Supporting Information

Microwave promoted ligand-free Pd-catalyzed C-H arylation on the C-5 position of 1,4-disubstituted 1,2,3-triazoles

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1. General Information

All the reactions were conducted using CEM Discover-SP microwave instrument. ^1H and ^{13}C NMR spectra were recorded with a MercuryPlus 300 (300 MHz) or a Bruker ACF400 spectrometer (400 MHz) in $\text{d}_6\text{-DMSO}$ or CDCl_3 with TMS as an internal standard. All reactions were monitored by TLC with HuanghaiGF 254 silica gel coated plates. Column chromatography was carried out using 300–400 mesh silica gel at medium pressure. Infrared spectra were taken on a Bruker Vertex Series FTIR (KBr) and are reported in reciprocal centimeters (cm^{-1}). Melting points were obtained using a Büchi melting point apparatus and are uncorrected. HRMS spectra were recorded on Waters Micromass Premier Q-TOF spectrometer.

2. General Procedures for Scope of C(5)–H arylation

To a 5mL microwave reaction tube were added 1,4-disubstituted 1,2,3-triazoles **1** (0.3 mmol), aryl iodides **2** (0.36mmol, 1.2equiv), Pd(OAc)₂ (7mg, 0.03mmol, 10 mol%), *t*BuCO₂H (6mg, 0.06mmol, 20 mol%), Cs₂CO₃ (195mg, 0.6mmol, 2.0 equiv), and DMA (2.0 mL). The mixture was conducted under 10 watt microwave for 1h. After consumption of the 1,4-disubstituted 1,2,3-triazoles monitored by TLC analysis, the mixture was added with H₂O (15 mL) and extracted with EtOAc (3 × 15 mL), and the combined organic layer was washed with brine (3 × 5 mL), dried over Na₂SO₄ and concentrated under reduced pressure to afford a crude product. Purification by column chromatography on silica gel afforded the desired 1,4,5-trisubstituted 1,2,3-triazoles **3**.

3. Formation of 4,5-disubstituted 1,2,3-triazoles by debenzylation in one-pot

To a 5mL microwave reaction tube were added 1,4-disubstituted 1,2,3-triazoles **1** (0.3 mmol), aryl iodides **2** (0.36mmol, 1.2equiv), Pd(OAc)₂ (7mg, 0.03mmol, 10 mol%), *t*BuCO₂H (6mg, 0.06mmol, 20 mol%), Cs₂CO₃ (195mg, 0.6mmol, 2.0 equiv), and DMA (2.0 mL). The mixture was conducted under 10 watt microwave for 1h. After consumption of **1** monitored by TLC analysis, the mixture was added by 2 equivalents of *t*BuOK and 1 mL DMSO and conducted under 10 watt microwave for another 0.5h until the debenzylation completed. The system was then added with H₂O (15 mL) and extracted with EtOAc (3 × 15 mL). The combined organic layer was washed with brine (3 × 5 mL), dried over Na₂SO₄ and concentrated under reduced pressure to afford a crude product. Purification by column chromatography on silica gel afforded the desired 4,5-disubstituted 1,2,3-triazoles **4**.

4. Spectral data of the compounds

1-Benzyl-4,5-diphenyl-1*H*-1,2,3-triazole (3a)¹

Light yellow solid; mp 95 – 97°C; ¹H NMR (400 MHz, CDCl₃): δ = 7.60 – 7.52 (m, 2H), 7.47 (t, *J* = 7.1 Hz, 1H), 7.41 (t, *J* = 7.5 Hz, 2H), 7.33 – 7.22 (m, 6H), 7.14 (d, *J* = 7.2 Hz, 2H), 7.02 (dd, *J* = 6.2, 2.7 Hz, 2H), 5.41 (s, 2H); IR (KBr): 3416, 3129, 1896, 1779, 1602, 1499, 1450, 1362, 1246, 1179, 1074, 1000, 983, 811, 795, 778, 694, 600, 558 cm⁻¹.

1-Benzyl-4-phenyl-5-(*p*-tolyl)-1*H*-1,2,3-triazole (3b)¹

Brown oil; ¹H NMR (400 MHz, CDCl₃): δ = 7.60 – 7.55 (m, 2H), 7.27 – 7.21 (m, 8H), 7.07 – 7.01 (m, 4H), 5.39 (s, 2H), 2.42 (s, 3H); IR (KBr): 3418, 3129, 3030, 2918, 1607, 1514, 1484, 1401, 1313, 1242, 1186, 1110, 1039, 984, 918, 773, 593, 563, 512 cm⁻¹.

1-Benzyl-4-phenyl-5-(*m*-tolyl)-1*H*-1,2,3-triazole (3c)²

Brown oil; ¹H NMR (400 MHz, DMSO): δ = 7.48 (d, *J* = 7.7 Hz, 2H), 7.46 – 7.13 (m, 8H), 7.13 – 6.77 (m, 4H), 5.45 (d, *J* = 7.6 Hz, 2H), 2.28 (d, *J* = 7.5 Hz, 3H); IR (KBr): 3131, 1603, 1495, 1443, 1351, 1329, 1244, 1210, 1093, 1071, 990, 916, 886, 812, 775, 604, 577, 519 cm⁻¹.

1-Benzyl-4-phenyl-5-(*o*-tolyl)-1*H*-1,2,3-triazole (3d)²

Light brown oil; ¹H NMR (400 MHz, CDCl₃): δ = 7.54 (dd, *J* = 7.7, 1.6 Hz, 2H), 7.41 (t, *J* = 7.1 Hz, 1H), 7.32 – 7.15 (m, 8H), 7.10 (d, *J* = 7.5 Hz, 1H), 6.94 (d, *J* = 6.7 Hz, 2H), 5.33 – 5.24 (m, 2H), 1.60 (s, 3H); IR (KBr): 3128, 2308, 1607, 1244, 1073, 1026, 983, 763, 720, 696 cm⁻¹.

1-Benzyl-5-(4-chlorophenyl)-4-phenyl-1*H*-1,2,3-triazole (3e)¹

Light brown oil; ¹H NMR (400 MHz, DMSO): δ = 7.58 – 7.48 (m, 2H), 7.45 (d, *J* = 7.4 Hz, 2H), 7.36 – 7.32 (m, 3H), 7.31 – 7.26 (m, 5H), 6.99 (d, *J* = 6.7 Hz, 2H), 5.52 – 5.43 (m, 2H); IR (KBr): 3421, 3129, 1604, 1500, 1091, 838, 776, 731, 695 cm⁻¹.

1-Benzyl-5-(3-chlorophenyl)-4-phenyl-1H-1,2,3-triazole (3f)

Brown solid; mp 89-91 °C; ^1H NMR (400 MHz, DMSO): δ = 7.59 (d, J = 7.7 Hz, 1H), 7.51 (d, J = 7.7 Hz, 1H), 7.48-7.39 (m, 3H), 7.36 – 7.23 (m, 7H), 6.98 (d, J = 5.1 Hz, 2H), 5.50 (s, 2H); ^{13}C NMR (100 MHz, DMSO): δ = 143.2, 134.9, 133.2, 132.0, 130.5, 129.9, 129.3, 129.1, 128.8, 128.3, 128.1, 128.1, 127.4, 126.7, 126.7, 125.8, 51.0; IR (KBr): 3418, 3128, 2308, 1602, 1568, 1498, 1349, 1130, 1096, 990, 814, 777, 693 cm^{-1} ; HRMS Calcd for $[\text{C}_{21}\text{H}_{16}\text{ClN}_3+\text{H}]^+$: 346.1106, Found: 346.1108.

1-Benzyl-5-phenyl-4-(*p*-tolyl)-1H-1,2,3-triazole (4g)¹

Brown solid; mp 125-127 °C; ^1H NMR (400 MHz, CDCl_3): δ = 7.50 – 7.44 (m, 2H), 7.44 – 7.37 (m, 3H), 7.25 (dd, J = 4.2, 2.5 Hz, 3H), 7.14 (dd, J = 8.2, 1.3 Hz, 2H), 7.10 – 6.87 (m, 4H), 5.40 (s, 2H), 2.29 (s, 3H); IR (KBr): 3421, 3129, 1620, 1516, 1454, 1356, 1248, 1072, 984, 824, 758, 729, 696, 569, 518 cm^{-1} .

1-Benzyl-4,5-di-*p*-tolyl-1H-1,2,3-triazole (3h)³

Light brown oil; ^1H NMR (400 MHz, DMSO): δ = 7.36 (d, J = 8.1 Hz, 2H), 7.27 (dd, J = 14.4, 6.7 Hz, 5H), 7.17 (d, J = 8.0 Hz, 2H), 7.09 (d, J = 8.0 Hz, 2H), 7.02 – 6.96 (m, 2H), 5.44 (s, 2H), 2.35 (s, 3H), 2.24 (s, 3H); IR (KBr): 3424, 3132, 1603, 1523, 1492, 1356, 1314, 1241, 1216, 1181, 1111, 1041, 983, 719, 702, 608, 563, 515 cm^{-1} .

1-Benzyl-5-(*m*-tolyl)-4-(*p*-tolyl)-1H-1,2,3-triazole (3i)

Light brown oil; ^1H NMR (400 MHz, DMSO): δ = 7.43 – 7.32 (m, 4H), 7.31 – 7.22 (m, 3H), 7.16 – 7.04 (m, 4H), 7.04 – 6.91 (m, 2H), 5.43 (s, 2H), 2.28 (s, 3H), 2.24 (s, 3H); ^{13}C NMR (100 MHz, DMSO): δ = 142.8, 138.0, 136.5, 135.2, 133.1, 129.8, 129.8, 128.6, 128.5, 128.4, 128.0, 127.5, 127.3, 126.7, 126.5, 125.6, 50.7, 20.3, 20.2; IR (KBr): 3419, 3129, 1610, 1514, 1000, 823, 731, 703, 687, 521 cm^{-1} ; HRMS Calcd for $[\text{C}_{23}\text{H}_{21}\text{N}_3+\text{H}]^+$: 340.1808, Found: 340.1809.

1-Benzyl-5-(4-chlorophenyl)-4-(*p*-tolyl)-1H-1,2,3-triazole (3j)

Light brown oil; ^1H NMR (400 MHz, CDCl_3): δ = 7.46 – 7.35 (m, 4H), 7.28 – 7.23 (m, 3H), 7.18 – 6.93 (m, 6H), 5.40 (s, 2H), 2.30 (d, J = 4.8 Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ = 144.8, 137.7, 135.8, 135.2, 132.2, 131.4, 129.4, 129.2, 128.7, 128.2, 127.6, 127.3, 126.6, 126.0, 52.0, 21.1; IR (KBr): 3419, 3129, 1621, 1515, 1480, 1091, 984, 824, 734, 517 cm^{-1} ; HRMS Calcd for $[\text{C}_{22}\text{H}_{18}\text{ClN}_3+\text{H}]^+$: 360.1262, Found: 360.1260.

1-Benzyl-4-(4-methoxyphenyl)-5-phenyl-1*H*-1,2,3-triazole (3k)¹

White solid; mp 120-121 °C; ¹H NMR (400 MHz, CDCl₃): δ = 7.50 – 7.38 (m, 5H), 7.25 (dd, *J* = 5.4, 2.6 Hz, 3H), 7.17 – 7.09 (m, 2H), 7.02 (dd, *J* = 6.6, 2.9 Hz, 2H), 6.82 – 6.76 (m, 2H), 5.40 (s, 2H), 3.76 (s, 3H); IR (KBr): 3130, 2837, 1612, 1563, 1515, 1482, 1352, 1302, 1109, 1036, 982, 841, 816, 791, 765, 726, 589, 570, 633 cm⁻¹.

1-Benzyl-4-(4-methoxyphenyl)-5-(*p*-tolyl)-1*H*-1,2,3-triazole (3l)³

Light yellow oil; ¹H NMR (400 MHz, CDCl₃): δ = 7.52 – 7.46 (m, 2H), 7.27 – 7.18 (m, 5H), 7.08 – 6.97 (m, 4H), 6.82 – 6.71 (m, 2H), 5.38 (s, 2H), 3.76 (s, 3H), 2.41 (s, 3H); IR (KBr): 3060, 2938, 2837, 1614, 1566, 1521, 1452, 1302, 1256, 1178, 1129, 1109, 984, 731, 695, 583, 563, 534, 456 cm⁻¹.

1-Benzyl-4-(4-methoxyphenyl)-5-(*m*-tolyl)-1*H*-1,2,3-triazole (3m)

Light yellow solid; mp 108-110 °C; ¹H NMR (400 MHz, CDCl₃): δ = 7.53 – 7.44 (m, 2H), 7.32 – 7.22 (m, 5H), 7.07 – 6.99 (m, 2H), 6.94 (d, *J* = 7.1 Hz, 1H), 6.87 (s, 1H), 6.84 – 6.72 (m, 2H), 5.37 (s, 2H), 3.76 (s, 3H), 2.29 (s, 3H); ¹³C NMR (100 MHz, CDCl₃): δ = 159.1, 144.2, 138.8, 135.5, 133.2, 130.6, 130.2, 128.9, 128.5, 128.0, 127.8, 127.8, 127.5, 127.1, 123.6, 113.8, 55.1, 52.0, 21.2; IR (KBr): 3419, 3131, 2956, 2835, 1614, 1562, 1455, 1352, 1175, 1109, 1038, 996, 841, 815, 794, 705, 675, 594, 576 cm⁻¹; HRMS Calcd for [C₂₃H₂₁N₃O+H]⁺: 356.1757, Found: 356.1755.

1-Benzyl-4-(4-methoxyphenyl)-5-(*o*-tolyl)-1*H*-1,2,3-triazole (3n)

Light brown solid; mp 105-106 °C; ¹H NMR (400 MHz, CDCl₃): δ = 7.54 – 7.43 (m, 2H), 7.40 (td, *J* = 7.5, 1.2 Hz, 1H), 7.29 – 7.25 (m, 1H), 7.25 – 7.14 (m, 4H), 7.09 (dd, *J* = 7.5, 0.9 Hz, 1H), 6.93 (dd, *J* = 7.8, 1.4 Hz, 2H), 6.83 – 6.69 (m, 2H), 5.36 – 5.22 (m, 2H), 3.74 (s, 3H), 1.60 (s, 3H). ¹³C NMR (100 MHz, CDCl₃): δ = 159.1, 144.3, 138.4, 134.7, 131.9, 130.6, 130.3, 129.9, 128.4, 128.1, 127.9, 127.4, 126.9, 126.43, 123.8, 113.8, 55.0, 52.1, 19.0; IR (KBr): 3130, 2835, 1612, 1564, 1515, 1481, 1345, 1306, 1180, 1027, 982, 838, 789, 770, 697, 610, 577, 532 cm⁻¹; HRMS Calcd for [C₂₃H₂₁N₃O+H]⁺: 356.1757, Found: 356.1756.

1-Benzyl-5-(4-chlorophenyl)-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (3o)

Light brown oil; ¹H NMR (400 MHz, CDCl₃): δ = 7.49 – 7.44 (m, 2H), 7.43 – 7.36 (m, 2H), 7.26 (td, *J* = 4.4, 2.9 Hz, 3H), 7.16 – 6.95 (m, 4H), 6.81 (d, *J* = 8.9 Hz, 2H), 5.40 (s, 2H), 3.77 (d, *J* = 4.1 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃): δ = 159.2, 144.6, 135.8, 135.2, 131.8, 131.4, 129.4, 128.7, 128.2, 128.0, 127.3, 126.4, 123.1, 113.9, 55.1, 52.0; IR (KBr): 3418, 3129, 2836, 2309, 1617, 1515, 1453, 1252, 1176, 1107, 1030, 836, 733,

699, 616, 566, 518 cm^{-1} ; HRMS Calcd for $[\text{C}_{22}\text{H}_{18}\text{ClN}_3\text{O}+\text{H}]^+$: 376.1211, Found: 376.1212.

1-Benzyl-4-(4-fluorophenyl)-5-phenyl-1H-1,2,3-triazole (3p)¹

Light brown oil; ^1H NMR (400 MHz, DMSO): δ = 7.61 – 7.44 (m, 5H), 7.31 (d, J = 6.4 Hz, 2H), 7.30 – 7.20 (m, 3H), 7.16 (t, J = 9.0 Hz, 2H), 7.07 – 6.90 (m, 2H), 5.47 (s, 2H); IR (KBr): 3418, 3127, 1610, 1514, 1454, 1352, 1228, 1158, 1025, 984, 841, 800, 729, 581, 525 cm^{-1} .

1-Benzyl-4-(4-fluorophenyl)-5-(*p*-tolyl)-1H-1,2,3-triazole (3q)

Yellow solid; mp 97-99 $^{\circ}\text{C}$; ^1H NMR (400 MHz, CDCl_3): δ = 7.58 – 7.48 (m, 2H), 7.28 – 7.21 (m, 5H), 7.15 – 7.02 (m, 3H), 7.01 (s, 1H), 6.99 – 6.84 (m, 2H), 5.39 (s, 2H), 2.43 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ = 163.5, 161.0, 143.6, 139.8, 135.4, 133.7, 129.9, 129.6, 128.6, 128.4, 128.1, 127.4, 124.4, 115.2, 51.9, 21.4; IR (KBr): 3066, 3028, 1607, 1518, 1491, 1453, 1351, 1302, 1181, 1123, 1096, 984, 849, 713, 619, 566, 529, 464 cm^{-1} ; HRMS Calcd for $[\text{C}_{22}\text{H}_{18}\text{FN}_3+\text{H}]^+$: 344.1558, Found: 344.1555.

1-Benzyl-4-(4-fluorophenyl)-5-(*m*-tolyl)-1H-1,2,3-triazole (3r)

Yellow solid; mp 96-98 $^{\circ}\text{C}$; ^1H NMR (400 MHz, CDCl_3): δ = 7.54 (dd, J = 8.9, 5.4 Hz, 2H), 7.33 – 7.22 (m, 5H), 7.03 (dd, J = 4.1, 1.8 Hz, 2H), 7.01 – 6.90 (m, 3H), 6.87 (s, 1H), 5.38 (s, 2H), 2.30 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ = 163.4, 161.0, 143.5, 138.9, 135.3, 133.7, 130.5, 130.4, 129.0, 128.5, 128.3, 128.0, 127.5, 127.0, 115.4, 115.2, 52.0, 21.2; IR (KBr): 3129, 3028, 2943, 1588, 1511, 1433, 1346, 1223, 1094, 1000, 880, 799, 705, 588, 530, 438 cm^{-1} ; HRMS Calcd for $[\text{C}_{22}\text{H}_{18}\text{FN}_3+\text{H}]^+$: 344.1558, Found:

344.1560.

1-Benzyl-5-(4-chlorophenyl)-4-(4-fluorophenyl)-1H-1,2,3-triazole (3s)

Brown oil; ^1H NMR (400 MHz, CDCl_3): δ = 7.53 – 7.47 (m, 2H), 7.46 – 7.33 (m, 2H), 7.29 – 7.23 (m, 3H), 7.13 (dd, J = 8.2, 1.3 Hz, 1H), 7.11 – 7.00 (m, 3H), 7.00 – 6.87 (m, 2H), 5.40 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ = 136.1, 135.2, 135.0, 131.3, 130.0, 129.7, 129.6, 129.2, 128.8, 128.5, 128.1, 127.4, 127.3, 115.2, 52.2; IR (KBr): 3128, 3029, 1607, 1481, 1350, 1221, 1158, 1092, 1014, 984, 844, 763, 700, 570, 463 cm^{-1} ; HRMS Calcd for $[\text{C}_{21}\text{H}_{15}\text{ClFN}_3+\text{H}]^+$: 364.1011, Found: 364.1010.

1-Benzyl-4-(4-chlorophenyl)-5-phenyl-1H-1,2,3-triazole (3t)⁴

Light yellow solid; mp 141-143 $^{\circ}\text{C}$; ^1H NMR (400 MHz, DMSO): δ = 7.54 – 6.48 (m, 3H), 7.45 (d, J = 8.8 Hz, 2H), 7.38 (d, J = 8.3 Hz, 2H), 7.32 (d, J = 7.6 Hz, 2H), 7.27 (d, J = 5.0 Hz, 3H), 7.01 – 6.92 (m, 2H), 5.47 (s, 2H); IR (KBr): 3421, 3130, 1629, 1499, 1234, 1088, 981, 838, 762, 698, 556, 523 cm^{-1} .

1-Benzyl-4-(2-fluorophenyl)-5-(*o*-tolyl)-1*H*-1,2,3-triazole (3u)

Brown oil; ^1H NMR (400 MHz, CDCl_3) δ 7.56 (t, J = 7.3 Hz, 1H), 7.34 (t, J = 7.5 Hz, 1H), 7.27 – 7.13 (m, 7H), 7.11 – 7.06 (m, 2H), 6.96 (s, 3H), 5.35 (s, 2H), 1.63 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3): δ = 140.8, 137.9, 134.8, 134.5, 130.4, 130.4, 130.2, 129.7, 129.7, 128.5, 128.1, 128.0, 126.8, 125.9, 124.1, 124.0, 115.9, 115.7, 52.3, 19.0; IR (KBr): 3435, 2927, 2359, 2068, 1837, 1603, 1383, 1219, 1101, 872, 762, 666, 556 cm^{-1} ; HRMS Calcd for $[\text{C}_{22}\text{H}_{18}\text{FN}_3+\text{H}]^+$: 344.1558, Found: 344.1559.

1-Benzyl-4-(3-bromophenyl)-5-(*o*-tolyl)-1*H*-1,2,3-triazole (3v)

Brown oil; ^1H NMR (400 MHz, CDCl_3): δ = 7.51 (s, 1H), 7.40 (t, J = 7.4 Hz, 1H), 7.31 – 7.18 (m, 9H), 7.10 (d, J = 7.3 Hz, 2H), 6.94 (s, 1H), 5.29 (s, 2H), 2.05 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ = 141.9, 141.3, 135.2, 134.6, 130.7, 130.3, 130.2, 130.0, 129.4, 128.5, 128.3, 128.2, 128.0, 127.1, 126.7, 126.5, 125.6, 124.2, 52.2, 20.1; IR (KBr): 3435, 2926, 2821, 2359, 2068, 1837, 1602, 1383, 1261, 1100, 871, 762, 667, 464 cm^{-1} ; HRMS Calcd for $[\text{C}_{22}\text{H}_{18}\text{BrN}_3+\text{H}]^+$: 404.0757, Found: 404.0756.

4-Phenyl-5-(*p*-tolyl)-1*H*-1,2,3-triazole (4a)⁵

Yellow oil; ^1H NMR (400 MHz, CDCl_3): δ = 7.63 – 7.49 (m, 2H), 7.43 (d, J = 8.1 Hz, 2H), 7.35 (dd, J = 6.7, 3.7 Hz, 3H), 7.15 (d, J = 7.9 Hz, 2H), 2.37 (s, 3H); IR (KBr): 3435, 2926, 2359, 2068, 1603, 1383, 1100, 871, 809, 667, 558, 464 cm^{-1} .

4,5-Di-*p*-tolyl-1*H*-1,2,3-triazole (4b)⁶

Light brown oil; ^1H NMR (400 MHz, CDCl_3): δ = 7.33 (d, J = 7.5 Hz, 4H), 7.03 (d, J = 7.7 Hz, 4H), 2.26 (s, 6H); IR (KBr): 3437, 2921, 2359, 2068, 1605, 1381, 1183, 1102, 818, 668, 612, 556, 465 cm^{-1} .

4-(4-Chlorophenyl)-5-phenyl-1*H*-1,2,3-triazole (4c)⁷

Brown oil; ^1H NMR (400 MHz, CDCl_3): δ = 7.49 (t, J = 8.1 Hz, 4H), 7.37 (d, J = 5.4 Hz, 3H), 7.31 (d, J = 8.0 Hz, 2H); IR (KBr): 3435, 2925, 2359, 2068, 1603, 1384, 1264, 1097, 832, 738, 668, 562, 465 cm^{-1} .

4-(4-Methoxyphenyl)-5-(*p*-tolyl)-1*H*-1,2,3-triazole (4d)⁸

Brown oil; ¹H NMR (400 MHz, CDCl₃): δ = 7.49 (d, *J* = 8.1 Hz, 2H), 7.21 (d, *J* = 7.6 Hz, 2H), 7.04 (d, *J* = 6.2 Hz, 3H), 6.80 (d, *J* = 8.1 Hz, 2H), 3.77 (s, 3H), 2.42 (s, 3H); IR (KBr): 3435, 2926, 2359, 2068, 1596, 1462, 1384, 1257, 1103, 872, 613, 557, 465 cm⁻¹.

5. ^1H and ^{13}C NMR spectra

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