

Supporting Information for

First direct access to 2-hydroxybenzophenones via Nickel-catalyzed cross-coupling of 2-hydroxybenzaldehydes with aryl iodides

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2-Hydroxybenzophenone (Table 2, Entry 1) [117-99-7]: IR (KBr): 3500, 1728 cm^{-1} . $^1\text{H-NMR}$ (250 MHz, CDCl_3) δ (ppm): 11.96 (s, 1H, OH), 7.62-7.40 (m, 7H, Ar), 7.02-6.98 (m, 1H, Ar), 6.83-6.77 (m, 2H, Ar). $^{13}\text{C-NMR}$ (62.9 MHz, CDCl_3) δ (ppm): 200.01, 158.02, 140.77, 133.85, 133.76, 132.95, 132.04, 127.96, 127.46, 120.01 (overlap, two peaks). Anal. Calcd for $\text{C}_{13}\text{H}_{10}\text{O}_2$: C, 78.77; H, 5.09. Found: C, 78.37; H, 4.96.

(2-Hydroxyphenyl)(*p*-tolyl)methanone (Table 2, Entry 3) [19434-30-1]: IR (KBr): 3434, 1650 cm^{-1} . $^1\text{H-NMR}$ (250 MHz, CDCl_3) δ (ppm): 11.97 (s, 1H, OH), 7.52-7.37 (m, 4H, Ar), 7.21 (d, 2H, $J = 8.0$ Hz, Ar), 6.97 (t, 1H, $J = 8.5$ Hz, Ar), 6.80-6.74 (m, 1H, Ar), 2.35 (s, 3H, CH_3). $^{13}\text{C-NMR}$ (62.9 MHz, CDCl_3) δ (ppm): 201.31, 163.11, 142.73, 136.07 (overlap, two peaks), 133.51, 129.46 (overlap, two peaks), 129.00, 118.53, 118.33, 30.18. Anal. Calcd for $\text{C}_{14}\text{H}_{12}\text{O}_2$: C, 79.22; H, 5.70. Found: C, 78.98; H, 5.83.

(2-Hydroxyphenyl)(4-nitrophenyl)methanone (Table 2, Entry 6) [68223-20-1]: IR (KBr): 3400, 1659 cm^{-1} . $^1\text{H-NMR}$ (250 MHz, CDCl_3) δ (ppm): 11.76 (s, 1H, OH), 8.34-7.83 (m, 6H, Ar), 7.71-7.65 (m, 2H, Ar). $^{13}\text{C-NMR}$ (62.9 MHz, CDCl_3) δ (ppm): 137.34, 133.03, 132.61 (overlap, two peaks), 129.97, 129.87, 124.99, 123.63, 119.13, 118.83. Anal. Calcd for $\text{C}_{13}\text{H}_9\text{NO}_4$: C, 64.20; H, 3.73; N, 5.76. Found: C, 64.00; H, 3.82; N, 5.70.

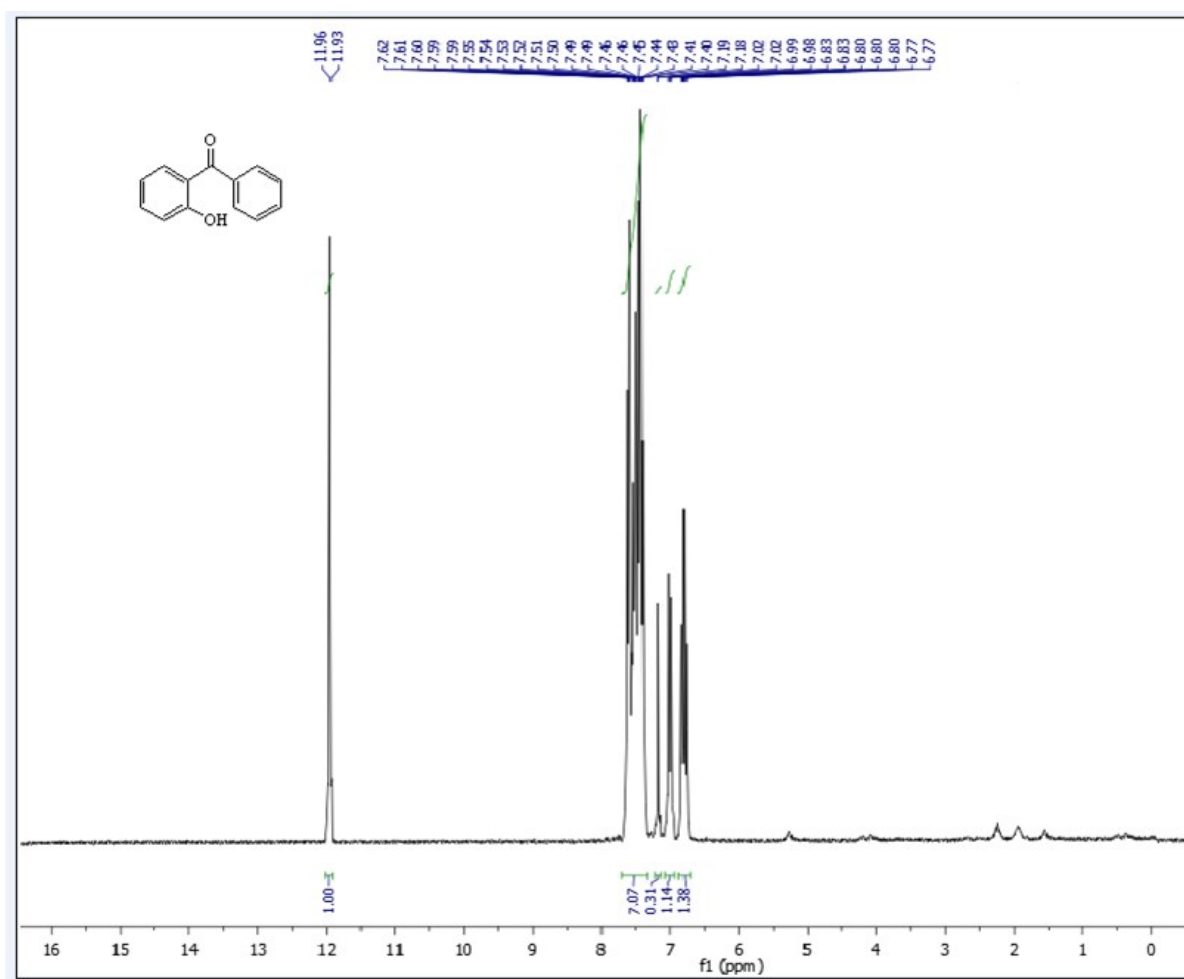
4-(2-Hydroxybenzoyl)benzonitrile (Table 2, Entry 7) [131117-91-4]: IR (KBr): 3500, 2200, 1650 cm^{-1} . $^1\text{H-NMR}$ (250 MHz, CDCl_3) δ (ppm): 12.00 (s, 1H, OH), 8.23-7.80 (m, 1H, Ar), 7.68-7.62 (m, 3H, Ar), 7.59-7.52 (m, 4H, Ar). $^{13}\text{C-NMR}$ (62.9 MHz, CDCl_3) δ (ppm): 202.85, 138.83, 132.77, 132.61 (overlap, two peaks), 124.99, 124.04 (overlap, two peaks), 119.37, 116.69 (overlap, two peaks), 116.09. Anal. Calcd for $\text{C}_{14}\text{H}_9\text{NO}_2$: C, 75.33; H, 4.06; N, 6.27. Found: C, 75.24; H, 4.10; N, 6.18.

(5-bromo-2-hydroxyphenyl)(phenyl)methanone (Table 2, Entry 9) [55082-33-2]: $^1\text{H-NMR}$ (250 MHz, CDCl_3) δ (ppm): 11.77 (s, 1H, OH), 7.49 (d, 1H, $J = 8.5$ Hz, Ar), 7.24 (m, 1H, Ar), 7.07 (d, 1H, $J = 8.4$ Hz, Ar), 6.97 (m, 2H, Ar), 6.85 (s, 1H, Ar), 6.56 (m, 2H, Ar). $^{13}\text{C-NMR}$ (62.9 MHz, CDCl_3) δ (ppm): 200.05, 158.11, 147.94, 140.55, 133.85, 133.46, 132.95, 131.25, 127.96, 127.58, 119.46.

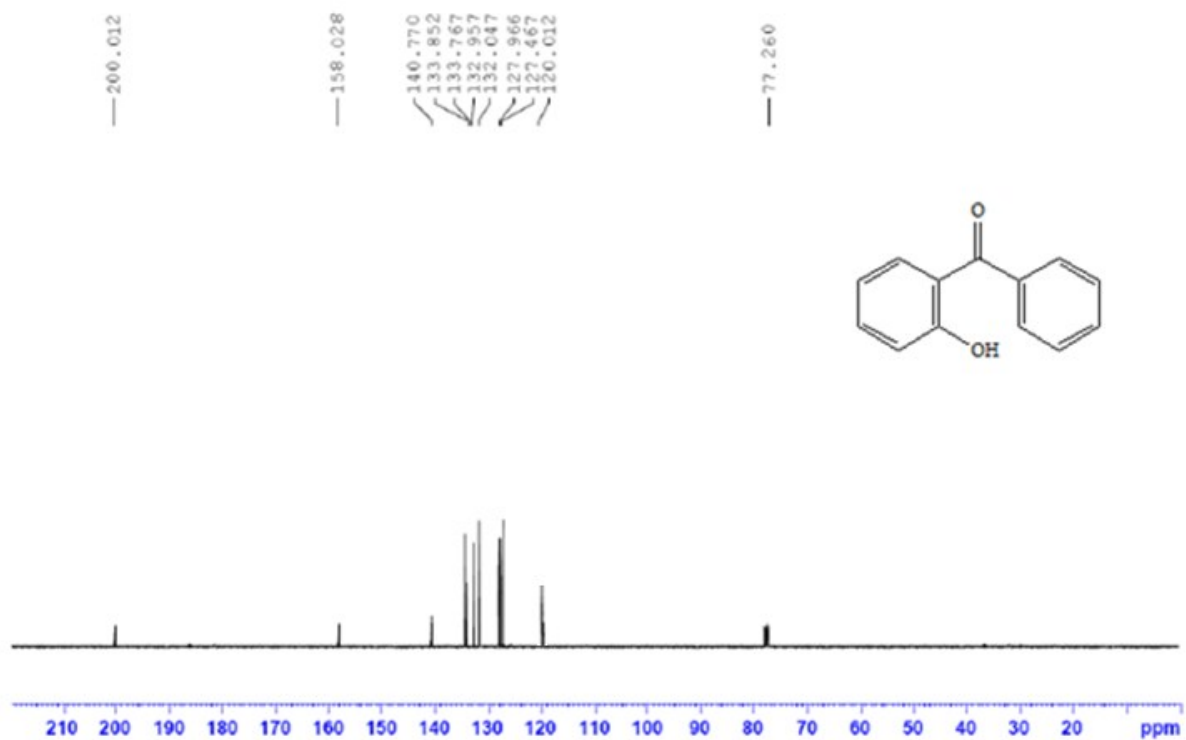
(5-bromo-2-hydroxyphenyl)(*p*-tolyl)methanone (Table 2, Entry 10) [215380-62-4]: $^1\text{H-NMR}$ (250 MHz, CDCl_3) δ (ppm): 11.63 (s, 1H, OH), 7.99 (m, 2H, Ar), 7.89 (m, 1H, Ar), 7.83 (m, 2H, Ar), 7.62 (s, 1H, Ar), 7.52 (m, 1H, Ar), 2.76 (s, 3H, CH_3). $^{13}\text{C-NMR}$ (62.9

MHz, CDCl₃) δ (ppm): 200.93, 160.88, 149.20, 141.59 (overlap, two peaks), 136.29, 132.26, 126.47, 124.16 (overlap, two peaks), 118.85, 29.16.

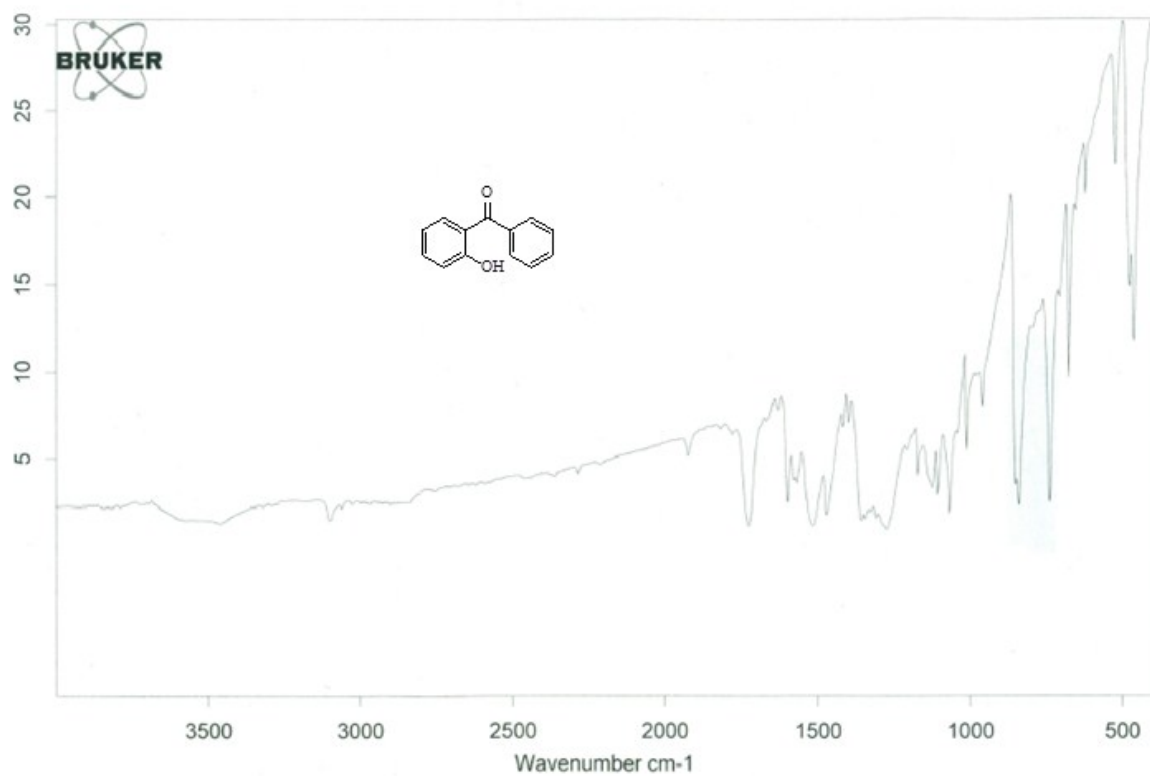
(5-bromo-2-hydroxyphenyl)(4-nitrophenyl)methanone (Table 2, Entry 11): ¹H-NMR (250 MHz, CDCl₃) δ (ppm): 11.95 (s, 1H, OH), 8.16 (m, 1H, Ar), 7.98 (m, 2H, Ar), 7.89 (d, 1H, *J* = 8.4 Hz, Ar), 7.83 (m, 2H, Ar), 7.63 (s, 1H, Ar). ¹³C-NMR (62.9 MHz, CDCl₃) δ (ppm): 205.65, 159.12, 147.81, 144.05, 134.36, 133.26, 133.00, 132.89, 129.96, 127.77, 121.38.



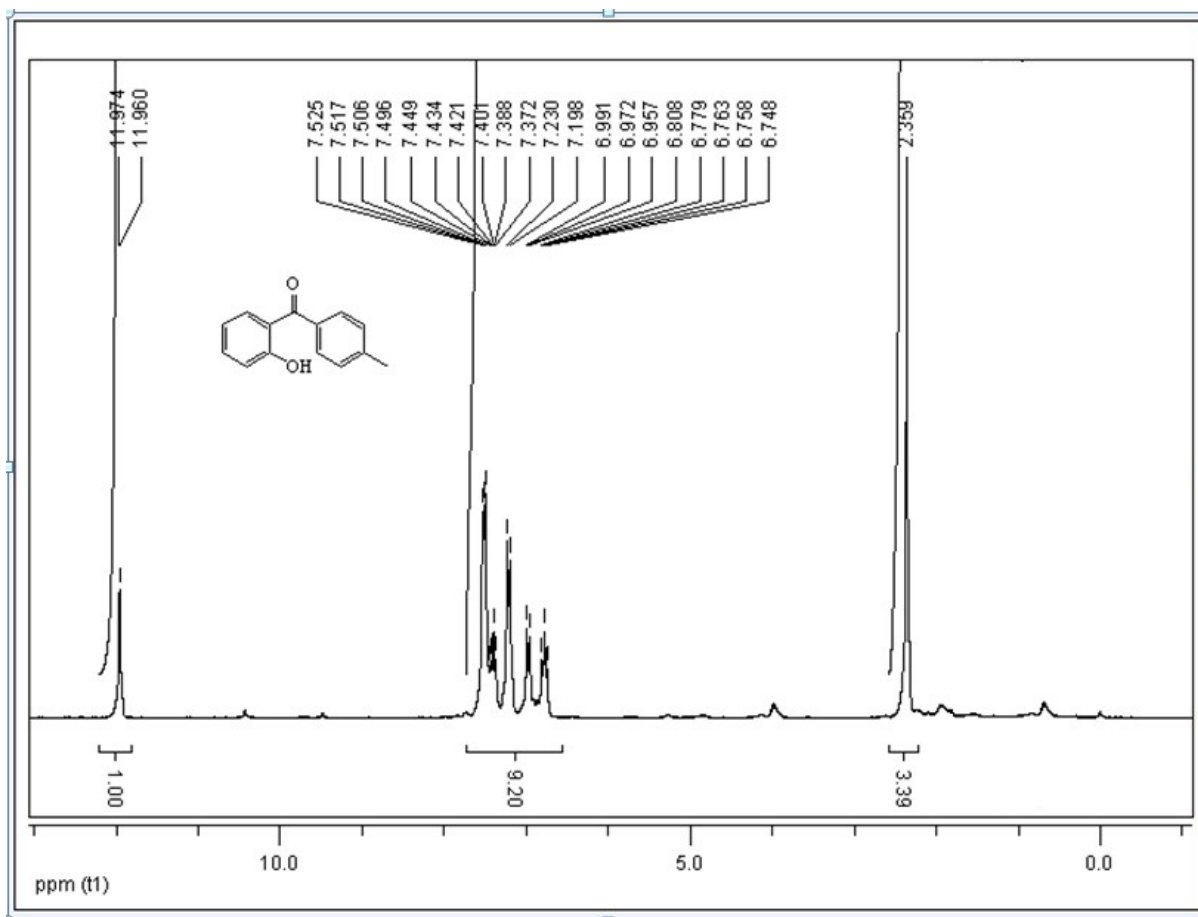
¹H-NMR of 2-Hydroxybenzophenone (Table 2, Entry 1)



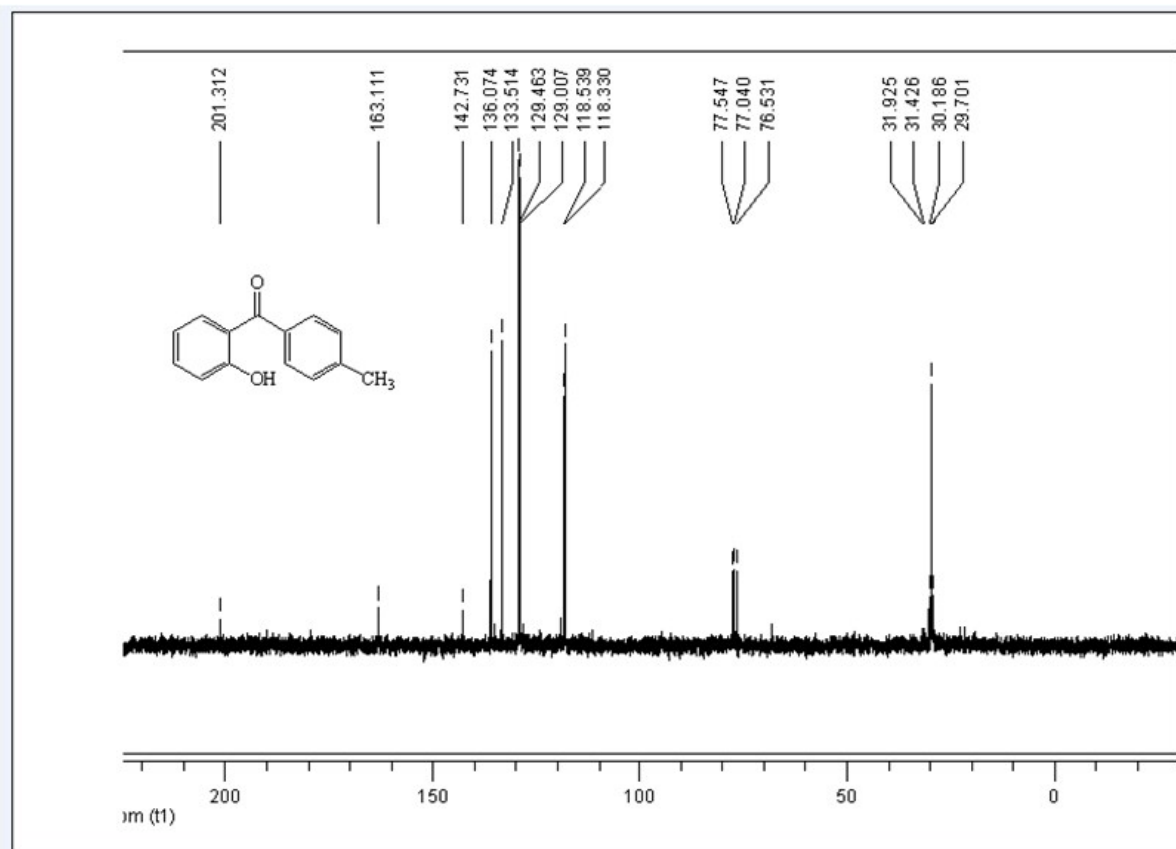
¹³C-NMR of 2-Hydroxybenzophenone (Table 2, Entry 1)



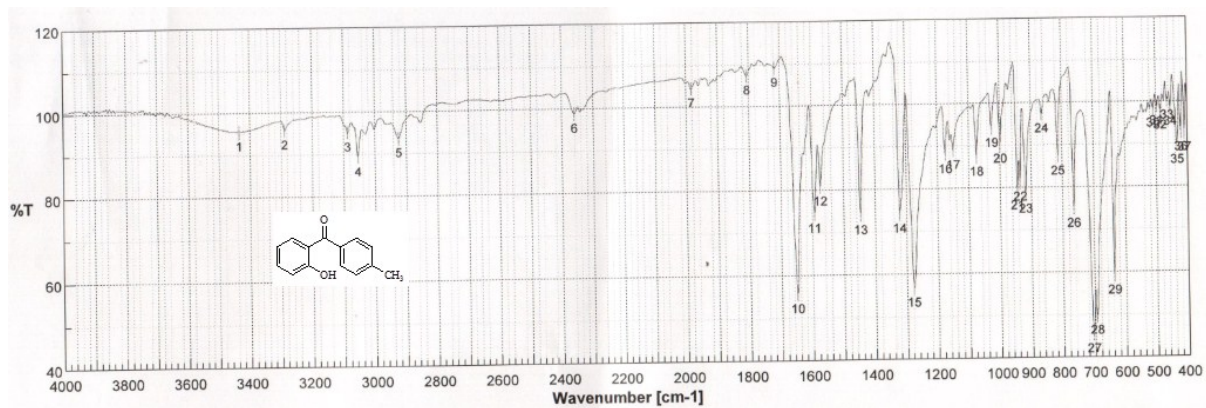
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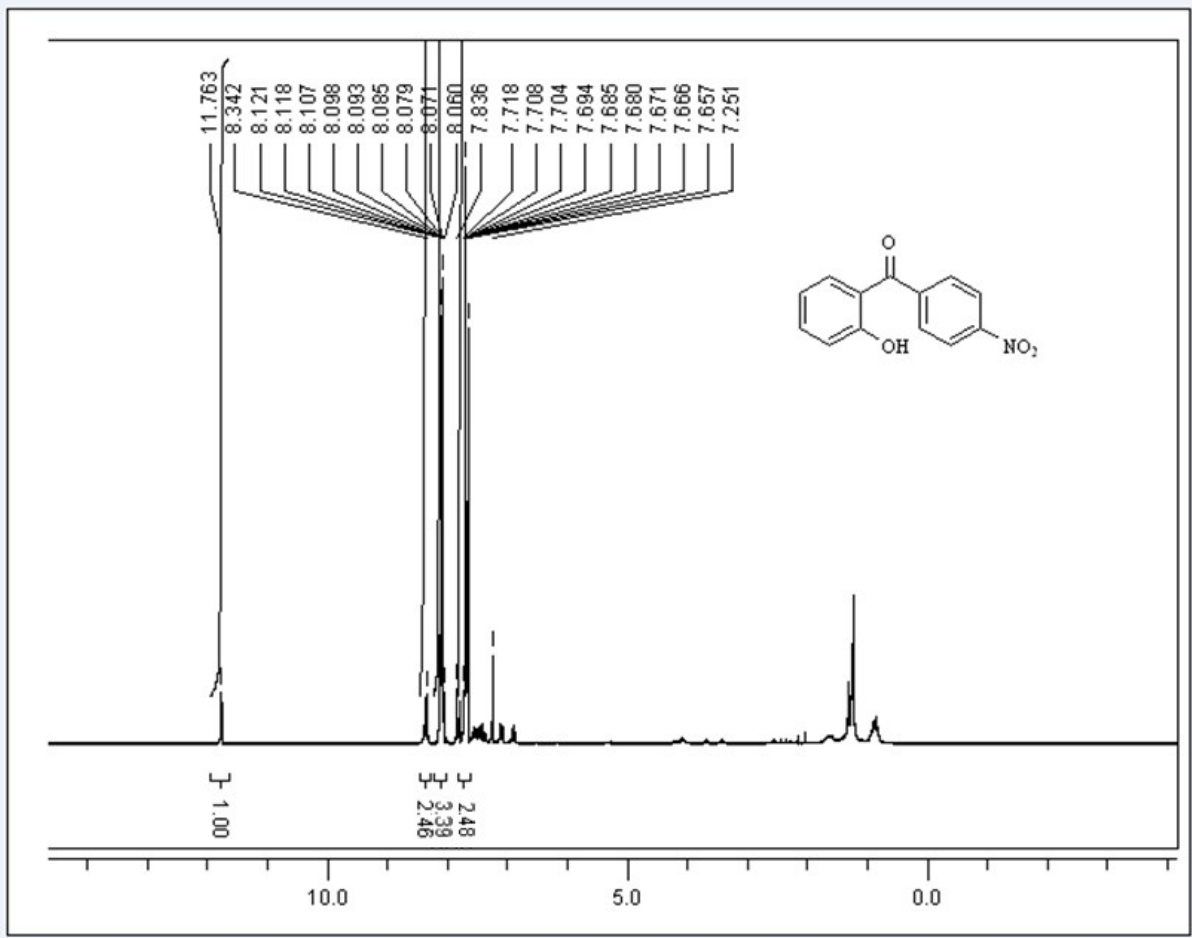
¹H-NMR of (2-Hydroxyphenyl)(*p*-tolyl)methanone (Table 2, Entry 3)



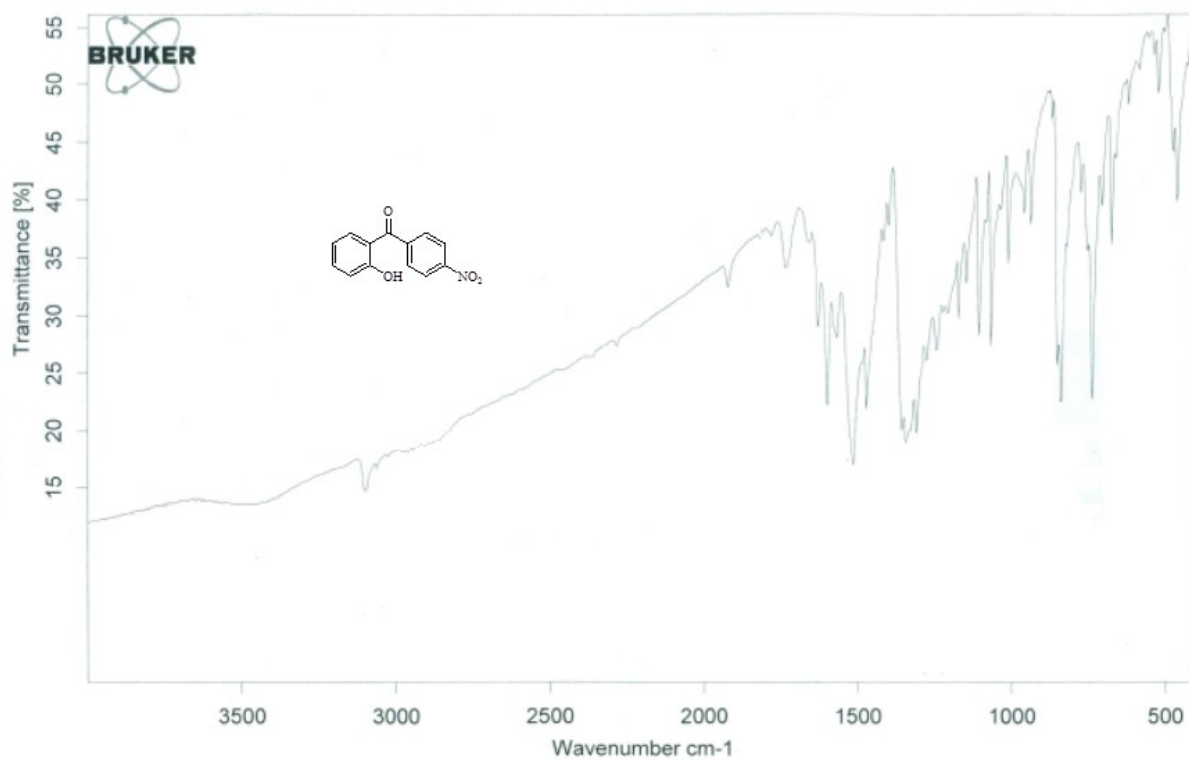
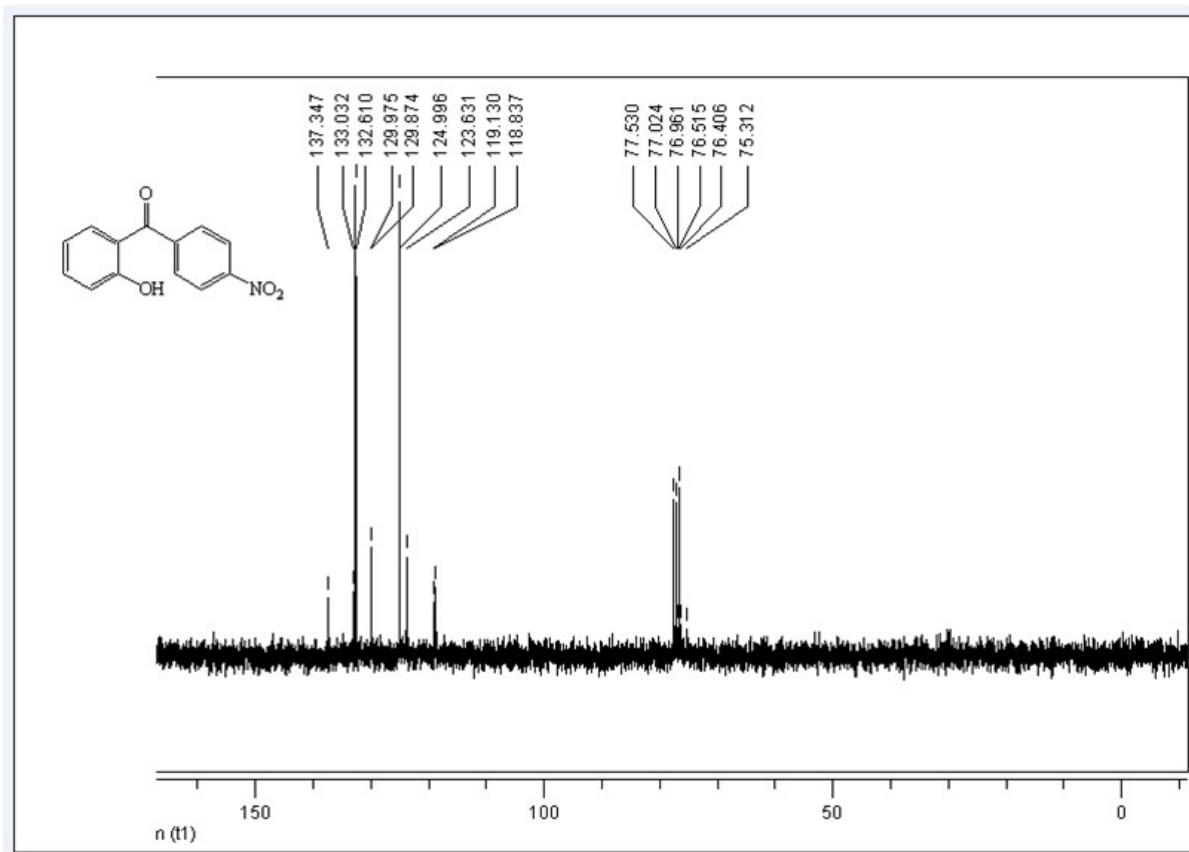
¹³C-NMR of (2-Hydroxyphenyl)(*p*-tolyl)methanone (Table 2, Entry 3)



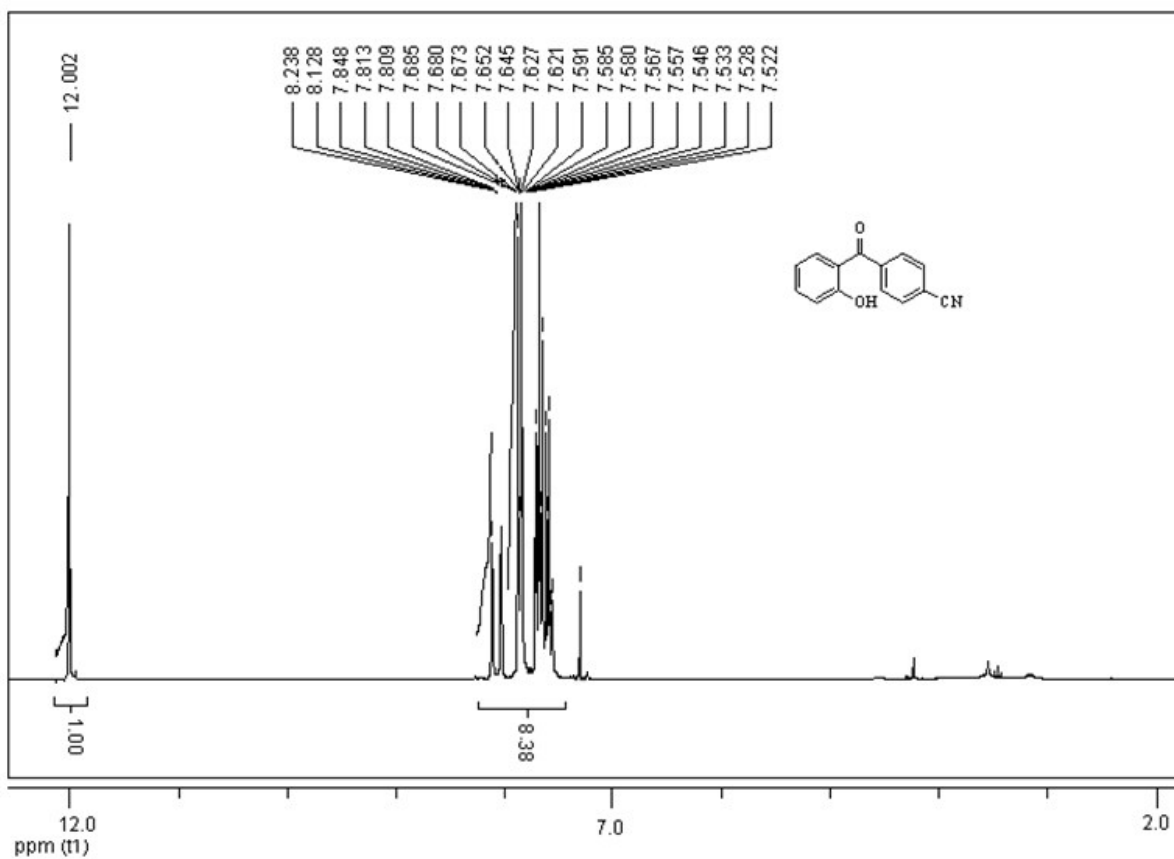
IR of (2-Hydroxyphenyl)(*p*-tolyl)methanone (Table 2, Entry 3)



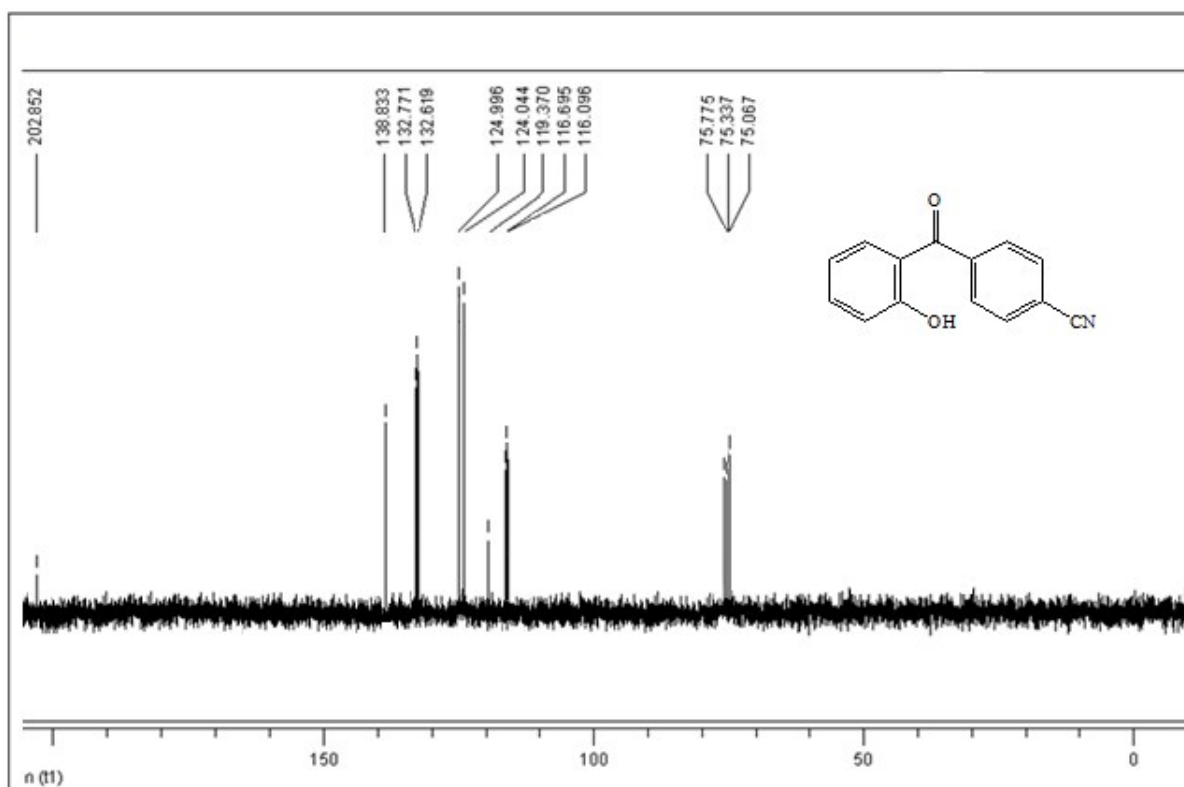
¹H-NMR of (2-Hydroxyphenyl)(4-nitrophenyl)methanone (Table 2, Entry 6)



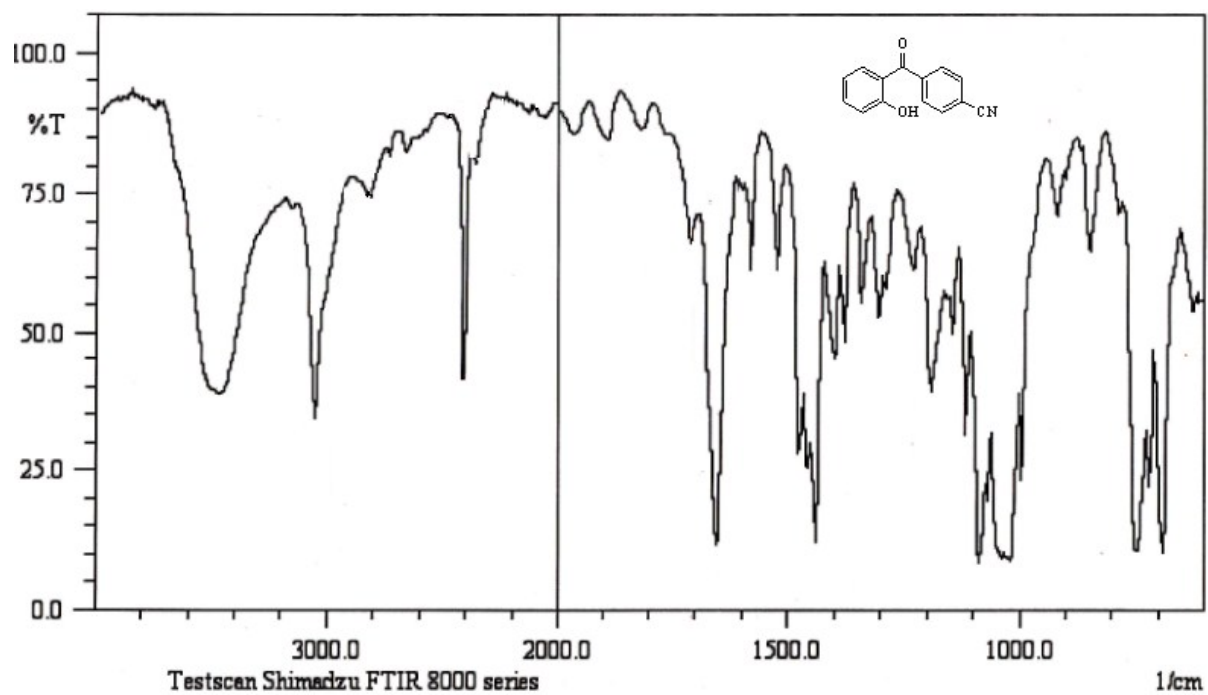
IR of (2-Hydroxyphenyl)(4-nitrophenyl)methanone (Table 2, Entry 6)



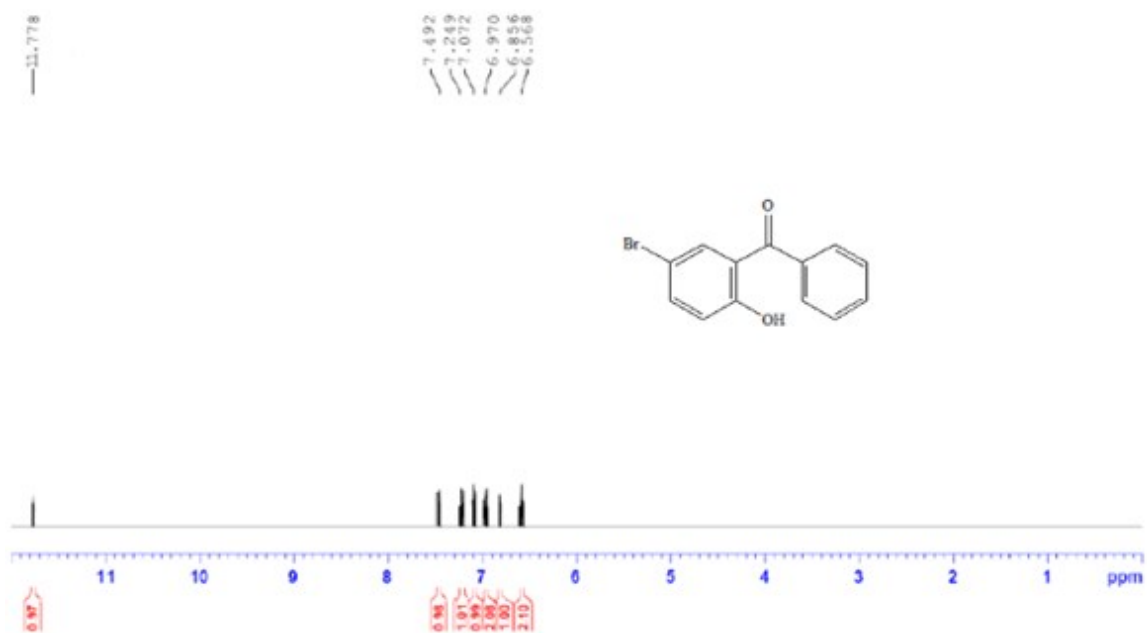
¹H-NMR of 4-(2-Hydroxybenzoyl)benzonitrile (Table 2, Entry 7)



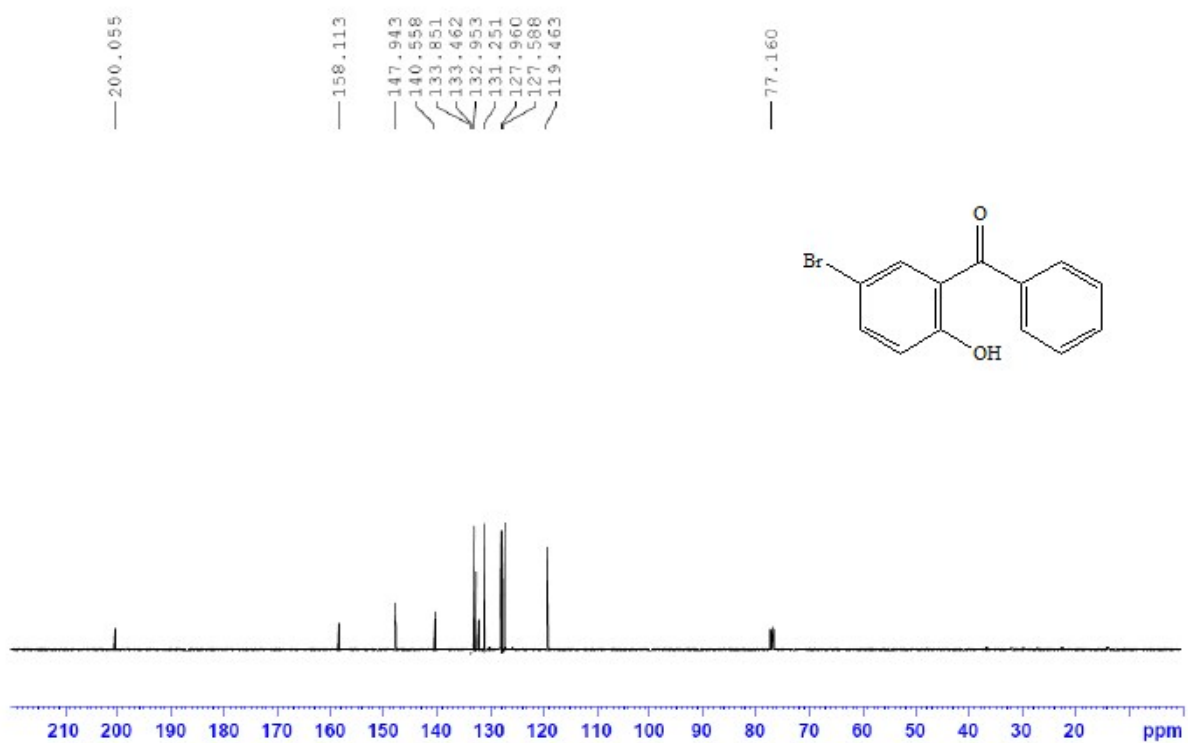
¹³C-NMR of 4-(2-Hydroxybenzoyl)benzonitrile (Table 2, Entry 7)



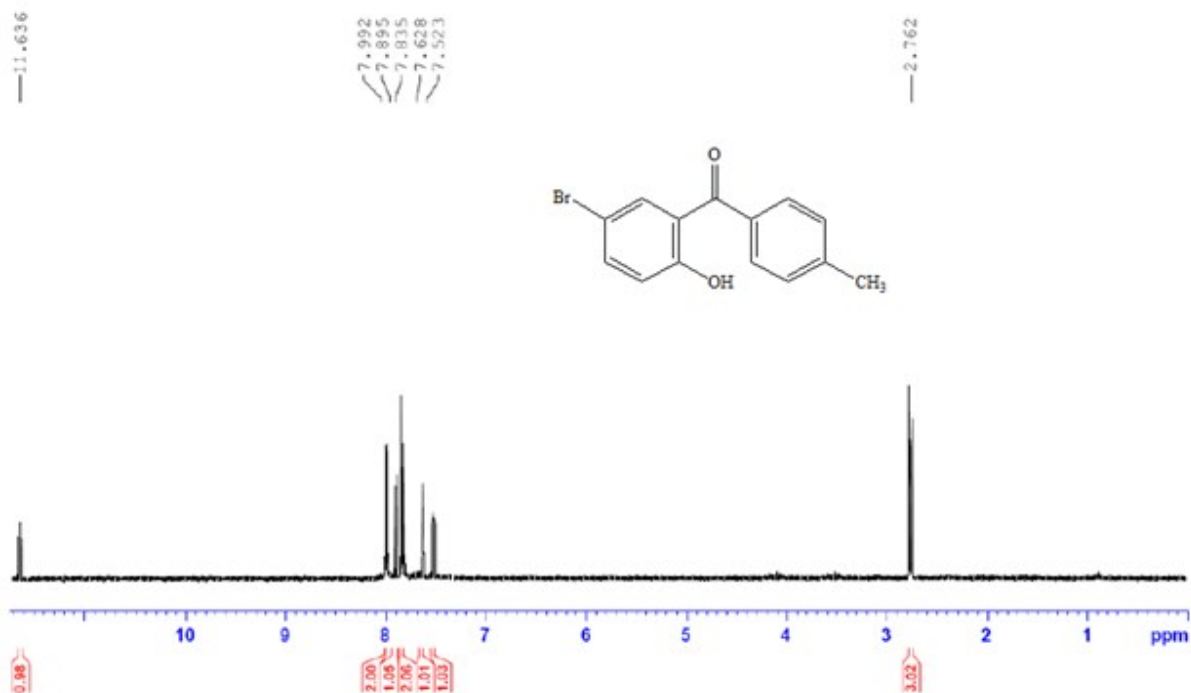
IR of 4-(2-Hydroxybenzoyl)benzonitrile (Table 2, Entry 7)



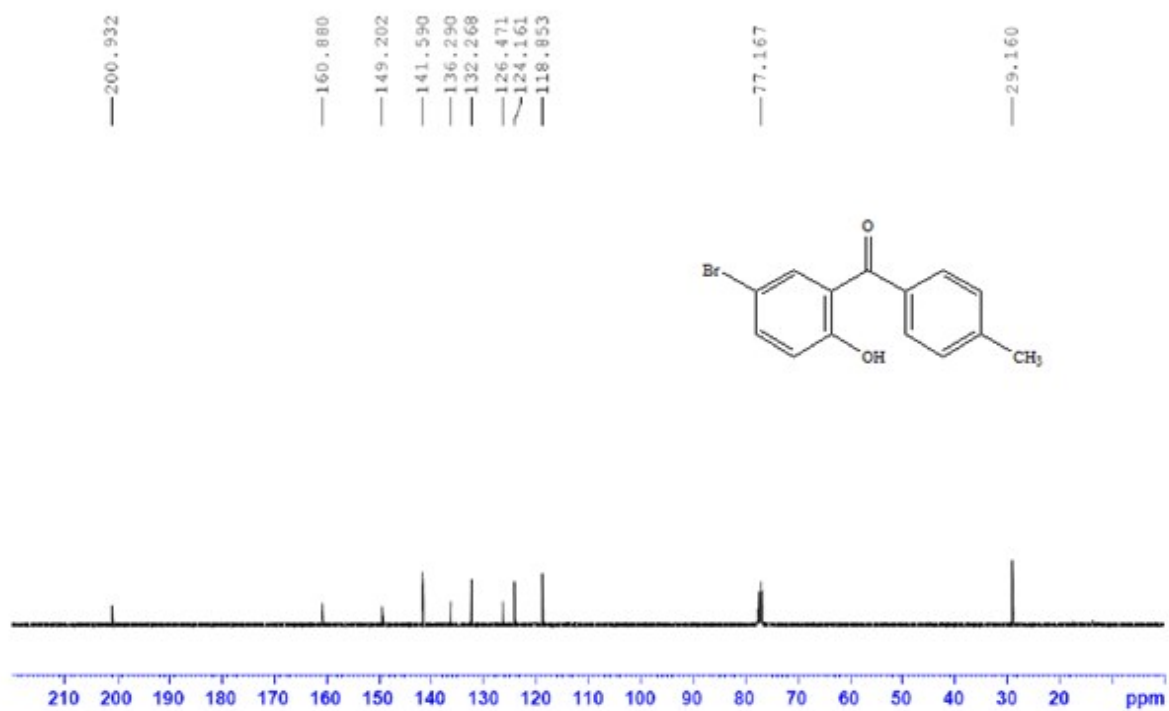
¹H-NMR of (5-bromo-2-hydroxyphenyl)(phenyl)methanone (Table 2, Entry 9)



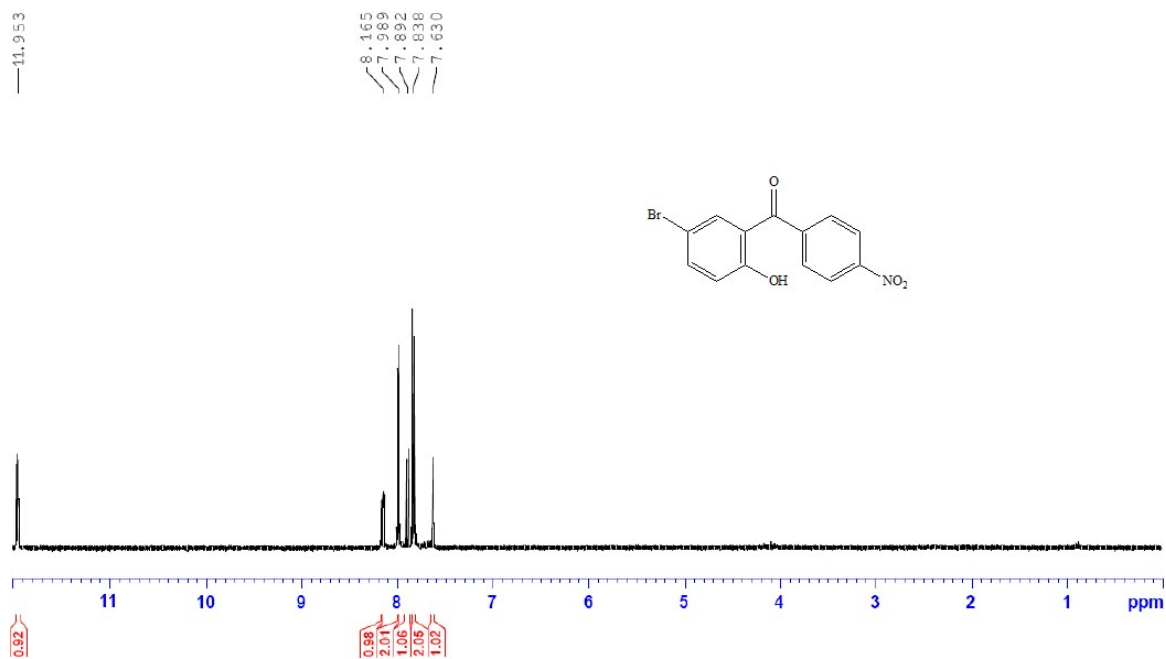
¹³C-NMR of (5-bromo-2-hydroxyphenyl)(phenyl)methanone (Table 2, Entry 9)



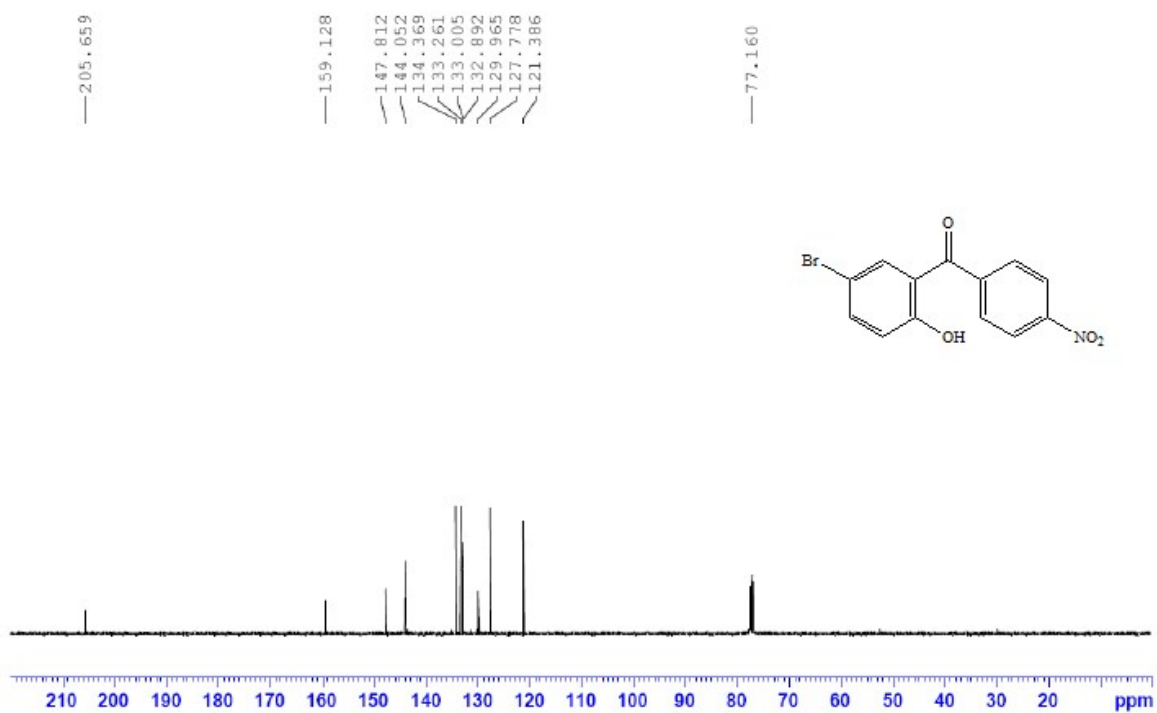
¹H-NMR of (5-bromo-2-hydroxyphenyl)(*p*-tolyl)methanone (Table 2, Entry 10)



¹³C-NMR of (5-bromo-2-hydroxyphenyl)(*p*-tolyl)methanone (Table 2, Entry 10)



¹H-NMR of (5-bromo-2-hydroxyphenyl)(4-nitrophenyl)methanone (Table 2, Entry 11)



¹³C-NMR of (5-bromo-2-hydroxyphenyl)(4-nitrophenyl)methanone (Table 2, Entry 11)