

## Supporting Information

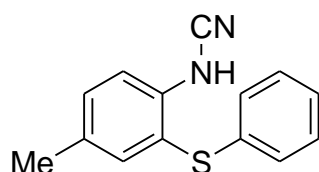
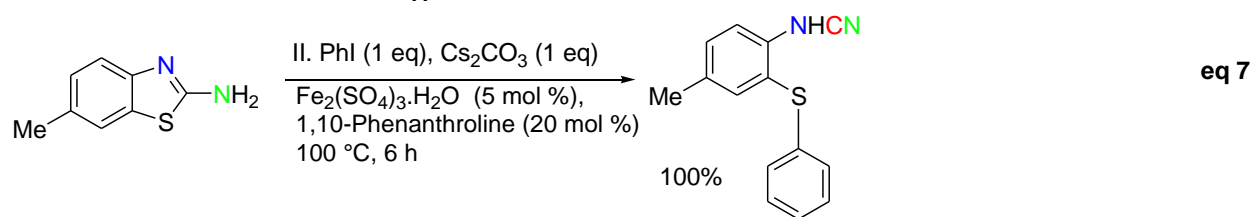
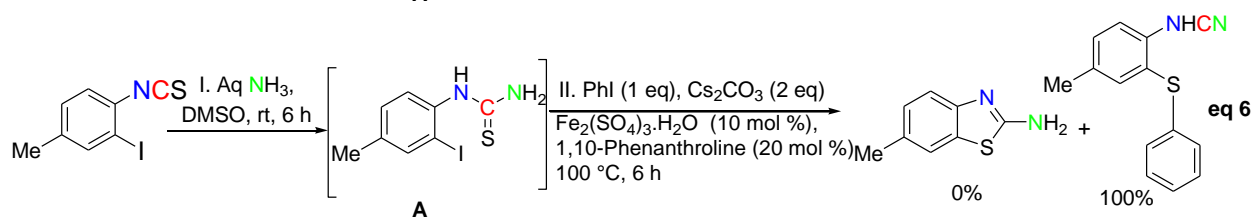
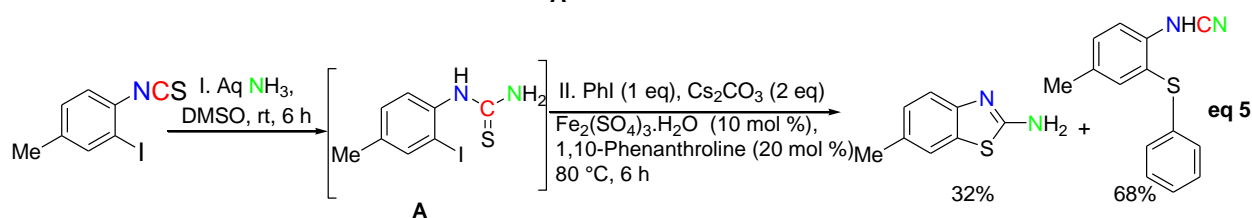
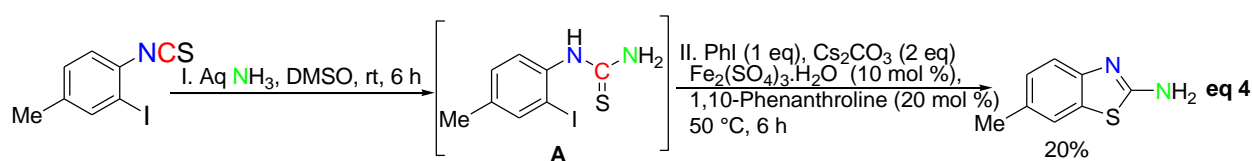
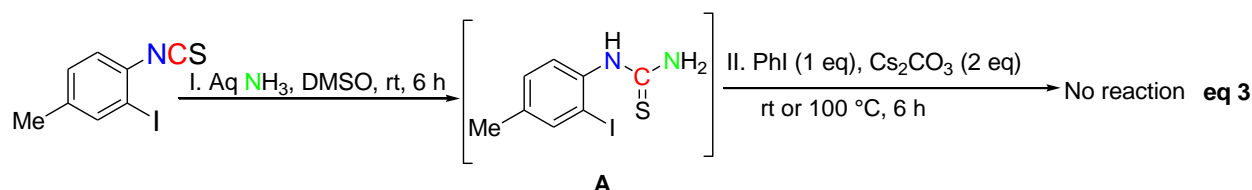
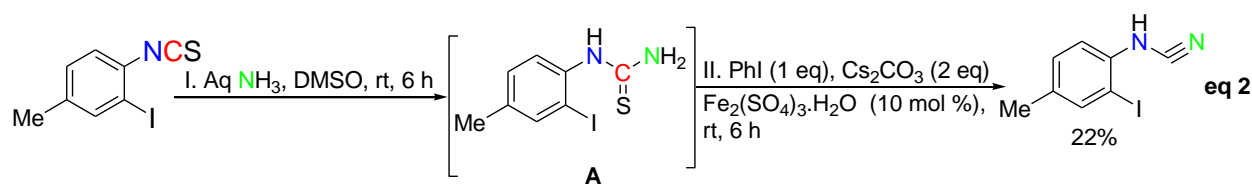
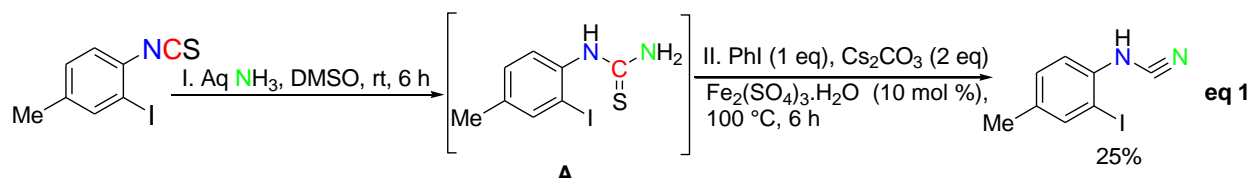
# Synthesis of 2-arylthio arylcyanamides from 2-iodoaryl isothiocyanates in one pot three component reaction

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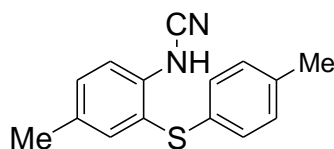
**General Information.** Iodobenzene, FeCl<sub>3</sub> (99%), Fe(NO<sub>3</sub>)<sub>3</sub>.H<sub>2</sub>O (99%), Fe<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub>.H<sub>2</sub>O (99%), FeCl<sub>2</sub> (98%), Et<sub>3</sub>N, Pyridine, sodium bicarbonate were purchased from Aldrich and used without further purification. The solvents were purchased and dried according to standard procedure prior to use. <sup>1</sup>H NMR (400 MHz) spectra were recorded with a Varian 400 spectrometer. Infrared (IR) spectra recorded on a Perkin Elmer Spectrum one FT-IR spectrometer. Elemental analyses were recorded with Perkin Elmer CHNS analyzer. Atomic absorption analyses were recorded with Perkin-Elmer 2280 atomic absorption (AA) spectrophotometer. 2-Iodo phenylisothiocyanates have been prepared by our recent reported literature<sup>1</sup> and aryl iodides were synthesized according to previous literature.<sup>2</sup>

**General Procedure for 2-(Phenylthio)phenylcyanamides:** To a stirred mixture of DMSO (2 ml) and *N*-2-iodo phenyl isothiocyanate (1 mmol, 520 mg), Aq NH<sub>3</sub> was added slowly and the reaction mixture stirred for 6 h at room temperature. After forming the thiourea (as per TLC), to that previous mixture iodobenzene (1 mmol, 203 mg), Cs<sub>2</sub>CO<sub>3</sub> (610 mg, 2 mmol), Fe<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub>.H<sub>2</sub>O (10 mol %, 41.7 mg) and 1,10-phenanthroline (20 mol %, 36 mg) were added and stirred at 100 °C for 6 h. Progress of the reaction was monitored by TLC using ethyl acetate and hexane (1:9). After finish the reaction, the reaction mixture was cooled to room temperature. Then, the solution was washed with ethyl acetate (7 ml) and water (3 mL) for 5 times. The organic layer was evaporated and crude reaction mixture was purified by silica gel (60-120 mesh) column chromatography using ethylacetate in hexane as eluent to obtain final product 2-(phenylthio)phenylcyanamide which was characterized by NMR (<sup>1</sup>H and <sup>13</sup>C), IR and elemental analysis.

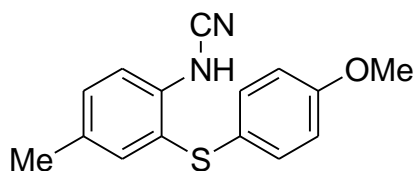


**4-Methyl-2-(phenylthio)phenylcyanamide** (Table 2, entry 1):<sup>3,4</sup> White solid; yield 95%; mp 126 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.40 (s, 1H), 7.30-7.19 (m, 5H), 7.04-7.01 (m, 2H), 6.81 (br s, 1H), 2.32 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 138.0, 137.4, 135.3, 134.1, 132.7, 129.6, 127.0, 126.7, 115.3, 110.0,

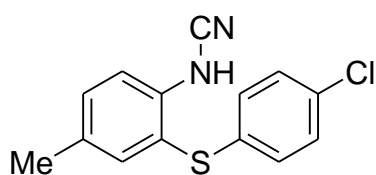
20.7; FT-IR (KBr) 3210, 2922, 2224, 1605, 1580, 1497, 1439, 1405, 1388, 1286, 1154, 1025  $\text{cm}^{-1}$ . Anal. Calcd. for  $\text{C}_{14}\text{H}_{12}\text{N}_2\text{S}$ : C, 69.97; H, 5.03; N, 11.66; S, 13.34. Found: C, 70.09; H, 5.02; N, 11.62; S, 13.27.



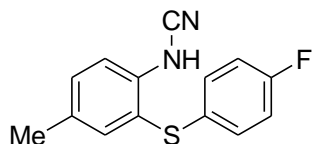
**2-(p-Tolylthio)-4-methylphenylcyanamide** (Table 2, entry 2):<sup>3,4</sup> Colour less solid; yield 95 %; mp 136-138  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.38 (s, 1H), 7.26-7.12 (m, 4H), 6.99 (d,  $J = 8.8$  Hz, 1H), 6.57-6.56 (m, 1H), 6.40 (br s, 1H), 2.36 (s, 3H), 2.16 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  143.1, 134.2, 133.4, 130.5, 130.0, 129.6, 129.0, 128.6, 122.6, 115.5, 111.1, 22.1, 20.9; FT-IR (KBr) 3210, 2968, 2877, 2226, 1752, 1656, 1599, 1578, 1489, 1365, 1272, 1154, 1011, 987  $\text{cm}^{-1}$ . Anal. Calcd. for  $\text{C}_{15}\text{H}_{14}\text{N}_2\text{S}$ : C, 70.83; H, 5.55; N, 11.01; S, 12.61. Found: C, 70.95; H, 5.53; N, 10.95; S, 12.57.



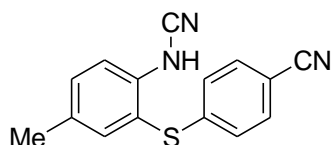
**2-(4-Methoxyphenylthio)-4-methylphenylcyanamide** (Table 2, entry 3):<sup>3</sup> Gummy liquid; yield 97%;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.33 (s, 1H), 7.23-7.18 (m, 2H), 7.10-7.07 (m, 2H), 6.83-6.80 (m, 3H), 3.78 (s, 3H), 2.30 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  159.2, 136.9, 136.6, 134.0, 131.9, 130.5, 125.3, 119.5, 115.3, 115.2, 110.7, 55.6, 20.7; FT-IR (KBr) 2925, 2851, 2227, 1594, 1492, 1283, 1247, 1173, 1097, 1031  $\text{cm}^{-1}$ . Anal. Calcd. for  $\text{C}_{15}\text{H}_{14}\text{N}_2\text{SO}$ : C, 66.64; H, 5.22; N, 10.36; S, 11.86. Found: C, 66.76; H, 5.19; N, 10.31; S, 11.80.



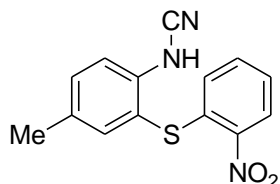
**2-(4-Chlorophenylthio)-4-methylphenylcyanamide** (Table 2, entry 4):<sup>3</sup> White solid; yield 91%; mp 105-106  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.38 (s, 1H), 7.29 (d,  $J = 0.8$  Hz, 1H), 7.27-7.21 (m, 3H), 6.95 (d,  $J = 8.4$  Hz, 2H), 6.78 (br s, 1H), 2.33 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  137.8, 137.2, 134.4, 133.1, 133.0, 132.7, 129.8, 128.4, 116.9, 115.5, 110.4, 20.7; FT-IR (KBr) 3183, 3028, 2921, 2960, 2853, 2232, 1892, 1605, 1580, 1563, 1495, 1473, 1387, 1288, 1262, 1155, 1090, 1051, 1008  $\text{cm}^{-1}$ . Anal. Calcd. for  $\text{C}_{14}\text{H}_{11}\text{N}_2\text{S}\text{Cl}$ : C, 61.20; H, 4.04; N, 10.20; S, 11.67. Found: C, 61.31; H, 4.01; N, 10.14; S, 11.60.



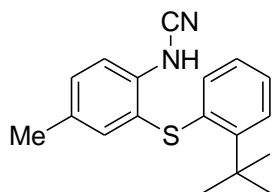
**2-(4-Fluorophenylthio)-4-methylphenylcyanamide** (Table 2, entry 5): White solid; yield 88%; mp 107-108 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.30 (s, 1H), 7.17 (d,  $J = 1.6$  Hz, 2H), 7.03-7.01 (m, 2H), 6.84 (br s, 1H), 6.60 (d,  $J = 7.6$  Hz, 2H), 2.28 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  146.4, 136.2, 133.8, 131.5, 131.3, 121.8, 120.6, 116.2, 115.2, 110.9, 20.7; FT-IR (KBr) 3199, 3132, 2923, 2853, 2233, 1711, 1683, 1604, 1523, 1495, 1449, 1290, 1154, 1115, 1028, 929  $\text{cm}^{-1}$ . Anal. Calcd. for  $\text{C}_{14}\text{H}_{11}\text{FN}_2\text{S}$ : C, 65.10; H, 4.29; F, 7.35; N, 10.84; S, 12.41. Found: C, 65.26; H, 4.28; N, 10.79; S, 12.35.



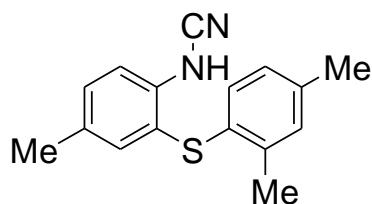
**4-((2-Cyanamide-5-methylphenyl)sulfanyl)benzonitrile** (Table 2, entry 6): White solid; yield 77%; mp 103-104 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.67 (d,  $J = 8$  Hz, 2H), 7.61-7.51 (m, 2H), 7.38 (s, 1H), 7.30-7.26 (m, 2H), 6.75 (br s, 1H), 2.30 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  137.8, 137.3, 134.3, 134.1, 128.9, 127.1, 126.9, 126.8, 126.1, 124.4, 116.8, 115.5, 20.7; FT-IR (KBr) 3210, 3060, 2935, 2899, 2242, 2222, 1717, 1670, 1579, 1488, 1413, 1388, 1270, 1243, 1023, 929  $\text{cm}^{-1}$ . Anal. Calcd. for  $\text{C}_{15}\text{H}_{11}\text{N}_3\text{S}$ : C, 67.90; H, 4.18; N, 15.84; S, 12.08. Found: C, 68.04; H, 4.16; N, 15.79; S, 12.01.



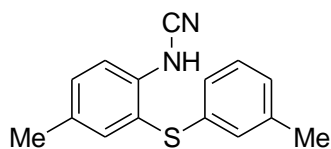
**2-(2-Nitrophenylthio)-4-methylphenylcyanamide** (Table 2, entry 7): White solid; yield 76%; mp 125-127 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.40 (d,  $J = 9.2$  Hz, 2H), 7.66-7.63 (m, 2H), 7.38 (s, 1H), 6.50 (d,  $J = 8.4$  Hz, 2H), 2.32 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  147.0, 141.9, 137.9, 132.9, 131.0, 129.3, 126.9, 125.2, 124.5, 122.7, 122.2, 110.0, 20.8; FT-IR (KBr) 3199, 3118, 2963, 2923, 2859, 2237, 1715, 1656, 1605, 1555, 1529, 1499, 1345, 1261, 1022, 929  $\text{cm}^{-1}$ . Anal. Calcd. for  $\text{C}_{14}\text{H}_{11}\text{N}_3\text{O}_2\text{S}$ : C, 58.93; H, 3.89; N, 14.73; O, 11.22; S, 11.24. Found: C, 59.08; H, 3.87; N, 14.68; S, 11.20.



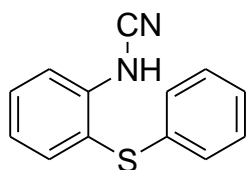
**2-(2-Tert-butylphenylthio)-4-methylphenylcyanamide** (Table 2, entry 8): White solid; yield 82%; mp 112-113 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.36 (s, 1H), 7.26-7.20 (m, 2H), 7.00 (d,  $J = 7.6$  Hz, 1H), 6.87 (d,  $J = 1.2$  Hz, 2H), 6.83 (br s, 1H), 6.79-6.76 (m, 2H), 2.26 (s, 3H), 1.43 (s, 9H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  138.2, 137.5, 137.1, 135.7, 133.9, 132.2, 131.6, 130.9, 129.0, 125.3, 122.2, 118.2, 115.2, 34.5, 30.5, 20.7; FT-IR (KBr) 3280, 3198, 2961, 2895, 2819, 2222, 1721, 1621, 1597, 1496, 1385, 1388, 1262, 1177, 1032, 943  $\text{cm}^{-1}$ . Anal. Calcd. for  $\text{C}_{18}\text{H}_{20}\text{N}_2\text{S}$ : C, 72.93; H, 6.80; N, 9.45; S, 10.82. Found: C, 73.05; H, 6.77; N, 9.41; S, 10.77.



**2-(2,4-Dimethylphenylthio)-4-methylphenylcyanamide** (Table 2, entry 9):<sup>3</sup> white solid; yield 90%;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.28-7.21 (m, 3H), 7.01 (s, 1H), 6.86 (d,  $J = 7.6$  Hz, 1H), 6.72 (br s, 1H), 6.57 (d,  $J = 8.0$  Hz, 1H), 2.36 (s, 3H), 2.30 (s, 3H), 2.27 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  137.1, 137.0, 136.7, 136.2, 134.2, 132.0, 131.7, 130.5, 127.9, 127.1, 117.8, 115.3, 110.7, 21.0, 20.7, 20.2; FT-IR (KBr) 2923, 2857, 2235, 2098, 1615, 1498, 1380, 1259, 1237, 1049  $\text{cm}^{-1}$ . Anal. Calcd. for  $\text{C}_{16}\text{H}_{16}\text{N}_2\text{S}$ : C, 71.61; H, 6.01; N, 10.44; S, 11.95. Found: C, 71.70; H, 5.98; N, 10.40; S, 11.92.

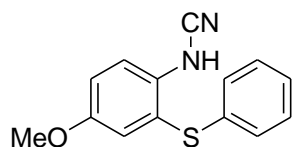


**2-(m-Tolylthio)-4-methylphenylcyanamide** (Table 2, entry 10): White solid; yield 92%; mp 121-122 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.36 (s, 1H), 7.26-7.19 (m, 2H), 7.00 (d,  $J = 7.6$  Hz, 2H), 6.87 (s, 1H), 6.83 (br s, 1H), 6.79-6.76 (m, 1H), 2.26 (s, 3H), 2.19 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  138.2, 137.5, 137.1, 135.7, 134.0, 132.2, 131.6, 130.9, 129.0, 123.2, 118.2, 115.2, 20.7, 20.0; FT-IR (KBr) 3144, 2984, 2917, 2859, 2230, 1604, 1584, 1498, 1449, 1413, 1391, 1289, 1270, 1213, 1153, 1057, 934  $\text{cm}^{-1}$ . Anal. Calcd. for  $\text{C}_{15}\text{H}_{14}\text{N}_2\text{S}$ : C, 70.83; H, 5.55; N, 11.01; S, 12.61. Found: C, 70.93; H, 5.54; N, 10.97; S, 12.56.

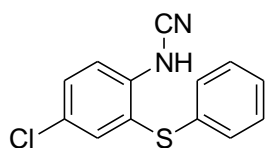


**2-(Phenylthio)phenylcyanamide** (Table 3, entry 1): White solid; yield 95%; mp 92-93 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.57-7.55 (dd,  $J = 1.6$  Hz, 7.6 Hz, 1H), 7.49-7.45 (td,  $J = 1.6$  Hz, 7.6 Hz, 1H), 7.34-

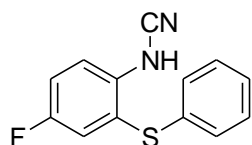
7.31 (dd,  $J = 1.2$  Hz, 8.4 Hz, 1H), 7.26-7.21 (m, 2H), 7.18-7.08 (m, 2H), 7.01-6.99 (m, 1H), 6.96-6.94 (d,  $J = 8.0$  Hz, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  139.9, 137.7, 135.1, 131.9, 129.6, 127.1, 126.7, 124.3, 117.5, 115.4, 110.3; FT-IR (KBr) 3148, 2964, 2917, 2237, 1590, 1578, 1490, 1438, 1409, 1288, 1261, 1078, 1023  $\text{cm}^{-1}$ . Anal. Calcd. for  $\text{C}_{13}\text{H}_{10}\text{N}_2\text{S}$ : C, 69.00; H, 4.45; N, 12.38; S, 14.17. Found: C, 69.10; H, 4.44; N, 12.35; S 14.11.



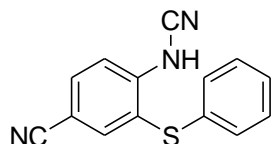
**4-Methoxy-2-(phenylthio)phenylcyanamide** (Table 3, entry 2): White solid; yield 95%; mp 132-133  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.49 (s, 1H), 7.26-7.18 (m, 4H), 6.82-6.79 (m, 3H), 3.77 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  159.6, 138.4, 136.7, 134.0, 132.7, 132.1, 120.1, 116.4, 115.6, 115.0, 110.9, 55.5; FT-IR (KBr) 3198, 3153, 2919, 2873, 2237, 1572, 1486, 1455, 1408, 1384, 1284, 1260, 1100, 1017, 934  $\text{cm}^{-1}$ . Anal. Calcd. for  $\text{C}_{14}\text{H}_{12}\text{N}_2\text{OS}$ : C, 65.60; H, 4.72; N, 10.93; O, 6.24; S, 12.51. Found: C, 65.76; H, 4.70; N, 10.88; S, 12.45.



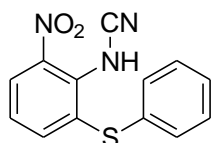
**4-Chloro-2-(phenylthio)phenylcyanamide** (Table 3, entry 3): White solid; yield 90%; mp 104-105  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.51 (s, 1H), 7.28-7.19 (m, 4H), 7.10-7.08 (m, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  139.1, 137.2, 134.3, 132.8, 131.1, 130.8, 130.0, 128.7, 115.2, 114.5, 110.7; FT-IR (KBr) 3255, 3199, 2232, 1677, 1607, 1581, 1548, 1453, 1401, 1367, 1265, 1155, 1018  $\text{cm}^{-1}$ . Anal. Calcd. for  $\text{C}_{13}\text{H}_9\text{ClN}_2\text{S}$ : C, 59.88; H, 3.48; Cl, 13.60; N, 10.74; S, 12.30 Found: C, 60.03; H, 3.46; N, 10.69; S, 12.24.



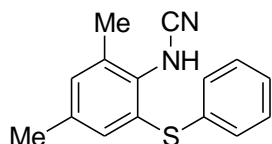
**4-Fluoro-2-(phenylthio)phenylcyanamide** (Table 3, entry 4): White solid; yield 83%; mp 109-110  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.46 (s, 1H), 7.26-7.08 (m, 2H), 6.57-6.55 (m, 3H), 6.92-6.90 (m, 2H), 6.74 (br s, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  146.7, 137.9, 136.5, 133.8, 133.4, 131.6, 117.3, 116.7, 116.4, 114.9, 111.1; FT-IR (KBr) 3157, 2224, 1658, 1599, 1516, 1428, 1411, 1242, 1197, 1065, 1022  $\text{cm}^{-1}$ . Anal. Calcd. for  $\text{C}_{13}\text{H}_9\text{FN}_2\text{S}$ : C, 63.92; H, 3.71; F, 7.78; N, 11.47; S, 13.13. Found: C, 64.08; H, 3.70; N, 11.40; S, 13.07.



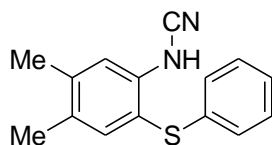
**4-(Cyanoamino)-3-(phenylthio)benzonitrile** (Table 3, entry 5): White solid; yield 75%; mp 119-120 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.53 (s, 1H), 7.29-7.22 (m, 5H), 7.16 (d,  $J = 6.8$  Hz, 2H), 6.97 (d,  $J = 7.2$  Hz, 2H), 6.84 (br s, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  139.2, 137.3, 134.2, 132.6, 130.5, 130.0, 129.7, 127.3, 115.0, 114.8, 111.0, 110.9, ; FT-IR (KBr) 3253, 3198, 2238, 2212, 1654, 1588, 1488, 1407, 1317, 1287, 1164, 1019, 927  $\text{cm}^{-1}$ . Anal. Calcd. for  $\text{C}_{14}\text{H}_9\text{N}_3\text{S}$ : C, 66.91; H, 3.61; N, 16.72; S, 12.76. Found: C, 67.01; H, 3.60; N, 16.68; S, 12.71.



**2-Nitro-6-(phenylthio)phenylcyanamide** (Table 3, entry 6): White solid; yield 70%; mp 130-131 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.07-8.04 (m, 2H), 7.55-7.26 (m, 6H), 6.80 (br s, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  149.0, 139.4, 137.4, 134.8, 133.6, 133.1, 130.5, 124.0, 115.5, 113.1, 110.4; FT-IR (KBr) 3153, 2237, 1717, 1667, 1601, 1572, 1486, 1408, 1314, 1284, 1260, 1100, 1017, 924  $\text{cm}^{-1}$ . Anal. Calcd. for  $\text{C}_{13}\text{H}_9\text{N}_3\text{O}_2\text{S}$ : C, 57.55; H, 3.34; N, 15.49; O, 11.79; S, 11.82. Found: C, 57.72; H, 3.32; N, 15.44; S, 11.75.

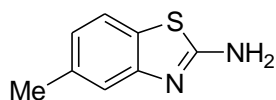


**2,4-Dimethyl-6-(phenylthio)phenylcyanamide** (Table 3, entry 7): White solid; yield 82%; mp 94 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.30 (s, 1H), 7.09 (s, 1H), 7.03 (d,  $J = 8.0$  Hz, 2H), 6.92-6.89 (m, 3H), 6.74 (br s, 1H), 2.28 (s, 3H), 2.27 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  141.5, 138.4, 137.7, 136.9, 133.2, 132.4, 130.6, 127.5, 116.8, 114.9, 111.1, 21.4, 20.4; FT-IR (KBr) 3201, 2922, 2858, 2232, 1607, 1581, 1453, 1410, 1389, 1268, 1155, 1018  $\text{cm}^{-1}$ . Anal. Calcd. for  $\text{C}_{15}\text{H}_{14}\text{N}_2\text{S}$ : C, 70.83; H, 5.55; N, 11.01; S, 12.61. Found: C, 70.94; H, 5.53; N, 10.97; S, 12.56.

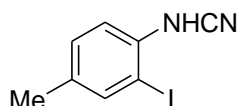


**4,5-Dimethyl-2-(phenylthio)phenylcyanamide** (Table 3, entry 8): White solid; yield 85%; mp 95 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.37 (s, 1H), 7.26-7.21 (m, 2H), 6.80 (d,  $J = 2.8$  Hz, 2H), 6.64 (d,  $J = 1.6$  Hz,

2H), 2.23 (s, 3H), 2.22 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  139.4, 137.8, 137.3, 134.6, 134.0, 132.4, 128.7, 124.9, 117.6, 115.3, 110.6, 21.4, 20.7; FT-IR (KBr) 3157, 2917, 2845, 2230, 1608, 1567, 1498, 1411, 1272, 1197, 1081, 1022  $\text{cm}^{-1}$ . Anal. Calcd. for  $\text{C}_{15}\text{H}_{14}\text{N}_2\text{S}$ : C, 70.83; H, 5.55; N, 11.01; S, 12.61. Found: C, 70.94; H, 5.53; N, 10.97; S, 12.56.



**5-methylbenzo[d]thiazol-2-amine:**<sup>5</sup> White solid; mp 129-130  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.40 (s, 1H), 7.31-7.27 (m, 1H), 7.13-7.09 (dt,  $J = 7.6, 1.2$  Hz, 1H), 5.62 (br s, 2H), 2.33 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  167.0, 151.9, 131.0, 125.5, 121.4, 120.6, 118.2, 20.7; FT-IR (KBr) 3348, 3286, 3199, 3063, 2899, 1701, 1645, 1511, 1209, 1112, 929  $\text{cm}^{-1}$ . Anal. Calcd. for  $\text{C}_8\text{H}_8\text{N}_2\text{S}$ : C, 58.51; H, 4.91; N, 17.06; S, 19.52. Found: C, 58.62; H, 4.89; N, 17.01; S 19.48.



**2-Iodo-4-methylphenylcyanamide:** Analytical TLC on silica gel, 1:19 ethyl acetate/hexane  $R_f = 0.8$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.63 (s, 1H), 7.10-7.15 (m, 2H), 2.30 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  142.3, 135.6, 132.4, 128.5, 124.6, 120.0, 94.3, 21.3; FT-IR (KBr) 3322, 3087, 2899, 2236, 1587, 1496, 1265, 1212, 1104, 941, 808, 578  $\text{cm}^{-1}$ . Anal. Calcd. for  $\text{C}_8\text{H}_7\text{IN}_2$ : C, 37.23; H, 2.73; N, 10.86. Found: C, 37.36; H, 2.71; N, 10.81.

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