

Supplementary Information

Hydrocyanation of Sulfonylimines Using Potassium Hexacyanoferrate(II) as an Eco-Friendly Cyanide Source

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The general procedure for the preparation of sulfonylimines

The mixture of 4-methylbenzenesulfonamide or benzenesulfonamide (20 mmol), aldehyde (22 mmol), anhydrous magnesium sulfate (5 mmol) and acetic acid (4 mmol) in 20 mL of toluene was refluxed at 110 °C for 15 h. The progress of the reaction was monitored by TLC. After the completion, the system was cooled to room temperature, and the solvent was removed under reduced pressure. The resulting solid was recrystallized from diethyl ether to give pure product. The analytical data for representative products are given below.

N-Benzylidene-4-methylbenzenesulfonamide (**1a**)

White solid; mp: 109-110 °C (lit. 112-113 °C).¹ ¹H NMR (400 MHz, CDCl₃) δ 2.32 (s, 3H, CH₃), 7.24 (d, 2H, J 8.4 Hz, Ar-H), 7.48 (t, 2H, J 7.8 Hz, Ar-H), 7.50 (t, 1H, J 6.4 Hz, Ar-H), 7.80-7.83 (m, 4H, Ar-H), 8.98 (s, 1H, CH). ¹³C NMR (100 MHz, CDCl₃) δ 21.8, 128.3, 129.8, 130.2, 131.5, 135.3, 140.1, 145.1, 170.6.

N-(4-Methylbenzylidene)-4-methylbenzenesulfonamide (**1b**)

White solid; mp: 111-113 °C (lit. 112-114 °C).² ¹H NMR (400 MHz, CDCl₃) δ 2.43 (s, 6H, CH₃), 7.27 (d, 2H, J 7.6 Hz, Ar-H), 7.35 (d, 2H, J 7.8 Hz, Ar-H), 7.83 (d, 2H, J 7.6 Hz, Ar-H), 7.91 (d, 2H, J 7.6 Hz, Ar-H), 8.97 (s, 1H, CH). ¹³C NMR (100 MHz, CDCl₃) δ 22.1, 126.9, 128.5, 129.9, 130.3, 130.4, 131.9, 135.8, 144.9, 170.5.

N-(4-Methoxybenzylidene)-4-methylbenzenesulfonamide (**1c**)

White solid; mp: 128-130 °C (lit. 128-129 °C).³ ¹H NMR (400 MHz, CDCl₃) δ 2.35 (s, 3H, CH₃), 3.77 (s, 3H, OCH₃), 6.92 (d, 2H, J 8.6 Hz, Ar-H), 7.28 (d, 2H, J 7.8 Hz, Ar-H), 7.80 (d, 2H, J 7.6 Hz, Ar-H), 7.84 (d, 2H, J 7.6 Hz,

Ar-H), 8.90 (s, 1H, CH). ¹³C NMR (100 MHz, CDCl₃) δ 22.3, 56.7, 115.4, 125.8, 128.6, 130.3, 134.4, 136.5, 145.1, 166.1, 170.0.

N-(2-Chlorobenzylidene)-4-methylbenzenesulfonamide (**1g**)

White solid; mp: 115-116 °C (lit. 114-116 °C).³ ¹H NMR (400 MHz, CDCl₃) δ 2.44 (s, 3H, CH₃), 7.28-7.91 (m, 8H, Ar-H), 9.12 (s, 1H, CH). ¹³C NMR (100 MHz, CDCl₃) δ 22.7, 126.8, 128.6, 129.2, 129.6, 131.3, 131.8, 134.4, 137.2, 168.2.

N-(Furan-2-ylmethylene)-4-methylbenzenesulfonamide (**1k**)

Brown solid; mp: 100-102 °C (lit. 101-102 °C).³ ¹H NMR (400 MHz, CDCl₃) δ 2.34 (s, 1H, CH₃), 6.78-7.77 (m, 7H, Ar-H), 8.85 (s, 1H, CH). ¹³C NMR (100 MHz, CDCl₃) δ 22.7, 112.8, 115.6, 126.8, 128.8, 131.1, 148.6, 151.8, 154.5, 157.2.

The general procedure for the hydrocyanation of sulfonylimines

The mixture of K₄[Fe(CN)₆] (0.1 mmol) and benzoyl chloride (0.6 mmol) was stirred at 160 °C for 3 h, then the reaction system was cooled to room temperature, and sulfonylimines (0.5 mmol) and potassium carbonate (0.1 mmol) in ethanol (8 mL) were added. The mixture was further stirred at room temperature for appropriate time indicated in Table 3. After completion of the reaction monitored by TLC, the resulting mixture was filtered to remove the solids. The liquor was concentrated, and the residues were isolated by column chromatography using petroleum ether and ethyl acetate (6:1) as eluent to give pure product. The analytical data for products are given below.

N-(Cyanophenylmethyl)-4-methylbenzenesulfonamide (**2a**)

White solid; mp 152-154 °C; IR (KBr) ν_{max} /cm⁻¹ 3254 (NH), 2245 (CN), 1334 (S=O asym), 1157 (S=O sym); ¹H NMR (400 MHz, CDCl₃) δ 2.46 (s, 3H, CH₃), 5.10 (d,

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1H, *J* 8.4 Hz, NH), 5.48 (d, 1H, *J* 8.4 Hz, CH), 7.36-7.46 (m, 7H, ArH), 7.82 (t, 2H, *J* 8.4 Hz, ArH); ¹³C NMR (100 MHz, CDCl₃) δ 21.6, 48.2, 116.2, 127.0, 127.3, 129.4, 129.9, 130.0, 132.0, 135.9, 144.7. Anal. calcd. for C₁₅H₁₄N₂O₂S: C, 62.92; H, 4.93; N, 9.78; found: C, 62.81; H, 4.95; N, 9.81.

***N*-(Cyano(4-tolyl)methyl)-4-methylbenzenesulfonamide (**2b**)**

White solid; mp 149-150 °C; IR (KBr) ν_{max} /cm⁻¹ 3270 (NH), 2248 (CN), 1336 (S=O asym), 1160 (S=O sym); ¹H NMR (400 MHz, CDCl₃) δ 2.28 (s, 3H, CH₃), 2.38 (s, 3H, CH₃), 5.09 (d, 1H, *J* 8.4 Hz, NH), 5.34 (d, 1H, *J* 8.4 Hz, CH), 7.12 (d, 2H, *J* 8.0 Hz, ArH), 7.23 (d, 2H, *J* 8.0 Hz, ArH), 7.28 (d, 2H, *J* 8.0 Hz, ArH), 7.72 (d, 2H, *J* 8.0 Hz, ArH); ¹³C NMR (100 MHz, CDCl₃) δ 21.1, 21.6, 47.9, 116.4, 127.0, 127.3, 129.1, 130.0, 136.1, 140.0, 144.6. Anal. calcd. for C₁₆H₁₆N₂O₂S: C, 63.98; H, 5.37; N, 9.33; found: C, 64.09; H, 5.36; N, 9.35.

***N*-(Cyano(4-methoxyphenyl)methyl)-4-methylbenzenesulfonamide (**2c**)**

White solid; mp 124-125 °C; IR (KBr) ν_{max} /cm⁻¹ 3271 (NH), 2248 (CN), 1337 (S=O asym), 1160 (S=O sym); ¹H NMR (400 MHz, CDCl₃) δ 2.37 (s, 3H, CH₃), 3.71 (s, 3H, OCH₃), 5.25 (d, 1H, *J* 8.4 Hz, NH), 5.32 (d, 1H, *J* 8.4 Hz, CH), 6.77-6.82 (m, 2H, ArH), 7.18-7.28 (m, 4H, ArH), 7.68-7.73 (m, 2H, ArH); ¹³C NMR (100 MHz, CDCl₃) δ 22.0, 48.0, 55.8, 115.0, 116.8, 124.4, 127.5, 128.8, 130.3, 136.4, 144.9, 160.9. Anal. calcd. for C₁₆H₁₆N₂O₃S: C, 60.74; H, 5.10; N, 8.85; found: C, 60.83; H, 5.09; N, 8.82.

***N*-(Cyano[4-(dimethylamino)phenyl)methyl)-4-methylbenzenesulfonamide (**2d**)**

White solid; mp 158-160 °C; IR (KBr) ν_{max} /cm⁻¹ 3297 (NH), 2247 (CN), 1335 (S=O asym), 1164 (S=O sym); ¹H NMR (400 MHz, CDCl₃) δ 2.48 (s, 3H, CH₃), 2.99 (s, 6H, N(CH₃)₂), 4.95 (d, 1H, *J* 8.0 MHz, NH), 5.37 (d, 1H, *J* 8.0 Hz, CH), 6.69 (d, 2H, *J* 8.0 Hz, ArH), 7.27 (d, 2H, *J* 8.0 Hz, ArH), 7.38 (d, 2H, *J* 8.0 Hz, ArH), 7.84 (d, 2H, *J* 8.0 Hz, ArH); ¹³C NMR (100 MHz, CDCl₃) δ 22.0, 40.3, 47.9, 112.6, 117.0, 127.2, 128.3, 129.9, 136.2, 144.9. Anal. calcd. for C₁₇H₁₉N₃O₂S: C, 61.98; H, 5.81; N, 12.76; found: C, 62.21; H, 5.83; N, 12.73.

***N*-(Benzo[*d*][1,3]dioxol-5-yl(cyano)methyl)-4-methylbenzenesulfonamide (**2e**)**

White solid; mp 166-168 °C; IR (KBr) ν_{max} /cm⁻¹ 3212 (NH), 2244 (CN), 1338 (S=O asym), 1159 (S=O sym); ¹H NMR (400 MHz, CDCl₃) δ 2.48 (s, 3H, CH₃), 5.10 (d, 1H, *J* 8.4 Hz, NH), 5.39 (d, 1H, *J* 8.4 Hz, CH), 6.03 (s, 2H, CH₂), 6.81 (d, 1H, *J* 8.4 Hz, ArH), 6.89 (s, 1H, CH, ArH), 6.95 (d, 1H, *J* 8.4 Hz, ArH), 7.39 (d, 2H, *J* 7.6 Hz,

ArH), 7.83 (d, 2H, *J* 7.6 Hz, ArH); ¹³C NMR (100 MHz, CDCl₃) δ 21.7, 48.0, 101.8, 107.5, 108.7, 116.3, 121.0, 125.6, 126.5, 127.3, 129.7, 130.1, 136.0, 144.7, 148.6, 149.0. Anal. calcd. for C₁₆H₁₄N₂O₂S: C, 58.17; H, 4.27; N, 8.48; found: C, 58.09; H, 4.26; N, 8.50.

***N*-(Cyano(4-fluorophenyl)methyl)-4-methylbenzenesulfonamide (**2f**)**

White solid; mp 122-124 °C; IR (KBr) ν_{max} /cm⁻¹ 3256 (NH), 2243 (CN), 1332 (S=O asym), 1156 (S=O sym); ¹H NMR (400 MHz, CDCl₃) δ 2.45 (s, 3H, CH₃), 5.43 (d, 1H, *J* 9.6 Hz, CH), 5.59 (bs, 1H, NH), 7.03-7.07 (m, 2H, ArH), 7.33-7.42 (m, 4H, ArH), 7.76 (d, 2H, *J* 8.0 Hz, ArH); ¹³C NMR (100 MHz, CDCl₃) δ 21.6, 47.5, 116.3, 127.2, 128.0, 129.1, 129.2, 130.0, 135.9, 144.8, 162.1, 164.6. Anal. calcd. for C₁₅H₁₃FN₂O₂S: C, 59.20; H, 4.31; N, 9.20; found: C, 59.14; H, 4.30; N, 9.16.

***N*-(2-Chlorophenyl)(cyano)methyl)-4-methylbenzenesulfonamide (**2g**)**

White solid; mp 112-114 °C; IR (KBr) ν_{max} /cm⁻¹ 3248 (NH), 2241 (CN), 1340 (S=O asym), 1159 (S=O sym); ¹H NMR (400 MHz, CDCl₃) δ 2.41 (s, 3H, CH₃), 5.67-5.70 (m, 2H, NH and CH), 7.24-7.34 (m, 5H, ArH), 7.49 (d, 1H, *J* 7.2 Hz, ArH), 7.72-7.74 (m, 2H, ArH); ¹³C NMR (100 MHz, CDCl₃) δ 21.5, 46.3, 115.8, 127.4, 127.9, 129.4, 130.0, 130.3, 130.7, 131.4, 133.1, 135.9, 144.6. Anal. calcd. for C₁₅H₁₃ClN₂O₂S: C, 56.16; H, 4.08; N, 8.73; found: C, 56.00; H, 4.09; N, 8.75.

***N*-(4-Chlorophenyl)(cyano)methyl)-4-methylbenzenesulfonamide (**2h**)**

White solid; mp 130-132 °C; IR (KBr) ν_{max} /cm⁻¹ 3262 (NH), 2249 (CN), 1342 (S=O asym), 1160 (S=O sym); ¹H NMR (400 MHz, CDCl₃) δ 2.46 (s, 3H, CH₃), 5.30 (d, 1H, *J* 9.2 Hz, NH), 5.45 (d, 1H, *J* 9.2 Hz, CH), 7.35-7.39 (m, 6H, ArH), 7.77 (d, 2H, *J* 8.4 Hz, ArH); ¹³C NMR (100 MHz, CDCl₃) δ 21.6, 47.5, 116.0, 127.2, 128.5, 129.5, 130.0, 130.6, 135.8, 136.0, 144.8. Anal. calcd. for C₁₅H₁₃ClN₂O₂S: C, 56.16; H, 4.08; N, 8.73; found: C, 56.22; H, 4.08; N, 8.72.

***N*-(Cyano(2,4-dichlorophenyl)methyl)-4-methylbenzenesulfonamide (**2i**)**

White solid; mp 136-137 °C; IR (KBr) ν_{max} /cm⁻¹ 3248 (NH), 2248 (CN), 1343 (S=O asym), 1158 (S=O sym); ¹H NMR (400 MHz, CDCl₃) δ 2.44 (s, 3H, CH₃), 5.51 (bs, 1H, NH), 5.64 (d, 1H, *J* 8.8 Hz, CH), 7.28-7.32 (m, 3H, ArH), 7.37 (s, 1H, ArH), 7.44 (d, 1H, *J* 8.4 Hz, ArH), 7.72 (d, 2H, *J* 8.0 Hz, ArH); ¹³C NMR (100 MHz, CDCl₃) δ 21.7, 45.7, 115.5, 127.3, 128.1, 128.4, 130.0, 130.3, 130.4, 133.9,

135.7, 137.0, 144.8. Anal. calcd. for $C_{15}H_{12}Cl_2N_2O_2S$: C, 50.72; H, 3.41; N, 7.89; found: C, 50.64; H, 3.42; N, 7.91.

N-[4-(Bromophenyl)(cyano)methyl]-4-methylbenzenesulfonamide (2j)

White solid; mp 150-151 °C; IR (KBr) $\nu_{\text{max}}/\text{cm}^{-1}$ 3262 (NH), 2248 (CN), 1343 (S=O asym), 1160 (S=O sym); ^1H NMR (400 MHz, CDCl_3) δ 2.45 (s, 3H, CH_3), 5.40 (d, 1H, J 9.6 Hz, NH), 5.51 (d, 1H, J 9.6 Hz, CH), 7.29 (d, 2H, J 8.4 Hz, ArH), 7.34 (d, 2H, J 8.4 Hz, ArH), 7.50 (d, 2H, J 8.4 Hz, ArH), 7.75 (d, 2H, J 8.4 Hz, ArH); ^{13}C NMR (100 MHz, CDCl_3) δ 21.7, 47.7, 115.9, 124.2, 127.3, 127.8, 128.8, 130.1, 130.6, 131.2, 132.6, 135.8, 144.9. Anal. calcd. for $C_{15}H_{13}BrN_2O_2S$: C, 49.33; H, 3.59; N, 7.67; found: C, 49.26; H, 3.60; N, 7.70.

N-[Cyano(furan-2-yl)methyl]-4-methylbenzenesulfonamide (2k)

White solid; mp 98-100 °C; IR (KBr) $\nu_{\text{max}}/\text{cm}^{-1}$ 3277 (NH), 2251 (CN), 1337 (S=O asym), 1161 (S=O sym); ^1H NMR (400 MHz, CDCl_3) δ 2.44 (s, 3H, CH_3), 5.37 (d, 1H, J 9.2 Hz, NH), 5.53 (d, 1H, J 9.2 Hz, CH), 6.34-6.35 (m, 1H, Fu-H), 6.47 (d, 1H, J 3.6 Hz, Fu-H), 7.34 (d, 2H, J 8.4 Hz, ArH), 7.38 (s, 1H, Fu-H), 7.77 (d, 2H, J 8.4 Hz, ArH); ^{13}C NMR (100 MHz, CDCl_3) δ 21.9, 42.4, 110.6, 111.0, 114.7, 127.3, 131.2, 135.9, 143.9, 144.5, 144.8. Anal. calcd. for $C_{13}H_{12}N_2O_3S$: C, 56.51; H, 4.38; N, 10.14; found: C, 56.66; H, 4.39; N, 10.13.

N-(1-Cyanopropyl)-4-methylbenzenesulfonamide (2l)

White solid; mp 52-54 °C; IR (KBr) $\nu_{\text{max}}/\text{cm}^{-1}$ 3283 (NH), 2249 (CN), 1333 (S=O asym), 1161 (S=O sym); ^1H NMR (400 MHz, CDCl_3) δ 0.95-0.96 (m, 3H, CH_3), 2.01-2.04 (m, 2H, CH_2), 2.44 (s, 3H, CH_3), 4.69 (d, 1H, J 9.2 Hz, CH), 5.12 (bs, 1H, NH), 7.26-7.36 (m, 2H, ArH), 7.77-7.79 (m, 2H, ArH); ^{13}C NMR (100 MHz, CDCl_3) δ 13.3, 21.3, 21.6, 51.2, 116.0, 126.0, 127.3, 129.9, 134.2, 136.2, 144.5. Anal. calcd. for $C_{11}H_{14}N_2O_2S$: C, 55.44; H, 5.92; N, 11.76; found: C, 55.58; H, 5.94; N, 11.80.

N-(1-Cyano-2-methylpropyl)-4-methylbenzenesulfonamide (2m)

White solid; mp 78-79 °C; IR (KBr) $\nu_{\text{max}}/\text{cm}^{-1}$ 3281 (NH), 2240 (CN), 1339 (S=O asym), 1162 (S=O sym); ^1H NMR (400 MHz, CDCl_3) δ 1.04 (d, 6H, J 6.8 Hz, CH_3), 1.99-2.07 (m, 1H, CH), 2.44 (s, 3H, CH_3), 4.01-4.05 (m, 1H, CH), 5.53 (bs, 1H, NH), 7.35 (d, 2H, J 7.6 Hz, ArH), 7.78 (d, 2H, J 7.6 Hz, ArH); ^{13}C NMR (100 MHz, CDCl_3) δ 17.8, 18.5, 21.7, 32.4, 50.6, 116.8, 127.2, 130.1, 136.0, 144.6. Anal. calcd. for $C_{12}H_{16}N_2O_2S$: C, 57.12; H, 6.39; N, 11.10; found: C, 57.04; H, 6.41; N, 11.06.

N-[Cyano(phenyl)methyl]benzenesulfonamide (2n)

White solid; mp 98-100 °C; IR (KBr) $\nu_{\text{max}}/\text{cm}^{-1}$ 3261 (NH), 2248 (CN), 1341 (S=O asym), 1169 (S=O sym); ^1H NMR (400 MHz, CDCl_3) δ 5.47 (d, 1H, J 9.2 Hz, NH), 5.79 (d, 1H, J 9.2 Hz, CH), 7.28-7.91 (m, 10H, ArH); ^{13}C NMR (100 MHz, CDCl_3) δ 48.2, 116.3, 127.1, 127.3, 129.4, 129.5, 129.9, 132.0, 133.7, 138.9. Anal. calcd. for $C_{14}H_{12}N_2O_2S$: C, 61.75; H, 4.44; N, 10.29; found: C, 61.66; H, 4.45; N, 10.25.

N-[Cyano(4-tolyl)methyl]benzenesulfonamide (2o)

White solid; mp 100-102 °C; IR (KBr) $\nu_{\text{max}}/\text{cm}^{-1}$ 3278 (NH), 2245 (CN), 1336 (S=O asym), 1163 (S=O sym); ^1H NMR (400 MHz, CDCl_3) δ 2.36 (s, 3H, CH_3), 5.43 (d, 1H, J 8.0 Hz, NH), 5.59 (d, 1H, J 8.0 Hz, CH), 7.18-7.31 (m, 4H, ArH), 7.55-7.93 (m, 5H, ArH); ^{13}C NMR (100 MHz, CDCl_3) δ 21.2, 48.0, 116.4, 127.0, 127.3, 129.0, 129.5, 130.0, 133.7, 139.0, 140.1. Anal. calcd. for $C_{15}H_{14}N_2O_2S$: C, 62.92; H, 4.93; N, 9.78; found: C, 62.99; H, 4.92; N, 9.76.

N-[(4-Chlorophenyl)(cyano)methyl]benzenesulfonamide (2p)

White solid; mp 122-124 °C; IR (KBr) $\nu_{\text{max}}/\text{cm}^{-1}$ 3229 (NH), 2238 (CN), 1333 (S=O asym), 1170 (S=O sym); ^1H NMR (400 MHz, CDCl_3) δ 5.44 (bs, 1H, NH), 5.50 (d, 1H, J 8.0 Hz, CH), 7.40 (s, 4H, ArH), 7.58-7.62 (m, 2H, ArH), 7.68-7.72 (m, 1H, ArH), 7.93 (d, 2H, J 8.0 Hz, ArH); ^{13}C NMR (100 MHz, CDCl_3) δ 47.7, 115.8, 127.3, 128.5, 129.6, 129.6, 130.5, 133.9, 136.2, 138.8. Anal. calcd. for $C_{14}H_{11}ClN_2O_2S$: C, 54.82; H, 3.61; N, 9.13; found: C, 54.77; H, 3.60; N, 9.16.

N-[(4-Bromophenyl)(cyano)methyl]benzenesulfonamide (2q)

White solid; mp 130-132 °C; IR (KBr) $\nu_{\text{max}}/\text{cm}^{-1}$ 3233 (NH), 2239 (CN), 1332 (S=O asym), 1169 (S=O sym); ^1H NMR (400 MHz, CDCl_3) δ 5.28 (d, 1H, J 9.2 Hz, NH), 5.50 (d, 1H, J 9.2 Hz, CH), 7.33-7.55 (m, 2H, ArH), 7.56-7.74 (m, 5H, ArH), 7.92-7.96 (m, 2H, ArH); ^{13}C NMR (100 MHz, CDCl_3) δ 47.7, 115.7, 124.4, 127.2, 128.7, 129.6, 130.9, 132.6, 133.9, 138.8. Anal. calcd. for $C_{14}H_{11}BrN_2O_2S$: C, 47.88; H, 3.16; N, 7.98; found: C, 47.74; H, 3.17; N, 7.95.

References

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3. Trost, B. M.; Marrs, C.; *J. Org. Chem.* **1991**, 56, 6468.

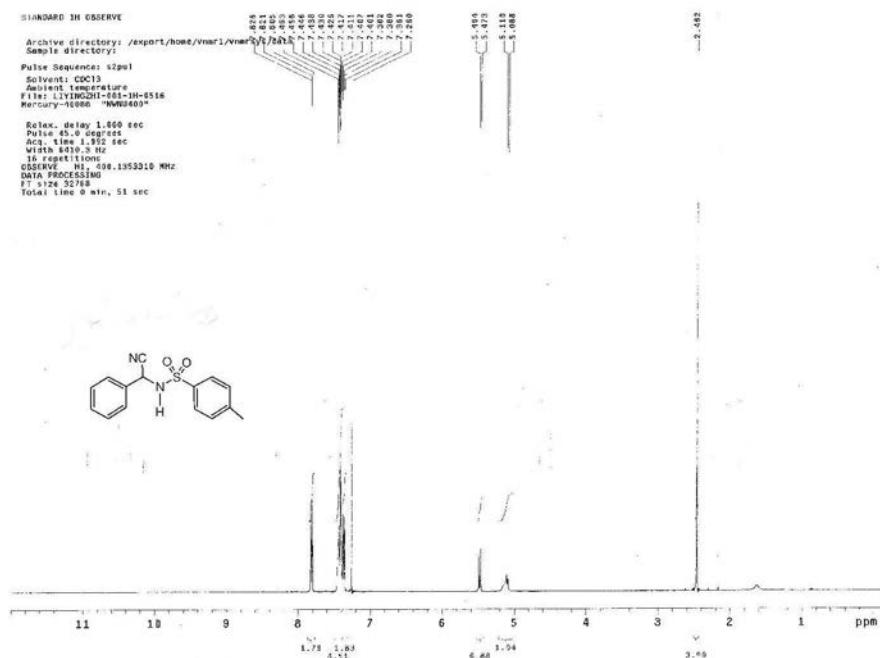


Figure S1. ¹H NMR spectrum (400 MHz, CDCl₃) of *N*-(cyanophenylmethyl)-4-methylbenzenesulfonamide (**2a**).

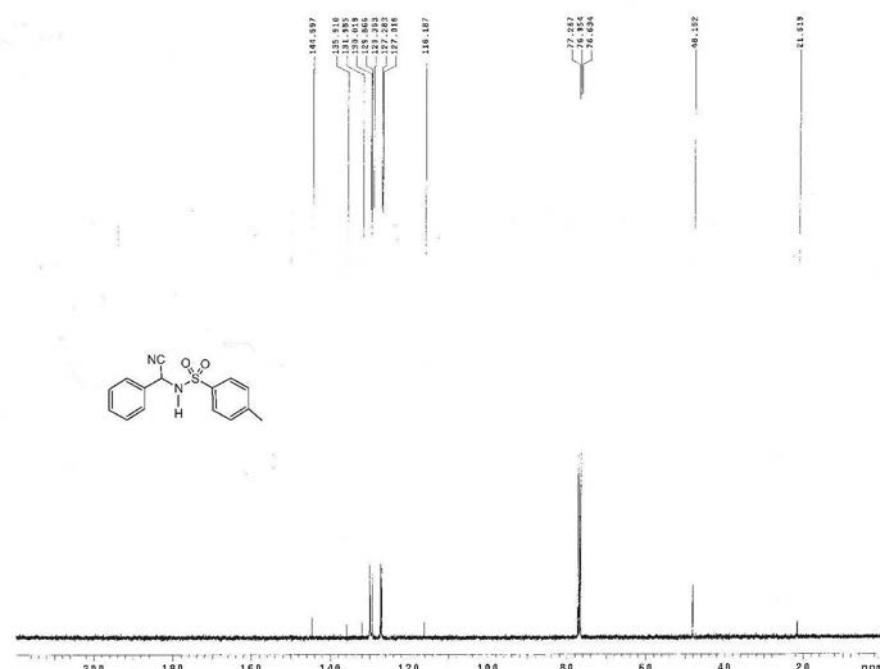


Figure S2. ¹³C NMR spectrum (100 MHz, CDCl₃) of *N*-(cyanophenylmethyl)-4-methylbenzenesulfonamide (**2a**).

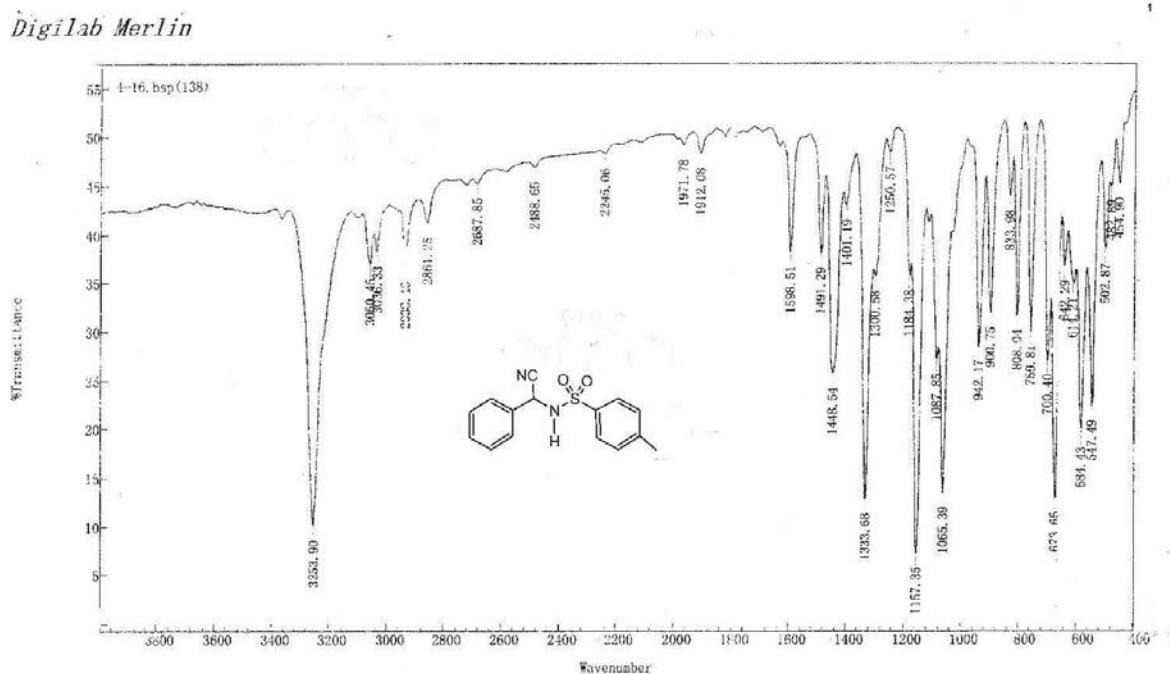


Figure S3. IR of *N*-(cyanophenylmethyl)-4-methylbenzenesulfonamide (**2a**).

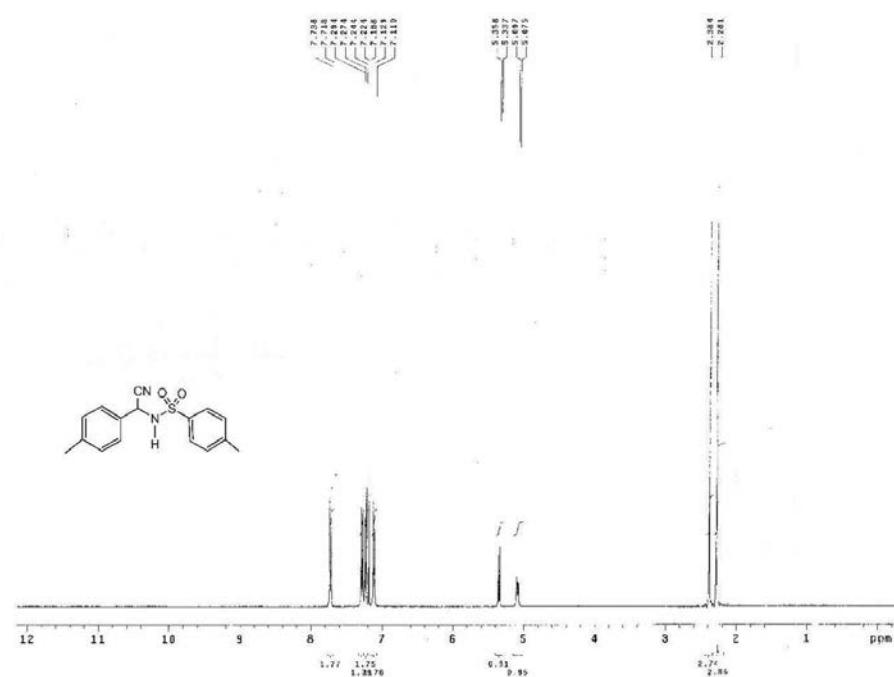


Figure S4. ^1H NMR spectrum (400 MHz, CDCl_3) of *N*-(cyano(4-tolyl)methyl)-4-methylbenzenesulfonamide (**2b**).

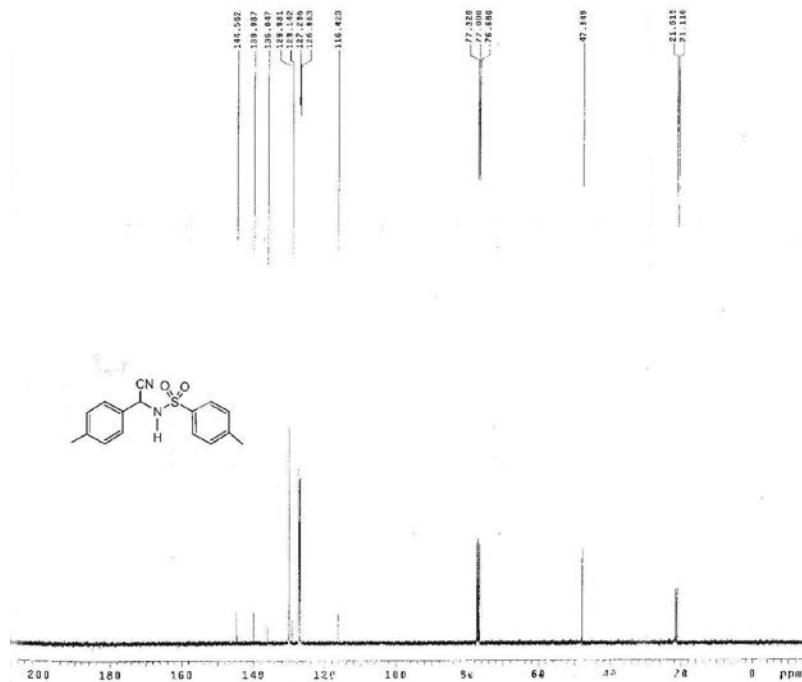


Figure S5. ¹³C NMR spectrum (100 MHz, CDCl₃) of *N*-[cyano(4-tolyl)methyl]-4-methylbenzenesulfonamide (**2b**).

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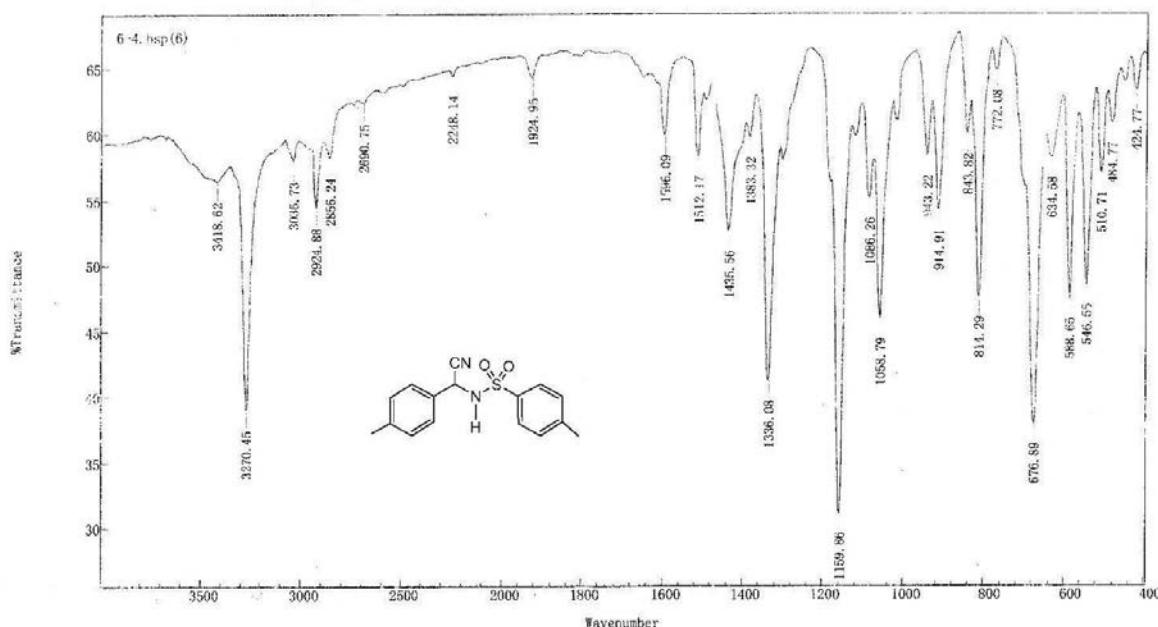
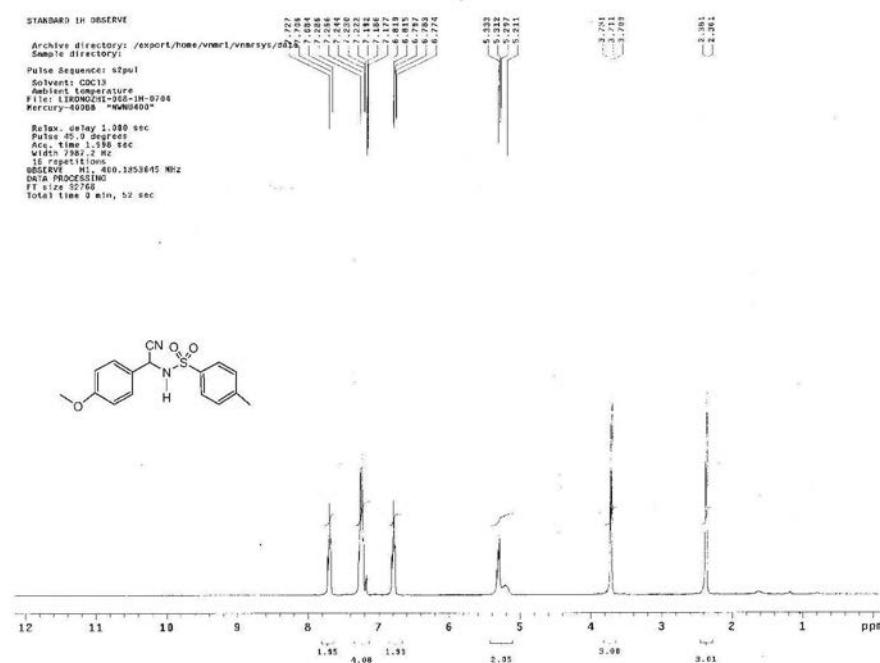


Figure S6. IR of *N*-[cyano(4-tolyl)methyl]-4-methylbenzenesulfonamide (**2b**).



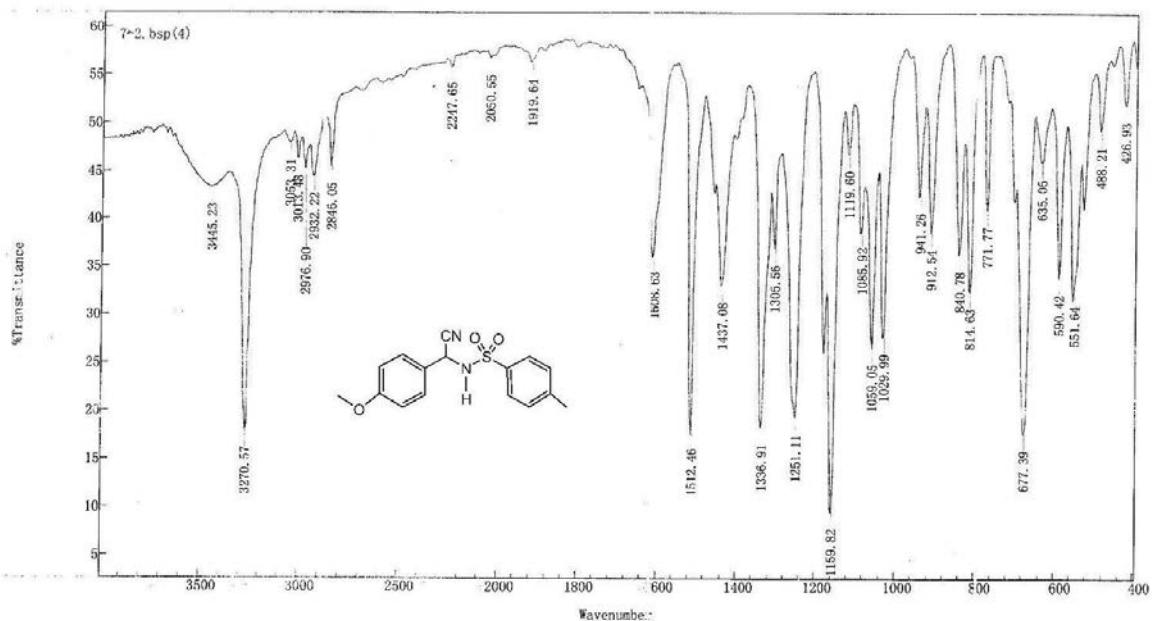
Digilab Merlin

Figure S9. IR of *N*-[cyano(4-methoxyphenyl)methyl]-4-methylbenzenesulfonamide (**2c**).

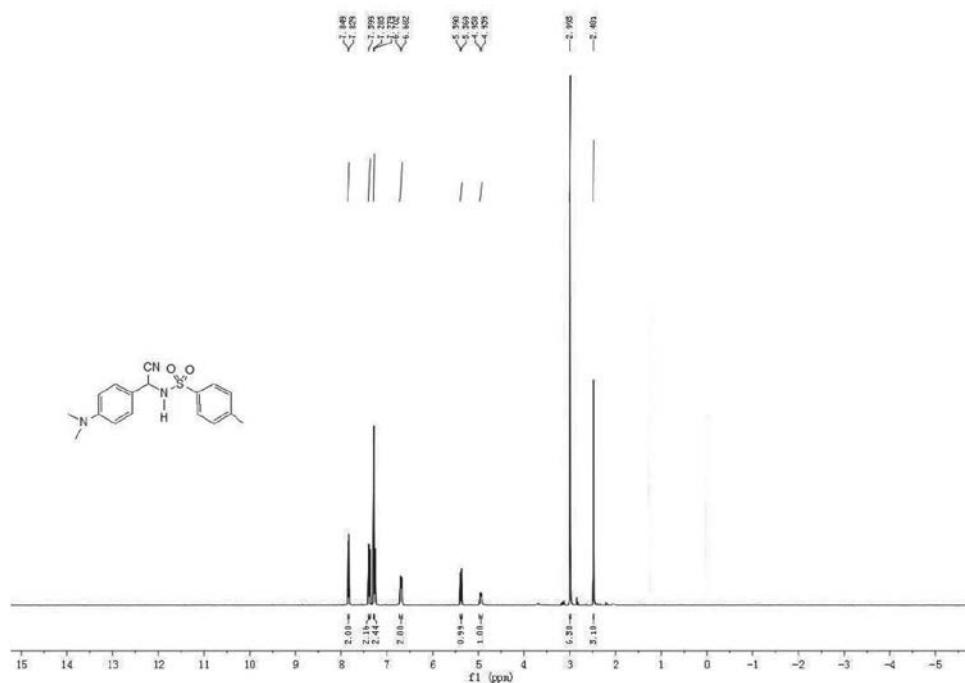


Figure S10. ¹H NMR spectrum (400 MHz, CDCl₃) of *N*-{cyano[4-(dimethylamino)phenyl]methyl}-4-methylbenzenesulfonamide (**2d**).

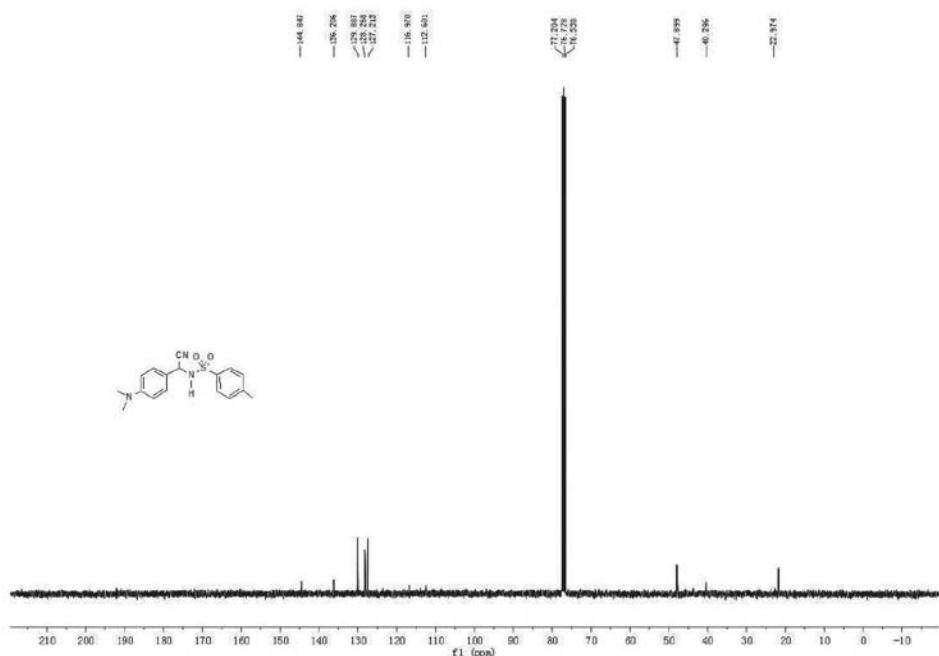


Figure S11. ^{13}C NMR spectrum (100 MHz, CDCl_3) of *N*-(cyano[4-(dimethylamino)phenyl]methyl)-4-methylbenzenesulfonamide (**2d**).

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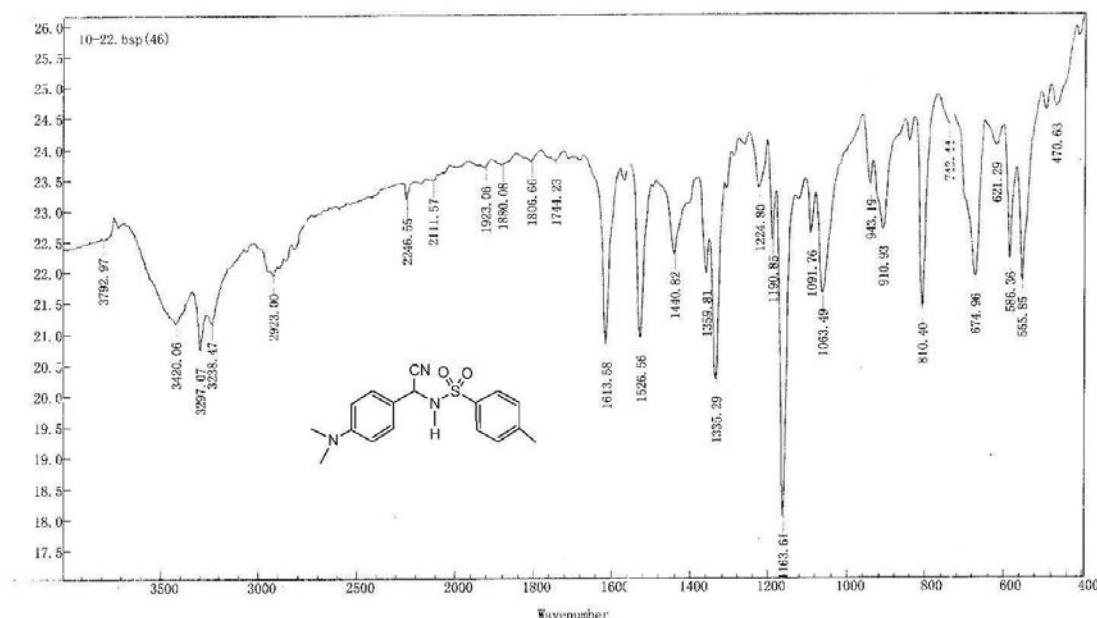


Figure S12. IR of *N*-{cyano[4-(dimethylamino)phenyl]methyl}-4-methylbenzenesulfonamide (**2d**).

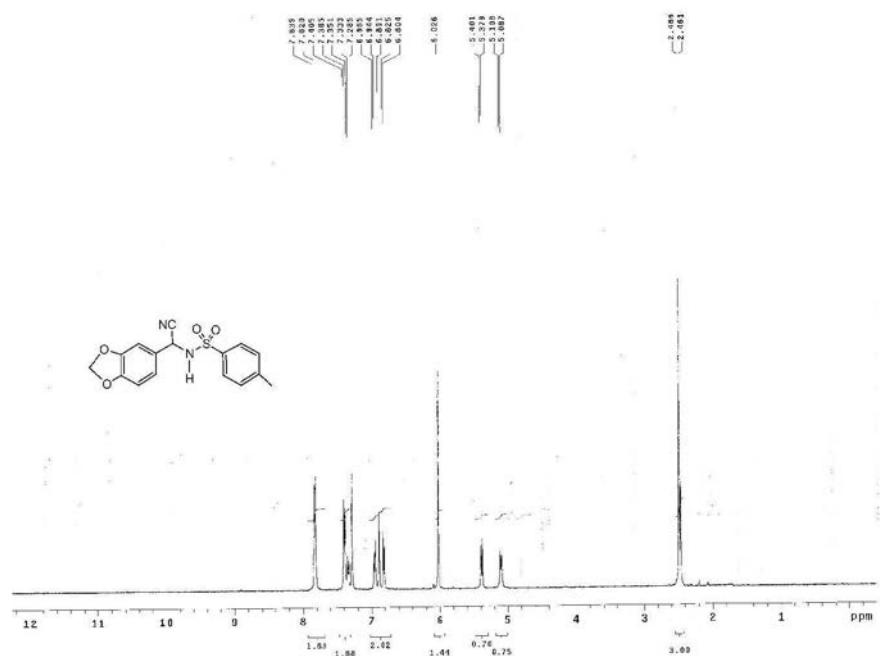


Figure S13. ^1H NMR spectrum (400 MHz, CDCl_3) of *N*-{benzo[*d*][1,3]dioxol-5-yl(cyano)methyl}-4-methylbenzenesulfonamide (**2e**).

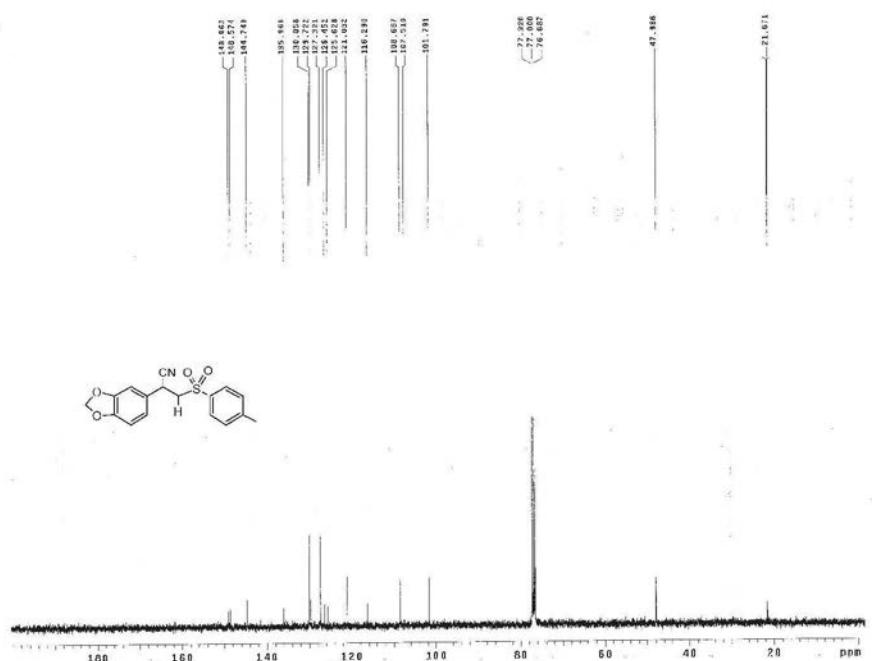
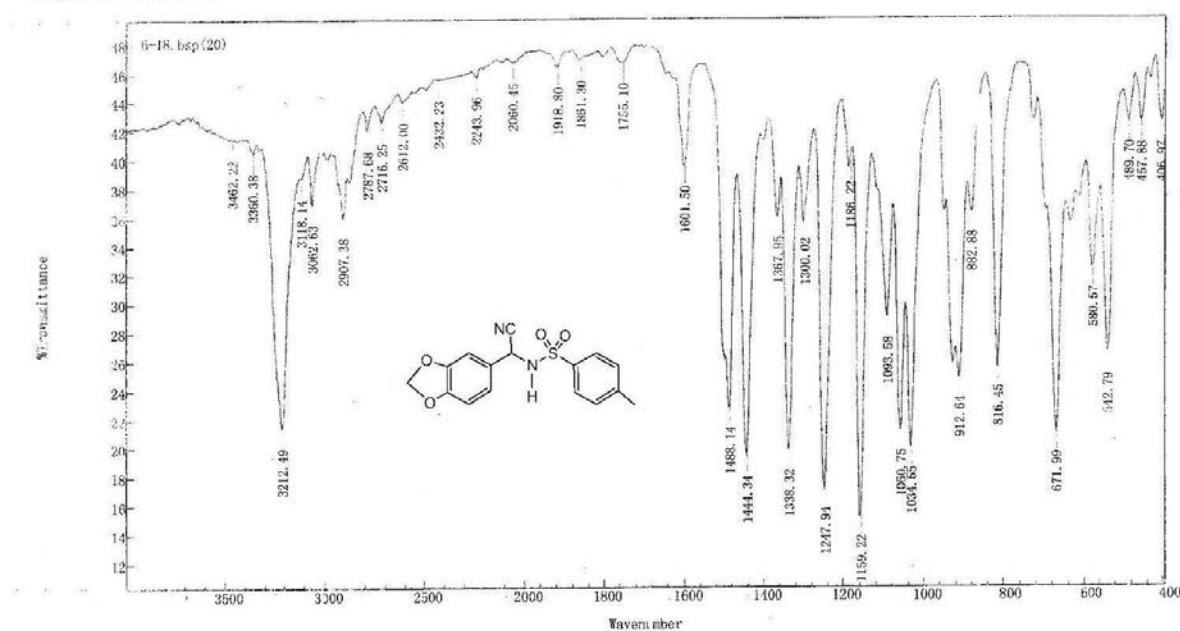
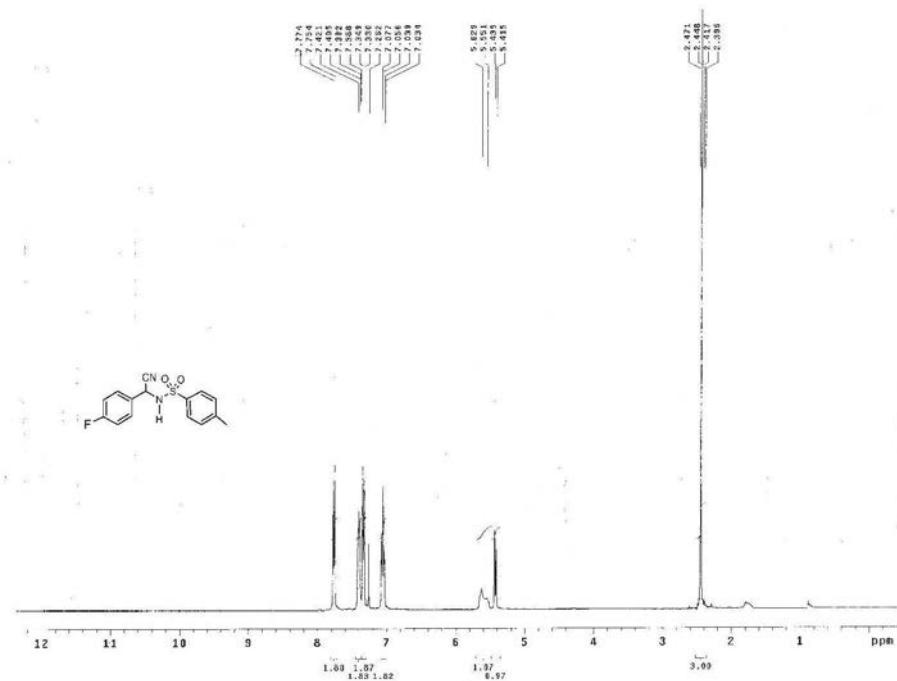


Figure S14. ^{13}C NMR spectrum (100 MHz, CDCl_3) of *N*-[benzo[*d*][1,3]dioxol-5-yl(cyano)methyl]-4-methylbenzenesulfonamide (**2e**).

Digilab Merlin**Figure S15.** IR of *N*-(benzo[*d*][1,3]dioxol-5-yl(cyano)methyl)-4-methylbenzenesulfonamide (**2e**).**Figure S16.** ¹H NMR spectrum (400 MHz, CDCl₃) of *N*-(cyano(4-fluorophenyl)methyl)-4-methylbenzenesulfonamide (**2f**).

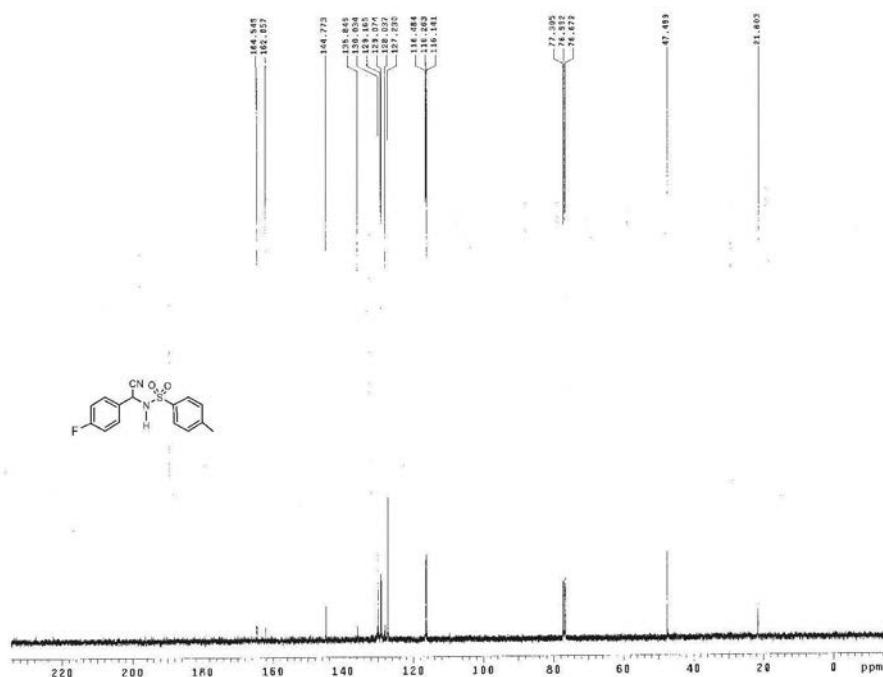


Figure S17. ¹³C NMR spectrum (100 MHz, CDCl₃) of *N*-[cyano(4-fluorophenyl)methyl]-4-methylbenzenesulfonamide (**2f**).

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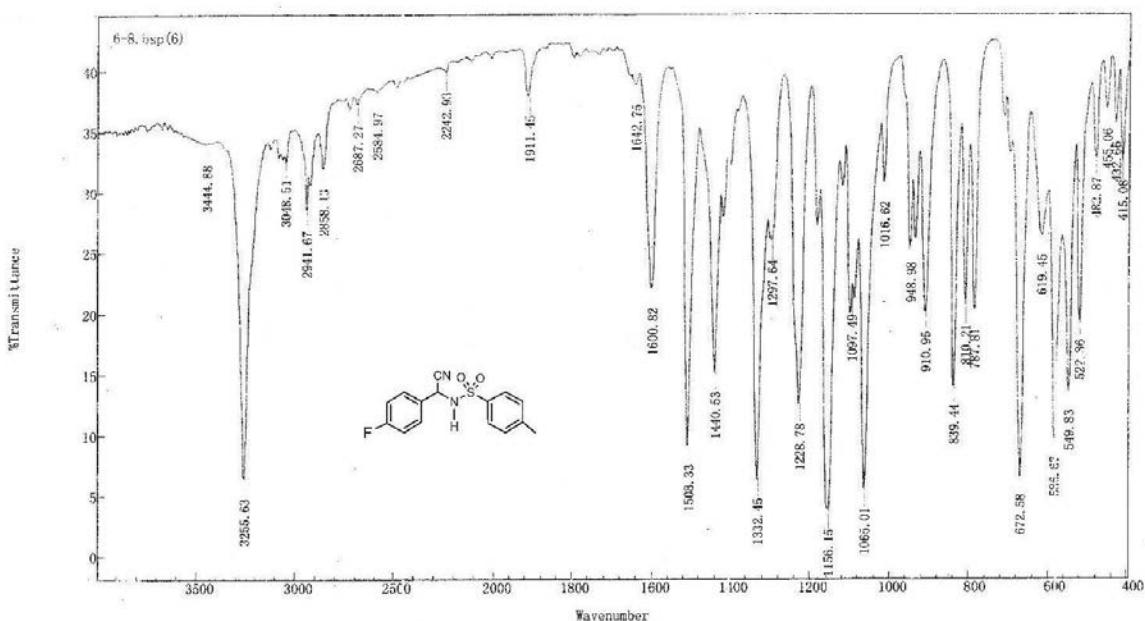


Figure S18. IR of *N*-[cyano(4-fluorophenyl)methyl]-4-methylbenzenesulfonamide (**2f**).

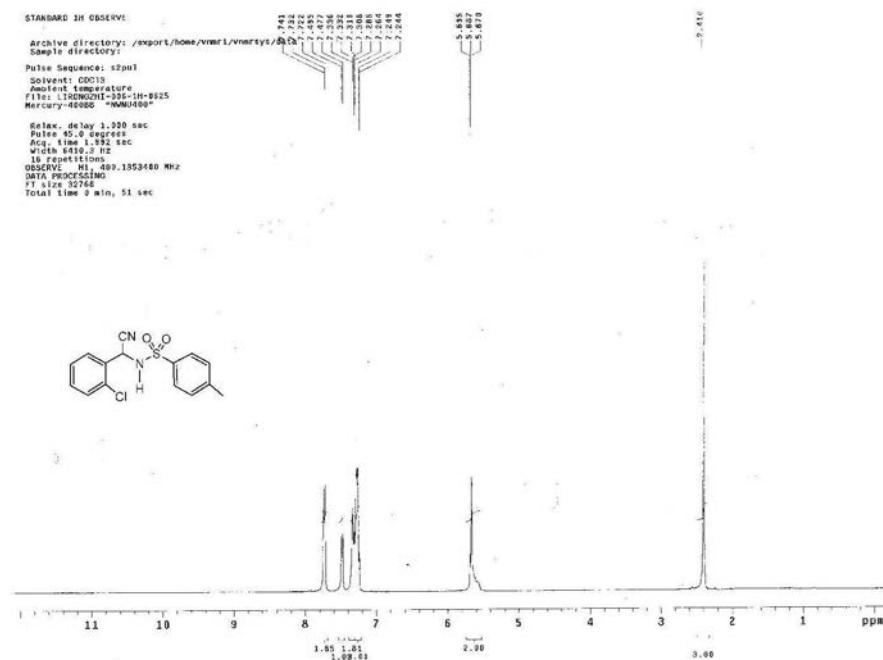


Figure S19. ¹H NMR spectrum (400 MHz, CDCl₃) of *N*-(2-chlorophenyl)(cyano)methyl]-4-methylbenzenesulfonamide (**2g**).

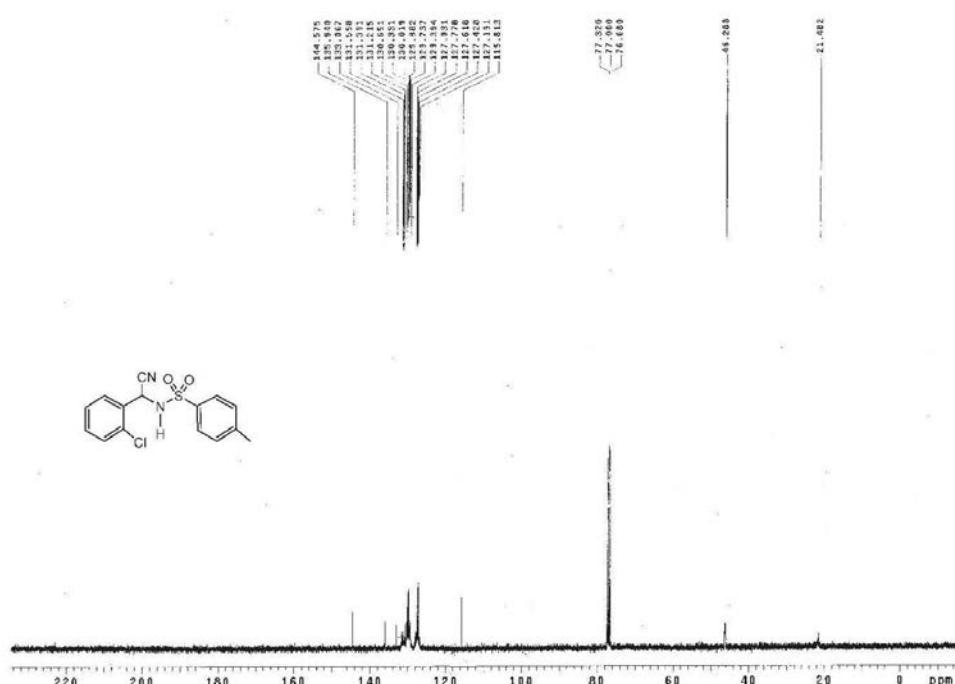


Figure S20. ¹³C NMR spectrum (100 MHz, CDCl₃) of *N*-(2-chlorophenyl)(cyano)methyl]-4-methylbenzenesulfonamide (**2g**).

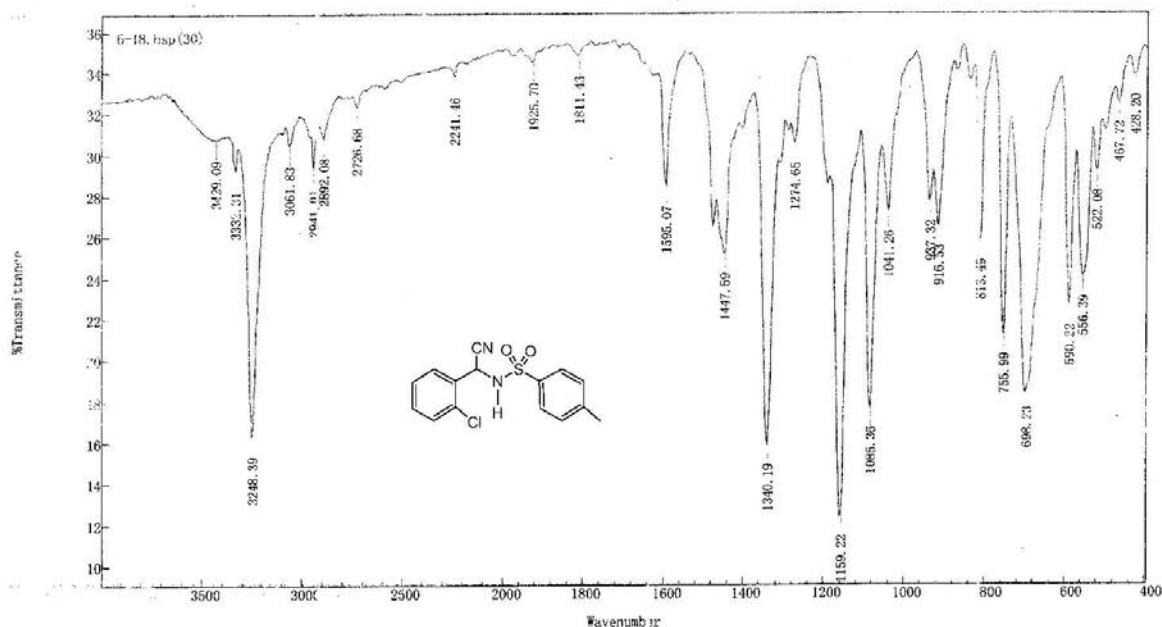
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Figure S21. IR of *N*-[(2-chlorophenyl)(cyano)methyl]-4-methylbenzenesulfonamide (**2g**).

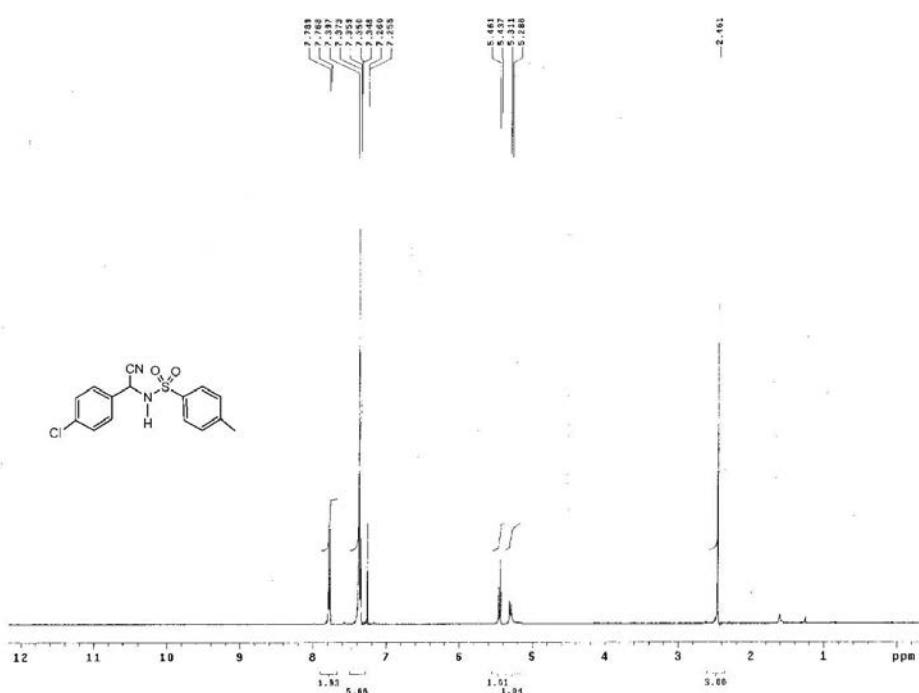


Figure S22. ¹H NMR spectrum (400 MHz, CDCl₃) of *N*-[4-chlorophenyl(cyano)methyl]-4-methylbenzenesulfonamide (**2h**).

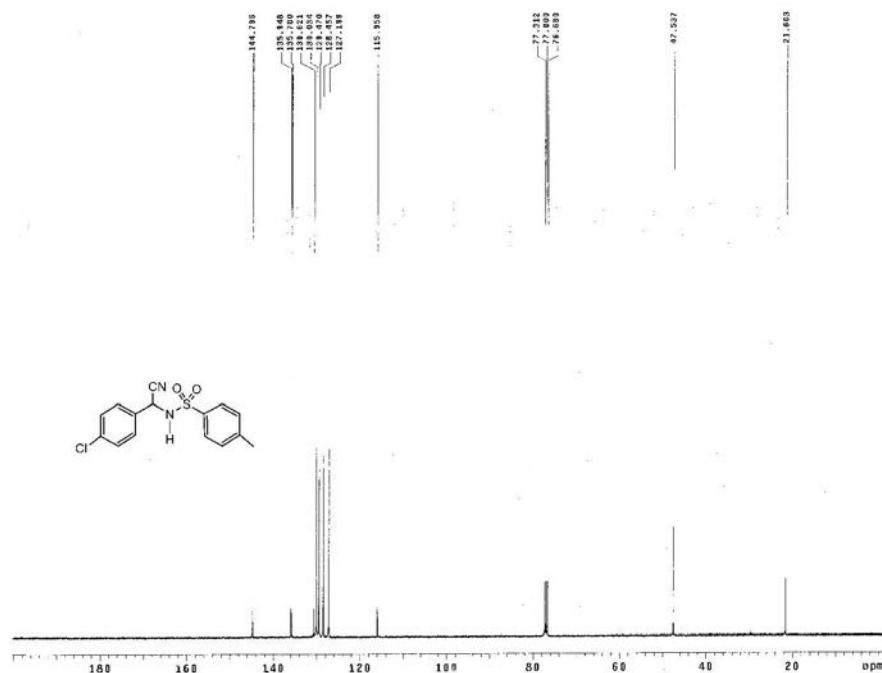


Figure S23. ¹³C NMR spectrum (100 MHz, CDCl_3) of *N*-[4-chlorophenyl(cyano)methyl]-4-methylbenzenesulfonamide (**2h**).

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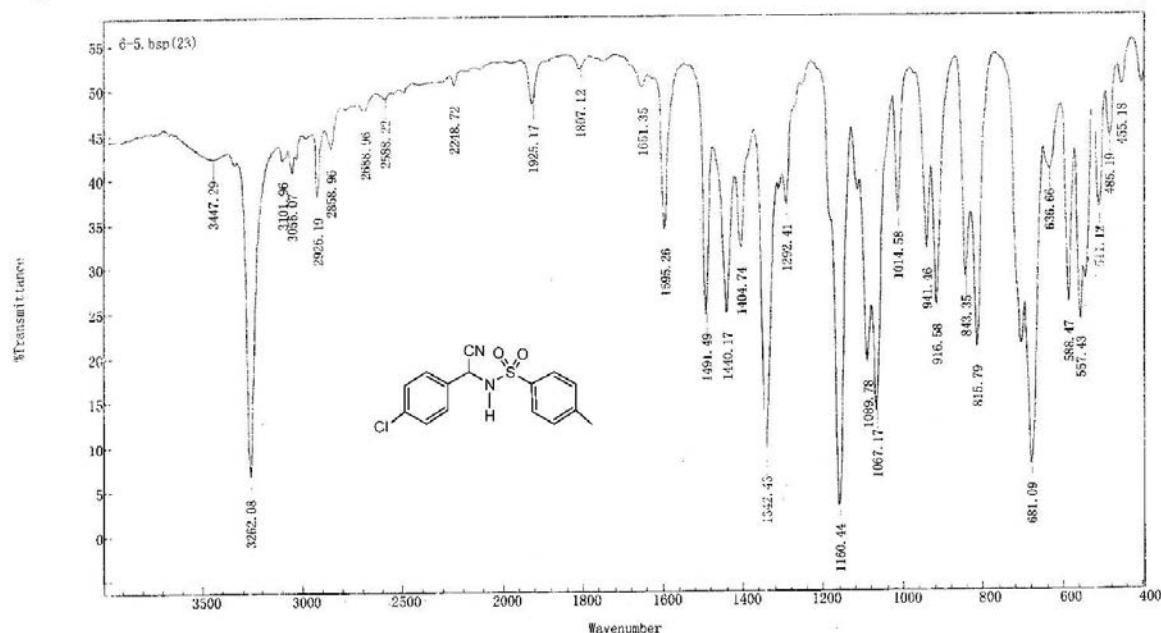


Figure S24. IR of *N*-[4-chlorophenyl(cyano)methyl]-4-methylbenzenesulfonamide (**2h**).

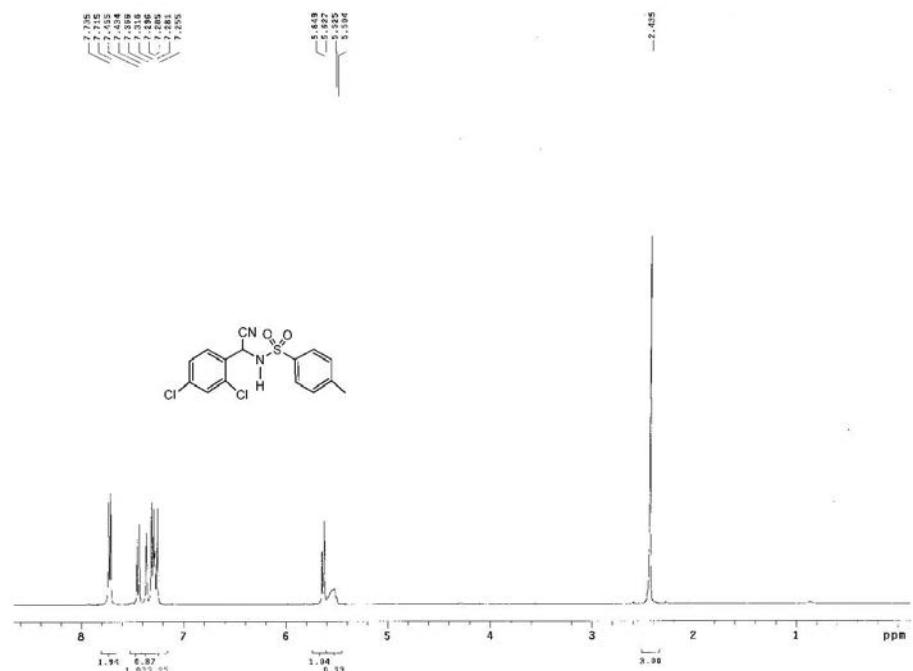


Figure S25. ^1H NMR spectrum (400 MHz, CDCl_3) of *N*-[cyano(2,4-dichlorophenyl)methyl]-4-methylbenzenesulfonamide (**2i**).

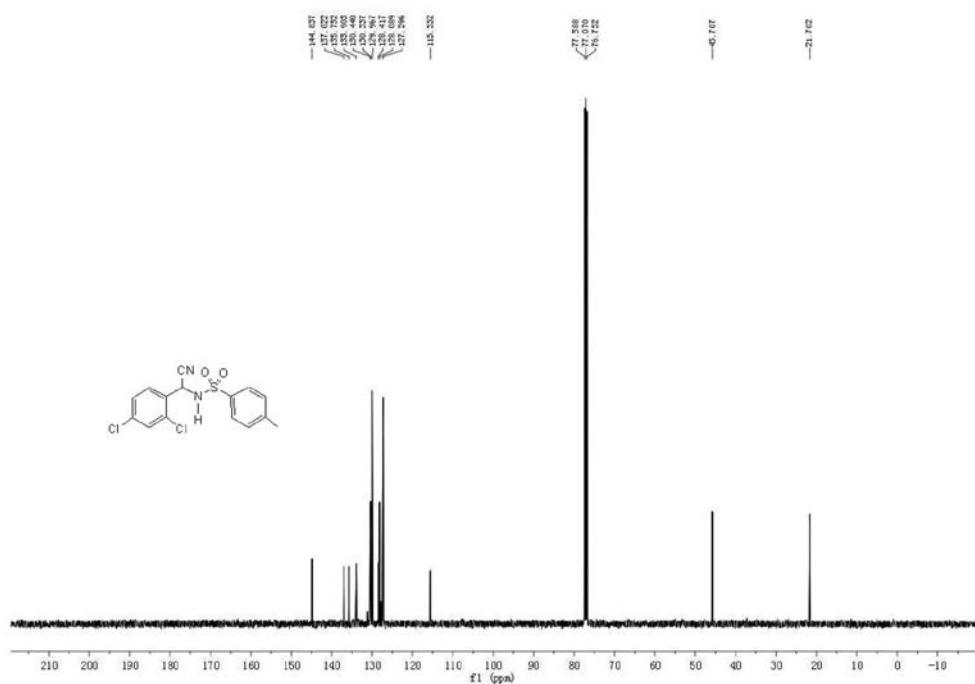
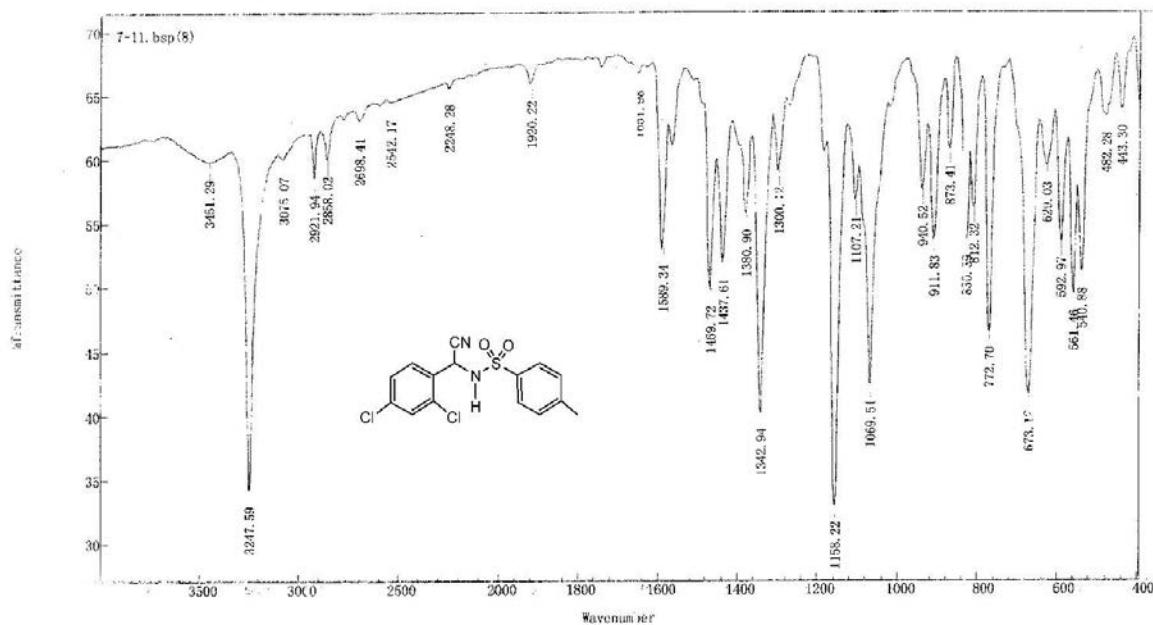
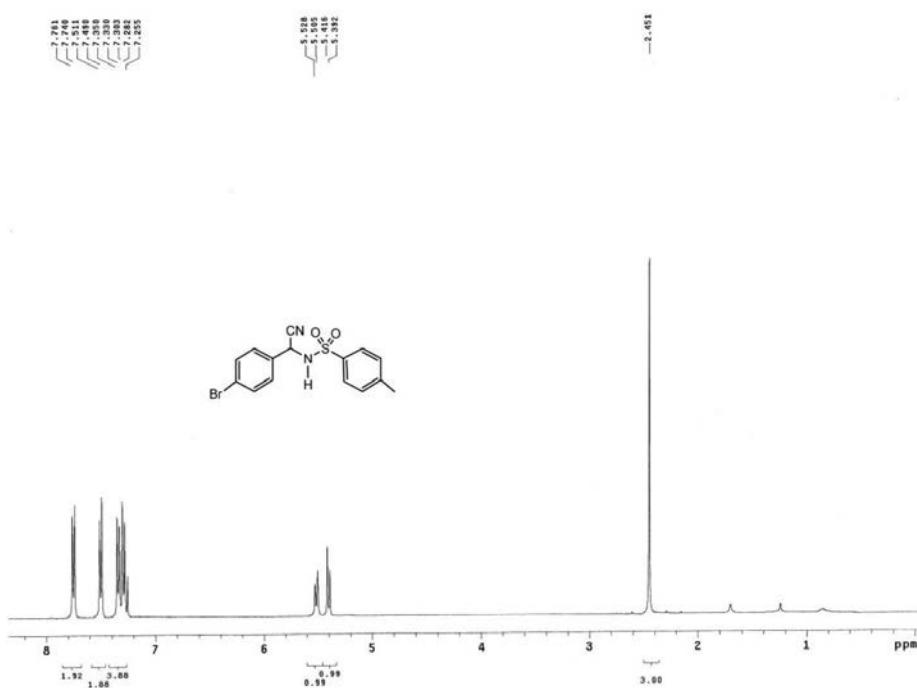


Figure S26. ^{13}C NMR spectrum (100 MHz, CDCl_3) of *N*-[cyano(2,4-dichlorophenyl)methyl]-4-methylbenzenesulfonamide (**2i**).

Vigilab Merlin**Figure S27.** IR of *N*-[cyano(2,4-dichlorophenyl)methyl]-4-methylbenzenesulfonamide (**2i**).**Figure S28.** ¹H NMR spectrum (400 MHz, CDCl₃) of *N*-[4-(bromophenyl)(cyano)methyl]-4-methylbenzenesulfonamide (**2j**).

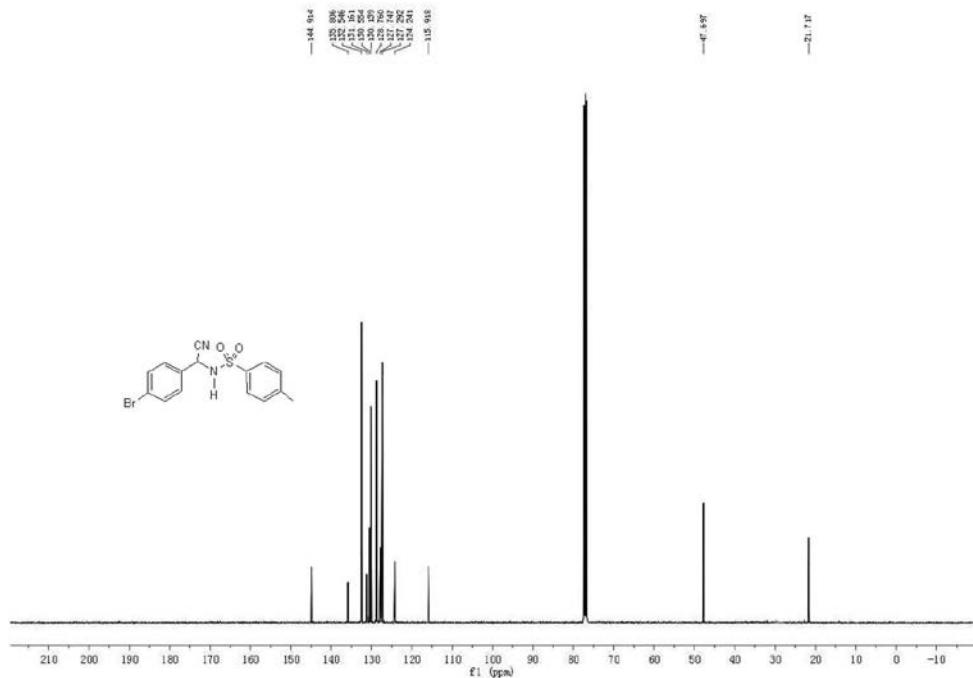


Figure S29. ^{13}C NMR spectrum (100 MHz, CDCl_3) of *N*-[4-(bromophenyl)(cyano)methyl]-4-methylbenzenesulfonamide (**2j**).

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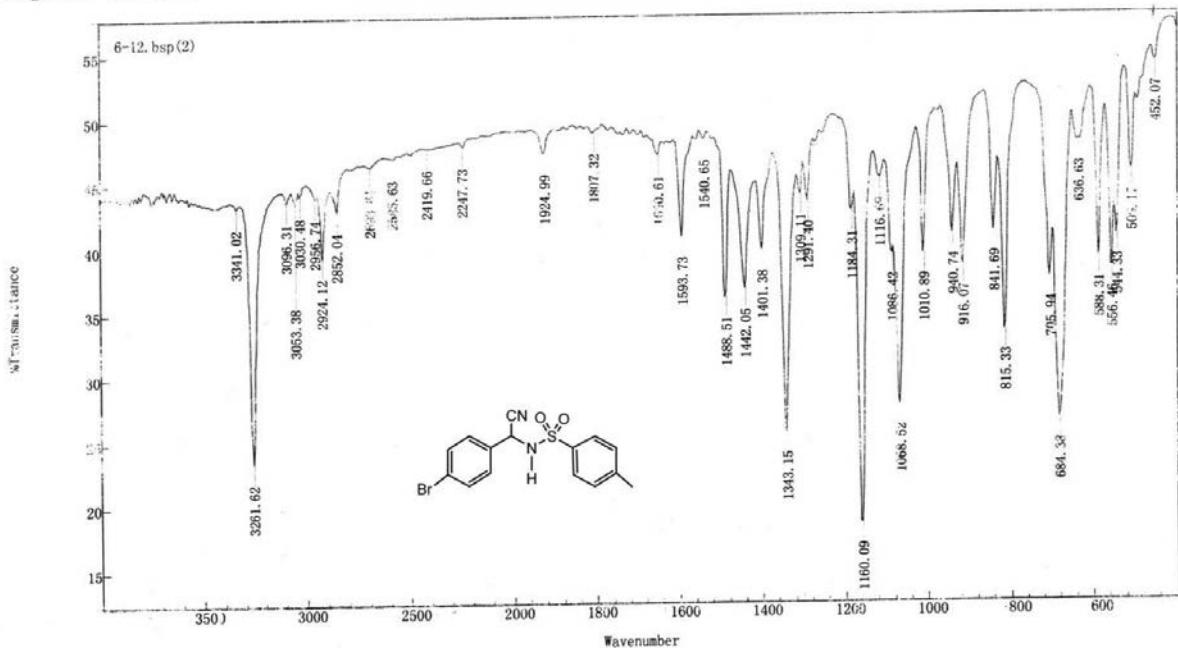


Figure S30. IR of *N*-[4-(bromophenyl)(cyano)methyl]-4-methylbenzenesulfonamide (**2j**).

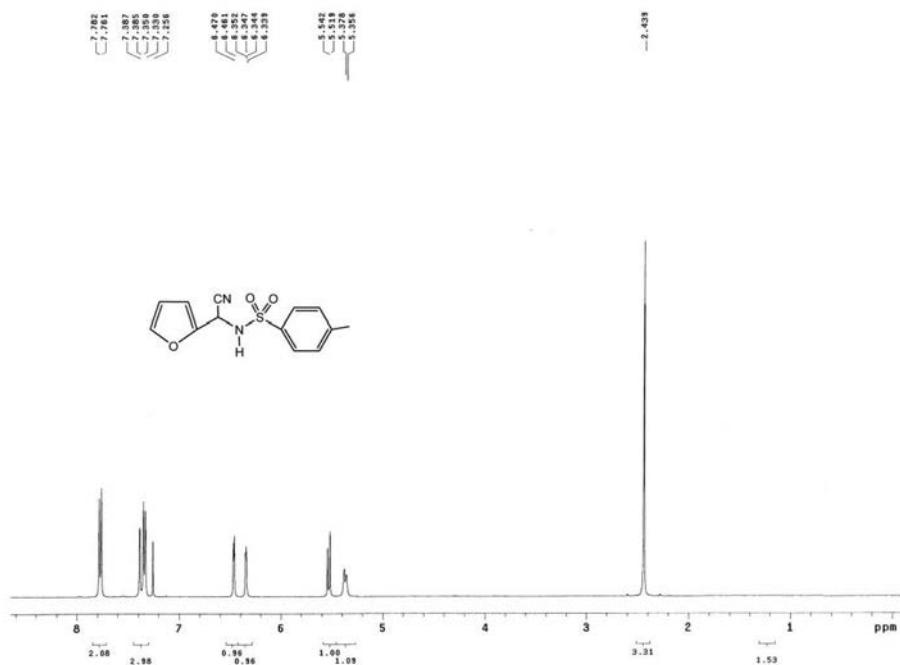


Figure S31. ¹H NMR spectrum (400 MHz, CDCl₃) of *N*-[cyano(furan-2-yl)methyl]-4-methylbenzenesulfonamide (**2k**).

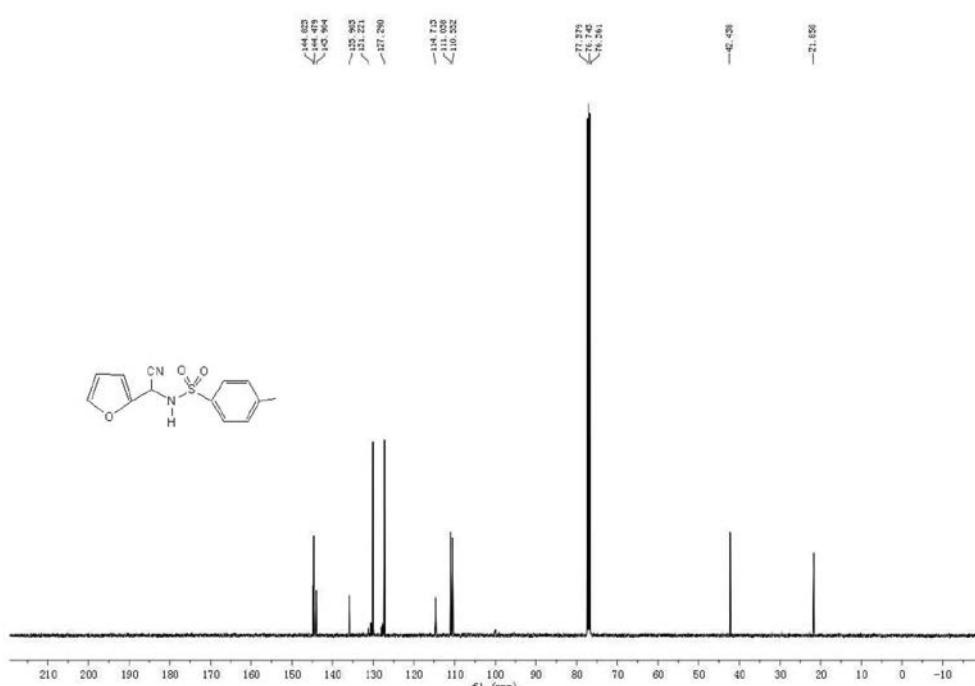


Figure S32. ¹³C NMR spectrum (100 MHz, CDCl₃) of *N*-[cyano(furan-2-yl)methyl]-4-methylbenzenesulfonamide (**2k**).

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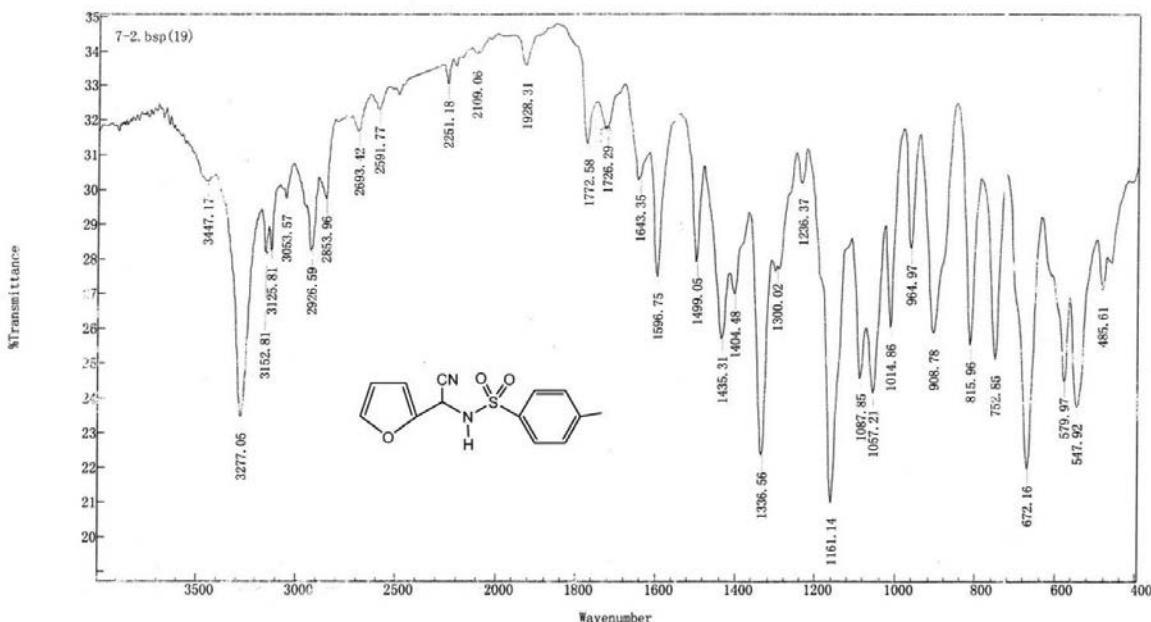


Figure S33. IR of *N*-[cyano(furan-2-yl)methyl]-4-methylbenzenesulfonamide (**2k**).

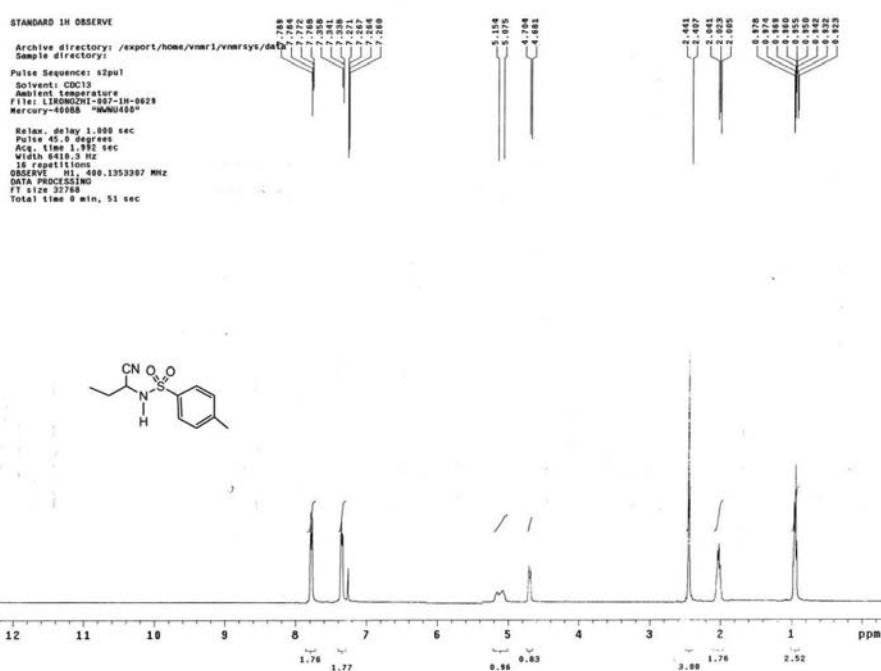


Figure S34. ^1H NMR spectrum (400 MHz, CDCl_3) *N*-(1-cyanopropyl)-4-methylbenzenesulfonamide (**2l**).

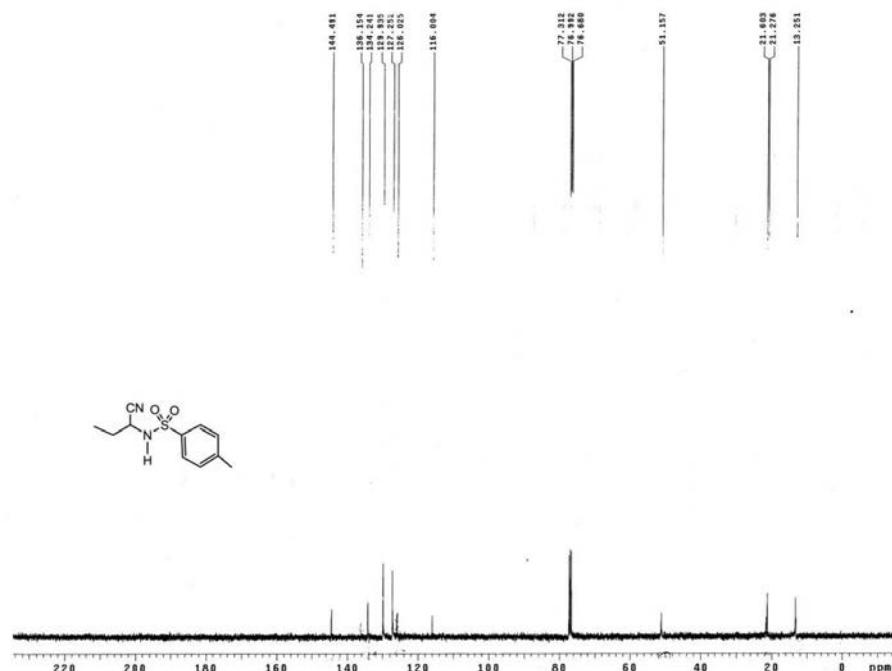


Figure S35. ¹³C NMR spectrum (100 MHz, CDCl₃) of *N*-(1-cyanopropyl)-4-methylbenzenesulfonamide (**2l**).

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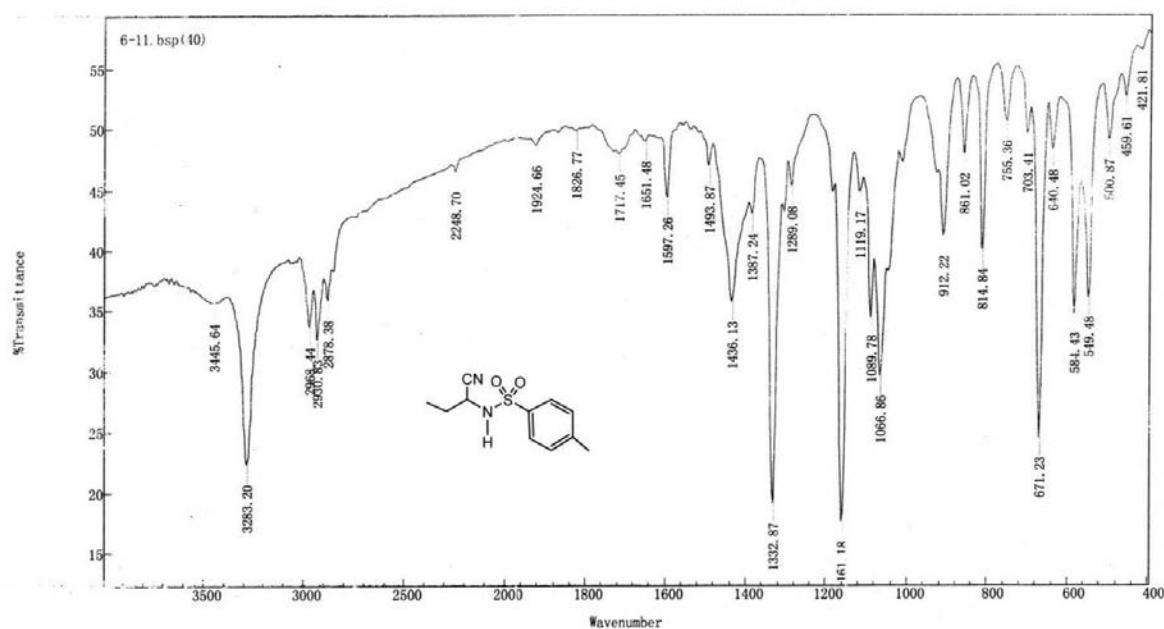


Figure S36. IR of *N*-(1-cyanopropyl)-4-methylbenzenesulfonamide (**2l**).

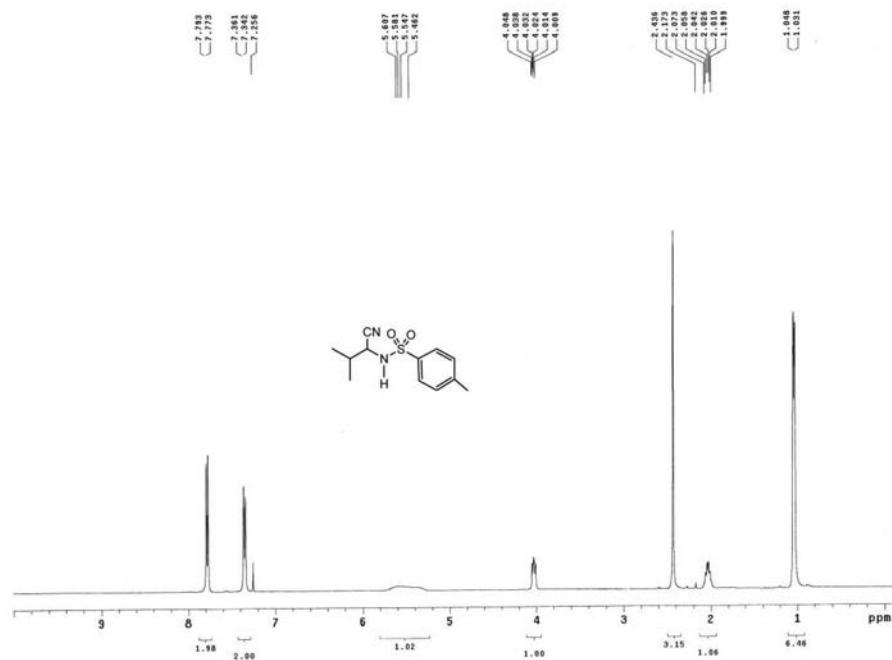


Figure S37. ¹H NMR spectrum (400 MHz, CDCl₃) of *N*-(1-cyano-2-methylpropyl)-4-methylbenzenesulfonamide (**2m**).

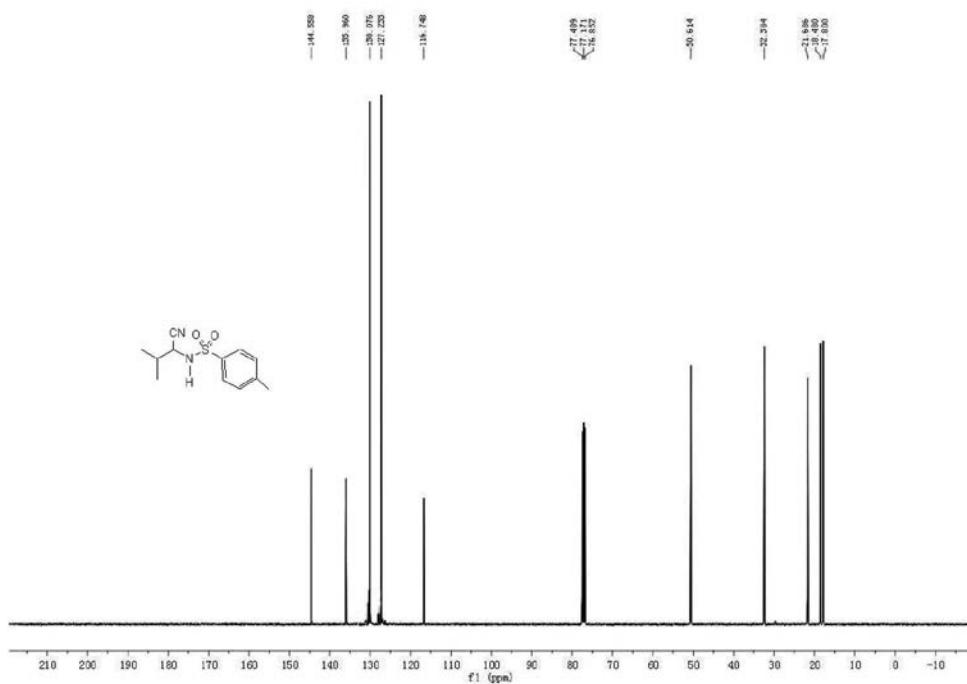
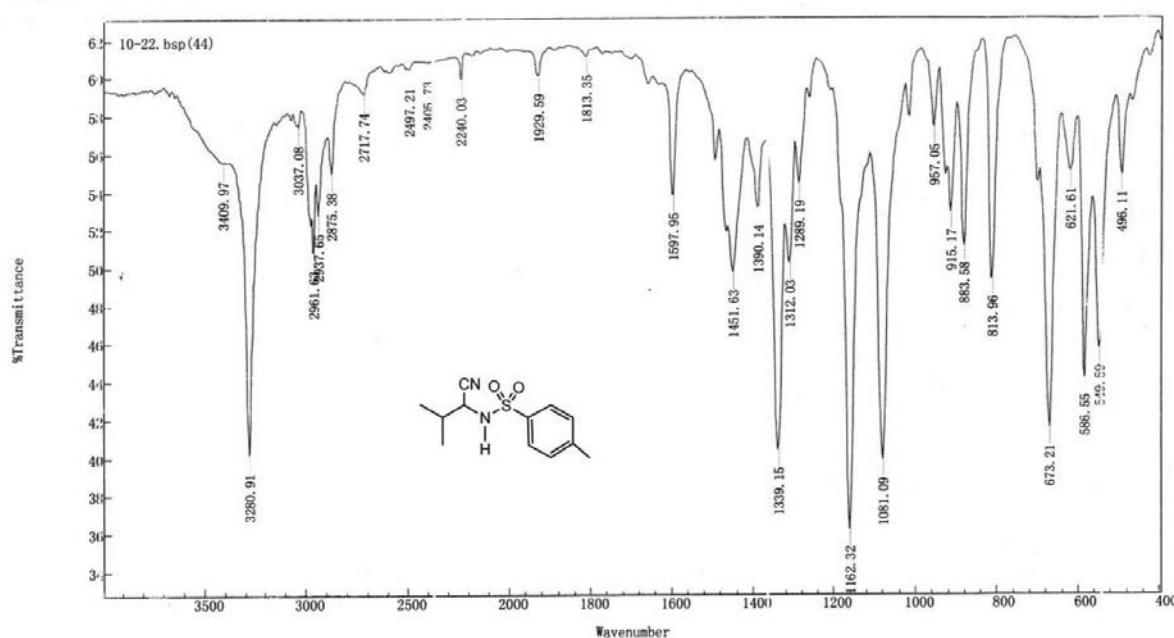
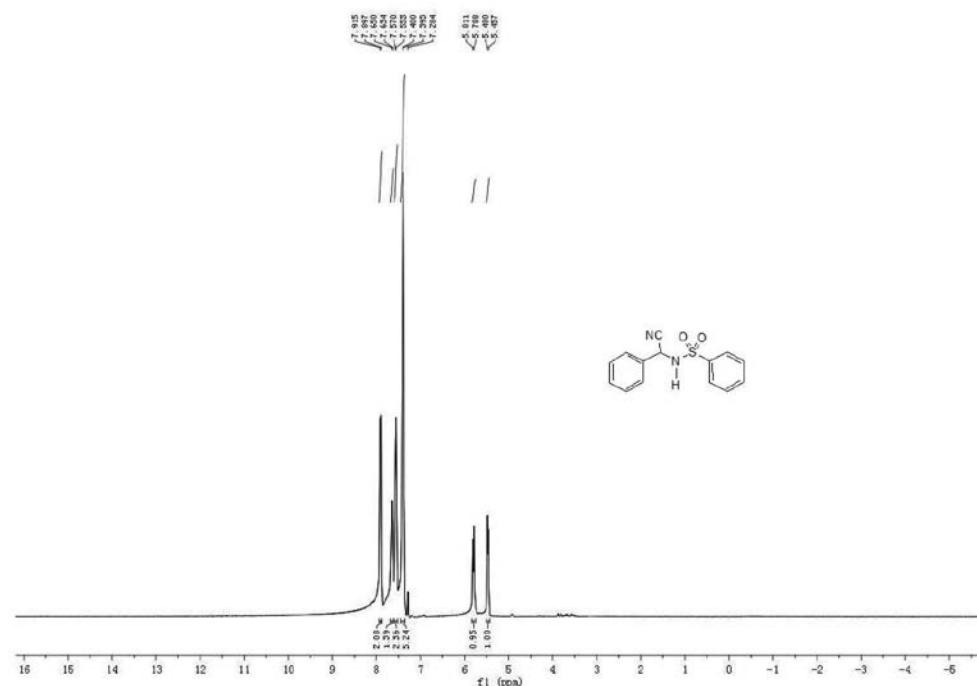


Figure S38. ¹³C NMR spectrum (100 MHz, CDCl₃) of *N*-(1-cyano-2-methylpropyl)-4-methylbenzenesulfonamide (**2m**).

Digilab Merlin**Figure S39.** IR of *N*-(1-cyano-2-methylpropyl)-4-methylbenzenesulfonamide (**2m**).**Figure S40.** ¹H NMR spectrum (400 MHz, CDCl₃) of *N*-[cyano(phenyl)methyl]benzenesulfonamide (**2n**).

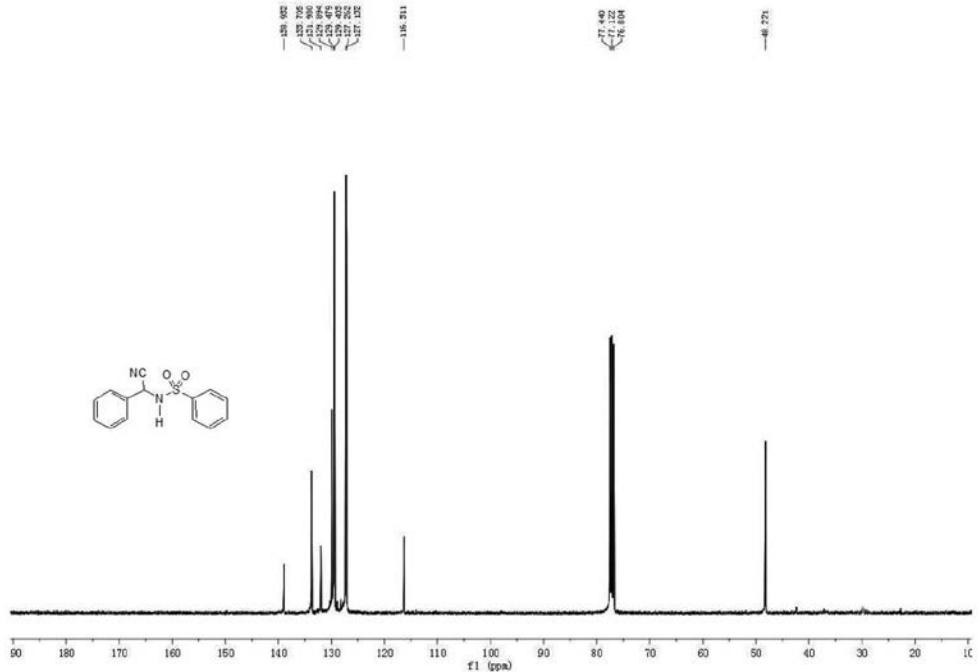


Figure S41. ^{13}C NMR spectrum (100 MHz, CDCl_3) of *N*-[cyano(phenyl)methyl]benzenesulfonamide (**2n**).

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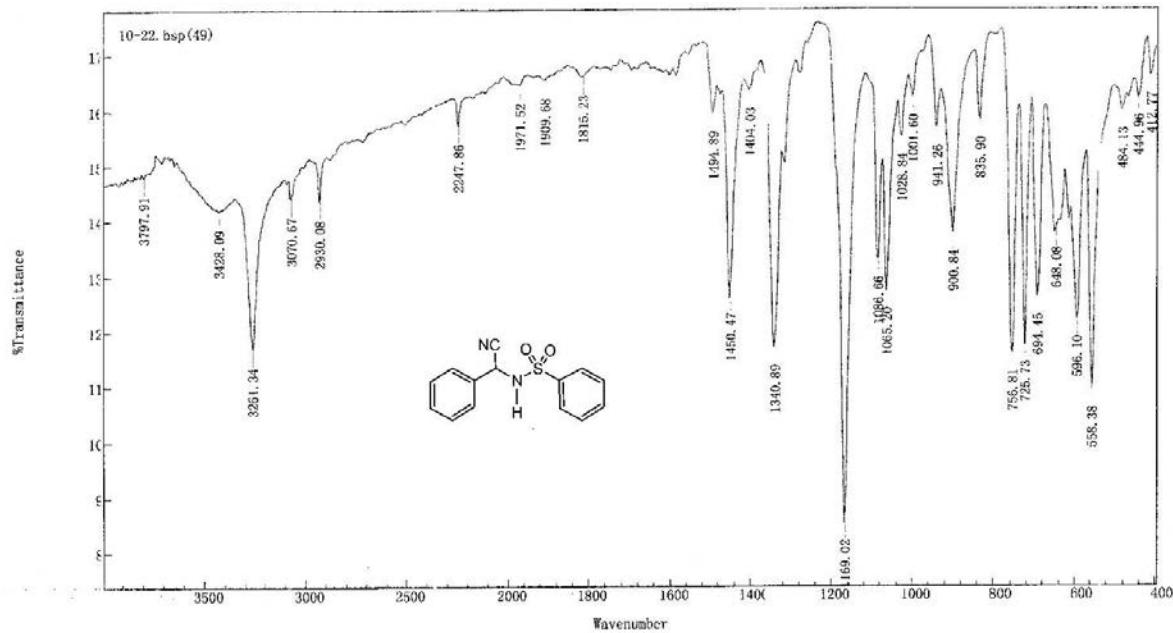


Figure S42. IR of *N*-[cyano(phenyl)methyl]benzenesulfonamide (**2n**).

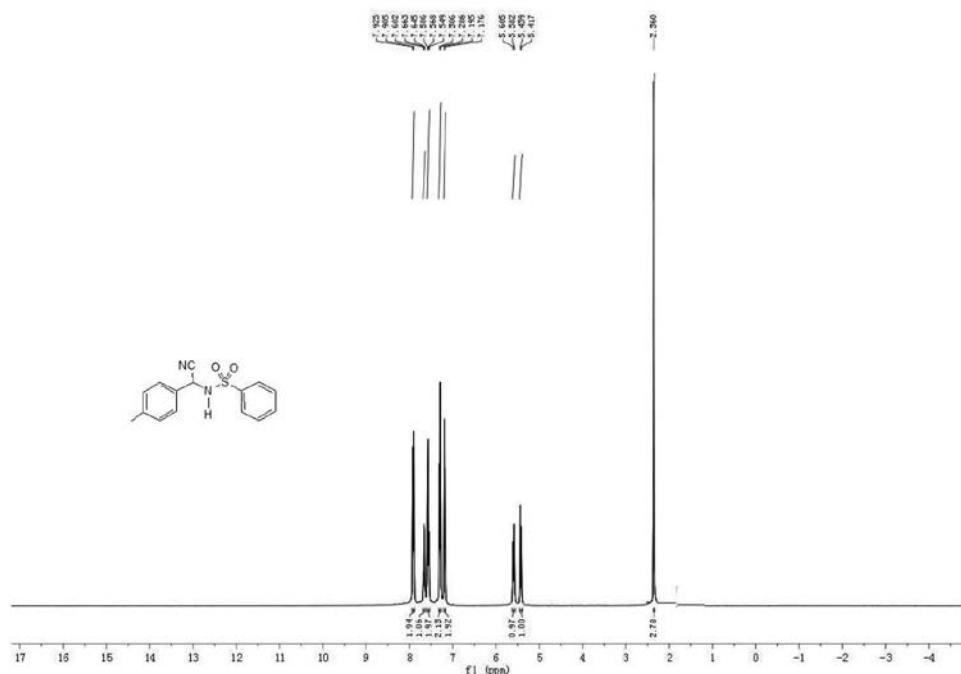


Figure S43. ¹H NMR spectrum (400 MHz, CDCl₃) of *N*-[cyano(4-tolyl)methyl]benzenesulfonamide (**2o**).

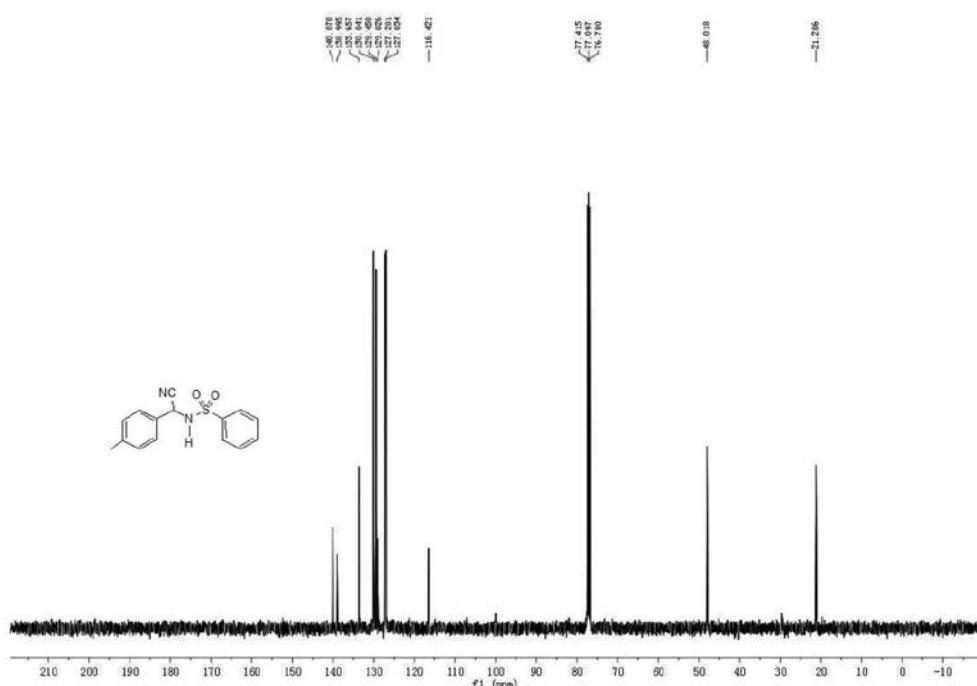


Figure S44. ¹³C NMR spectrum (100 MHz, CDCl₃) of *N*-[cyano(4-tolyl)methyl]benzenesulfonamide (**2o**).

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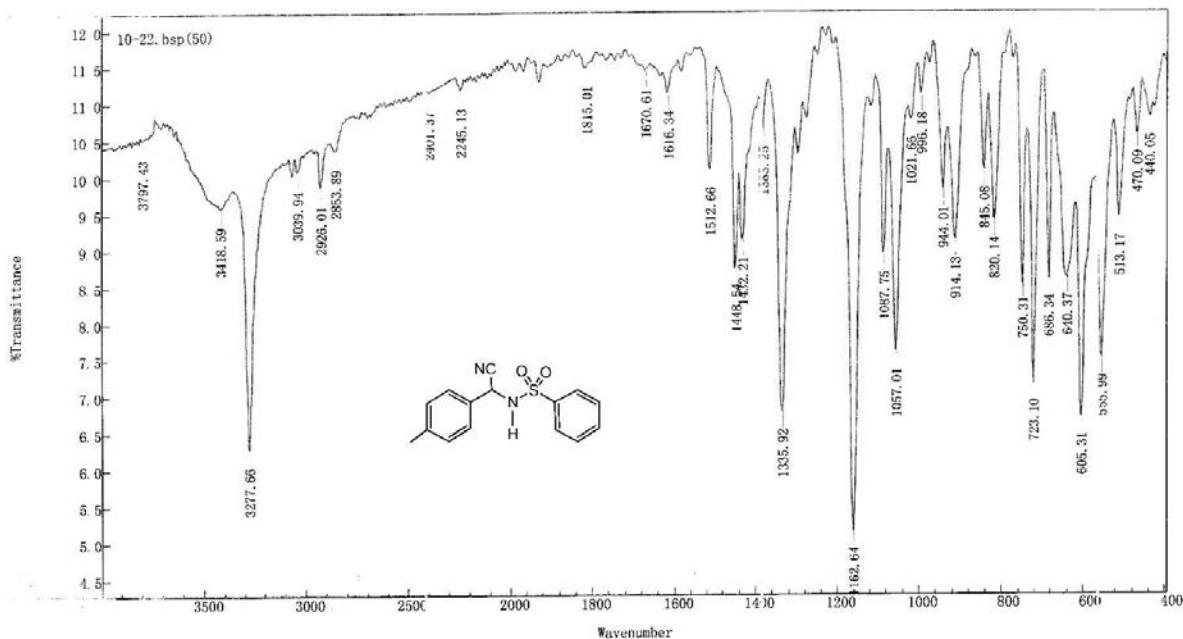


Figure S45. IR of *N*-[cyano(4-tolyl)methyl]benzenesulfonamide (**2o**).

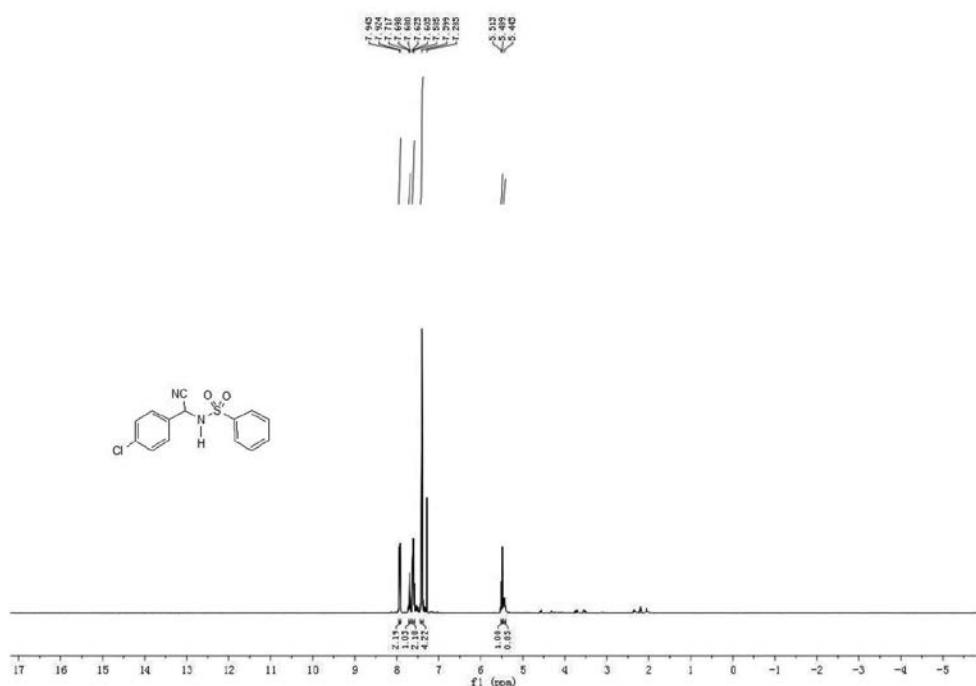


Figure S46. ^1H NMR spectrum (400 MHz, CDCl_3) of *N*-[(4-chlorophenyl)(cyano)methyl]benzenesulfonamide (**2p**).

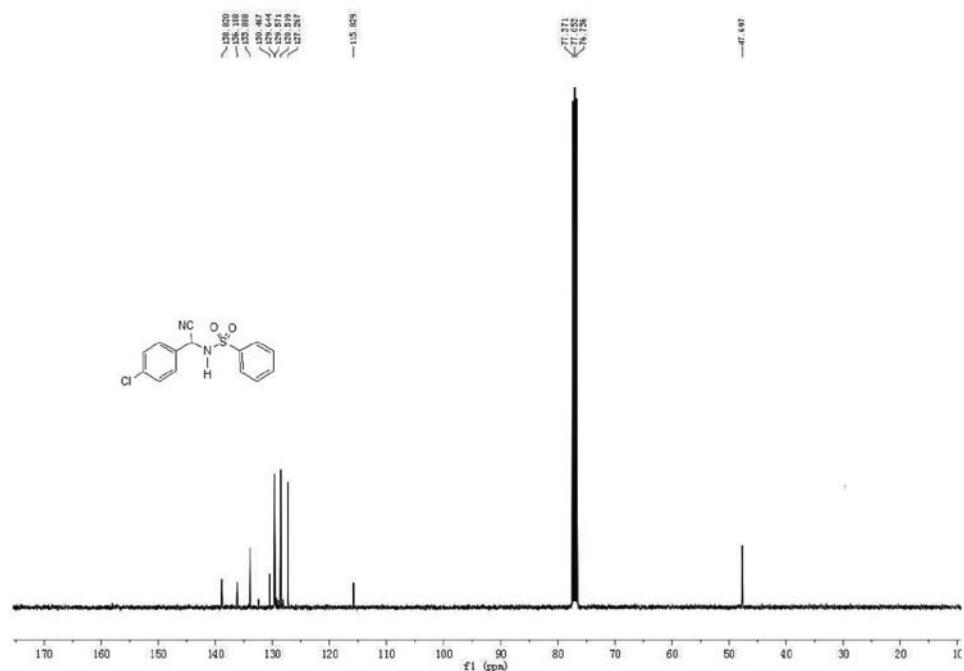


Figure S47. ^{13}C NMR spectrum (100 MHz, CDCl_3) of *N*-[(4-chlorophenyl) (cyano)methyl]benzenesulfonamide (**2p**).

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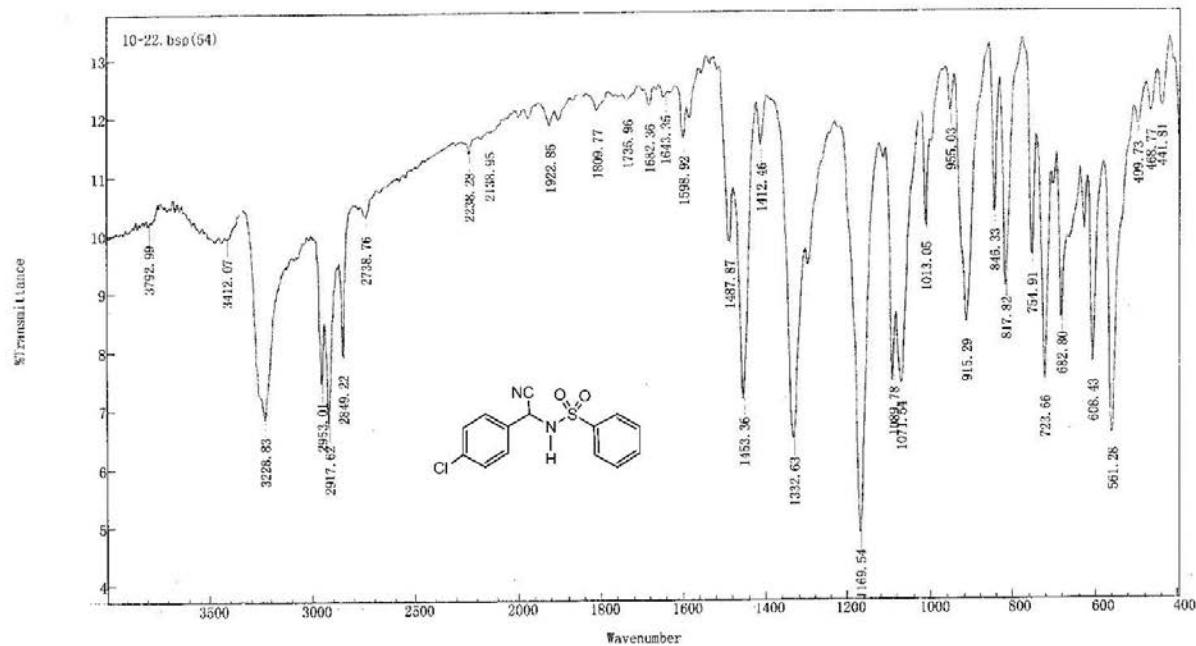


Figure S48. IR of *N*-[(4-chlorophenyl)(cyano)methyl]benzenesulfonamide (**2p**).

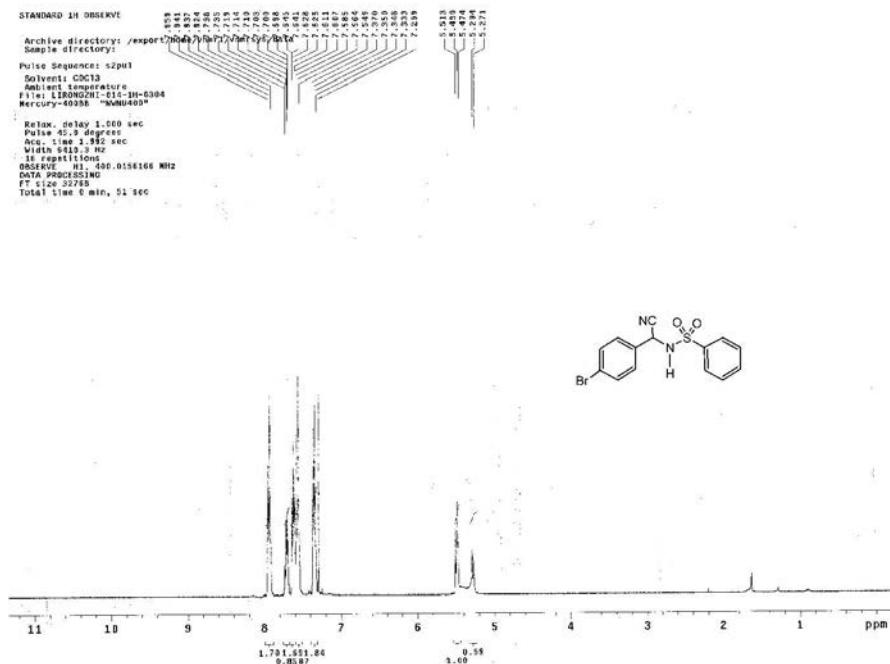


Figure S49. ¹H NMR spectrum (400 MHz, CDCl₃) of *N*-[(4-bromophenyl)(cyano)methyl]benzenesulfonamide (**2q**).

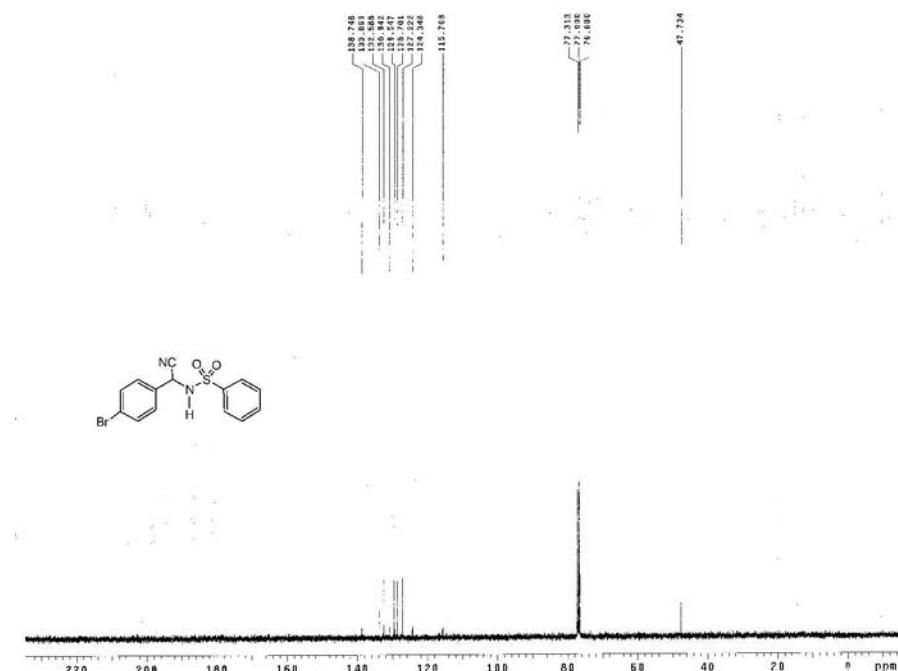


Figure S50. ¹³C NMR spectrum (100 MHz, CDCl₃) of *N*-[(4-bromophenyl)(cyano)methyl]benzenesulfonamide (**2q**).

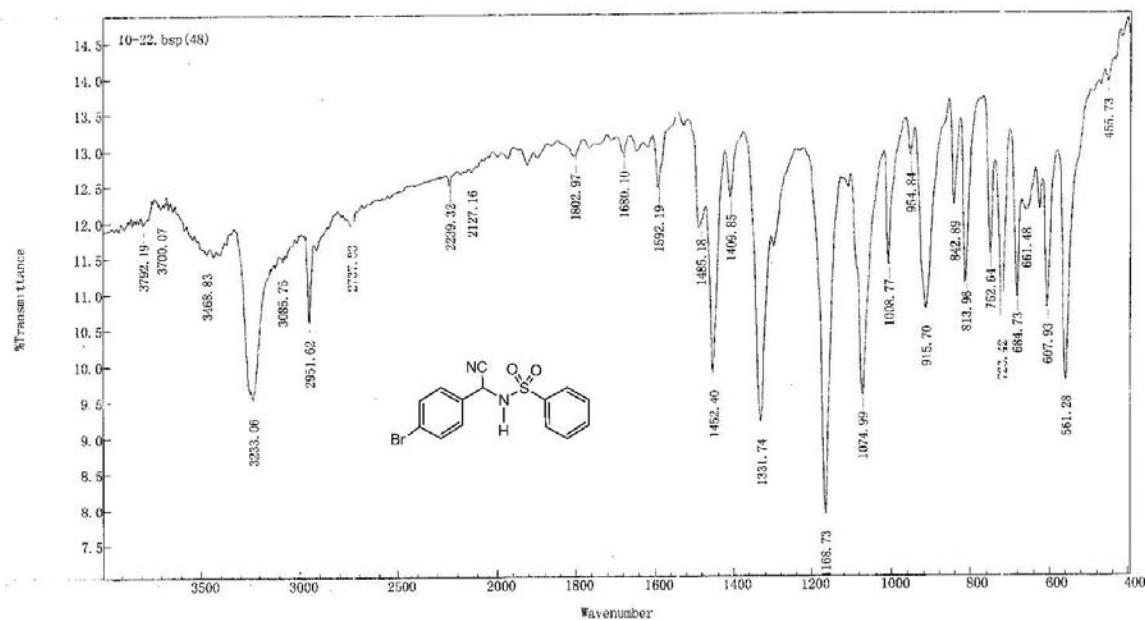
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Figure S51. IR of *N*-[(4-bromophenyl)(cyano)methyl]benzenesulfonamide (**2q**).