

Supporting Information

Fabrication and characterization of magnetic trimetallic mesoporous nanocomposite: As an effective nanocatalyst for synthesis of bisphenol derivatives

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General method for the synthesis of bisphenol derivatives

Bisphenol derivatives were synthesized via the condensation reaction of aldehydes (2.0 mmol) with 2,4-dimethylphenol (6.0 mmol) in the presence of an $\text{CoNiFe}_2\text{O}_4@\text{C}$ solid acid nanocatalyst. The reaction was carried out under solvent-free conditions at 100 °C in an oil bath. The progress of the reaction was monitored by thin-layer chromatography (TLC) using ethyl acetate/petroleum ether (7:3) as the eluent. Upon completion of the reaction, the mixture was allowed to cool to room temperature. The crude product was crystallized from boiling water and ethanol. After precipitation, the product was extracted with n-hexane to obtain the bisphenol derivatives in high purity. The final product was dried at 90 °C for 24 h. The structures of the synthesized bisphenol derivatives were confirmed by FT-IR spectroscopy, ^1H NMR spectroscopy, ^{13}C NMR spectroscopy and melting point analysis.

The spectral data of bisphenol derivatives

6,6'-((4-nitrophenyl)methylene)bis(2,4-dimethylphenol) (3a): White solid; m.p = 135-137 °C (Lit. m.p 136-138 °C); IR (KBr)/ ν (cm^{-1}): 3503, 3302, 2917, 1598, 1520, 1479, 1344, 1215, 1141, 863; ^1H NMR (DMSO-d_6 , 400 MHz)/ δ (ppm): 2.07 (6H, s, CH_3), 2.13 (6H, s, CH_3), 6.26 (1H, s, Ar_3CH), 6.30 (2H, s, OH), 6.79 (2H, s, DMP), 7.23 (2H, d, J = 8.0 Hz, DMP), 8.14 (4H, d, J = 8.0 Hz, aldehyde).

6,6'-((4-chlorophenyl)methylene)bis(2,4-dimethylphenol) (3b): White solid; m.p = 159-161 °C (Lit. m.p 158-160 °C); IR (KBr)/ ν (cm⁻¹): 3502, 3470, 3024, 2914, 1602, 1479, 1334, 1254, 1185, 1138, 856; ¹H NMR (DMSO-d₆, 400 MHz)/ δ (ppm): 2.06 (6H, s, CH₃), 2.12 (6H, s, CH₃), 6.14 (1H, s, Ar₃CH), 6.30 (2H, s, OH), 6.75 (2H, s, DMP), 6.99 (2H, d, DMP), 7.30 (2H, d, *J* = 8.0 Hz, aldehyde), 8.02 (2H, s, aldehyde).

6,6'-((4-bromophenyl)methylene)bis(2,4-dimethylphenol) (3c): White solid; m.p = 241-243 °C (Lit. m.p >240 °C); IR (KBr)/ ν (cm⁻¹): 3472, 2914, 1602, 1475, 1395, 1333, 1254, 1184, 1139, 1072, 855; ¹H NMR (DMSO-d₆, 400 MHz)/ δ (ppm): 2.06 (6H, s, CH₃), 2.12 (6H, s, CH₃), 6.12 (1H, s, Ar₃CH), 6.30 (2H, s, OH), 6.74 (2H, s, DMP), 6.94 (2H, d, *J* = 8.0 Hz, DMP), 7.43 (2H, d, *J* = 8.0 Hz, aldehyde), 8.01 (2H, s, aldehyde).

6,6'-((3-nitrophenyl)methylene)bis(2,4-dimethylphenol) (3d): White solid; m.p = 140-142 °C (Lit. m.p 141-143 °C); IR (KBr)/ ν (cm⁻¹): 3436, 3083, 2915, 1607, 1526, 1481, 1347, 1216, 1094, 861; ¹H NMR (DMSO-d₆, 400 MHz)/ δ (ppm): 2.08 (6H, s, CH₃), 2.13 (6H, s, CH₃), 6.28 (1H, s, Ar₃CH), 6.33 (2H, s, OH), 6.79 (2H, s, DMP), 7.46 (1H, d, *J* = 8.0 Hz, DMP), 7.58 (1H, t, aldehyde), 7.77 (1H, s, DMP), 8.05 (1H, d, *J* = 8.0 Hz, aldehyde), 8.12 (2H, s, aldehyde).

6,6'-((4-fluorophenyl)methylene)bis(2,4-dimethylphenol) (3e): White solid; m.p = 126-128 °C; IR (KBr)/ ν (cm⁻¹): 3497, 3307, 3005, 2918, 1806, 1476, 1383, 1218, 1147, 1021, 899; ¹H NMR (DMSO-d₆, 400 MHz)/ δ (ppm): 2.06 (6H, s, CH₃), 2.12 (6H, s, CH₃), 6.16 (1H, s, Ar₃CH), 6.31 (2H, s, OH), 6.74 (2H, s, DMP), 7.01 (2H, d, *J* = 8.0 Hz, DMP), 7.06 (2H, d, *J* = 8.0 Hz, aldehyde), 8.02 (2H, s, aldehyde).

6,6'-((phenyl)methylene)bis(2,4-dimethylphenol) (3f): White solid; m.p = 110-112 °C (Lit. m.p 113-115 °C); IR (KBr)/ ν (cm⁻¹): 3611, 3021, 2918, 1481, 1384, 1297, 1188, 1145, 865, 703; ¹H NMR (DMSO-d₆, 400 MHz)/ δ (ppm): 2.06 (6H, s, CH₃), 2.11 (6H, s, CH₃), 6.16 (1H, s, Ar₃CH), 6.31 (2H, s, OH), 6.73 (2H, s, DMP), 6.99 (2H, d, *J* = 8.0 Hz, DMP), 7.14 (2H, t, *J* = 8.0 Hz, aldehyde), 7.24 (1H, t, *J* = 8.0 Hz, aldehyde), 7.97 (2H, s, aldehyde).

6,6'-((Hexanal)methylene)bis(2,4-dimethylphenol) (3g): White solid; m.p = 148-149 °C; IR (KBr)/ ν (cm⁻¹): 3462, 3295, 2924, 2861, 1479, 1291, 1182, 1023, 859; ¹H NMR (DMSO-d₆, 400 MHz)/ δ (ppm): 0.82 (3H, t, CH₃-aldehyde), 1.17-1.26 (6H, m, CH₂-aldehyde), 1.87-1.93 (2H, m, CH₂-aldehyde), 2.11 (6H, s, CH₃), 2.14 (6H, s, CH₃), 4.52 (1H, t, *J* = 8.0 Hz, Ar₃CH), 6.68 (2H, s,

OH), 6.82 (2H, s, DMP), 8.22 (2H, s, DMP); ^{13}C NMR (100 MHz, DMSO- d_6) δ (ppm): 14.40, 17.20, 20.95, 22.46, 27.72, 31.76, 34.28, 35.85, 124.53, 125.73, 128.31, 129.00, 132.09, 150.13.

6,6'-((2,4-Dichlorophenyl)methylene)bis(2,4-dimethylphenol) (3h): White solid; m.p = 182-184 °C (Lit. m.p 183-185 °C); IR (KBr)/ ν (cm^{-1}): 3500, 3471, 3020, 2917, 1591, 1474, 1381, 1255, 1183, 1139, 859; ^1H NMR (DMSO- d_6 , 400 MHz)/ δ (ppm): 2.06 (6H, s, CH_3), 2.12 (6H, s, CH_3), 6.22 (2H, s, OH), 6.37 (1H, s, Ar_3CH), 6.76 (2H, s, DMP), 6.84 (1H, d, $J = 8.0$ Hz, DMP), 7.31 (1H, d, $J = 8.0$ Hz, DMP), 7.53 (1H, s, aldehyde), 8.06 (2H, s, aldehyde).

6,6'-((4-Cyanophenyl)methylene)bis(2,4-dimethylphenol) (3i): White solid; m.p = 190-192 °C; IR (KBr)/ ν (cm^{-1}): 3579, 3461, 2994, 2917, 2227, 1603, 1479, 1381, 1203, 1027, 857; ^1H NMR (DMSO- d_6 , 400 MHz)/ δ (ppm): 2.06 (6H, s, CH_3), 2.12 (6H, s, CH_3), 6.21 (1H, s, Ar_3CH), 6.27 (2H, s, OH), 6.77 (2H, s, DMP), 7.16 (2H, d, $J = 8.0$ Hz, DMP), 7.72 (2H, d, $J = 8.0$ Hz, aldehyde), 8.09 (2H, s, aldehyde); ^{13}C NMR (100 MHz, DMSO- d_6) δ (ppm): 17.19, 20.91, 44.06, 108.84, 119.57, 124.73, 127.68, 128.09, 130.00, 130.52, 132.37, 150.72, 151.30.

6,6'-((4-Methoxyphenyl)methylene)bis(2,4-dimethylphenol) (3j): White solid; m.p = 178-179 °C; IR (KBr)/ ν (cm^{-1}): 3443, 3017, 2911, 1602, 1475, 1231, 1183, 1140, 855; ^1H NMR (DMSO- d_6 , 400 MHz)/ δ (ppm): 2.06 (6H, s, CH_3), 2.11 (6H, s, CH_3), 3.71 (3H, s, CH_3), 6.08 (1H, s, Ar_3CH), 6.32 (2H, s, OH), 6.72 (2H, s, DMP), 6.82 (2H, d, $J = 8.0$ Hz, DMP), 6.90 (2H, d, $J = 8.0$ Hz, aldehyde), 8.09 (2H, s, aldehyde); ^{13}C NMR (100 MHz, DMSO- d_6) δ (ppm): 17.20, 20.99, 42.76, 55.37, 113.75, 124.36, 127.28, 128.09, 129.42, 130.54, 132.11, 136.59, 150.64, 157.63.

6,6'-((3-Methylphenyl)methylene)bis(2,4-dimethylphenol) (3k): White solid; m.p = 136-137 °C; IR (KBr)/ ν (cm^{-1}): 3351, 3018, 2919, 1601, 1480, 1326, 1191, 1031, 866; ^1H NMR (DMSO- d_6 , 400 MHz)/ δ (ppm): 2.06 (6H, s, CH_3), 2.11 (6H, s, CH_3), 3.23 (3H, s, CH_3), 6.12 (1H, s, Ar_3CH), 6.32 (2H, s, OH), 6.72 (2H, s, DMP), 6.76 (1H, d, $J = 8.0$ Hz, DMP), 6.96 (1H, d, $J = 8.0$ Hz, DMP), 7.12 (1H, t, $J = 8.0$ Hz, aldehyde), 7.94 (2H, s, aldehyde); ^{13}C NMR (100 MHz, DMSO- d_6) δ (ppm): 17.20, 21.00, 21.61, 43.51, 124.36, 126.74, 127.27, 128.20, 129.48, 130.33, 131.80, 137.18, 144.85, 150.65.

6,6'-((Heptanal)methylene)bis(2,4-dimethylphenol) (3l): White solid; m.p = 169-171 °C; IR (KBr)/ ν (cm^{-1}): 3460, 3308, 2924, 2858, 1478, 1292, 1176, 1021, 857; ^1H NMR (DMSO- d_6 , 400 MHz)/ δ (ppm): 0.83 (3H, t, $J = 8.0$ Hz, aldehyde), 1.17-1.28 (8H, m, aldehyde), 1.87-1.93 (2H, m,

aldehyde), 2.10 (6H, s, CH₃), 2.14 (6H, s, CH₃), 4.51 (1H, t, *J* = 8.0 Hz, Ar₃CH), 6.68 (2H, s, OH), 6.82 (2H, s, DMP), 8.21 (2H, s, DMP).

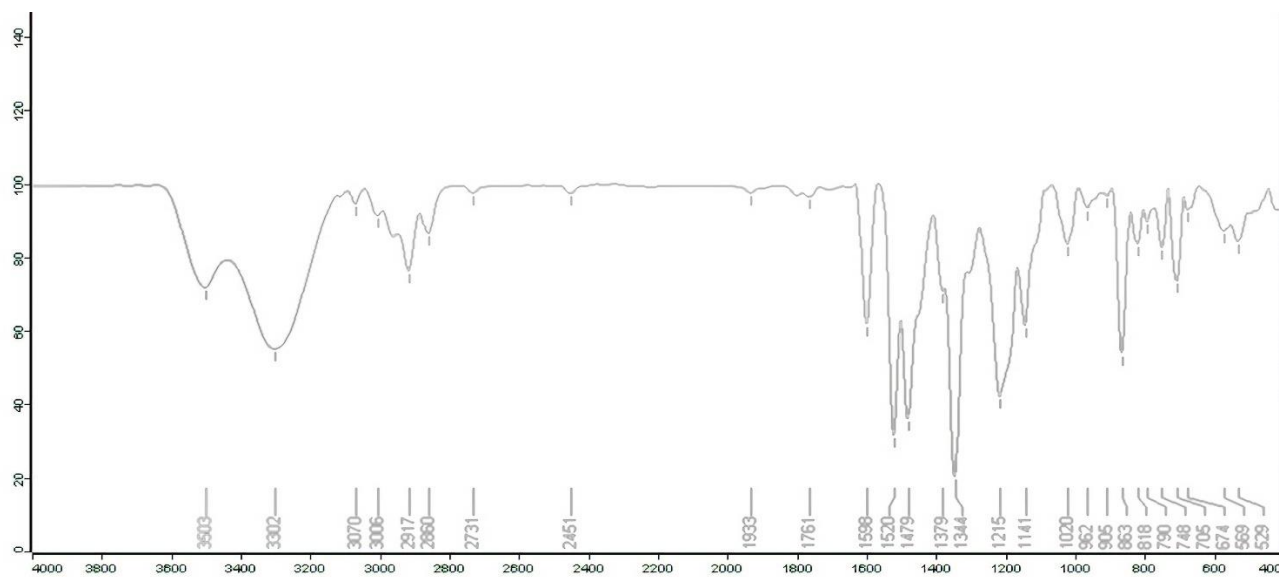


Fig. 1S. FT-IR of 6,6'-((4-nitrophenyl)methylene)bis(2,4-dimethylphenol) (3a)

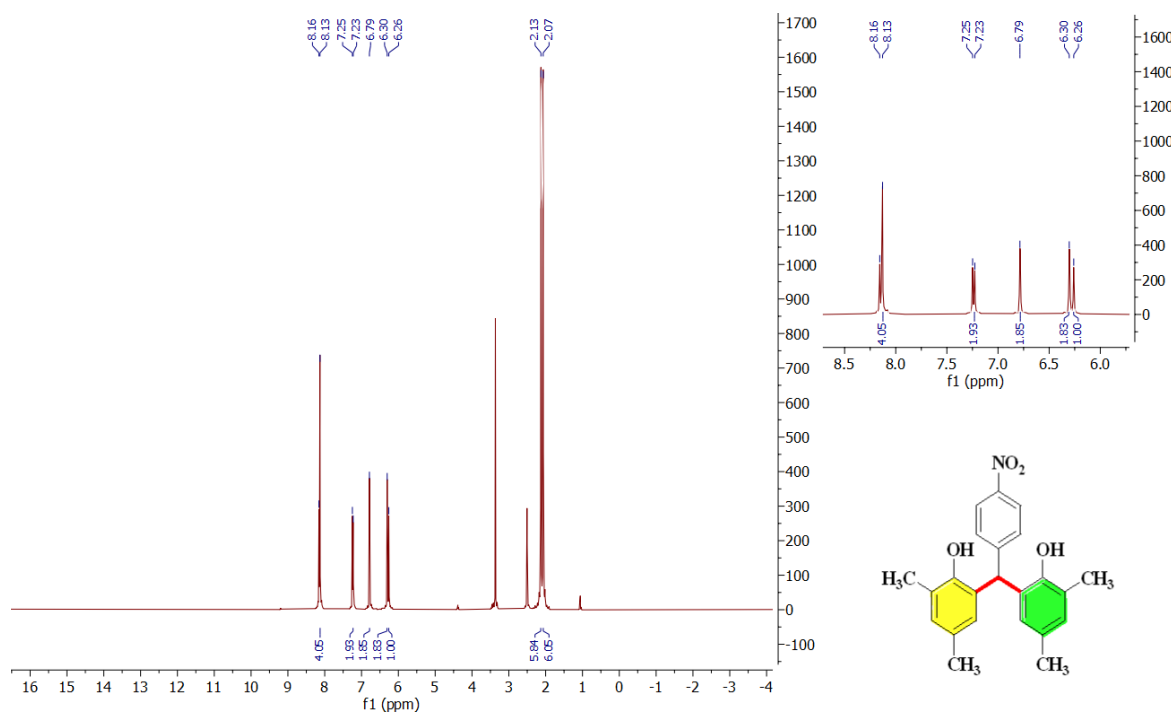


Fig. 2S. ¹H NMR of 6,6'-((4-nitrophenyl)methylene)bis(2,4-dimethylphenol) (3a)

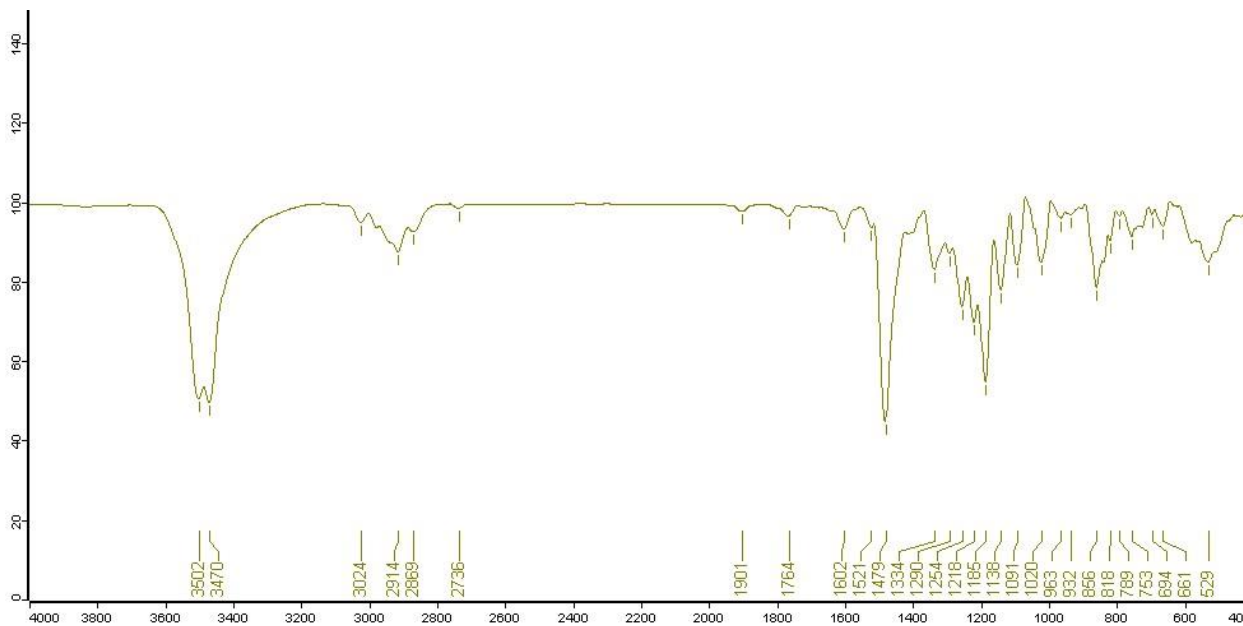


Fig. 3S. FT-IR of 6,6'-((4-chlorophenyl)methylene)bis(2,4-dimethylphenol) (3b)

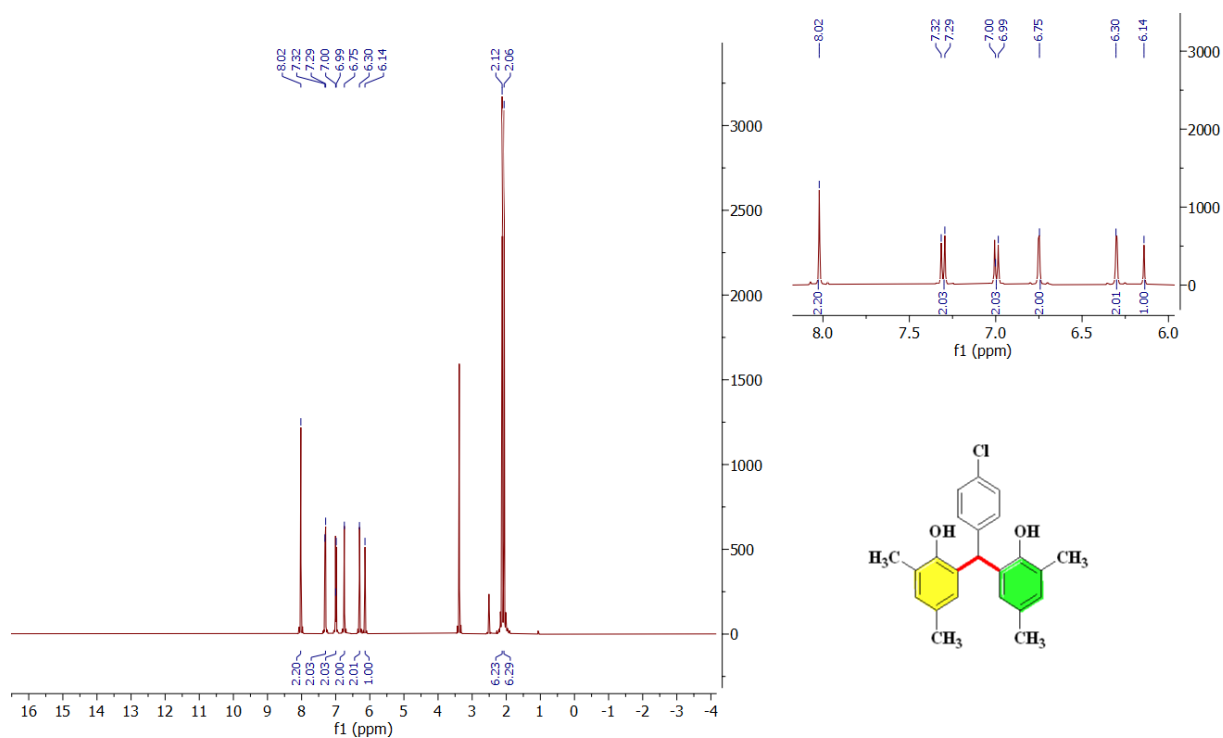


Fig. 4S. ^1H NMR of 6,6'-((4-chlorophenyl)methylene)bis(2,4-dimethylphenol) (3b)

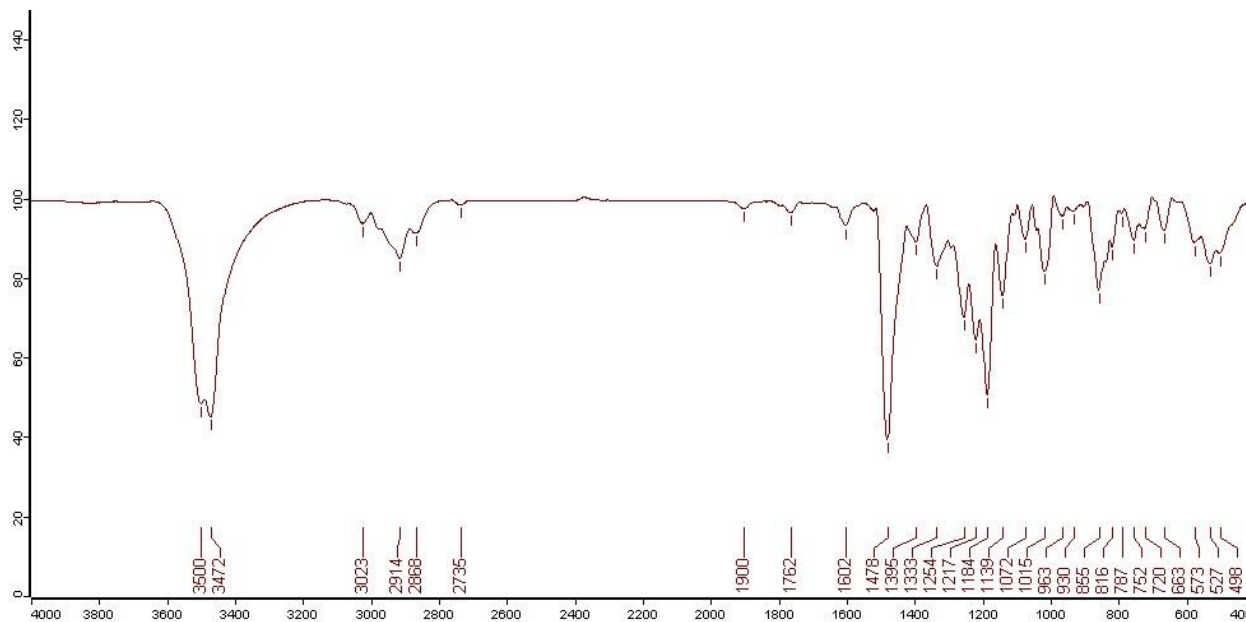


Fig. 5S. FT-IR of 6,6'-((4-bromophenyl)methylene)bis(2,4-dimethylphenol) (3c)

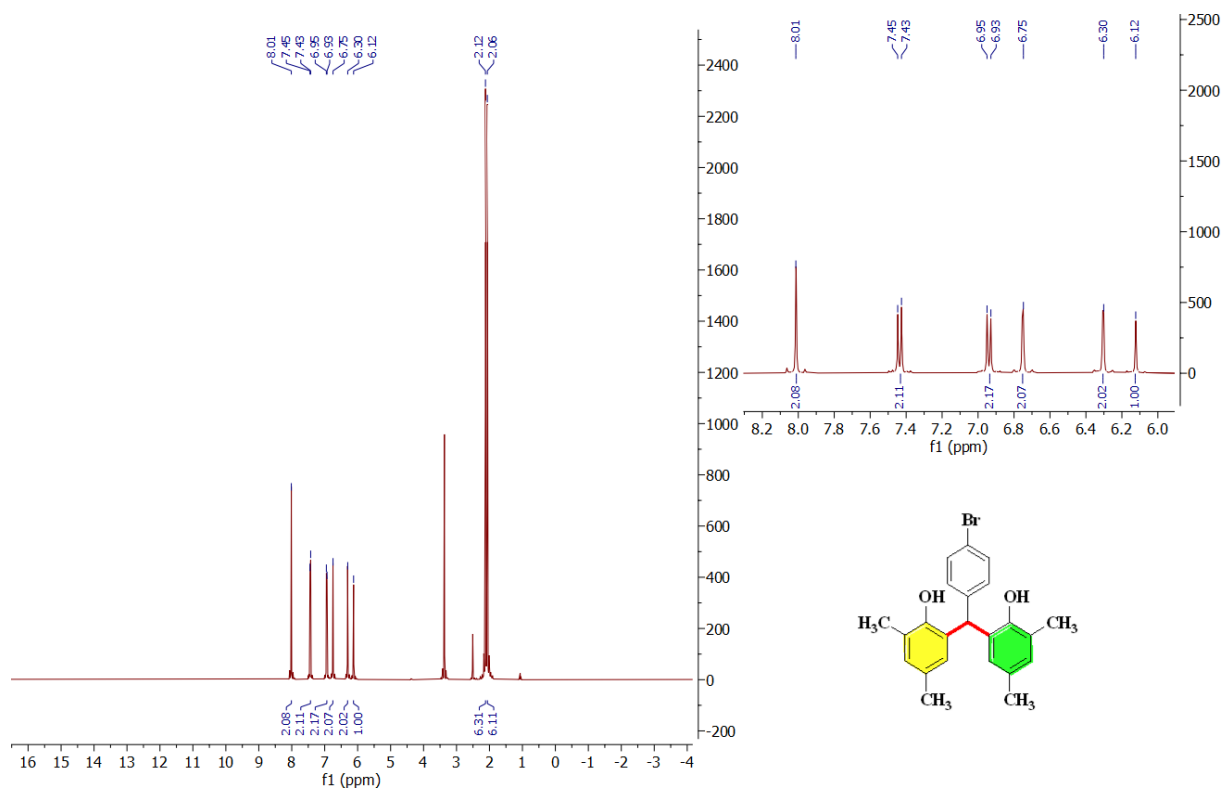


Fig. 6S. ^1H NMR of 6,6'-((4-bromophenyl)methylene)bis(2,4-dimethylphenol) (3c)

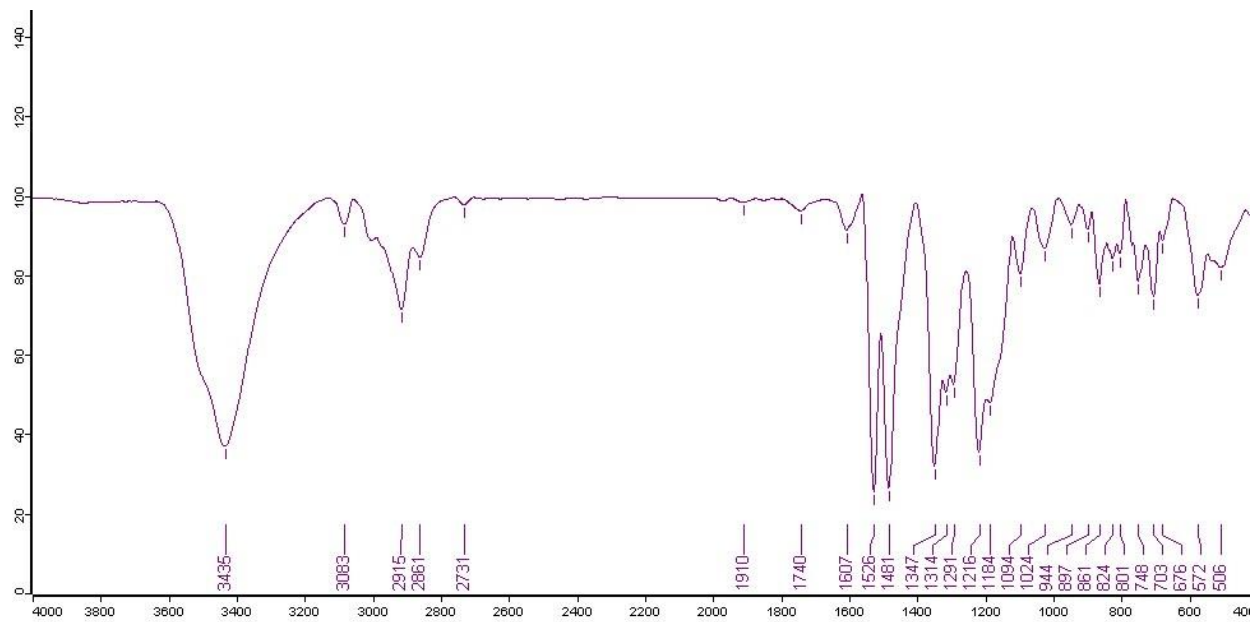


Fig. 7S. FT-IR of 6,6'-((3-nitrophenyl)methylene)bis(2,4-dimethylphenol) (3d)

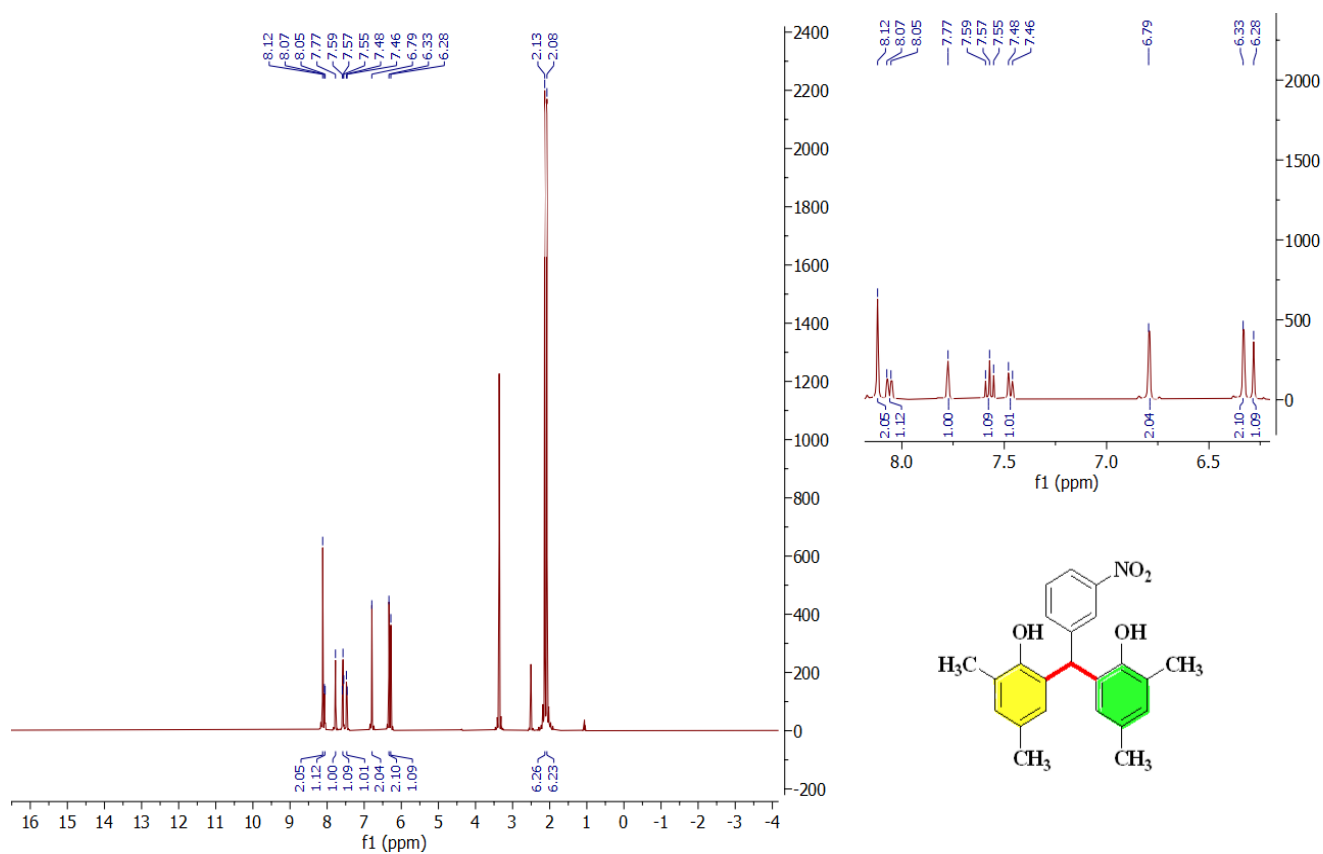


Fig. 8S. ^1H NMR of 6,6'-((3-nitrophenyl)methylene)bis(2,4-dimethylphenol) (3d)

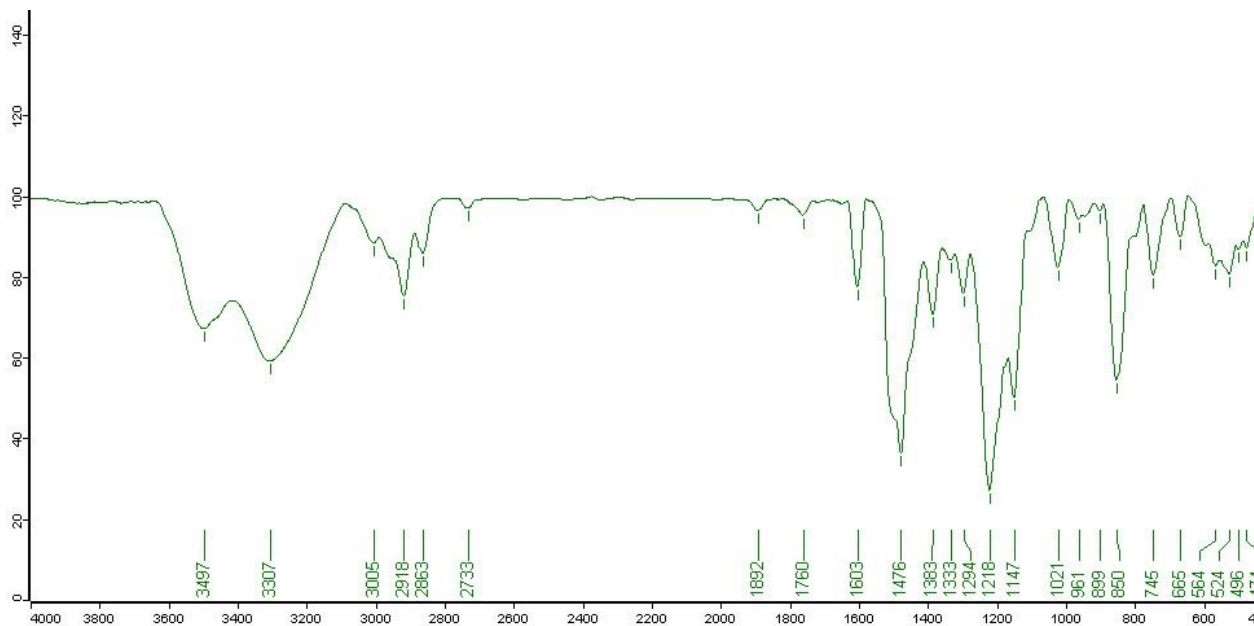


Fig. 9S. FT-IR of 6,6'-((4-fluorophenyl)methylene)bis(2,4-dimethylphenol) (3e)

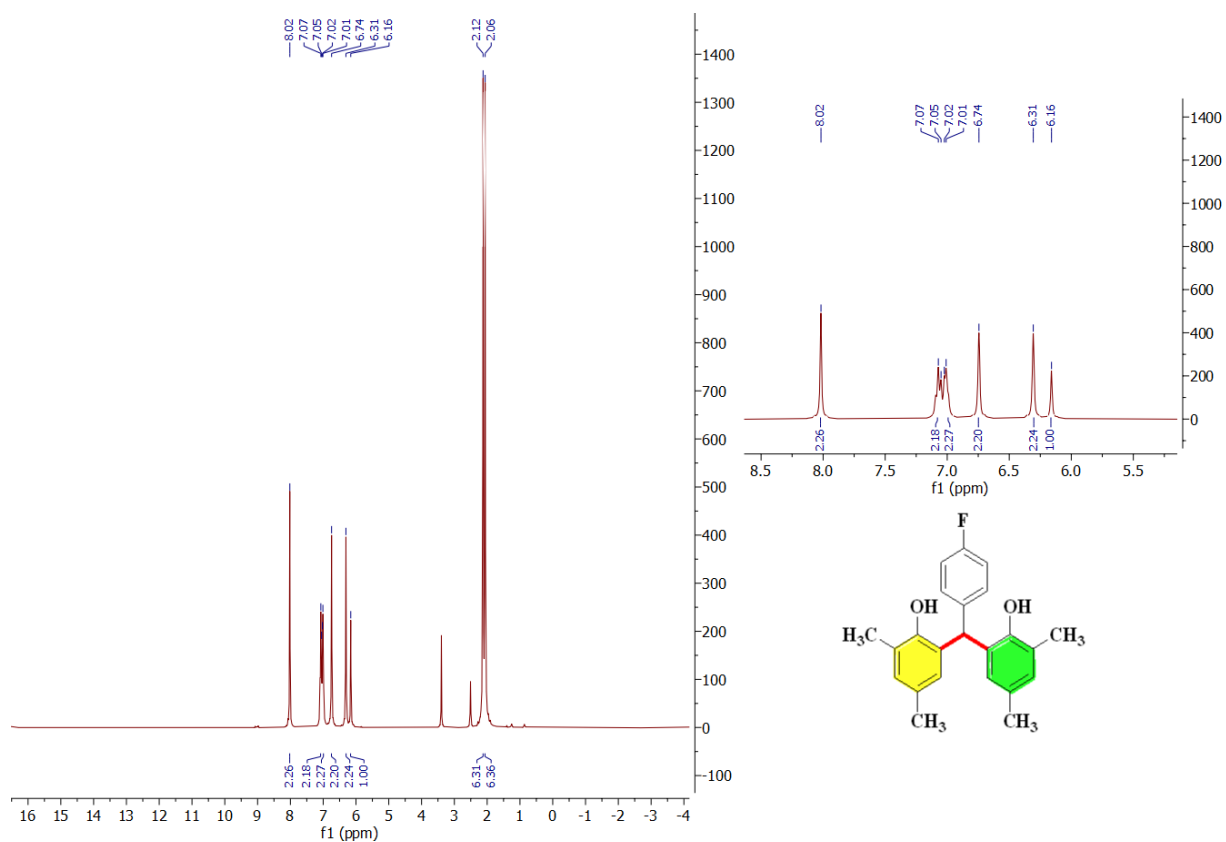


Fig. 10S. ^1H NMR of 6,6'-((4-fluorophenyl)methylene)bis(2,4-dimethylphenol) (3e)

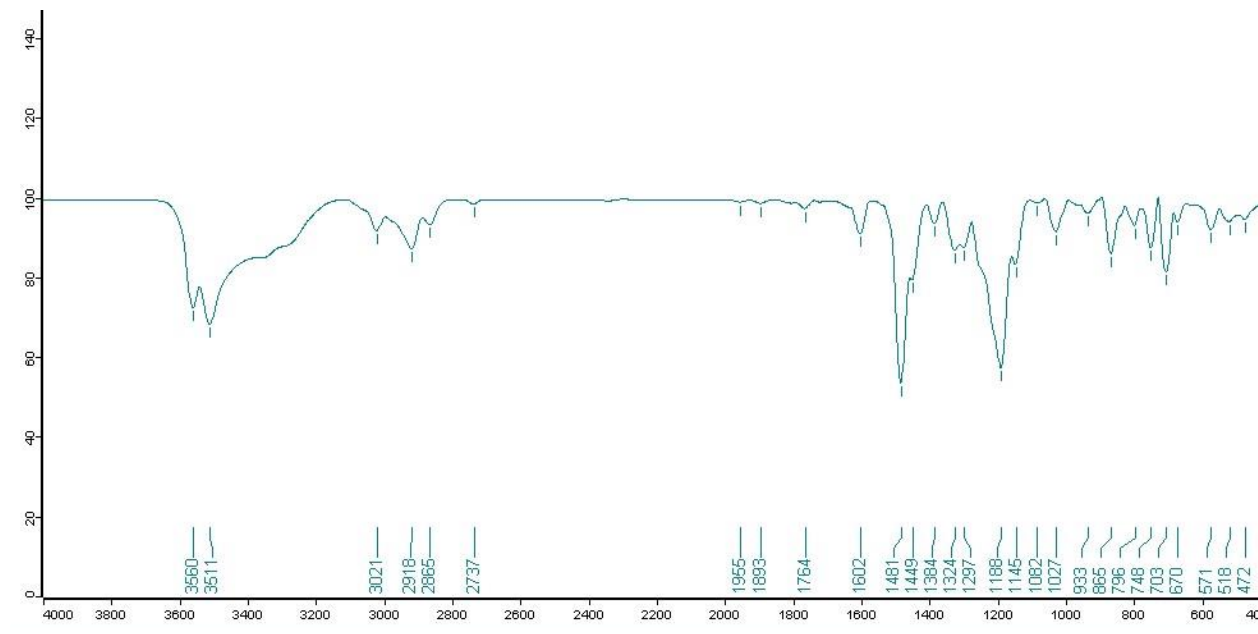


Fig. 11S. FT-IR of 6,6'-((phenyl)methylene)bis(2,4-dimethylphenol) (3f)

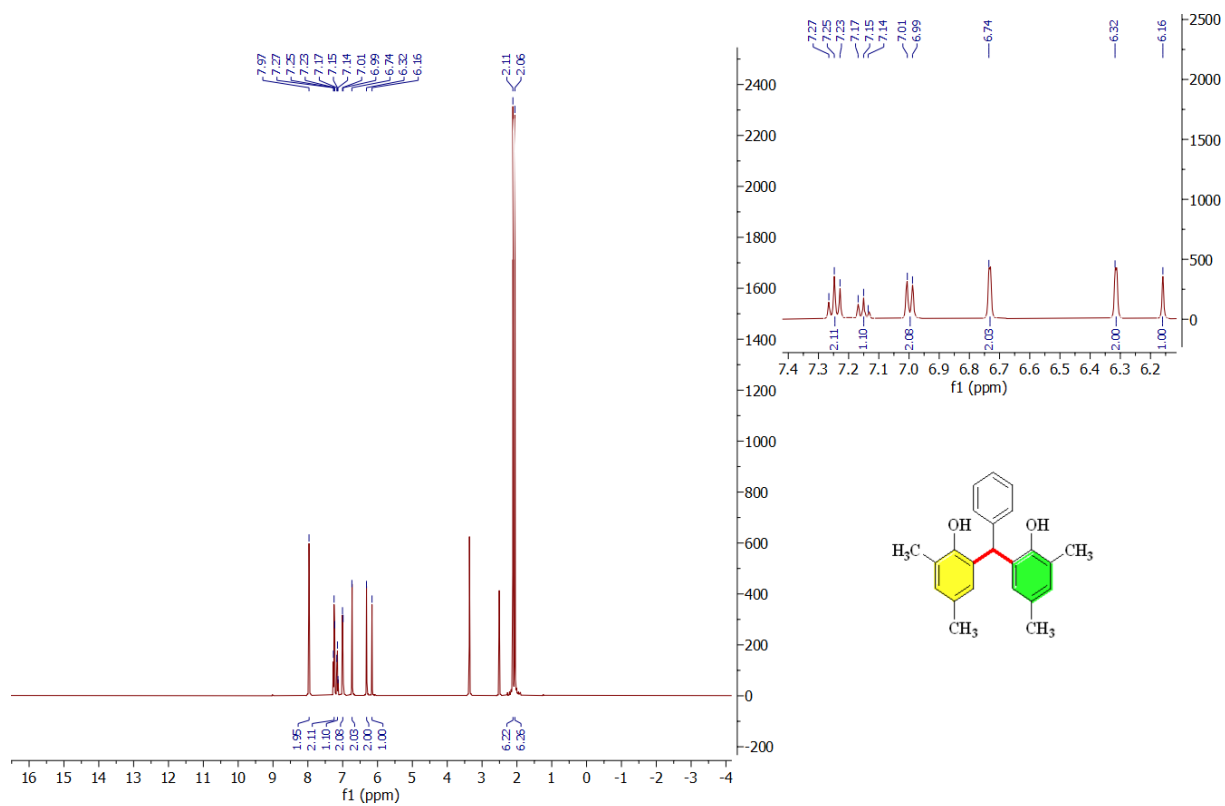


Fig. 12S. ^1H NMR of 6,6'-((phenyl)methylene)bis(2,4-dimethylphenol) (3f)

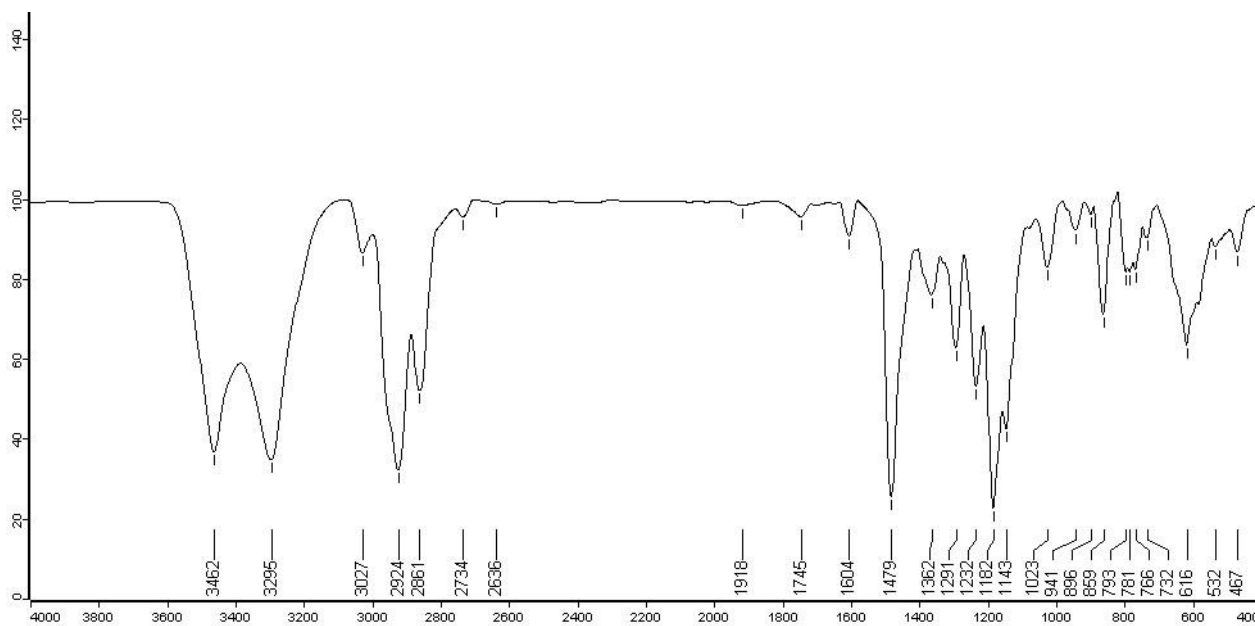


Fig. 13S. FT-IR of 6,6'-((Hexanal)methylene)bis(2,4-dimethylphenol) (3g)

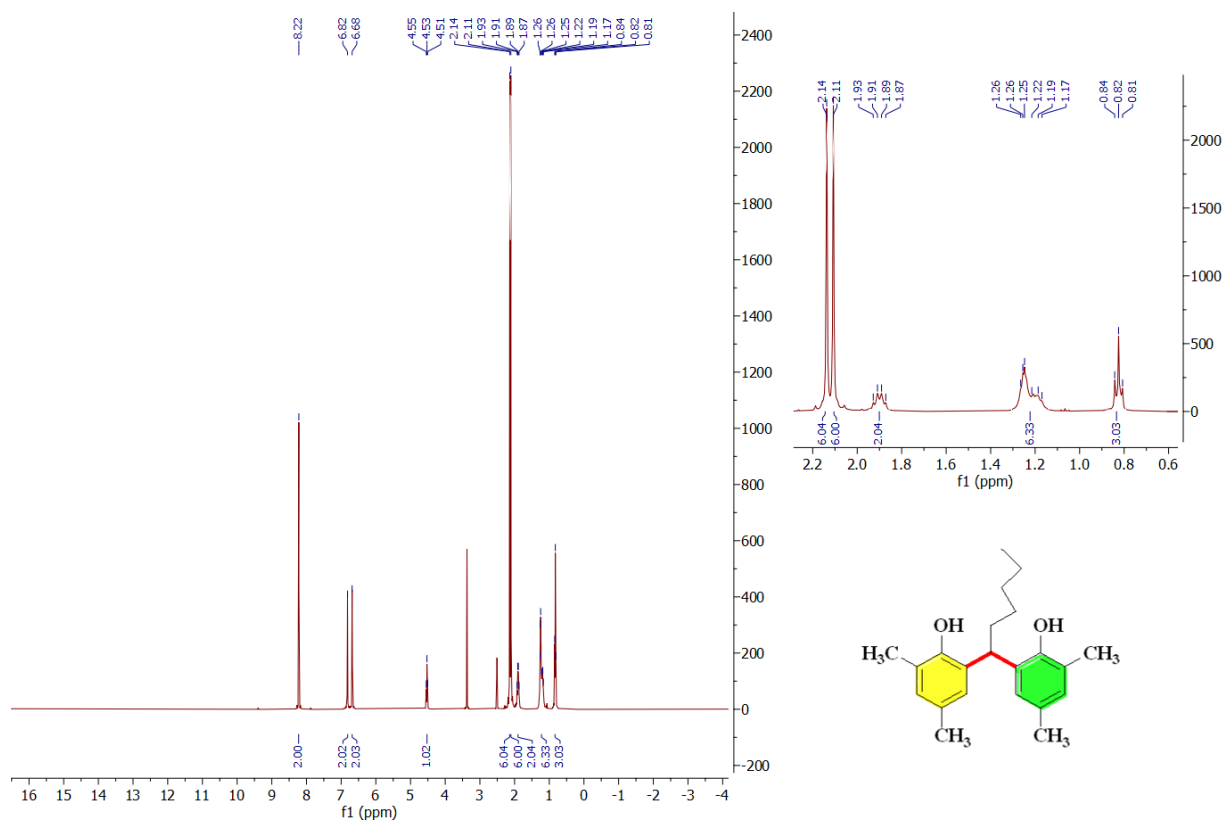


Fig. 14S. ^1H NMR of 6,6'-((Hexanal)methylene)bis(2,4-dimethylphenol) (3g)

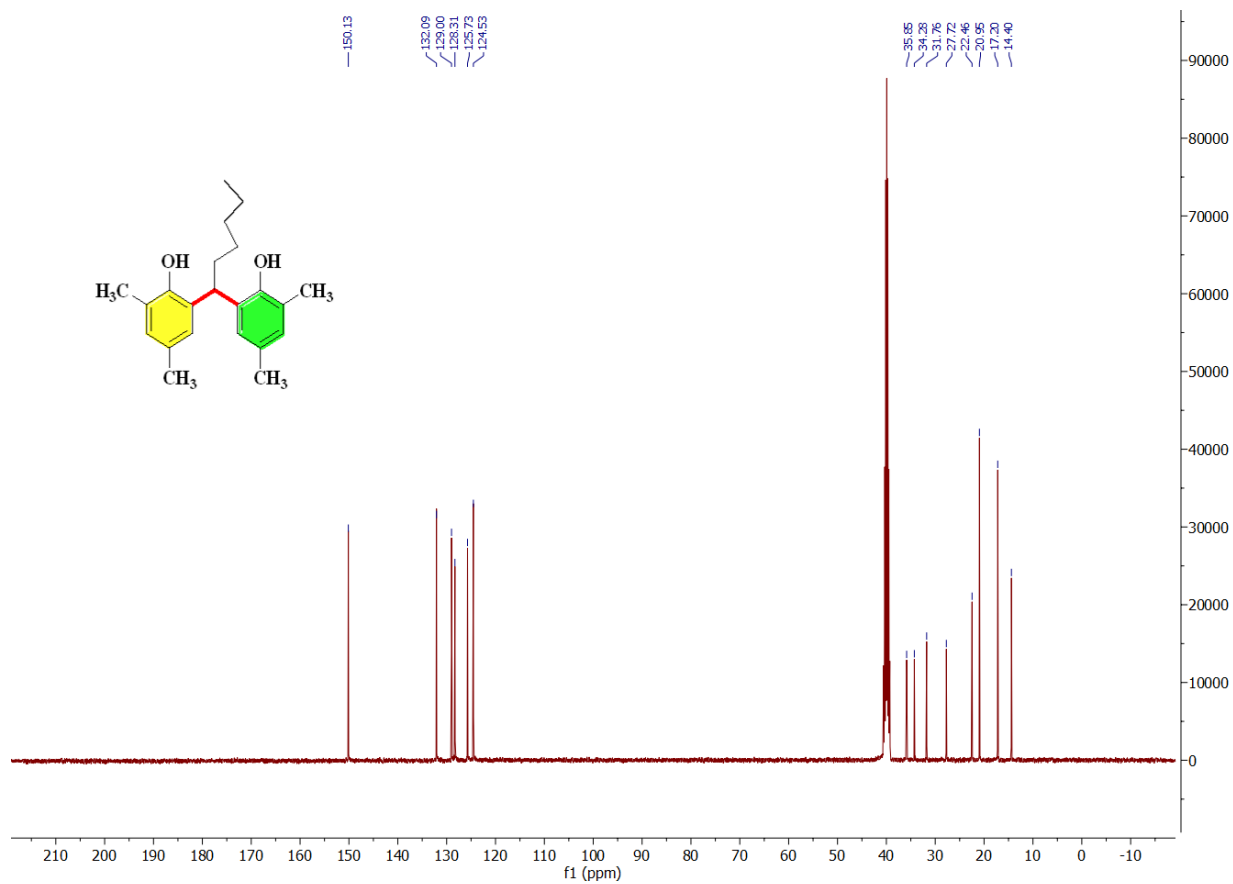


Fig. 15S. ¹³C NMR of 6,6'-((Hexanal)methylene)bis(2,4-dimethylphenol) (3g)

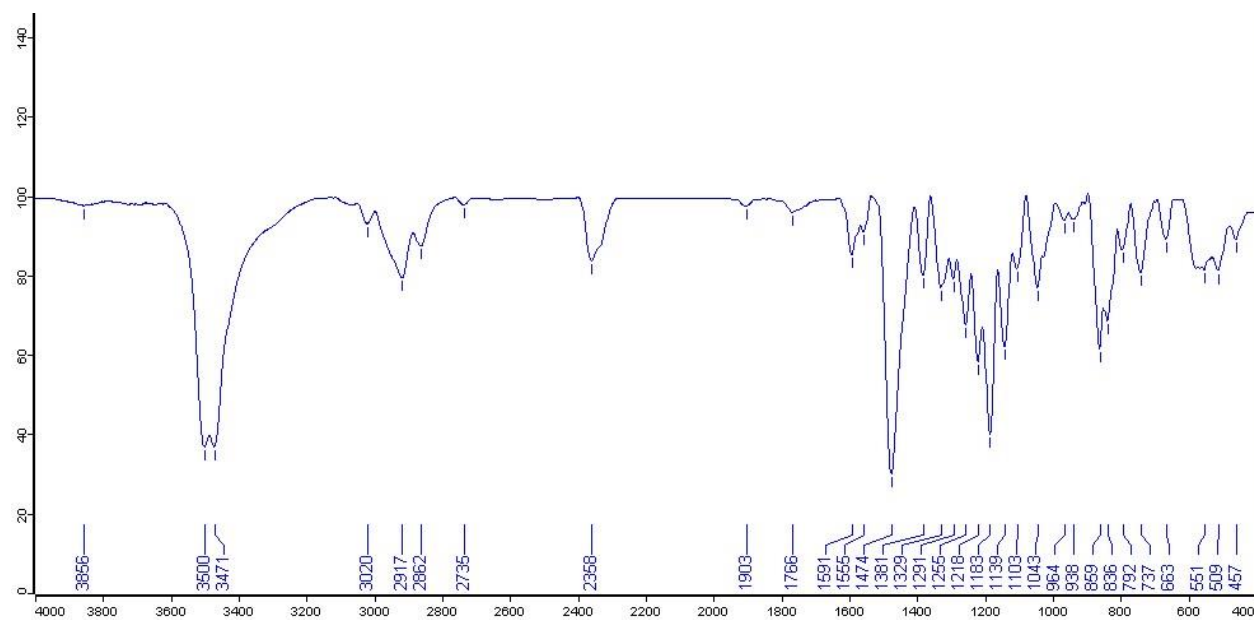


Fig. 16S. FT-IR of 6,6'-((2,4-Dichlorophenyl)methylene)bis(2,4-dimethylphenol) (3h)

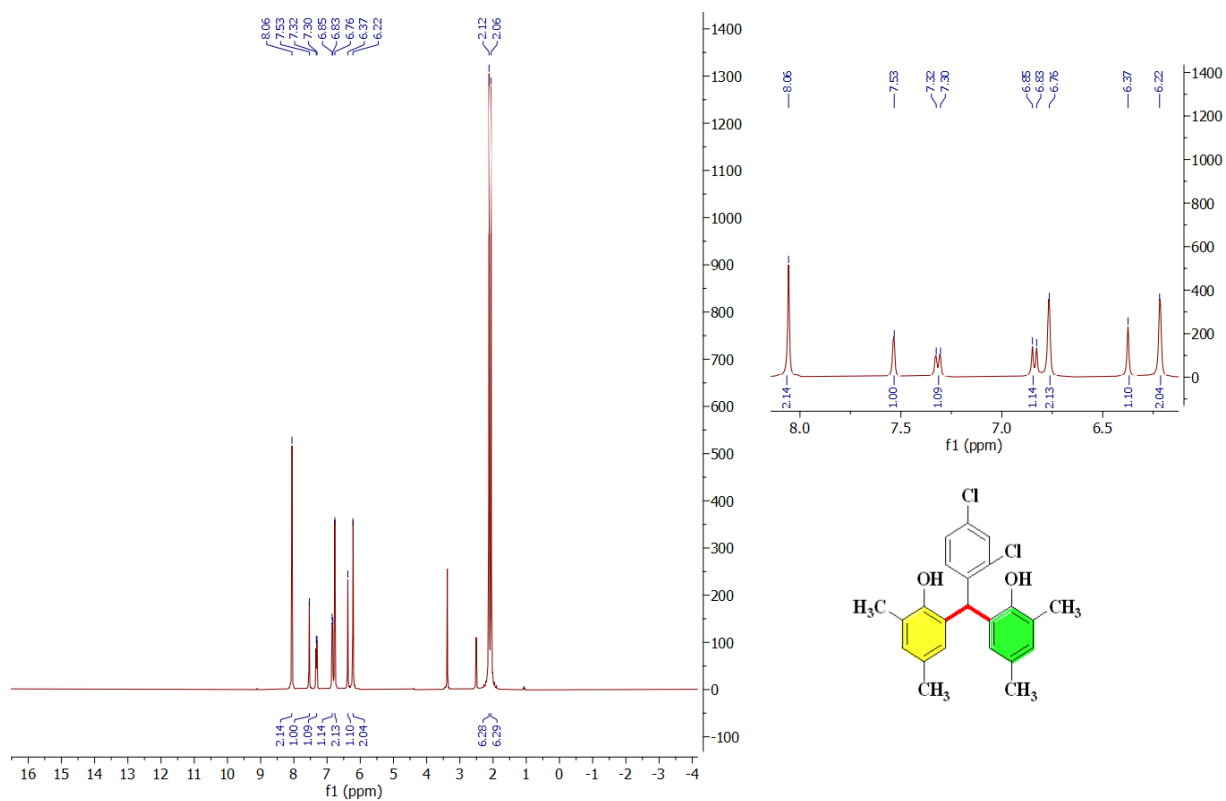


Fig. 17S. ¹H NMR of 6,6'-((2,4-Dichlorophenyl)methylene)bis(2,4-dimethylphenol) (3h)

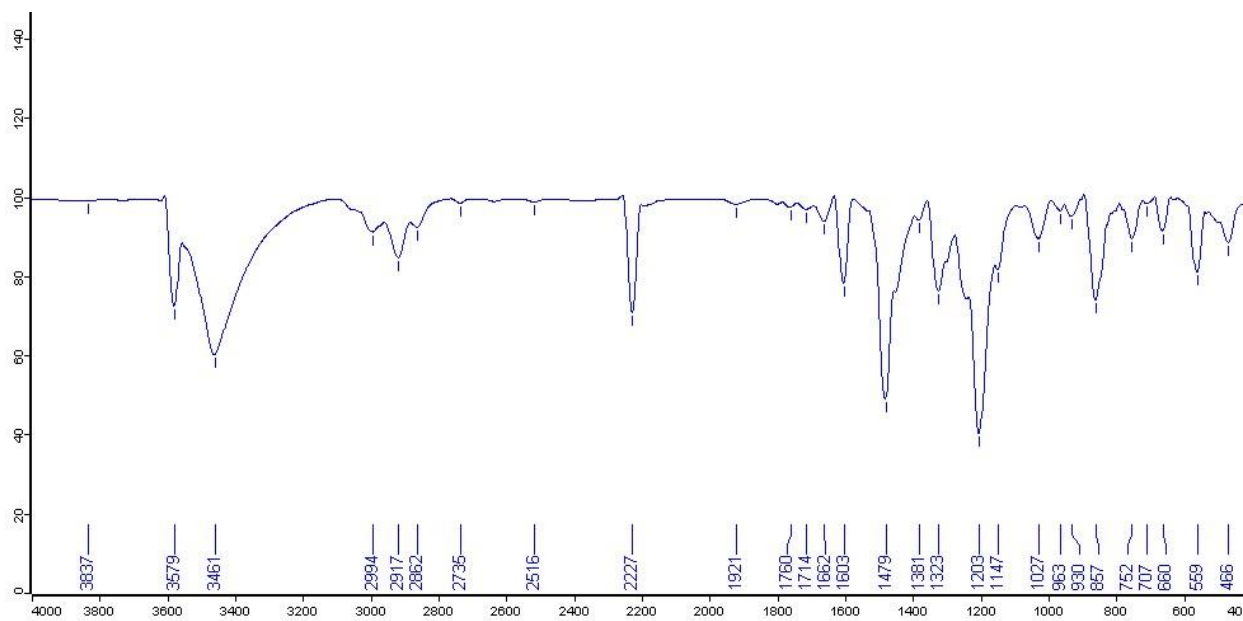


Fig. 18S. FT-IR of 6,6'-((4-Cyanophenyl)methylene)bis(2,4-dimethylphenol) (3i)

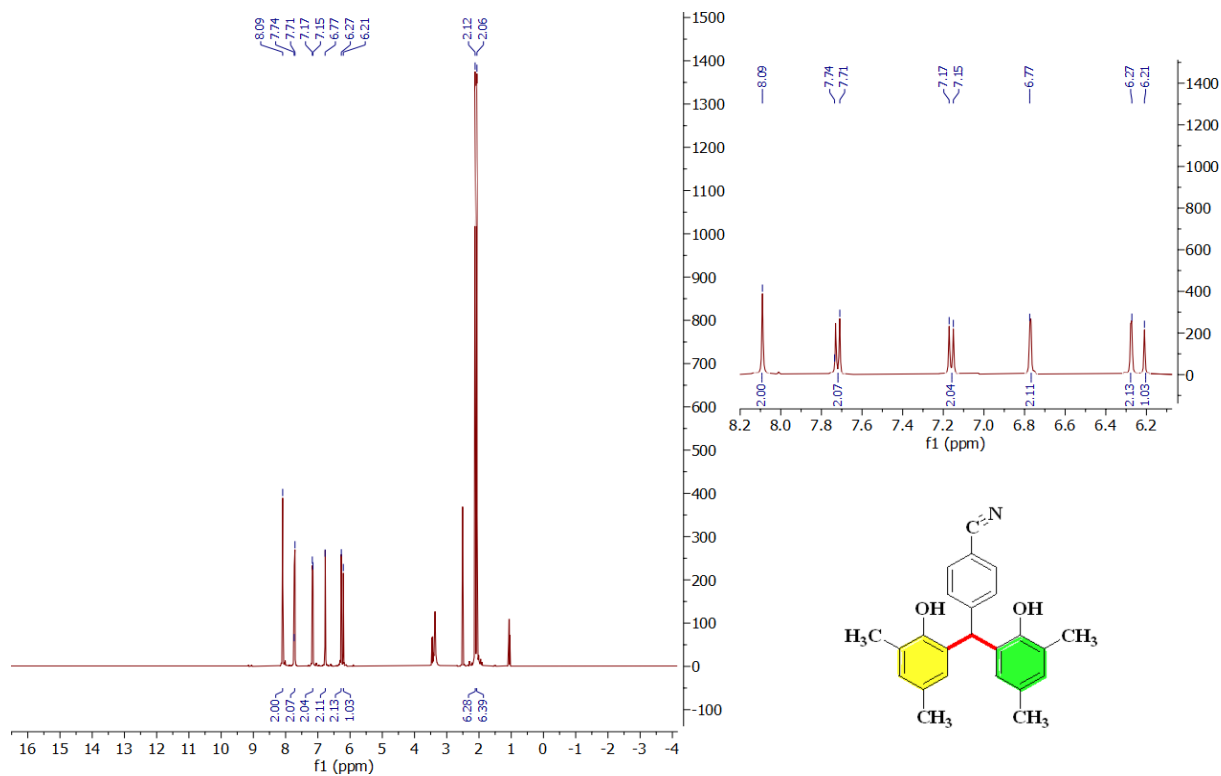


Fig. 19S. ¹H NMR of 6,6'-((4-Cyanophenyl)methylene)bis(2,4-dimethylphenol) (3i)

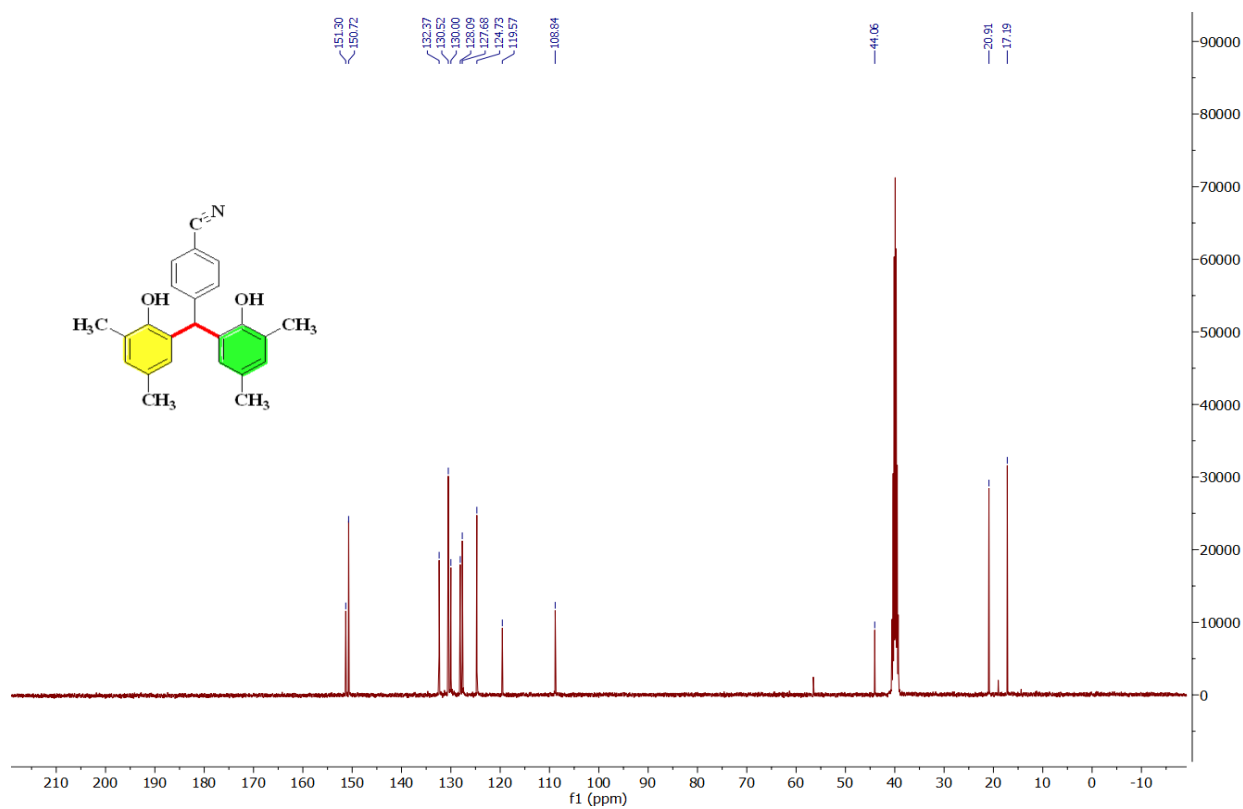


Fig. 20S. ¹³C NMR of 6,6'-((4-Cyanophenyl)methylene)bis(2,4-dimethylphenol) (3i)

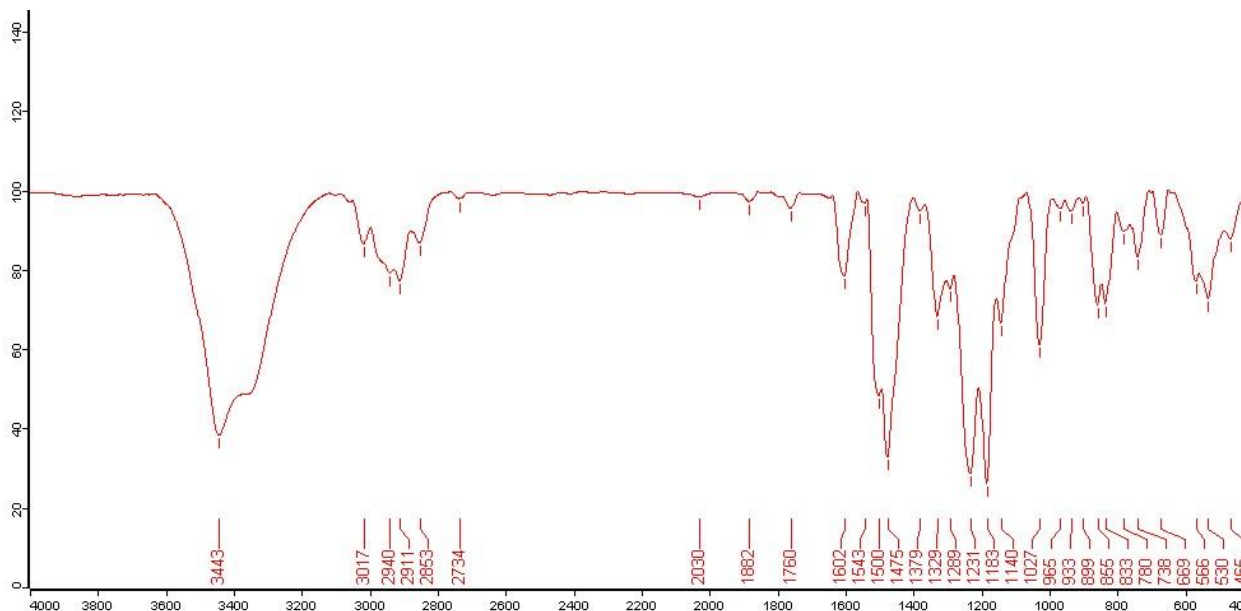


Fig. 21S. FT-IR of 6,6'-((4-Methoxyphenyl)methylene)bis(2,4-dimethylphenol) (3j)

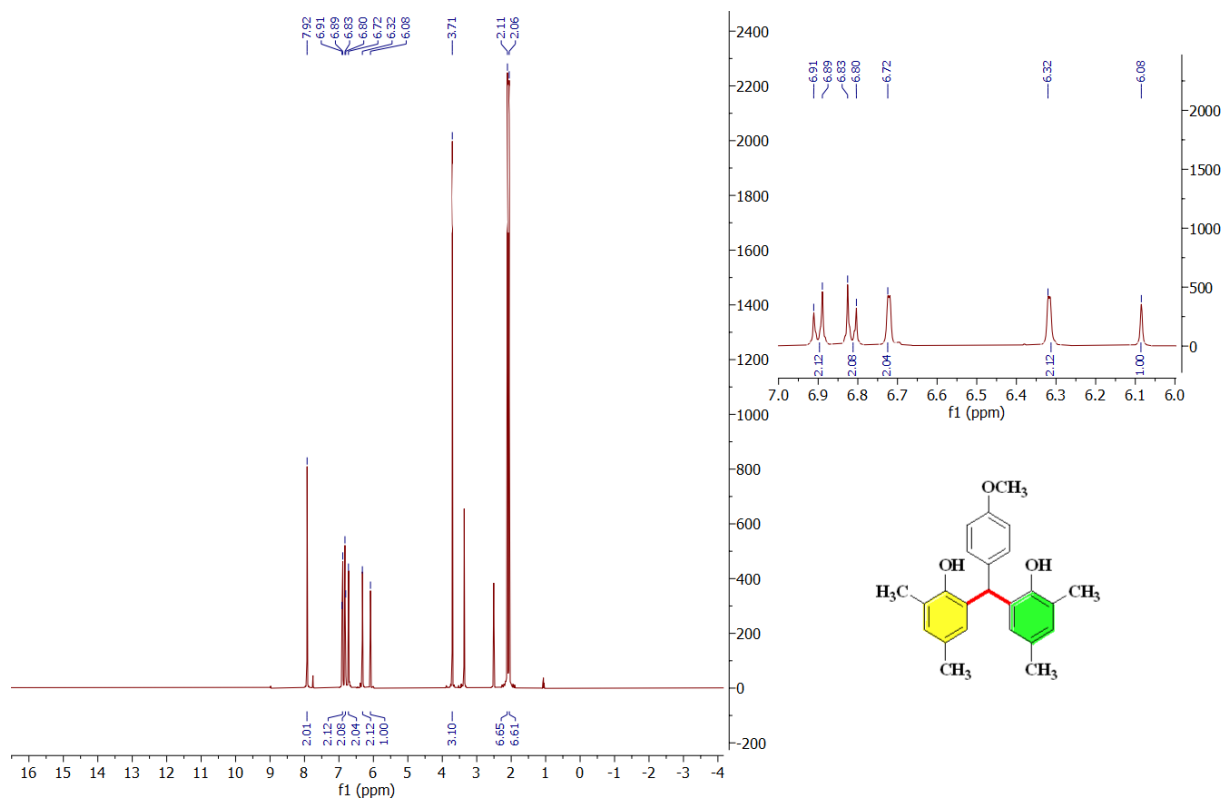


Fig. 22S. ^1H NMR of 6,6'-((4-Methoxyphenyl)methylene)bis(2,4-dimethylphenol) (3j)

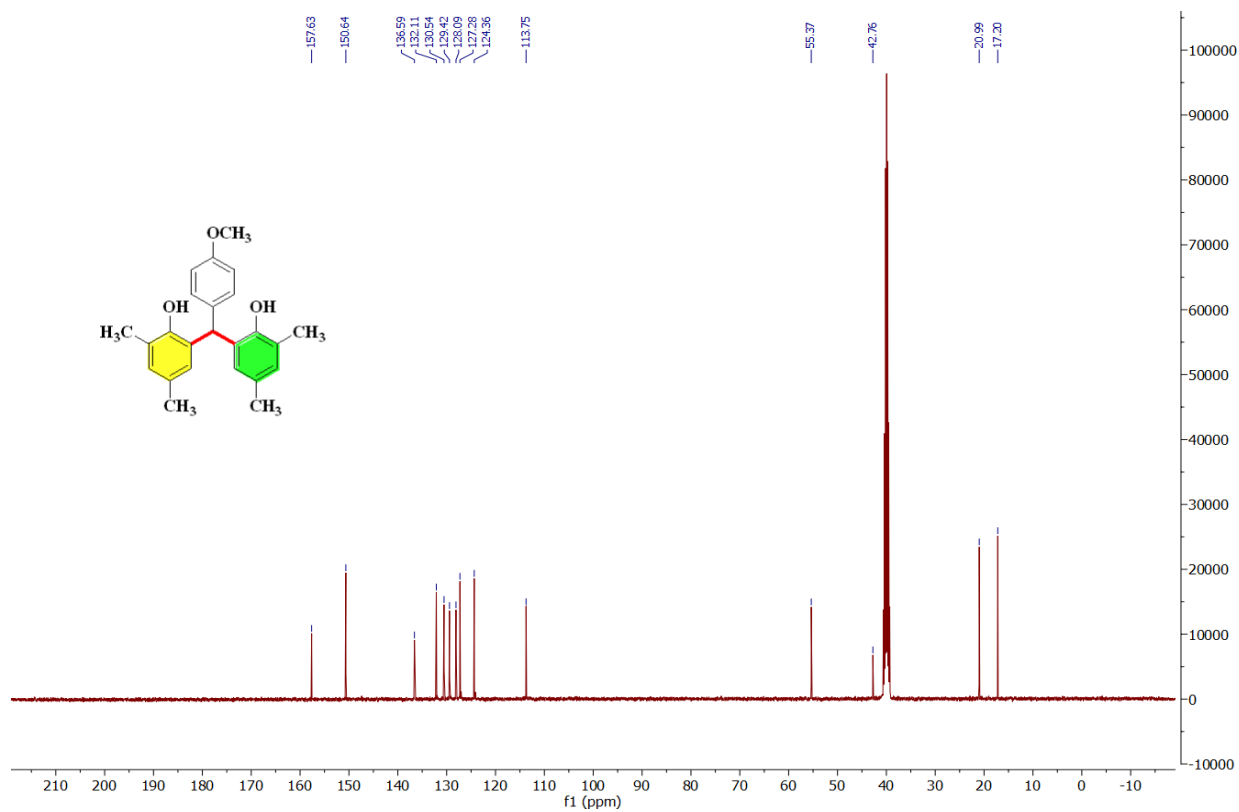


Fig. 23S. ¹³C NMR of 6,6'-((4-Methoxyphenyl)methylene)bis(2,4-dimethylphenol) (3j)

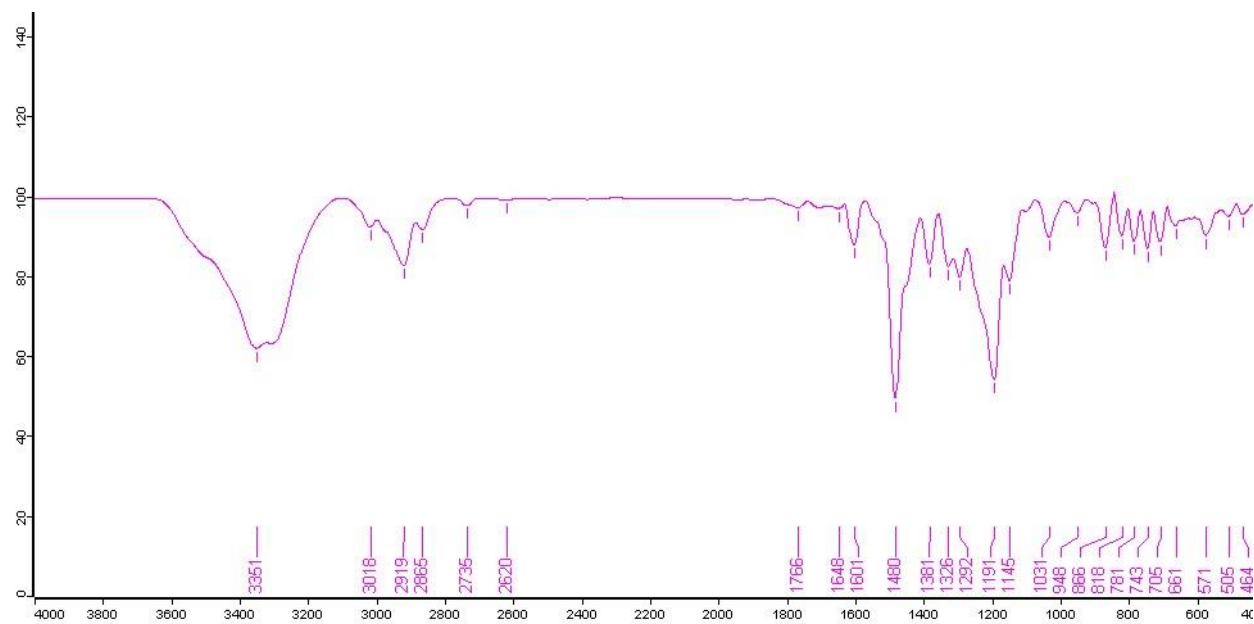


Fig. 24S. FT-IR of 6,6'-((3-Methylphenyl)methylene)bis(2,4-dimethylphenol) (3k)

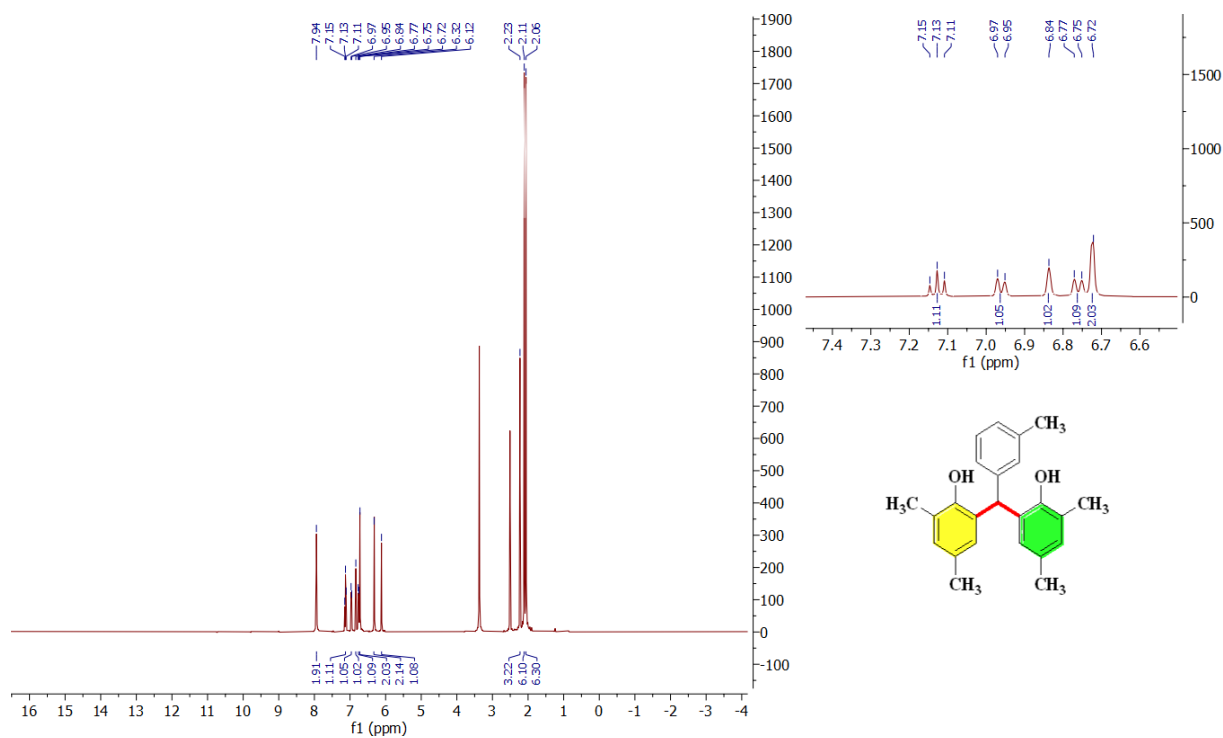


Fig. 25S. ¹H NMR of 6,6'-((3-Methylphenyl)methylene)bis(2,4-dimethylphenol) (3k)

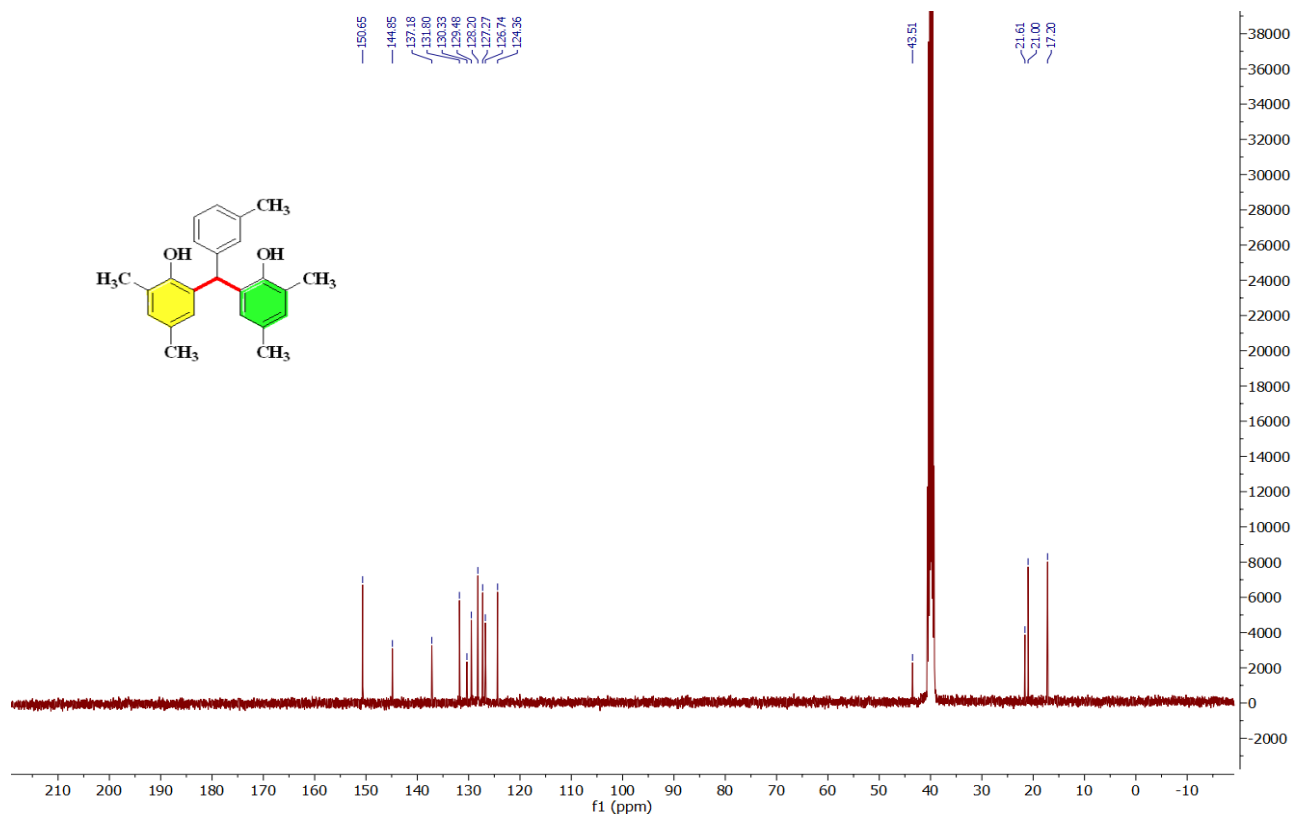


Fig. 26S. ¹³C NMR of 6,6'-((3-Methylphenyl)methylene)bis(2,4-dimethylphenol) (3k)

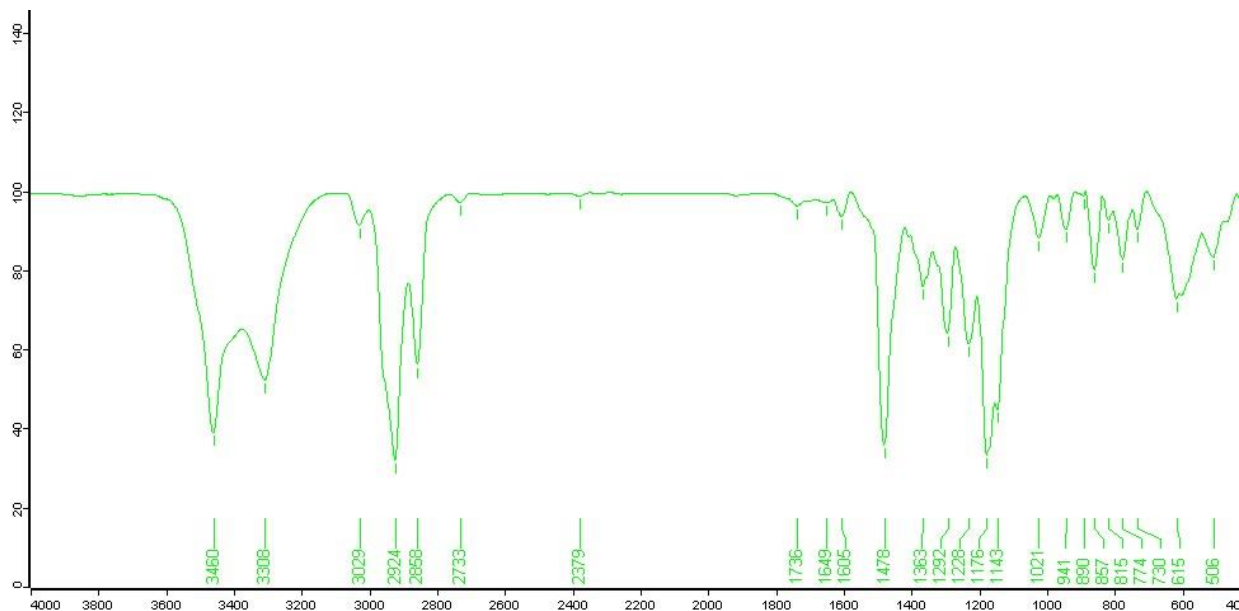


Fig. 27S. FT-IR of 6,6'-((Heptanal)methylene)bis(2,4-dimethylphenol) (3l)

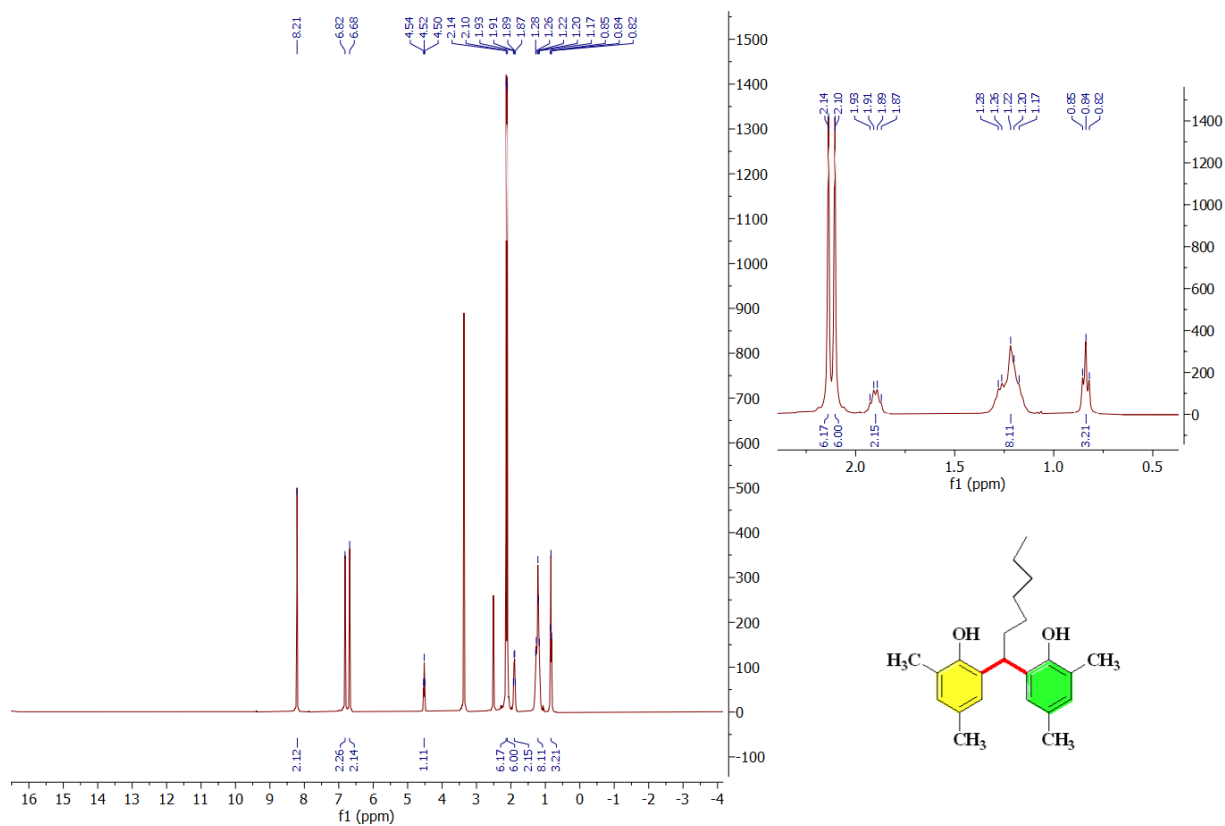


Fig. 28S. ¹H NMR of 6,6'-((Heptanal)methylene)bis(2,4-dimethylphenol) (3l)