

Supporting information

Preparation and characterization of functionalized nickel ferrite nanoparticles with thioether and using as solid acid nanocatalyst for the synthesis of 2-aryl benzimidazoles

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General procedure for the synthesis of 2-aryl substituted benzimidazoles

This process involved mixing aromatic aldehyde (1 mmol), *o*-phenylenediamine 0.1 g (1 mmol), solid iodine 0.06 g (2.4 mmol), and NiFe₂O₄@SiO₂-Pr-S-nBu-SO₃H catalyst (20 mg) in acetonitrile in a 50 mL round bottom flask until well combined. The reaction flask was placed on a stirrer at room temperature for an appropriate time. Thin-layer chromatography (TLC) was used to monitor the advancement of the reaction. Once the reaction was finished, the resulting product was separated by filtration and washed several times with cold methanol. Pure benzimidazole was obtained through a recrystallization process using methanol. Synthesized compounds were determined with melting point, FT-IR, and ¹H NMR analyses.

FT-IR and ¹H NMR Spectra of synthesized 2-aryl benzimidazoles derivatives:

2-Phenyl-1H-benzimidazole (4a); Yellow solid; M.P.: 289-290 °C (lit. m.p.: 290-292 °C); IR (KBr, ν , cm⁻¹): 3432, 1612, 1437, 1498, 3075, 1252; ¹H NMR (400 MHz, DMSO-*d*₆) δ (ppm): 7.48 (t, *J* = 7.6 Hz, 1H, Ar), 7.54-7.60 (m, 4H, Ar), 8.07-8.17 (m, 4H, Ar).

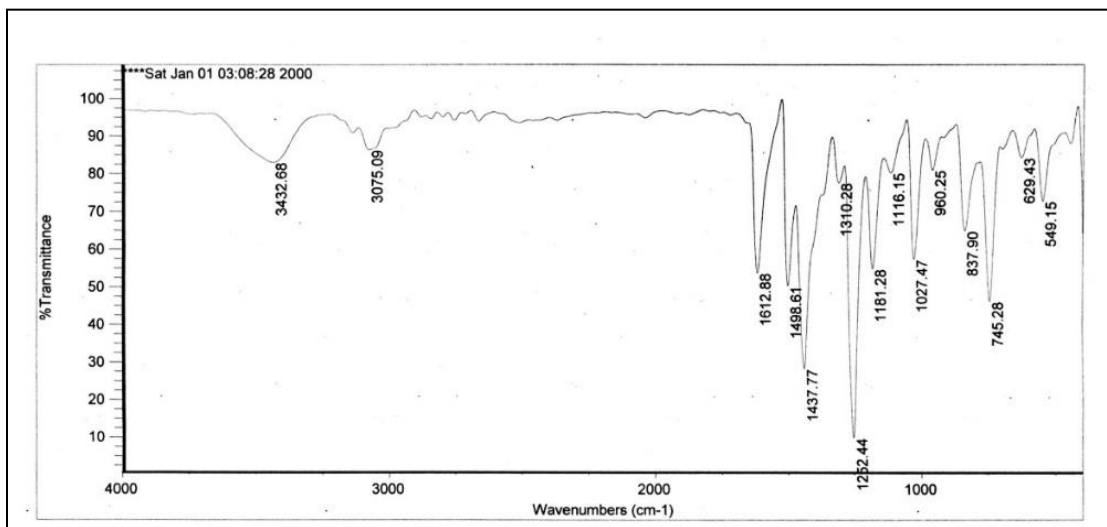


Figure 1S. The FT-IR spectrum

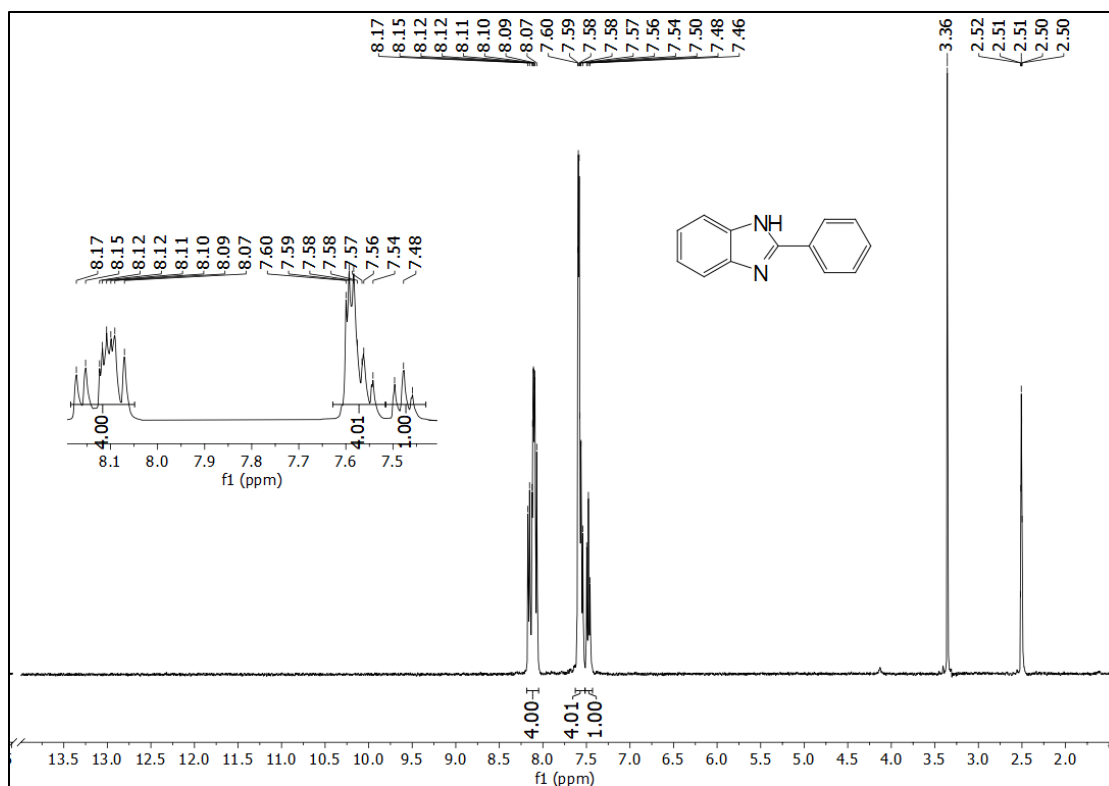


Figure 2S. The ¹H NMR spectrum

2-(2-Nitrophenyl)-1H-benzimidazole (4b): Yellow solid; 260-263 °C (lit. m.p.: 265-267 °C); IR (KBr, ν , cm^{-1}): 3438, 1603, 1530, 1437, 2917, 1337; ¹H NMR (400 MHz, DMSO-*d*₆) δ (ppm): 7.53 (s, 2H, Ar), 7.85 (s, 2H, Ar), 7.99 (q, $J = 7.9$ Hz, 1H, Ar), 8.47-8.61 (m, 2H, Ar), 9.06 (d, $J = 7.7$ Hz, 1H, Ar).

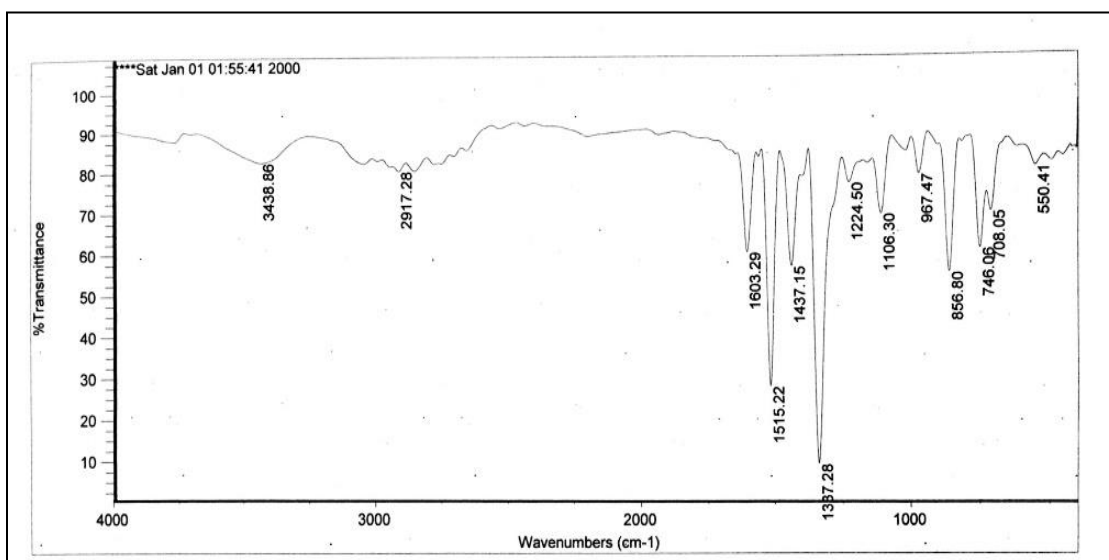


Figure 3S. The FT-IR spectrum

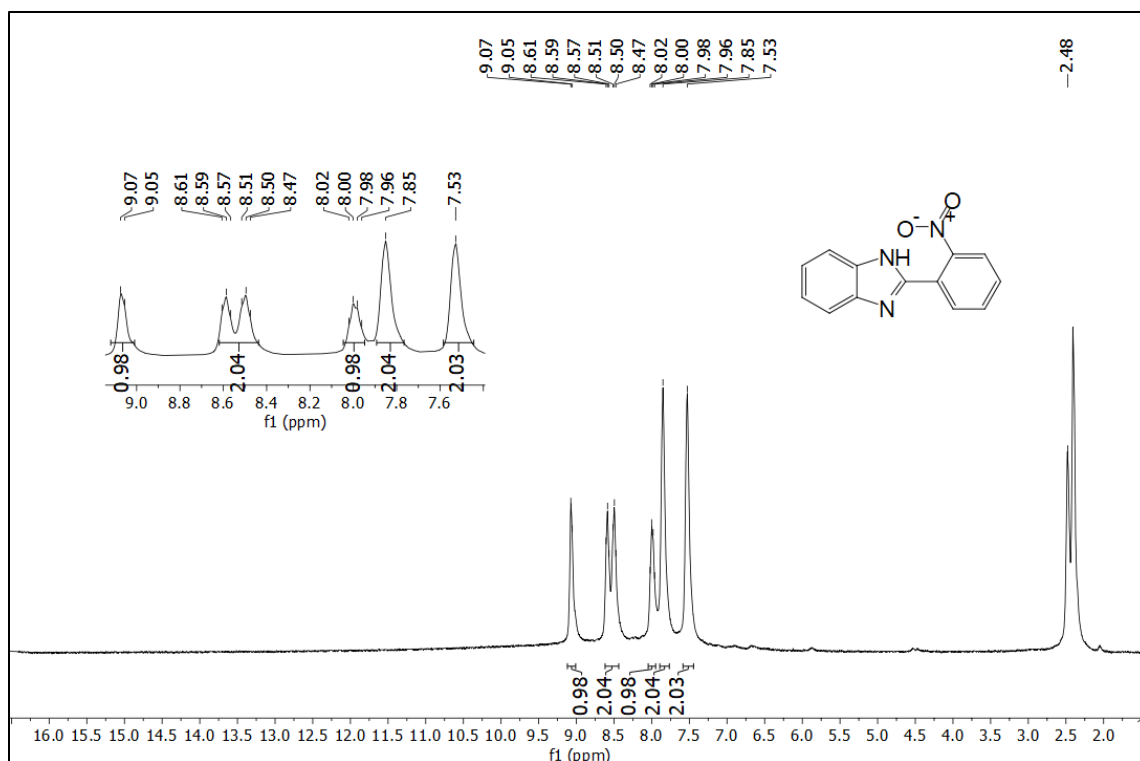


Figure 4S. The ^1H NMR spectrum

2-(4-Nitrophenyl)-1H-benzimidazole (4c); Yellow solid; M.P.: 307-309 °C (lit. m.p.: 310-312 °C); IR (KBr, ν , cm^{-1}): 3297, 1606, 1546, 1492, 1324; ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ (ppm): 7.29 (dt, $J = 7.1, 3.6$ Hz, 2H, Ar), 7.68 (dt, $J = 6.9, 3.6$ Hz, 2H, Ar), 8.43 (s, 4H, Ar).

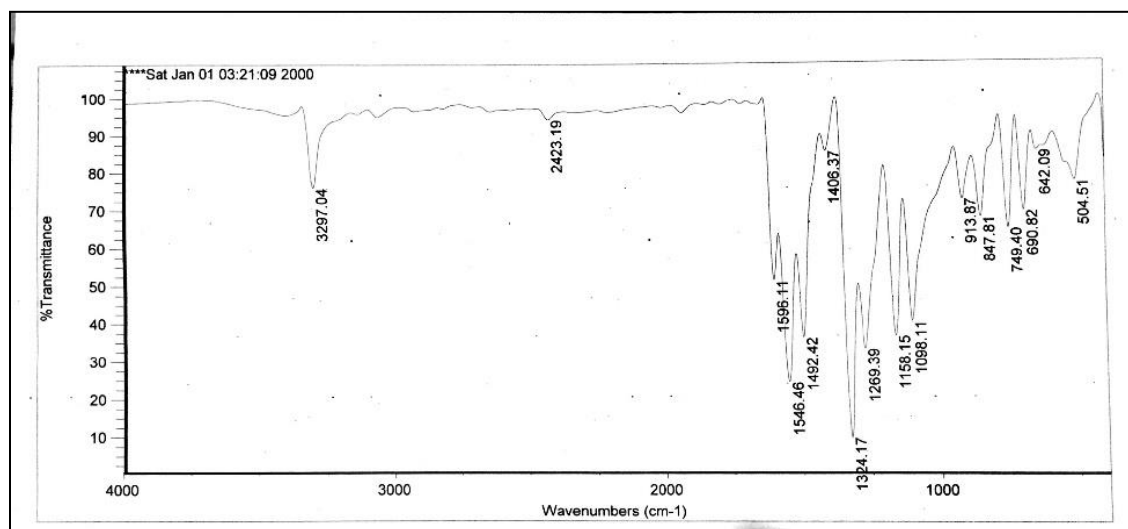


Figure 5S. The FT-IR spectrum

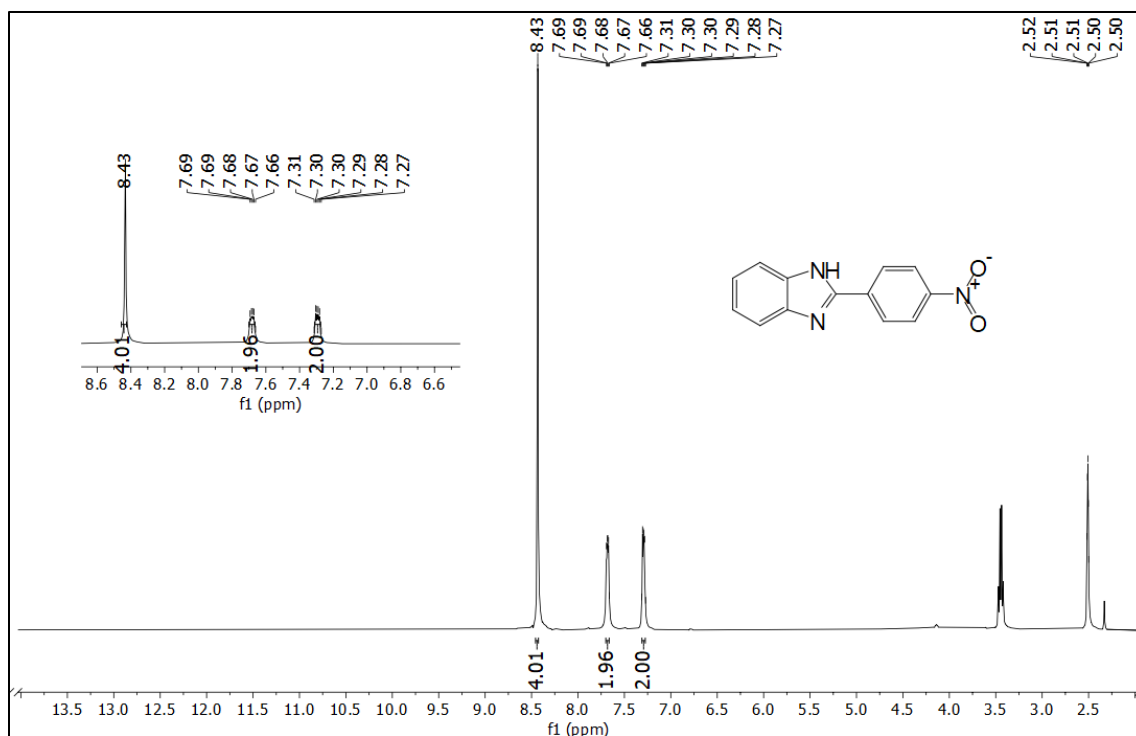


Figure 6S. The ¹H NMR spectrum

2-(2-Methylphenyl)-1H-benzimidazole (4d); Yellow solid; M.P.: 215-218 °C (lit. m.p.: 220-222 °C); IR (KBr, ν , cm^{-1}): 3049, 1624, 1447, 1403, 2969, 1360; ¹H NMR (400 MHz, DMSO-*d*₆) δ (ppm): 2.41 (s, 3H, Me), 7.19 (dd, $J = 6.2, 3.2$ Hz, 2H, Ar), 7.30 (d, $J = 7.5$ Hz, 1H, Ar), 7.43 (t, $J = 7.6$ Hz, 1H, Ar), 7.58 (s, 2H, Ar), 7.96 (d, $J = 7.6$ Hz, 1H, Ar) 8.02 (s, 1H, Ar), 12.85 (s, 1H, Ar).

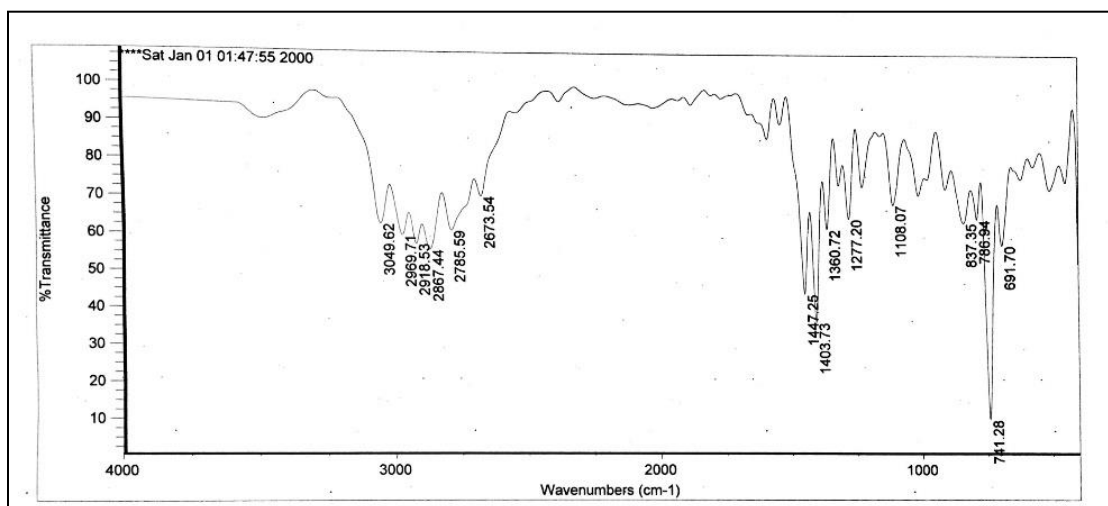


Figure 7S. The FT-IR spectrum

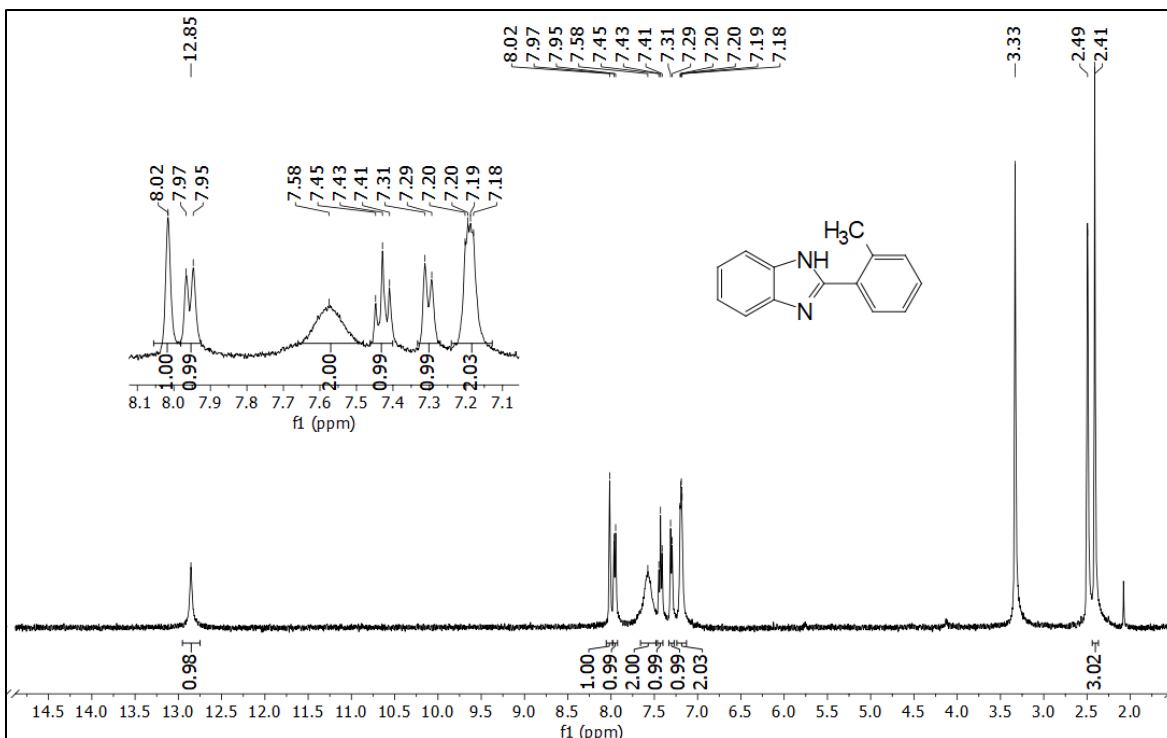


Figure 8S. The ¹H NMR spectrum

2-(4-Chlorophenyl)-1H-benzimidazole (4e); Yellow solid; M.P.: 287-290 °C (lit. m.p.: 292-294 °C); IR (KBr, ν , cm^{-1}): 3404, 1597, 1489, 1431, 3053, 1272; ¹H NMR (400 MHz, DMSO-*d*₆) δ (ppm): 7.16-7.29 (m, 2H, Ar), 7.49-7.56 (m, 1H, Ar), 7.61-7.71 (m, 3H, Ar), 8.19 (d, $J = 8.6$ Hz, 2H, Ar), 13 (s, 1H, NH).

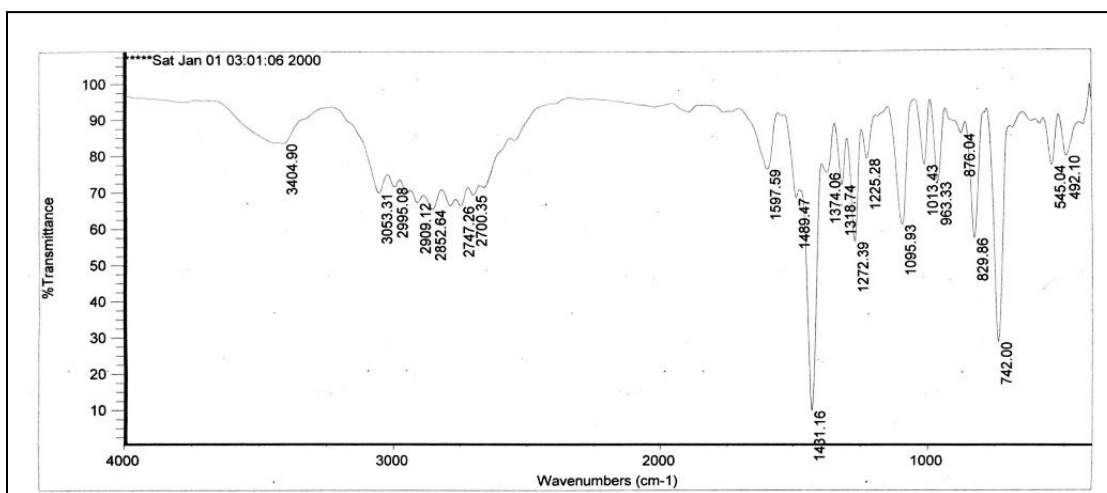


Figure 9S. The FT-IR spectrum

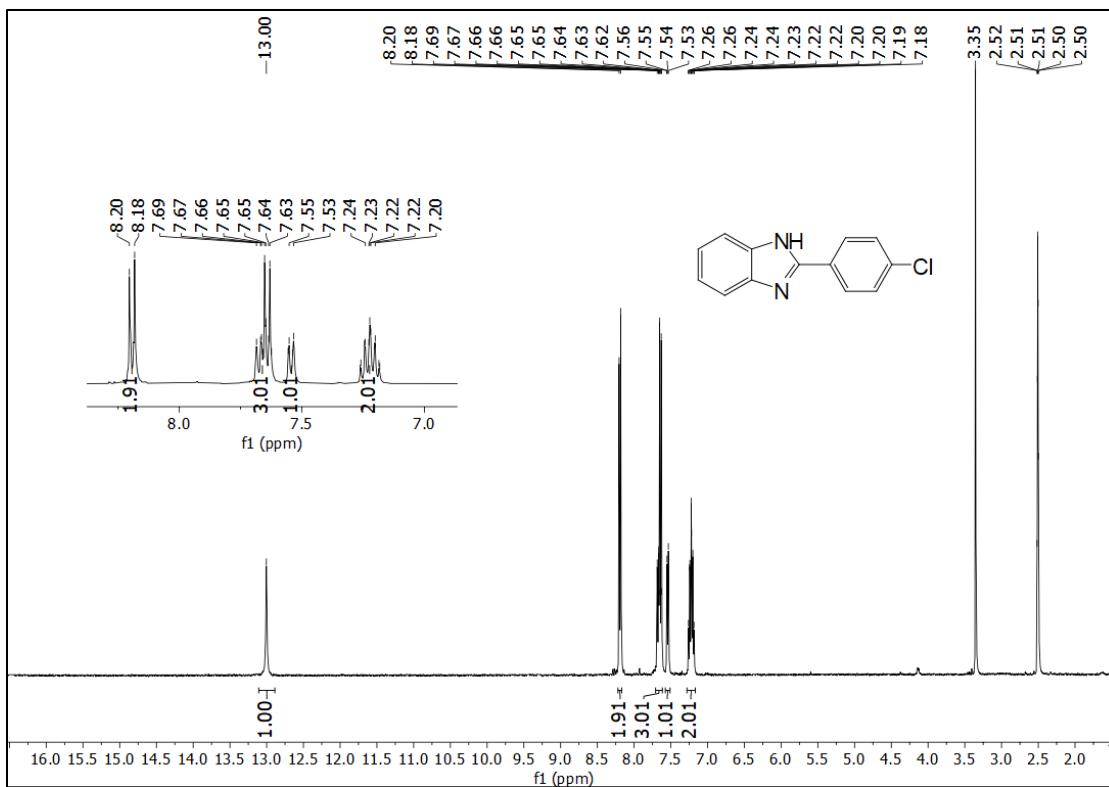


Figure 10S. The ¹H NMR spectrum

2-(3-Hydroxyphenyl)-1H-benzimidazole (4f); Yellow solid; M.P.: 250-252 °C (lit. m.p.: 245-247 °C); IR (KBr, ν , cm^{-1}): 3282, 1592, 1445, 1432, 2905, 1228; ¹H NMR (400 MHz, DMSO-*d*₆) δ (ppm): 6.88-6.91 (m, 1H, Ar), 7.18-7.22 (m, 2H, Ar), 7.34 (t, $J = 7.8$ Hz, 1H, Ar), 7.57-7.61 (m, 4H, Ar), 9.74 (s, 1H, O-H), 12.84 (s, 1H, NH).

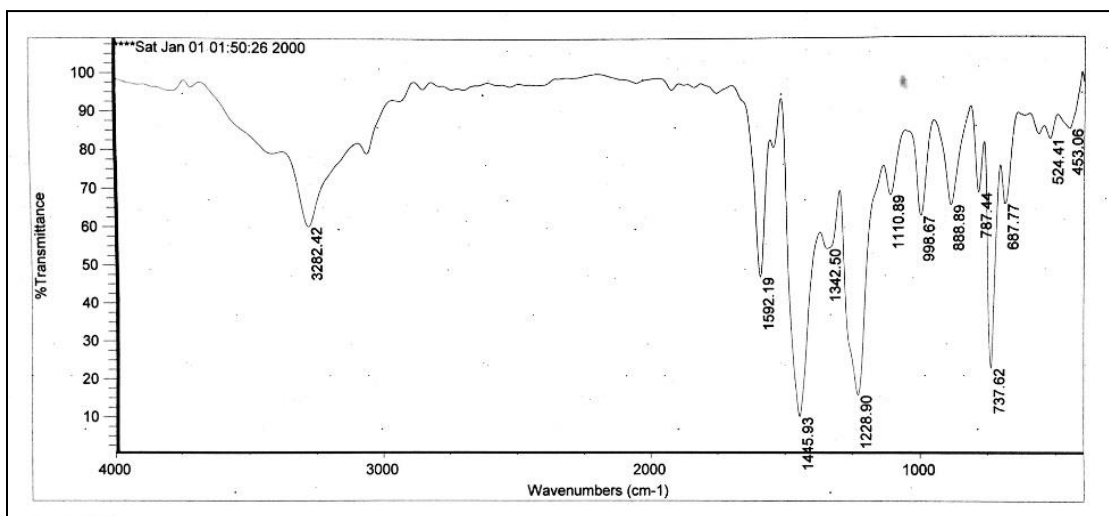


Figure 11S. The FT-IR spectrum

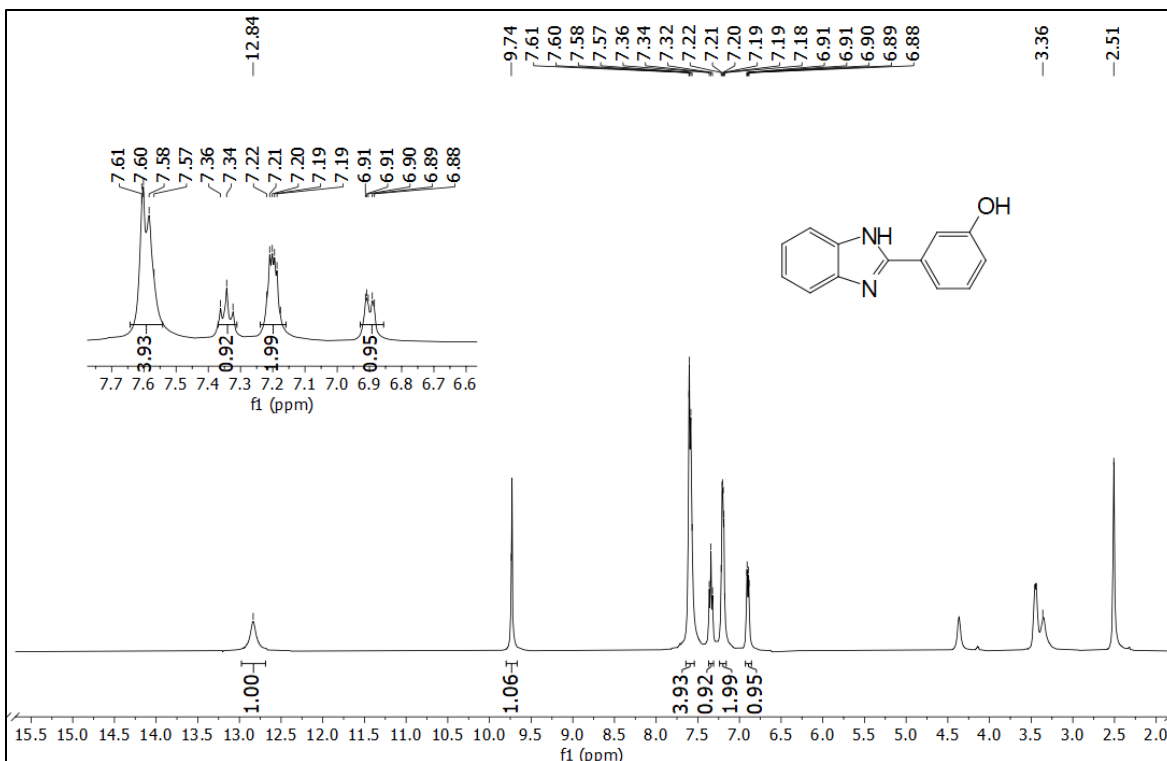


Figure 12S. The ¹H NMR spectrum

2-(2-Hydroxyphenyl)benzimidazole (4g); White solid; M.P.: 250-252 °C (lit. m.p.: 242-244 °C); IR (KBr, ν , cm^{-1}): 3245, 1592, 1533, 1489, 1264; ¹H NMR (400 MHz, DMSO-*d*₆) δ (ppm): 7.01-7.05 (m, 2H, Ar), 7.28-7-7.31 (m, 2H, Ar), 7.39 (t, $J = 7.8$ Hz, 1H, Ar), 7.64-7.68 (m, 2H, Ar), 8.06 (d, $J = 7.8$ Hz, 1H, Ar), 13.20 (s, 1H, O-H), 13.20 (s, 1H, N-H).

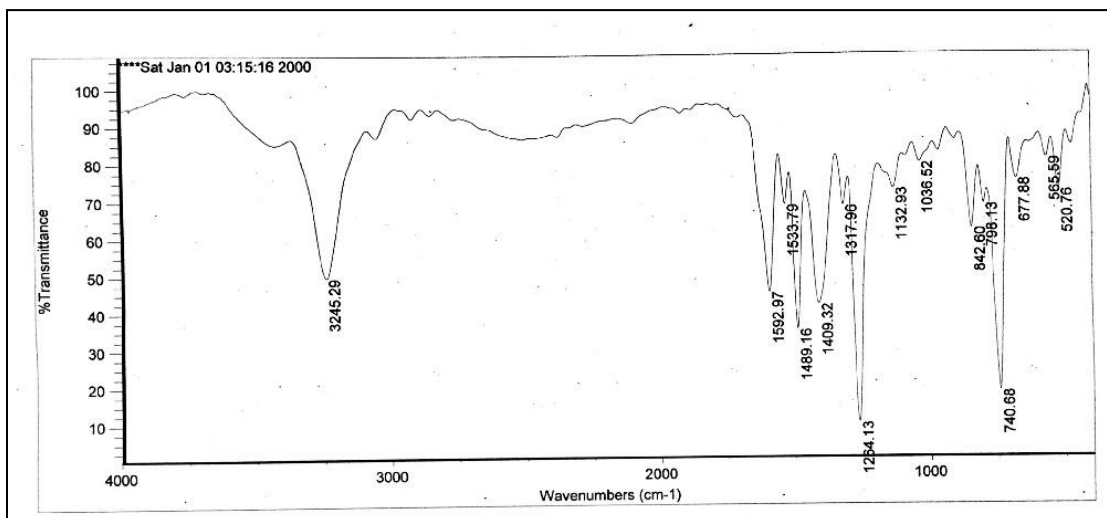


Figure 13S. The FT-IR spectrum

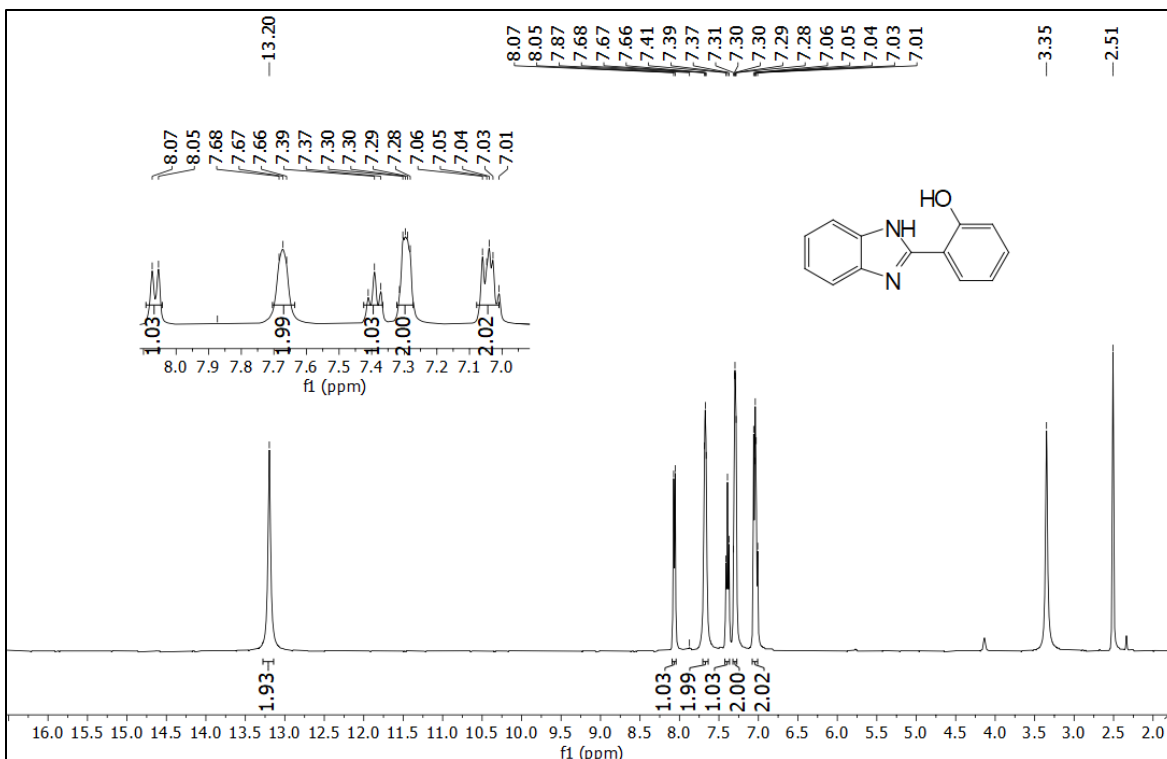


Figure 14S. The ¹H NMR spectrum

2-(P-tolyl)-1H-benzimidazole (4h); White solid; M.P.: 260-262 °C (lit. m.p.: 260-261 °C) (37); IR (KBr, ν , cm^{-1}): 3435, 1622, 1498, 1436, 3057, 2920, 1273; ¹H NMR (400 MHz, DMSO-*d*₆) δ (ppm): 2.38 (s, 3H, Me) 7.18 (dd, $J = 6.2$ Hz, 3.1 Hz, 2H, Ar), 7.34 (d, $J = 7.9$ Hz, 2H, Ar), 7.57 (s, 2H, Ar), 8.06 (d, $J = 7.9$ Hz, 2H, Ar), 12.81 (s, 1H, N-H).

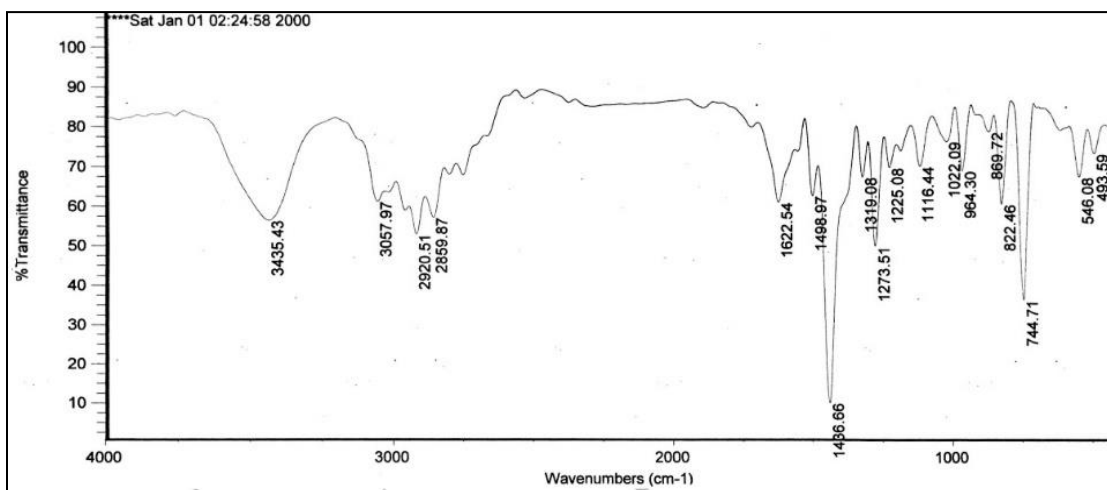


Figure 15S. The FT-IR spectrum

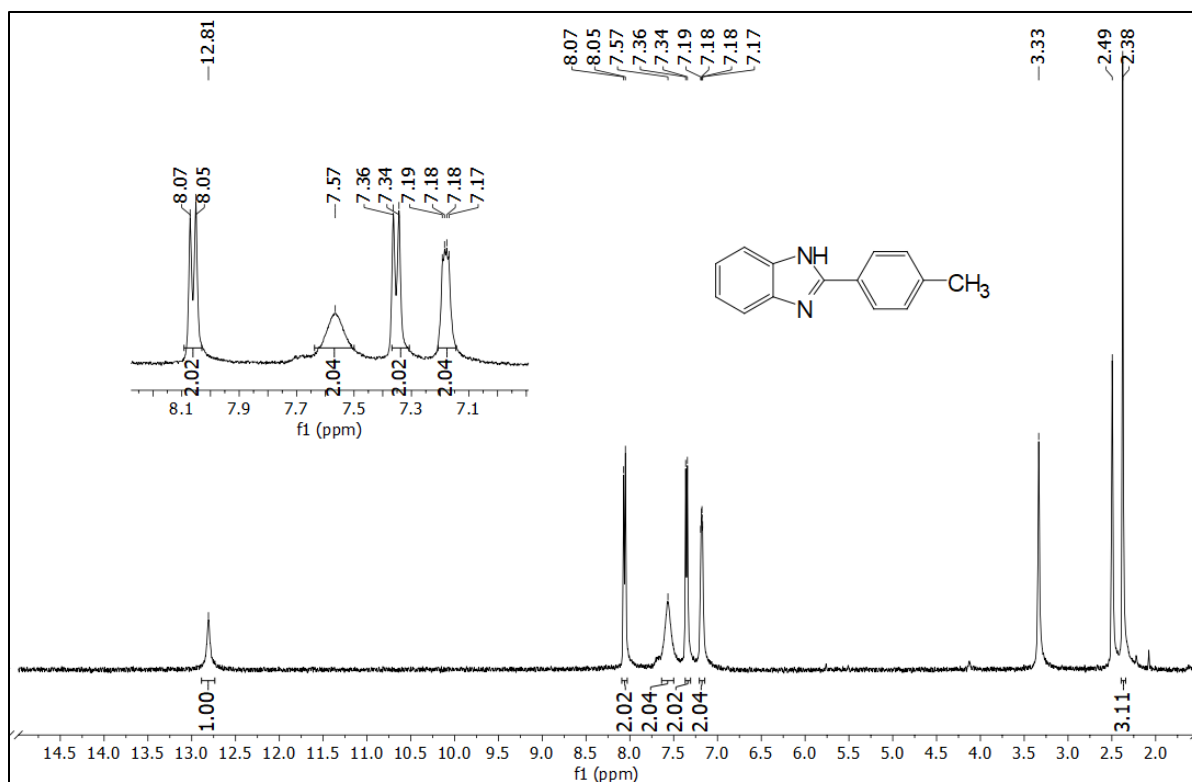


Figure 16S. The ^1H NMR spectrum

2-(4-Methoxyphenyl)-1H-benzimidazole (4i) Yellow solid; M.P.: 228-230 °C (lit. m.p.: 245-247 °C); IR (KBr, ν , cm^{-1}): 3442, 1628, 1527, 1477, 3072, 2858, 1235; ^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ (ppm): 3.79 (s, 3H, OMe), 7.05-7.16 (m, 4H, Ar), 7.52 (s, 2H, Ar), 8.06-8.12 (m, 2H, Ar), 12.71 (s, 1H, NH).

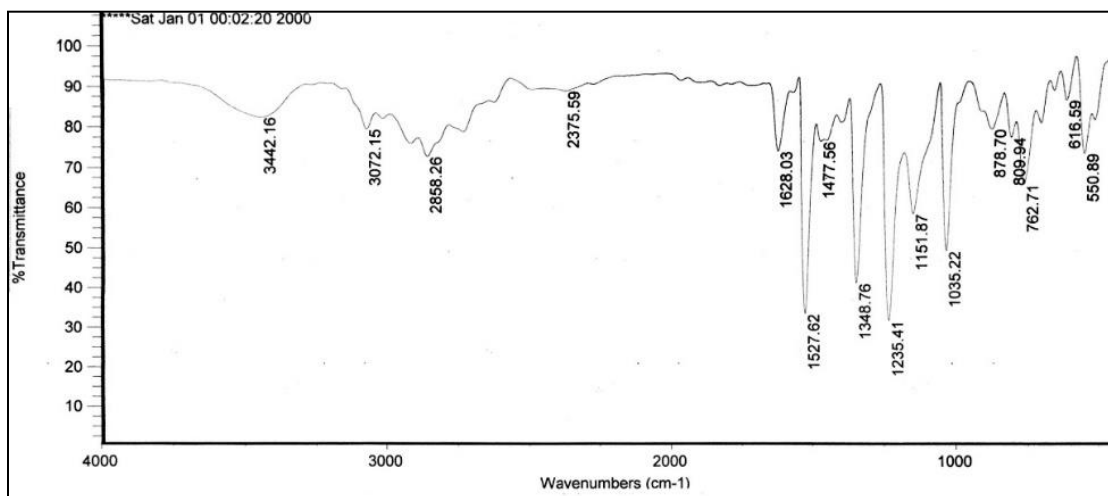


Figure 17S. The FT-IR spectrum

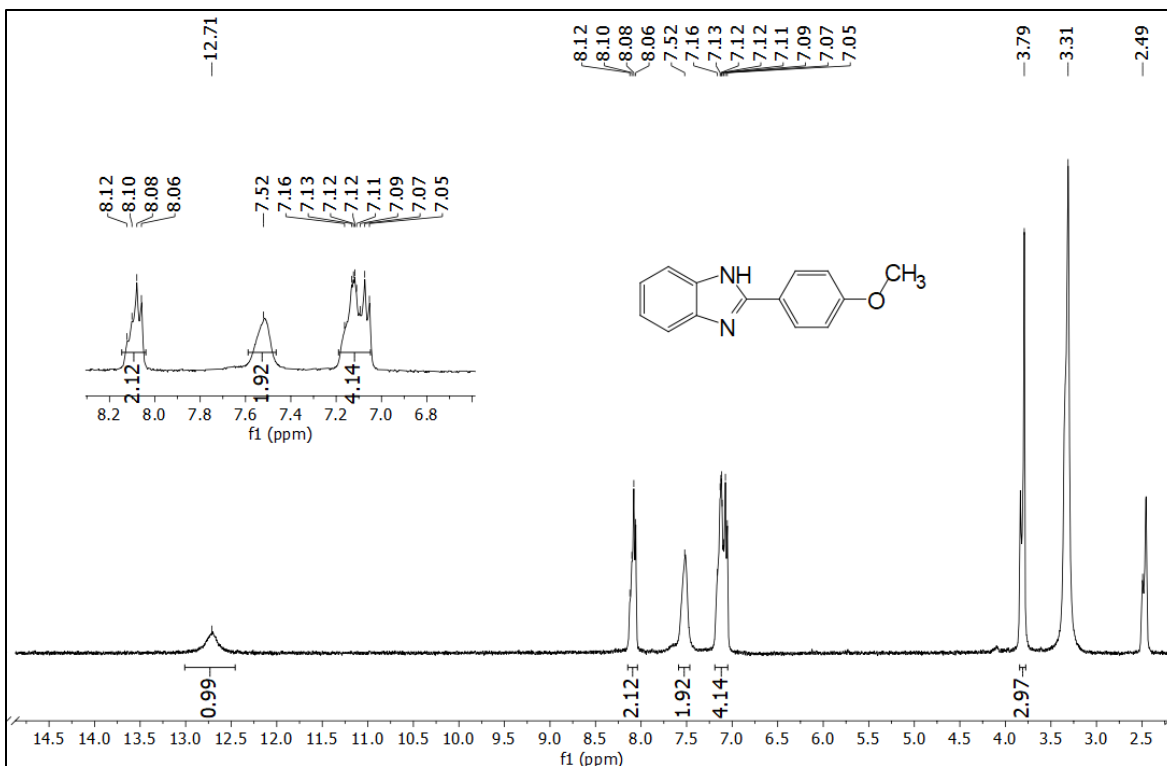


Figure 18S. The ¹H NMR spectrum

2-(5-Bromo-2-hydroxyphenyl)-1H-benzimidazole (4j); White solid; M.P.: 250-253 °C (lit. m.p.: 258-261 °C); IR (KBr, ν , cm^{-1}): 3335, 1582, 1485, 1381, 3054, 2925, 1254; ¹H NMR (400 MHz, DMSO-*d*₆) δ (ppm): 7.02 (d, J = 8.8 Hz, 1H, Ar), 7.29-7.31 (m, 2H, Ar), 7.52 (dd, J = 8.7, 2.5 Hz, 1H, Ar), 7.64-7.71 (m, 2H, Ar), 8.29 (d, J = 2.4 Hz, 1H, Ar), 13.30 (s, 1H, O-H), 13.30 (s, 1H, N-H).

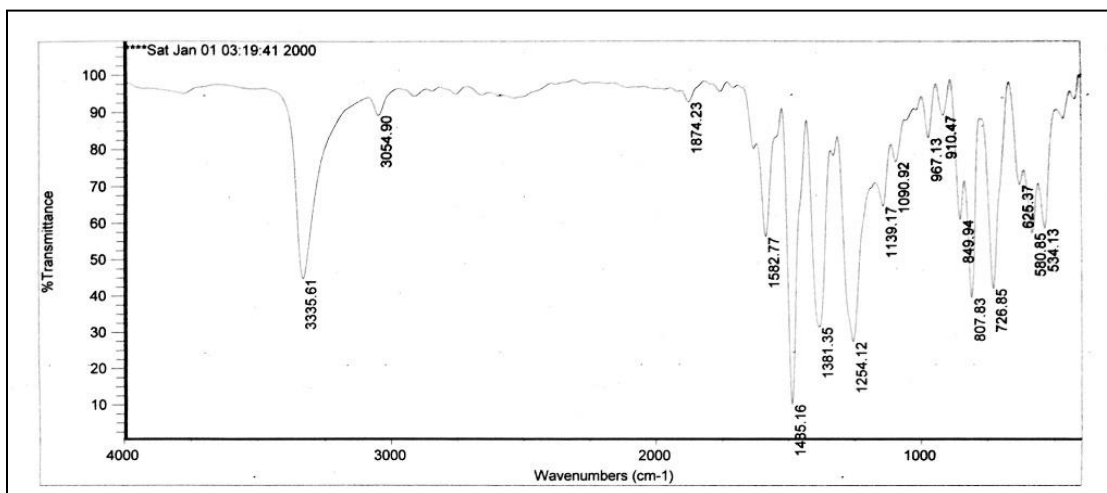


Figure 19S. The FT-IR spectrum

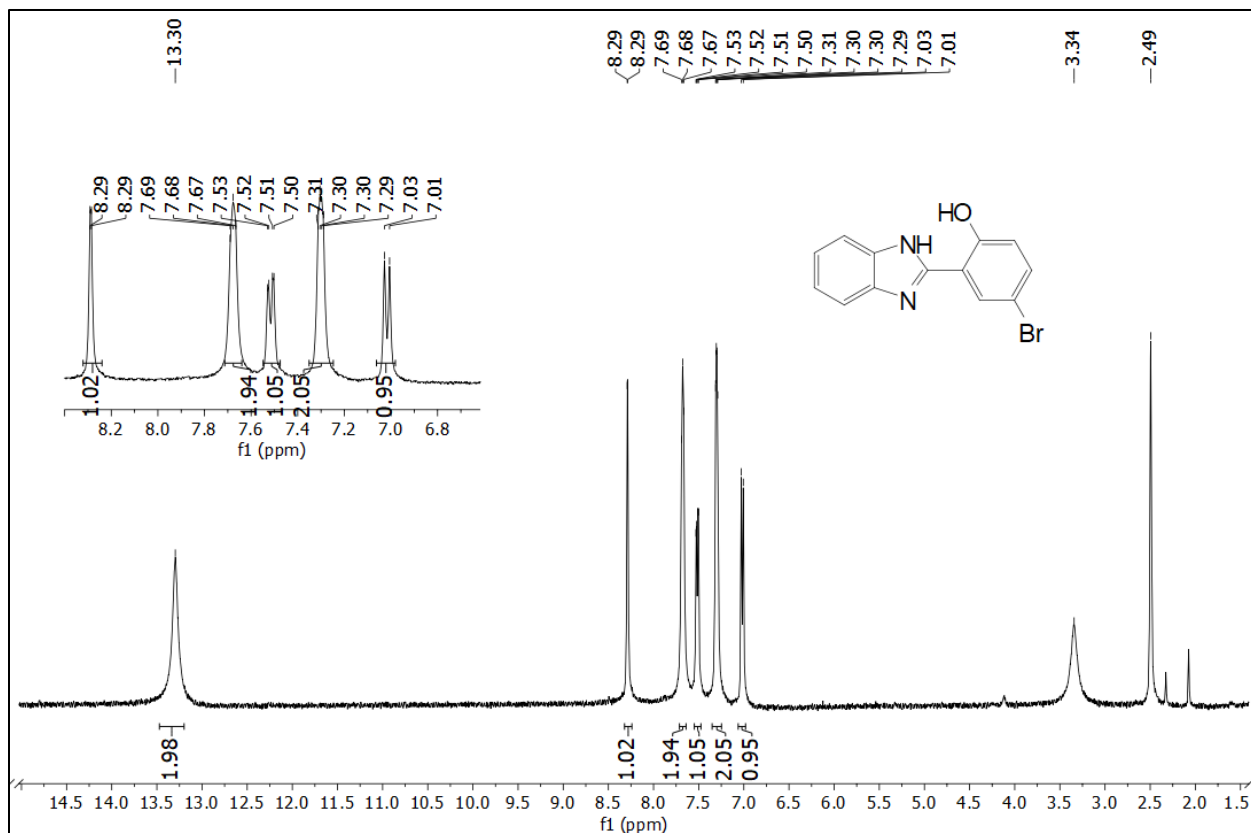


Figure 20S. The ¹H NMR spectrum

2-(3-Chlorophenyl)-1H-benzimidazole (4k); Yellow solid; M.P.: 232-234 °C (lit. m.p.: 235-237 °C); IR (KBr, ν , cm^{-1}): 3432, 1622, 1559, 1458, 3005, 1361; ¹H NMR (400 MHz, DMSO-*d*₆) δ (ppm): 7.21 (s, 2H, Ar), 7.56 (s, 4H, Ar), 8.17 (d, $J = 32.7$ Hz, 2H, Ar), 13.03 (s, 1H, N-H).

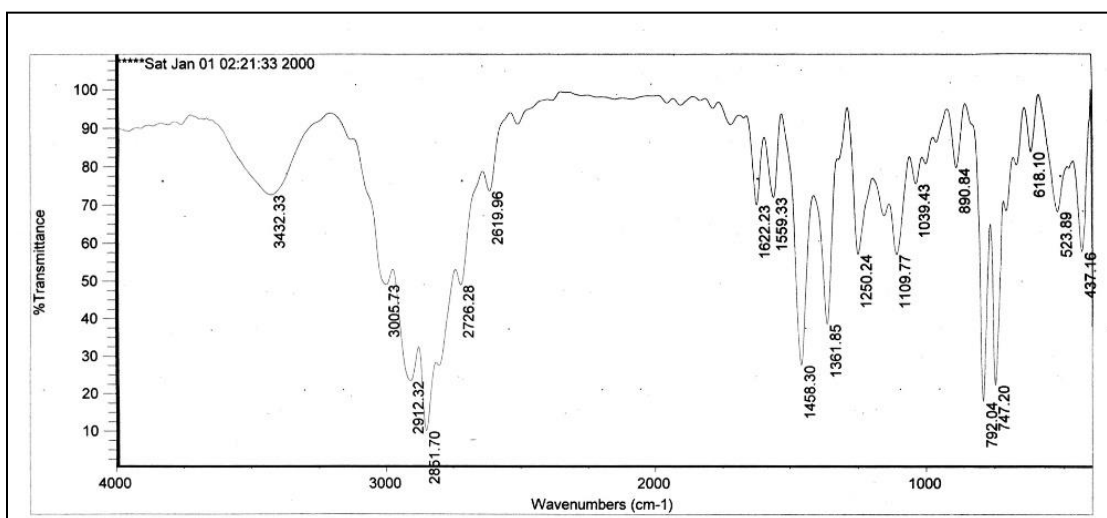


Figure 21S. The FT-IR spectrum

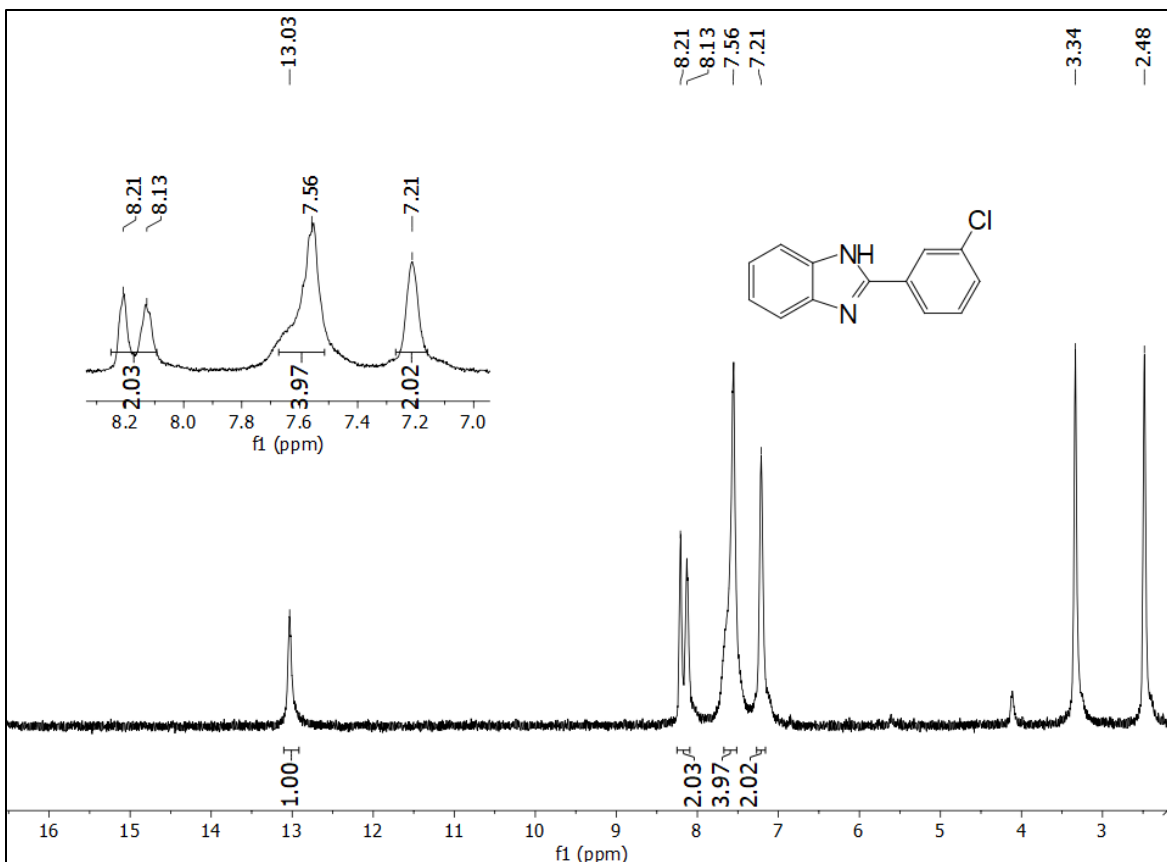


Figure 22S. The ^1H NMR spectrum

2-(4-Bromo-phenyl)-benzimidazole (4I); White solid; M.P.: 292-295 °C (lit. m.p.: 297-299 °C) (37); IR (KBr, ν , cm^{-1}): 3450, 1594, 1430, 3055, 1318; ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ (ppm): 7.20-7.24 (m, 2H, Ar), 7.61 (s, 2H, Ar), 7.77 (d, $J = 8.3$ Hz, 2H, Ar), 8.12 (d, $J = 8.4$ Hz, 2H, Ar), 13.0 (s, 1H, N-H).

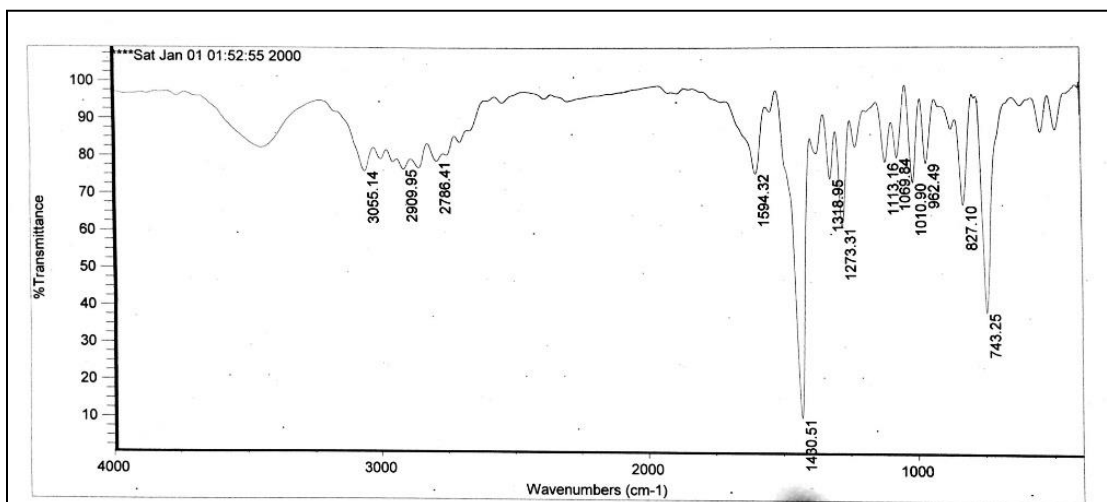


Figure 23S. The FT-IR spectrum

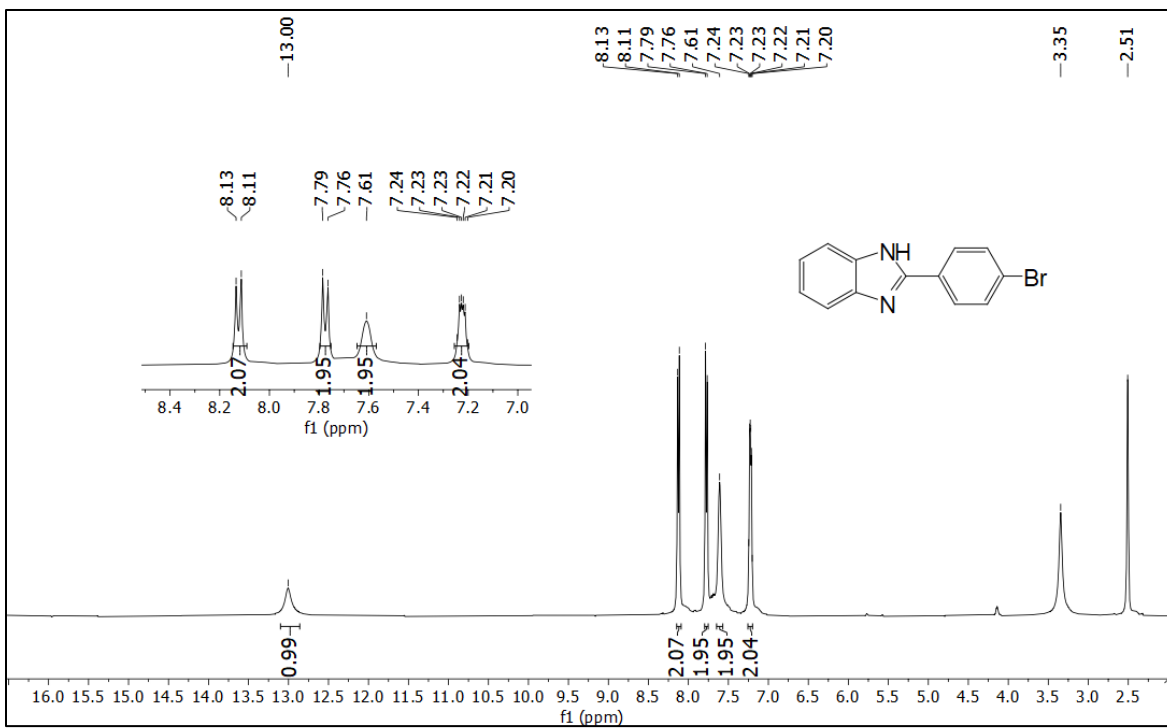


Figure 24S. The ^1H NMR spectrum