NMR spectra 4-tertiary butylphenol**Figure S20.** (Table 2, entry 7) ^{13}C NMR spectra 4-tertiary butylphenol**Figure S21.** (Table 2, entry 8) Mass spectra 4-chloro 2-methyl phenol

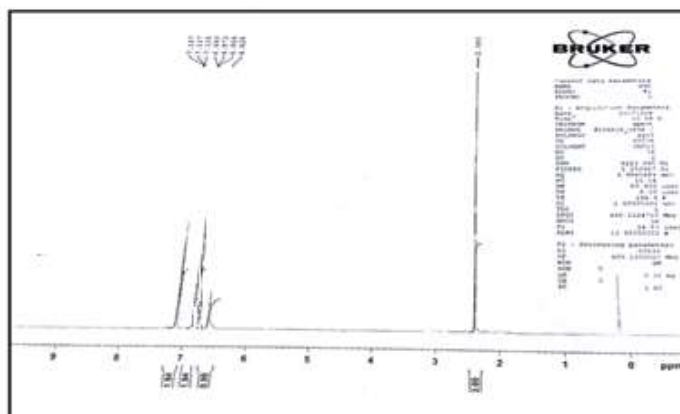
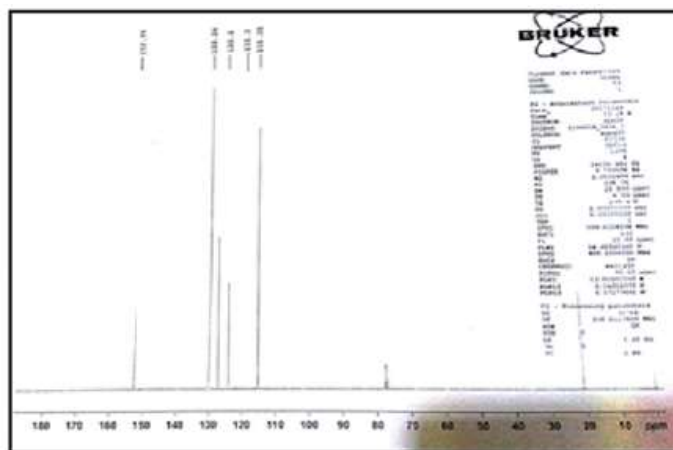
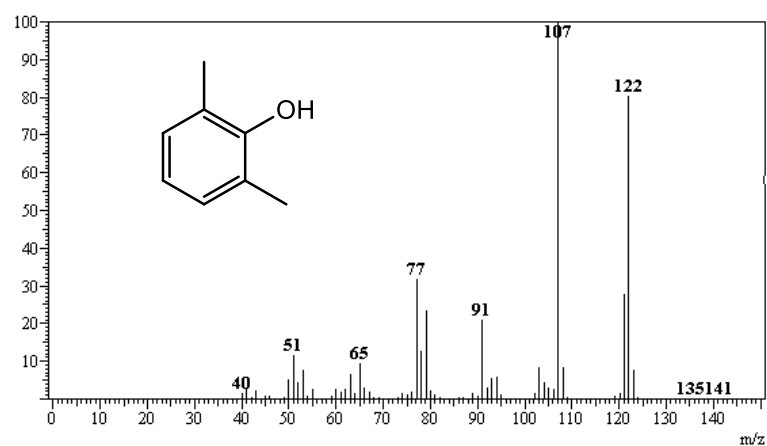
Figure S22. (Table 2, entry 8) ^1H NMR spectra 4-chloro 2-methyl phenol**Figure S23.** (Table 2, entry 8) ^{13}C NMR spectra 4-chloro 2-methyl phenol**Figure S24.** (Table 2, entry 9) Mass spectra 2,6 dimethyl phenol

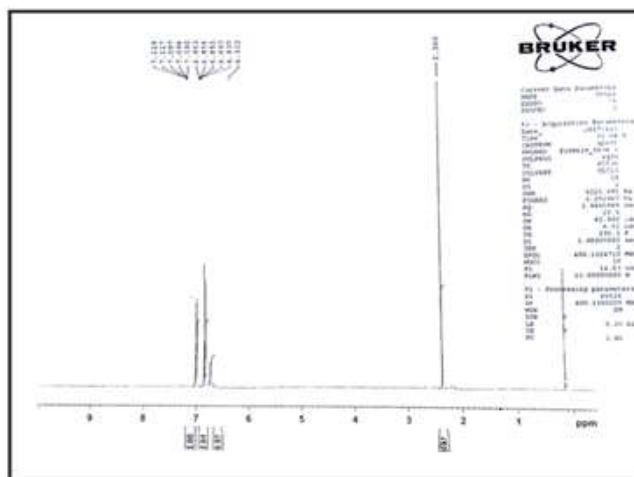
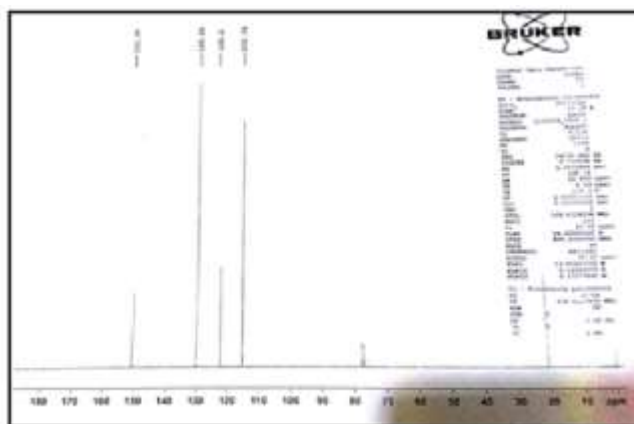
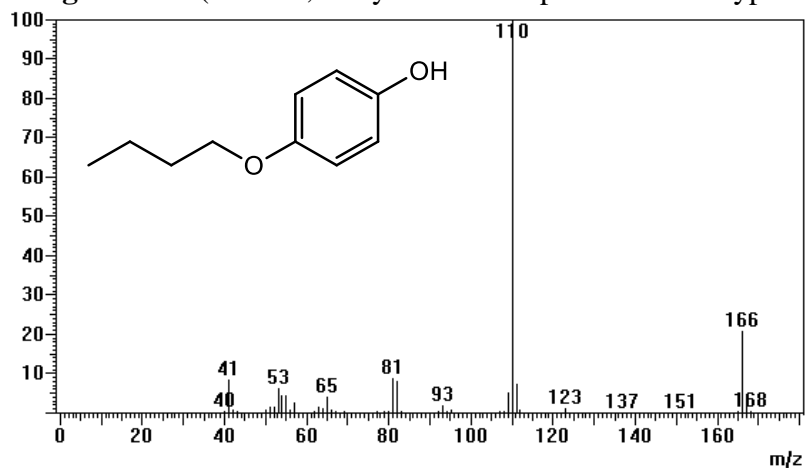
Figure S25. (Table 2, entry 9) ^1H NMR spectra 2,6 dimethyl phenol**Figure S26.** (Table 2, entry 9) ^{13}C NMR spectra 2,6 dimethyl phenol**Figure S27.** (Table 2, entry 10n) Mass spectra 4-butoxyphenol

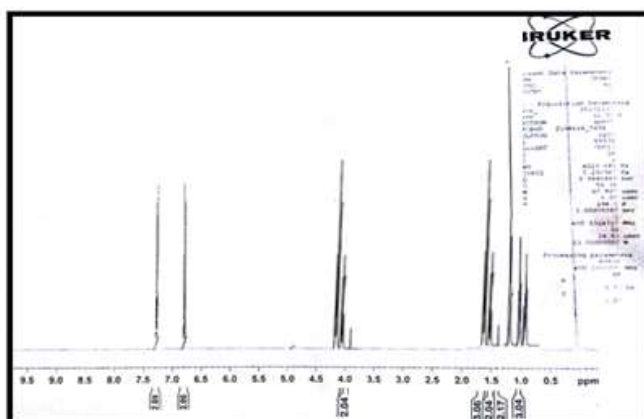
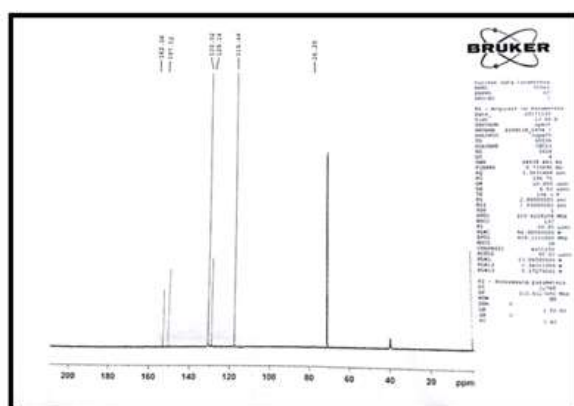
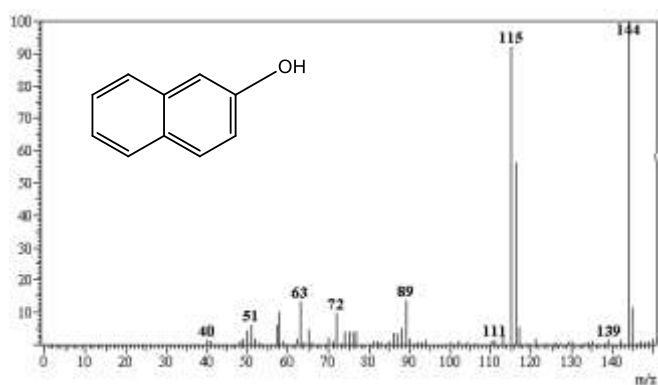
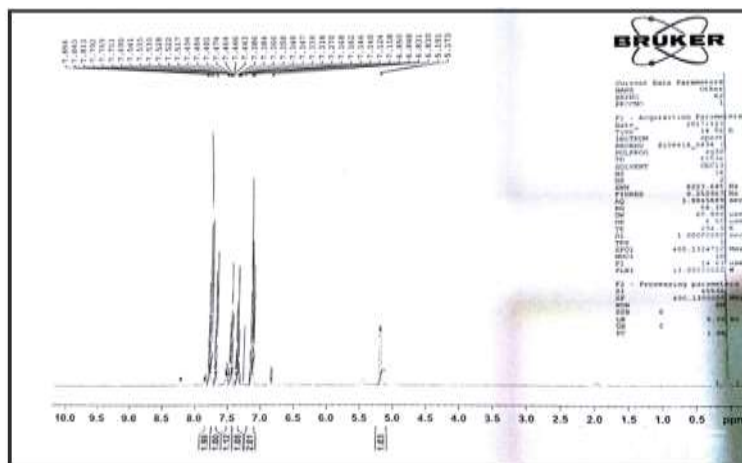
Figure S28. (Table 2, entry 10) ^1H NMR spectra 4-butoxyphenol**Figure S29.** (Table 2, entry 10) ^{13}C NMR spectra 4-butoxyphenol**Figure S30.** (Table 2, entry 11) Mass spectra 2-naphthol

Figure S31. (Table 2, entry 11) ^1H NMR spectra 2-naphthol**Figure S32.** (Table 2, entry 11) ^{13}C NMR spectra 2-naphthol