Supporting Information
A Convenient Preparation of Heteroaryl Sulfonamides and Sulfonyl Fluorides
from Heteroaryl Thiols

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General Information: ^1H , ^{13}C and ^{19}F NMR, spectra were recorded on a 400 MHz spectrometer. Mass spectral data were recorded using atmospheric pressure chemical ionization (APCI) or on a gas chromatograph fitted with a mass selective detector using electron impact ionization (EI). Infrared spectra were recorded on a FT-IR. Melting points are uncorrected. Elemental analyses were within 0.4% of the calculated values. Thin layer chromatography was carried out with 0.25 mm silica gel plates. All final products were characterized by ^1H , ^{13}C , and ^{19}F NMR, APCI MS, melting point and combustion analyses. All evaporations were carried out on a rotary evaporator at *ca.* 30 Torr. Commercial reagents were used as received without additional purification. Solvents were commercial anhydrous grades and were used without further drying

N-Benzyl benzo[d]thiazole-2-sulfonamide (3e): ^1H NMR ($\text{DMSO-}d_6$) δ 9.21 (t, J = 6 Hz, 1 H), 8.23 (d, J = 7 Hz, 1 H), 8.16 (d, J = 7 Hz, 1 H), 7.67 – 7.61 (m, 2 H), 7.27 - 7.14 (m, 5 H), 4.26 (d, J = 6 Hz, 2 H); ^{13}C NMR ($\text{DMSO-}d_6$): δ 167.9, 152.6, 137.9, 136.4, 128.9, 128.3, 127.9, 125.1, 123.9, 47.2. APCI MS: m/z 305 ($\text{M}+\text{H}$) $^+$. Anal. Calcd for $\text{C}_{14}\text{H}_{12}\text{N}_2\text{O}_2\text{S}_2$: C, 55.24; H, 3.97; N, 9.20. Found: C, 55.01; H, 3.74; N, 9.11.

N-Benzyl pyridine-2-sulfonamide (3f): ^1H NMR (CDCl_3) δ 8.65 (m, 1 H), 7.96 (d, J = 8 Hz, 1 H), 7.87 (t, J = 8 Hz, 1 H), 7.45 (m, 1 H), 7.28 - 7.20 (m, 5 H), 5.30 (br t, 1 H), 4.24 (d, J = 6 Hz, 2 H); ^{13}C NMR ($\text{DMSO-}d_6$): δ 158.8, 150.6, 139.3, 138.7, 128.8, 128.2, 127.7, 127.5, 122.2, 47.2. APCI MS: m/z 249 ($\text{M}+\text{H}$) $^+$. Anal. Calcd for $\text{C}_{12}\text{H}_{12}\text{N}_2\text{O}_2\text{S}$: C, 58.05; H, 4.87; N, 11.28. Found: C, 58.06; H, 4.74; N, 11.01.

Methyl 2-[(benzylamino)sulfonyl]nicotinate (3g): ^1H NMR ($\text{DMSO-}d_6$) δ 8.75 (m, 1 H), 8.59 (t, J = 6 Hz, 1 H), 8.12 (d, J = 8 Hz, 1 H), 7.71 (m, 1 H), 7.26 - 7.17 (m, 5 H), 4.13 (d, J = 6 Hz, 2 H), 3.81 (s, 3 H); ^{13}C NMR ($\text{DMSO-}d_6$): δ 167.0, 155.2, 151.4, 138.7, 138.3, 128.9, 128.2, 127.8, 127.3, 53.7, 47.3. APCI MS: m/z 307 ($\text{M}+\text{H}$) $^+$. Anal. Calcd for $\text{C}_{14}\text{H}_{14}\text{N}_2\text{O}_4\text{S}$: C, 54.89; H, 4.61; N, 9.14. Found: C, 54.31; H, 4.30; N, 9.06.

N-Benzyl-5-chloro-4-hydroxy-6-phenylpyrimidine-2-sulfonamide (5): ^1H NMR (CDCl_3): δ ; ^{13}C NMR (CDCl_3): δ . APCI MS: m/z 376, 378 ($\text{M}+\text{H}$, Cl isotope pattern) $^+$. Anal. Calcd for $\text{C}_{17}\text{H}_{14}\text{ClN}_3\text{O}_3\text{S}$: C, 54.33; H, 3.75; N, 11.18. Found: C, 54.71; H, 3.47; N, 11.11.

N-Benzyl quinoline-2-sulfonamide (3k): ^1H NMR ($\text{DMSO-}d_6$) δ 8.61 (d, J = 8 Hz, 1 H), 8.58 (br, 1 H), 8.09 (d, J = 8 Hz, 2 H), 7.95 (d, J = 9 Hz, 1 H), 7.90 (dd, J = 5, 2 Hz, 1 H), 7.75 (m, 1

H), 7.25 - 7.09 (m, 5 H), 4.22 (br s, 2 H); ^{13}C NMR (CDCl_3): δ 158.7, 147.0, 139.9, 138.6, 132.0, 129.9, 129.5, 129.1, 129.0, 128.8, 128.2, 127.7, 118.5, 47.3. APCI MS: m/z 299 ($\text{M}+\text{H}$) $^+$. Anal. Calcd for $\text{C}_{16}\text{H}_{14}\text{N}_2\text{O}_2\text{S}$: C, 64.41; H, 4.73; N, 9.39. Found: C, 64.15; H, 4.52; N, 9.20.

N-Benzyl-3-cyano-4,6-dimethylpyridine-2-sulfonamide (3l): ^1H NMR (CDCl_3) δ 7.26 - 7.21 (m, 6 H), 5.37 (br t, 1 H), 4.36 (d, $J = 6$ Hz, 2 H), 2.58 (s, 3 H), 2.56 (s, 3 H); ^{13}C NMR (CDCl_3): δ 162.0, 159.5, 154.5, 136.3, 128.8, 128.4, 128.2, 126.9, 113.6, 48.5, 24.4, 20.9. APCI MS: m/z 302 ($\text{M}+\text{H}$) $^+$. Anal. Calcd for $\text{C}_{15}\text{H}_{15}\text{N}_3\text{O}_2\text{S}$: C, 59.78; H, 5.02; N, 13.94. Found: C, 59.58; H, 4.76; N, 13.94.

N-Benzyl-thiazole-2-sulfonamide (3m): ^1H NMR (CDCl_3) δ 7.92 (d, $J = 3$ Hz, 1 H), 7.59 (d, $J = 3$ Hz, 1 H), 7.31 - 7.23 (m, 5 H), 5.42 (br t, 1 H), 4.34 (d, $J = 6$ Hz, 2 H); ^{13}C NMR ($\text{DMSO}-d_6$): δ 166.8, 145.0, 138.0, 129.0, 128.2, 128.0, 126.8, 47.1. APCI MS: m/z 255 ($\text{M}+\text{H}$) $^+$. Anal. Calcd for $\text{C}_{10}\text{H}_{10}\text{N}_2\text{O}_2\text{S}_2$: C, 47.23; H, 3.96; N, 11.01. Found: C, 47.29; H, 3.75; N, 10.98.

Methyl 6-[(benzylamino)sulfonyl]nicotinate (3n): ^1H NMR (CDCl_3) δ 9.20 (d, $J = 2$ Hz, 1 H), 8.43 (dd, $J = 8, 2$ Hz, 1 H), 8.01 (d, $J = 8$ Hz, 1 H), 7.28 - 7.20 (m, 5 H), 5.28 (br t, 1 H), 4.28 (d, $J = 6$ Hz, 2 H), 3.99 (s, 3 H); ^{13}C NMR (CDCl_3): δ 151.2, 139.5, 128.9, 128.6, 128.3, 128.2, 121.9, 53.2, 48.1. APCI MS: m/z 307 ($\text{M}+\text{H}$) $^+$. Anal. Calcd for $\text{C}_{14}\text{H}_{14}\text{N}_2\text{O}_4\text{S}$: C, 54.89; H, 4.61; N, 9.14. Found: C, 54.53; H, 4.58; N, 9.03.

N-Benzyl 2-phenyl-2H-tetrazole-5-sulfonamide (3c): ^1H NMR ($\text{DMSO}-d_6$) δ 9.83 (br, 1 H), 7.68 - 7.60 (m, 5 H), 7.34 - 7.23 (m, 5 H), 4.29 (s, 2 H); ^{13}C NMR ($\text{DMSO}-d_6$): δ 157.8, 137.5, 134.0, 132.0, 130.2, 129.1, 128.3, 128.2, 126.7, 47.3. APCI MS: m/z 316 ($\text{M}+\text{H}$) $^+$. Anal. Calcd for $\text{C}_{14}\text{H}_{13}\text{N}_5\text{O}_2\text{S}$: C, 53.32; H, 4.16; N, 22.21. Found: C, 53.18; H, 3.98; N, 22.06.

N-Benzyl 4-methylpyrimidine-2-sulfonamide (3d): ^1H NMR (CDCl_3) δ 8.67 (d, $J = 5$ Hz, 1 H), 7.28 - 7.22 (m, 6 H), 5.22 (br t, 1 H), 4.39 (d, $J = 6$ Hz, 2 H), 2.60 (s, 3 H); ^{13}C NMR ($\text{DMSO}-d_6$): δ 170.0, 166.2, 158.7, 138.7, 128.9, 128.8, 128.2, 127.8, 123.7, 47.5, 24.3. APCI MS: m/z 264 ($\text{M}+\text{H}$) $^+$. Anal. Calcd for $\text{C}_{12}\text{H}_{13}\text{N}_3\text{O}_2\text{S}$: C, 54.74; H, 4.98; N, 15.96. Found: C, 54.65; H, 4.84; N, 15.32.

N-Benzyl 1-methyl-1H-imidazole-2-sulfonamide (3i): ^1H NMR (CDCl_3) δ 7.35 - 7.26 (m, 5 H), 7.00 (d, $J = 1$ Hz, 1 H), 6.90 (d, $J = 1$ Hz, 1 H), 6.06 (br t, 1 H), 4.38 (d, $J = 6$ Hz, 2 H), 3.88 (s, 3 H); ^{13}C NMR (CDCl_3): δ 154.3, 136.4, 128.9, 128.3, 128.2, 128.1, 124.9, 48.3, 46.1. APCI MS:

m/z 252 ($M+H$)⁺. Anal. Calcd for C₁₁H₁₃N₃O₂S: C, 52.57; H, 5.21; N, 16.72. Found: C, 52.66; H, 5.15; N, 16.28.

N-Benzyl-6-methoxypyridazine-3-sulfonamide (3o): ¹H NMR (DMSO-*d*₆) δ 8.70 (t, 1 H), 7.93 (d, *J* = 10 Hz, 1 H), 7.35 (d, *J* = 9 Hz, 1 H), 7.26 - 7.08 (m, 5 H), 4.17 (d, *J* = 7 Hz, 2 H), 4.08 (s, 3 H); ¹³C NMR (DMSO-*d*₆): δ 176.4, 159.6, 138.3, 129.0, 128.9, 128.3, 127.8, 119.3, 56.0, 47.2. APCI MS: m/z 280 ($M+H$)⁺. Anal. Calcd for C₁₂H₁₃N₃O₃S: C, 51.60; H, 4.69; N, 15.04. Found: C, 51.80; H, 4.39; N, 15.06.

N-benzyl-5-methyl-4-phenyl-4H-1,2,4-triazole-3-sulfonamide (3p): ¹H NMR (DMSO-*d*₆) δ 9.08 (br, 1 H), 7.55 (m, 3 H), 7.45 (m, 2 H), 7.33 - 7.23 (m, 5 H), 4.21 (s, 2 H), 2.18 (s, 3 H); ¹³C NMR (DMSO-*d*₆): δ 155.8, 153.9, 138.3, 133.8, 130.8, 130.2, 129.0, 128.3, 128.2, 128.0, 47.4, 11.4. APCI MS: m/z 329 ($M+H$)⁺. Anal. Calcd for C₁₆H₁₆N₄O₂S: C, 58.52; H, 4.91; N, 17.06. Found: C, 58.22; H, 4.75; N, 17.20.

N-Benzyl pyridine-4-sulfonamide (3q): ¹H NMR (CD₃OD) δ 8.91 (d, *J* = 7 Hz, 2 H), 8.15 (d, *J* = 7 Hz, 2 H), 7.19 (m, 5 H), 4.25 (s, 2 H); ¹³C NMR (DMSO-*d*₆): δ 147.4, 137.7, 128.9, 128.4, 128.0, 121.9, 46.8. APCI MS: m/z 249 ($M+H$)⁺. Anal. Calcd for C₁₂H₁₂N₂O₂S HCl: C, 50.61; H, 4.60; N, 9.84. Found: C, 50.48; H, 4.28; N, 9.77.

N-Benzyl-1H-benzimidazole-2-sulfonamide (3t): ¹H NMR (CD₃OD) δ 7.69 (br, 1 H), 7.54 (br, 1 H), 7.35 (br, 2 H), 7.19 (m, 2 H), 7.15 (m, 2 H), 7.09 (m, 1 H); APCI MS: m/z 288 ($M+H$)⁺. Anal. Calcd for C₁₄H₁₃N₃O₂S: C, 58.52%; H, 4.56%; N, 14.62%. Found: C, 58.23%; H, 4.50%; N, 14.35%.

4,6-Dimethylpyrimidine-2-sulfonyl fluoride (8b): ¹H NMR (CDCl₃): δ 7.34 (s, 1 H); 2.64 (6 H). ¹³C NMR (CDCl₃): δ 170.4, 124.7, 24.2. ¹⁹F NMR (CDCl₃): Φ* -181.5. IR: 1573, 1411, 1383, 1233, 1190 cm⁻¹. EI MS: m/z 190 (M^+). Anal. Calcd for C₆H₇FN₂O₂S: C, 37.89; H, 3.71; N, 14.73; F, 9.99. Found: C, 37.97; H, 3.62; N, 14.80; F, 9.66.

1,3-benzothiazole-2-sulfonyl fluoride (8e): ¹H NMR (CDCl₃): δ 8.31 (dd, *J* = 6, 2 Hz, 1 H), 8.05 (dd, *J* = 7, 1 Hz, 1 H), 7.70 (m, 2 H). ¹³C NMR (CDCl₃): δ 152.1, 137.6, 129.6, 128.7, 126.5, 122.5. ¹⁹F NMR (CDCl₃): Φ* -166.2. IR: 1551, 1462, 1422, 1319, 1212 cm⁻¹. EI MS: m/z 217 (M^+). Anal. Calcd for C₇H₄FN₂O₂S₂: C, 38.70; H, 1.86; N, 6.45; F, 8.75. Found: C, 38.75; H, 1.67; N, 6.38; F, 8.48.

Pyridine-2-sulfonyl fluoride (8f): ^1H NMR (CDCl_3): δ 8.83 (m, 1 H); 8.12 (d, $J = 8$ Hz, 1 H); 8.05 (m, 1 H); 7.71 (m, 1 H). ^{13}C NMR (CDCl_3): δ 151.3, 138.9, 129.5, 124.4. ^{19}F NMR (CDCl_3): Φ^* -174.6. IR: 1582, 1407, 1260, 1213 cm^{-1} . EI MS: m/z 161 (M^+). Anal. Calcd for $\text{C}_5\text{H}_4\text{FNO}_2\text{S}$: C, 37.27; H, 2.50; N, 8.69; F 11.79. Found: C, 36.98; H, 2.39; N, 8.56; F, 11.21.

Quinoline-2-sulfonyl fluoride (8k): ^1H NMR (CDCl_3): δ 8.50 (d, $J = 9$ Hz, 1 H), 8.31 (d, $J = 9$ Hz, 1 H), 8.11 (d, $J = 9$ Hz, 1 H), 7.97 (m, 1 H), 7.92 (m, 1 H), 7.80 (m, 1 H). ^{13}C NMR (CDCl_3): δ 147.8, 139.7, 132.3, 130.9, 130.7, 130.0, 128.1, 118.8. ^{19}F NMR (CDCl_3): Φ^* -173.7. IR: 1574, 1497, 1408, 1208 cm^{-1} . EI MS: m/z 211 (M^+). Anal. Calcd for $\text{C}_9\text{H}_6\text{FNO}_2\text{S}$: C, 51.18; H, 2.86; N, 6.63; F, 8.99. Found: C, 51.40; H, 2.57; N, 6.58; F, 8.52.

6-Methoxypyridazine-3-sulfonyl fluoride (8o): ^1H NMR (CDCl_3): δ 8.04 (d, $J = 9$ Hz, 2H), 7.25 (d, $J = 9$ Hz, 1 H), 4.25 (s, 3 H); ^{13}C NMR (CDCl_3): δ 167.5, 129.3, 118.7, 59.2. ^{19}F NMR (CDCl_3): Φ^* -170.3. IR: 1575, 1420, 1400, 1308, 1224 cm^{-1} . EI MS: m/z 192 (M^+). Anal. Calcd for $\text{C}_5\text{H}_5\text{FN}_2\text{O}_3\text{S}$: C, 31.25; H, 2.62; N, 14.58; F, 9.89. Found: C, 31.73; H, 2.33; N, 14.25; F, 9.54.