Supporting Information

Chemoselective Nitration of Aromatic Sulfonamides with tert-Butyl Nitrite

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General: Reactions were run in dry glassware and no special precautions were taken to exclude air unless otherwise noted. Solvents and reagents were used as supplied and were not purified prior to use. Reactions were monitored by TLC using EMD TLC silica gel 60 F254 aluminum backed plates (UV visualization), and by analytical HPLC-MS using a Waters 2695 Separations Module, a Waters 996 Photodiode Array Detector and a Waters Micromass ZQ mass spectrometer. Purifications were performed using a Biotage Isolera One flash chromatography system equipped with Biotage SNAP KP-Sil silica gel cartridges. NMR spectra were recorded on a Bruker Avance III 400 Mhz spectrometer, a Bruker Avance III 500 MHz spectrometer or a Bruker Avance II TCI 600 MHz spectrometer, as noted in the characterization data for each compound.

2-amino-N-(quinazolin-8-yl)benzenesulfonamide (1)

Quinazolin-8-amine¹ (200 mg, 1.38 mmol, 1.0 eq) was dissolved in pyridine (14 mL, 0.1 M), cooled to 0 °C and treated with 4-nitrobenzenesulfonyl chloride (397 mg, 1.79 mmol, 1.3 eq). The reaction immediately turned dark orange. After 0.5 h the reaction was warmed to room temperature and stirred for 18 h, after which the pyridine was evaporated. The resulting red oil was taken up in EtOAc (50 mL) and water was added (20 mL). The layers were separated and the aqueous phase was extracted with EtOAc (2
x 20 mL). The organic layers were combined, washed with brine (20 mL), dried over Na$_2$SO$_4$, filtered and concentrated. The crude product was purified by flash chromatography to afford 2-nitro-N-(quinazolin-8-yl)benzenesulfonamide (226 mg, 0.684 mmol, 50%) as an orange solid.

2-nitro-N-(quinazolin-8-yl)benzenesulfonamide (226 mg, 0.684 mmol, 1.0 eq) was suspended in EtOH/H$_2$O (7 mL/1.5 mL, 0.08 M) and treated with NH$_4$Cl (366 mg, 6.84 mmol, 10.0 eq) and iron powder (286 mg, 5.13 mmol, 7.5 eq). The mixture was stirred and heated to reflux for 30 minutes, after which the reaction was complete. The reaction mixture was hot filtered through a pad of Celite to give a clear orange solution. The filter cake was washed with hot EtOH until the filtrate was colorless. The resulting EtOH solution was concentrated, and the residue was taken up in EtOAc (25 mL). The EtOAc solution was washed with NaHCO$_3$ (25 mL, saturated, aqueous). The layers were separated and the aqueous layer was extracted with EtOAc (3 × 20 mL). The organic layers were combined, dried over Na$_2$SO$_4$, filtered and concentrated to give compound 1 (132 mg, 0.440 mmol, 64%) as a light brown solid. $^1$H NMR (400 MHz, d$_6$-DMSO) δ = 10.42 (bs, 1H), 9.57 (s, 1H), 9.31 (s, 1H), 7.76 (d, J = 8.2 Hz, 1H), 7.74 (dd, J = 7.8, 1.1 Hz, 1H), 7.67 (dd, J = 8.1, 1.5 Hz, 1H), 7.63 (dd, J = 8.0, 8.0 Hz, 1H), 7.20 (dd, J = 7.6, 7.6 Hz, 1H), 6.69 (d, J = 8.2 Hz, 1H), 6.55 (dd, J = 7.5, 7.5 Hz, 1H), 6.24 (bs, 2H).

$^{13}$C NMR (150 MHz, d$_6$-DMSO) δ = 160.7 (CH), 154.0 (CH), 146.6 (C$_4$), 140.5 (C$_4$), 134.2 (CH), 133.7 (C$_4$), 129.6 (CH), 128.1 (CH), 124.8 (C$_4$), 121.3 (C$_4$), 119.3 (CH), 118.1 (CH), 116.9 (CH), 114.6 (CH).

4-nitro-7-phenylquinazoline-2’-8-sultam (3)

Aniline 1 (50 mg, 0.166 mmol, 1.0 eq) was suspended in AcOH (3 mL, 0.06 M) and dissolved by heating with a heat gun. This solution was placed in an oil bath pre-heated to 45 °C. Once the internal temperature of the solution was stabilized at 45 °C it was treated with tert-butyl nitrite (30 µL, 0.255 mmol, 1.5 eq) dropwise over 3 minutes. The reaction was stirred for 30 minutes after which it was cooled to 0 °C whereupon an orange precipitate formed. Water (5 mL) was added to further encourage precipitation, and the solid was isolated by suction filtration. This crude product was purified by flash chromatography to afford 3 (R$_f$ = 0.2 in 10 % MeOH/DCM, 20 mg, 36%) as a yellow solid along with a trace amount of compound 2. $^1$H NMR (400 MHz, d$_6$-DMSO) δ = 10.30 (s, 1H), 9.29 (s, 1H), 9.25 (s, 1H), 8.24 (d, J = 8.1 Hz, 1H), 7.88 (dd, J = 7.8, 1.2 Hz, 1H), 7.72-7.67 (m, 1H), 7.63-7.58 (m, 1H). N-H proton not observed. $^{13}$C NMR (150 MHz, d$_6$-DMSO) δ = 155.4 (CH), 153.7 (CH), 152.4 (C$_4$), 145.6
Regiochemical assignment of compound 3

![Diagram](image)

no nOE’s observed for 10.30 or 9.29

H (10.30), H (9.29), H (9.25) and H (8.24) were identified by a series of COSY, HSQC and HMBC NMR experiments. A strong NOE of 7% between H (9.25) and H (8.24) confirms the para relationship between the nitro group and the sulfonamide. Were the nitro group meta with the sulfonamide, this NOE would not be observed, and one would be expected between H (9.29) and H (9.25).

4-methyl-N-phenylbenzenesulfonamide (4)

![Structure](image)

Aniline hydrochloride (5.00 g, 38.6 mmol, 1.0 eq) was dissolved in pyridine (200 mL, 0.19 M) and treated with tosyl chloride (7.44 g, 39.0 mmol, 1.0 eq) in portions over 5 minutes. The mixture was heated at reflux for 16 h, after which it was cooled to room temperature and the pyridine was evaporated. The crude product was taken up in EtOAc (300 mL) and this solution was washed with HCl (1 M, 100 mL), water (100 mL) and brine (100 mL). The organic solution was then dried over Na$_2$SO$_4$, filtered and concentrated to give 4 (9.26 g, 37.4 mmol, 96% yield) as a white solid. $^1$H NMR (400 MHz, d$_6$-DMSO) δ = 10.20 (s, 1H), 7.63 (d, J = 8.3 Hz, 2H), 7.33 (d, J = 7.9 Hz, 2H), 7.23-7.19 (m, 2H), 7.09-7.06 (m, 2H), 7.02-6.98 (m, 1H), 2.32 (s, 3H).

4-methyl-N-(4-nitrophenyl)benzenesulfonamide (5a) and
4-methyl-N-(2-nitrophenyl)benzenesulfonamide (5b)

Optimized reaction conditions, Table 1, entry 14
Sulfonamide 4 (247 mg, 1.00 mmol, 1.0 eq) was dissolved in acetonitrile (10mL, 0.1M) and heated to 45 °C. The reaction was treated with tert-butyl nitrite (177 µL, 1.49 mmol, 1.5 eq) while stirring at 45 °C. After 6 h the sulfonamide 4 had been consumed (TLC and analytical HPLC-MS analysis), and the reaction was cooled to room temperature. Volatiles were removed in vacuo, and the resulting crude products were purified using flash chromatography to yield pure 5a (135 mg, 0.462 mmol, 46 %) and 5b (115 mg, 0.394 mmol, 39 %).

5a: Yellow solid. Rf = 0.24, 30 % EtOAc/hexanes. 1H NMR (400 MHz, d6-DMSO) δ = 11.20 (s, 1H), 8.13 (d, J = 9.3 Hz, 2H), 7.76 (d, J = 8.3 Hz, 2H), 7.39 (d, J = 8.3 Hz, 2H), 7.30 (d, J = 9.3 Hz, 2H), 2.34 (m, 3H).

13C NMR (100 MHz, d6-DMSO) δ = 144.3 (C4), 144.1 (C4), 142.5 (C4), 136.0 (C4), 130.0 (2 × CH), 126.8 (2 × CH), 125.4 (2 × CH), 117.9 (2 × CH), 21.0 (CH3).

5b: Yellow solid. Rf = 0.47, 30 % EtOAc/hexanes. 1H NMR (400 MHz, d6-DMSO) δ = 10.22 (s, 1H), 7.92 (dd, J = 8.2, 1.5 Hz, 1H), 7.64-7.59 (m, 3H), 7.38-7.34 (m, 3H), 7.26 (dd, J = 8.2, 1.2 Hz, 1H), 2.36 (m, 3H).

13C NMR (100 MHz, d6-DMSO) δ = 143.8 (C4), 143.1 (C4), 136.3 (C4), 134.2 (CH), 130.3 (C4), 129.8 (2 × CH), 126.8 (2 × CH), 126.2 (CH), 125.5 (CH), 125.3 (CH), 21.0 (CH3).

General procedure for the sulfonylation of substituted anilines – Table 2 starting materials
The aniline (1.0 eq) was dissolved in pyridine (0.2 M) and treated with the appropriate sulfonyl chloride (1.0 eq) in portions over 5 minutes. The mixture was heated at reflux until the reaction was complete (as determined by TLC and/or analytical HPLC-MS analysis), after which it was cooled to room temperature and the pyridine was evaporated. The crude product was taken up in EtOAc and this solution was washed with HCl (1 M), water and brine. The organic solution was then dried over Na2SO4, filtered and concentrated to give a crude product that was purified by flash chromatography.

The following sulfonylated anilines have been previously described in the literature:
Table 2, entry 1, starting material: N-(4-methoxyphenyl)-4-methylbenzenesulfonylamine2
Table 2, entry 2, starting material: 4-methyl-N-p-tolylbenzenesulfonylamine2
Table 2, entry 3, starting material: N-(4-chlorophenyl)-4-methylbenzenesulfonylamine3
Table 2, entry 4, starting material: ethyl 4-(4-methylphenylsulfonylamido)benzoate4
Table 2, entry 5, starting material: N-(4-cyanophenyl)-4-methylbenzenesulfonylamine4
Table 2, entry 6, starting material: 4-methyl-N-(4-(trifluoromethyl)phenyl)benzenesulfonylamine5
Table 2, entry 7, starting material: 4-methyl-N-(4-nitrophenyl)benzenesulfonamide

Table 2, entry 8, starting material: N-phenylmethanesulfonamide

Table 2, entry 9, starting material: 4-nitro-N-phenylbenzenesulfonamide

Table 2, entry 10, starting material

4-methyl-N-(2-(trifluoromethyl)phenyl)benzenesulfonamide

Brown solid. Rf = 0.53, 30% ethyl acetate/hexanes. 1H NMR (500 MHz, CDCl3) δ = 7.83 (d, J = 8.5 Hz, 1H), 7.66 (d, J = 8.5 Hz, 2H), 7.54 – 7.48 (m, 2H), 7.25 – 7.17 (m, 3H), 6.86 (s, 1H), 2.38 (s, 3H). 13C NMR (125 MHz, CDCl3) δ = 144.4 (C4), 135.7 (C4), 134.5 (C4), 133.1 (CH), 129.6 (CH), 127.3 (CH), 126.5 (q, JCF = 5.5 Hz, CH), 124.7 (CH), 123.6 (q, JCF = 272.9 Hz, CF3), 122.9 (CH), 120.6 (q, JCF = 29.7, C4), 21.6 (CH3). MS (ESI): M-H+ = 314.0 Calculated at 314.1.

Table 2, entry 11, starting material

4-methyl-N-(3-(trifluoromethyl)phenyl)benzenesulfonamide

White solid. Rf = 0.35, 30% ethyl acetate/hexanes. 1H NMR (500 MHz, CDCl3) δ = 7.70 (d, J = 8.5 Hz, 2H), 7.39 – 7.22 (m, 7H), 2.39 (s, 1H). 13C NMR (125 MHz, CDCl3) δ = 144.4 (C4), 137.3 (C4), 135.6 (C4), 131.8 (q, JCF = 32.7 Hz, C4), 129.93 (CH), 129.85 (CH), 127.3 (CH), 124.0 (CH), 123.5 (q, JCF = 272.5 Hz, CF3), 121.7 (q, JCF = 3.6 Hz, CH), 117.5 (q, JCF = 3.6 Hz, CH), 21.5 (CH3). MS (ESI): M-H+ = 314.0 Calculated at 314.1.

Competition experiment # 3 starting material

4-(((4-methylphenyl)sulfonyl)methyl)phenol

Brown solid. Rf = 0.50, 10% Methanol/dichloromethane. 1H NMR (500 MHz, d6-DMSO) δ = 9.65 (s, 1H), 9.29 (s, 1H), 7.53 (d, J = 8.5 Hz, 2H), 7.31 (d, J = 8.5 Hz, 2H), 6.83 (d, J = 8.9 Hz, 2H), 6.59 (d, J = 8.9 Hz, 2H), 2.32 (s, 3H). 13C NMR (125 MHz, d6-DMSO) δ = 155.2 (C4), 143.3 (C4), 131.2 (C4), 129.9
(CH), 129.1 (C₄), 127.2 (CH), 124.4 (CH), 116.0 (CH), 21.4 (CH₃) MS (ESI): M-H⁺ = 264.2 Calculated at 362.3.

**General procedure for the nitration of sulfonamides using tert-butyl nitrite**

The sulfonamide (1.0 eq) was dissolved in acetonitrile (0.1 M) and heated to 45 °C. The reaction was treated with tert-butyl nitrite (1.5 eq) while continuing to be stirred at 45 °C. When the reaction was complete (as determined by TLC and/or analytical HPLC-MS analysis) the reaction was cooled to room temperature and the volatiles were removed by evaporation under reduced pressure. The resulting crude products(s) were purified by flash chromatography.

**Table 2, entry 1**

**N-(4-methoxy-2-nitrophenyl)-4-methylbenzenesulfonamide**

Yellow solid. Rₕ = 0.61, 30% EtOAc/hexanes. ¹H NMR (500 MHz, CDCl₃) δ = 9.26 (s, 1H), 7.80 (d, J = 9.2 Hz, 1H), 7.61 (d, J = 8.5 Hz, 2H), 7.49 (d, J = 3.0 Hz, 1H), 7.22 (d, J = 8.0 Hz, 2H), 7.2 (dd, J = 9.2, 3.0 Hz, 1H), 3.82 (s, 3H), 2.38 (s, 3H). ¹³C NMR (125 MHz, CDCl₃) δ = 156.2 (C₄), 144.5 (C₄), 139.0 (C₄), 135.5 (C₄), 129.8 (CH), 127.1 (CH), 126.6 (CH), 124.8 (C₄), 123.0 (CH), 109.0 (CH), 56.0 (CH₃), 21.6 (CH₃). MS (ESI): M-H⁺ = 321.1. Calculated at 321.1.

**Table 2, entry 2**

**4-methyl-N-(4-methyl-2-nitrophenyl)benzenesulfonamide**

Yellow solid. Rₕ = 0.64, 30% ethyl acetate/hexanes. ¹H NMR (500 MHz, CDCl₃) δ = 9.63 (s, 1H), 7.88 (d, J = 2.1 Hz, 1H), 7.74 (d, J = 8.5 Hz, 1H), 7.69 (d, J = 8.5 Hz, 2H), 7.39 (dd, J = 8.5, 2.1 Hz, 2H), 7.24 (d, J = 8.5 Hz, 2H), 2.38 (s, 3H), 2.34 (s, 3H). ¹³C NMR (125 MHz, CDCl₃) δ = 144.6 (C₄), 137.3 (C₄), 136.7 (CH), 135.7 (C₄), 134.45 (C₄), 131.2 (C₄), 129.9 (CH), 127.2 (CH), 125.9 (CH), 121.6 (CH), 21.5 (CH₃), 20.4 (CH₃). MS (ESI): M-H⁺ = 305.1. Calculated at 305.1.

**Table 2, entry 3**

**N-(4-chloro-2-nitrophenyl)-4-methylbenzenesulfonamide**
Yellow solid. $R_f = 0.74$, 30% ethyl acetate/hexanes. $^1$H NMR (500 MHz, CDCl$_3$) $\delta =$ 9.75 (s, 1H), 9.12 (d, J = 8.6 Hz, 2H), 7.74 (d, J = 8.9, 2.5 Hz, 1H), 7.37 (d, J = 8.6 Hz, 2H), 2.42 (s, 3H).

$^{13}$C NMR (125 MHz, CDCl$_3$) $\delta =$ 145.1 (C$_4$), 137.1 (C$_4$), 135.8 (CH), 135.4 (C$_4$), 132.6 (C$_4$), 130.1 (CH), 129.3 (C$_4$), 127.2 (CH), 125.8 (CH), 122.3 (CH), 21.6 (CH$_3$). MS (ESI): M-H$^+$ = 325.1 and 326.9. Calculated at 325.0 and 327.0.

Table 2, entry 4

ethyl 4-(4-methylphenylsulfonylamido)-3-nitrobenzoate

Yellow solid. $R_f = 0.60$, 30% ethyl acetate/hexanes. $^1$H NMR (500 MHz, CDCl$_3$) $\delta =$ 10.19 (s, 1H), 8.80 (d, J = 2.1 Hz, 1H), 8.19 (dd, J = 8.9, 2.1 Hz, 1H), 7.88 (d, J = 8.9 Hz, 1H), 7.80 (d, J = 8.5, 2H), 7.30 (d, J = 8.5 Hz, 2H), 4.38 (q, J = 7.1 Hz, 2H), 2.40 (s, 3H), 1.39 (t, J = 7.1 Hz, 3H).

$^{13}$C NMR (125 MHz, CDCl$_3$) $\delta =$ 163.9 (C$_4$), 145.3 (C$_4$), 137.5 (C$_4$), 136.3 (CH), 135.6 (C$_4$), 135.4 (C$_4$), 130.1 (CH), 127.9 (CH), 127.4 (CH), 125.5 (C$_4$), 119.4 (CH), 61.8 (CH$_2$), 21.6 (CH$_3$), 14.2 (CH$_3$). MS (ESI): M-H$^+$ = 363.1. Calculated at 363.1.

Table 2, entry 5

N-(4-cyano-2-nitrophenyl)-4-methylbenzenesulfonamide

Yellow solid. $R_f = 0.54$, 30% ethyl acetate/hexanes. $^1$H NMR (500 MHz, CDCl$_3$) $\delta =$ 10.24 (s, 1H), 8.48 (d, J = 1.8 Hz, 1H), 7.95 (d, J = 8.7 Hz, 1H), 7.83 (d, J = 8.5 Hz, 2H), 7.79 (dd, J = 8.7, 1.8 Hz, 1H), 7.34 (d, J = 8.5 Hz, 2H), 2.43 (s, 3H).

$^{13}$C NMR (125 MHz, CDCl$_3$) $\delta =$ 145.7 (C$_4$), 138.2 (CH), 137.9 (C$_4$), 135.3 (C$_4$), 135.1 (C$_4$), 130.7 (CH), 130.3 (CH), 127.4 (CH), 120.0 (CH), 116.2 (C$_4$), 106.8 (C$_4$), 21.64 (CH$_3$). MS (ESI): M-H$^+$ = 316.2. Calculated at 316.0.

Table 2, entry 6

4-methyl-N-(2-nitro-4-(trifluoromethyl)phenyl)benzenesulfonamide
Yellow solid. Rf = 0.72, 30% ethyl acetate/hexanes. 1H NMR (500 MHz, d6-DMSO) δ = 10.72 (s, 1H), 8.27 (d, J = 8.7, 1H), 7.98 (dd, J = 8.7, 1.8 Hz, 1H), 7.77 (d, J = 8.5 Hz, 2H), 7.61 (d, J = 8.7 Hz, 1H), 7.38 (d, J = 8.5 Hz, 2H), 2.34 (s, 3H).

13C NMR (125 MHz, d6-DMSO) δ = 144.3 (C4), 141.0 (C4), 136.0 (C4), 134.4 (C4), 130.8 (q, 3JCF = 2.7 Hz, CH), 130.0 (CH), 127.0 (CH), 125.0 (q, 3JCF = 33.6, C4), 123.9 (CH), 123.2 (q, 3JCF = 3.6, CH), 122.9 (q, 1JCF = 272.5 Hz, CF3), 21.0 (CH3). MS (ESI): M-H+ = 359.0. Calculated at 359.0.

**Table 2, entry 7**

N-(2,4-dinitrophenyl)-4-methylbenzenesulfonamide

Yellow solid. Rf = 0.56, 30% ethyl acetate/hexanes. 1H NMR (500 MHz, d6-DMSO) δ = 8.65 (d, J = 2.5 Hz, 1H), 8.40 (dd, J = 9.2, 2.5 Hz, 1H), 7.81 (d, J = 8.5 Hz, 2H), 7.64 (d, J = 9.2 Hz, 1H), 7.42 (d, J = 8.5 Hz, 2H), 2.37 (s, 3H). 13C NMR (125 MHz, d6-DMSO) δ = 144.4 (C4), 142.2 (C4), 125.5 (CH), 117.5 (CH), 40.2 (CH3). MS (ESI): M-H+ = 336.1. Calculated at 336.0.

**Table 2, entry 8**

N-(4-nitrophenyl)methanesulfonamide (8a) and N-(2-nitrophenyl)methanesulfonamide (8b)

8a: Yellow solid. Rf = 0.18, 50% ethyl acetate/hexanes. 1H NMR (500 MHz, d6-DMSO) δ = 10.74 (s, 1H), 8.22 (d, J = 9.2, 2H), 7.36 (d, J = 9.2 Hz, 2H), 3.18 (s, 3H). 13C NMR (125 MHz, d6-DMSO) δ = 145.0(C4), 142.2 (C4), 125.5 (CH), 117.5 (CH), 40.2 (CH3). MS (ESI): M-H+ = 215.2. Calculated at 215.0

8b: Yellow Solid. Rf = 0.36, 50% ethyl acetate/hexanes. 1H NMR (500 MHz, CDCl3) δ = 9.77 (s, 1H), 8.28 (d, J = 8.5 Hz, 1H), 7.90 (d, J = 8.5 Hz, 1H), 7.70 (t, J = 8.5 Hz, 1H), 7.25 (t, J = 8.5 Hz, 1H), 3.17 (s, 3H). 13C NMR (125 MHz, CDCl3) δ = 136.2 (CH), 134.3 (C4), 126.6 (CH), 123.6 (CH), 119.5 (CH), 40.7 (CH3). MS (ESI): M-H+ = 215.2. Calculated at 215.0.
Table 2, entry 9

4-nitro-N-(4-nitrophenyl)benzenesulfonamide (9a) and
4-nitro-N-(2-nitrophenyl)benzenesulfonamide (9b)

9a: Yellow Solid. \( R_f = 0.30, 10\% \) ethyl acetate/toluene. \(^1\)H NMR (500 MHz, d\textsubscript{6}-DMSO) \( \delta = 11.57 \) (s, 1H), 8.40 (d, 8.9 Hz, 2H), 8.15 (9.4 Hz, 2H), 8.11 (d, \( J = 9.2 \) Hz, 2H), 7.34 (d, \( J = 9.2 \) Hz, 2H). \(^{13}\)C NMR (125 MHz, d\textsubscript{6}-DMSO) \( \delta = 150.2 \) (C\textsubscript{4}), 144.2 (C\textsubscript{4}), 143.4 (C\textsubscript{4}), 143.1 (C\textsubscript{4}), 128.3 (CH), 125.5 (CH), 125.0 (CH), 119.6 (CH). MS (ESI\textsuperscript{-}): M-H\(^+\) = 322.2. Calculated at 322.0.

9b: White Solid. \( R_f = 0.70, 10\% \) ethyl acetate/toluene. \(^1\)H NMR (500 MHz, CDCl\textsubscript{3}) \( \delta = 9.93 \) (s, 1H), 8.33 (d, \( J = 8.9 \) Hz, 2H), 8.15 (dd, \( J = 8.5 \), 1.6 Hz, 1H), 8.05 (d, \( J = 8.9 \) Hz, 2H), 7.87 (dd, \( J = 8.5 \), 1.4 Hz, 1H), 7.66 (m, 1H), 7.26 (m, 1H). \(^{13}\)C NMR (125 MHz, CDCl\textsubscript{3}) \( \delta = 144.3 \) (C\textsubscript{4}), 136.1 (CH), 132.7 (C\textsubscript{4}), 128.5 (CH), 126.4 (CH), 124.92 (CH), 124.6 (CH), 121.4 (CH). MS (ESI\textsuperscript{-}): M-H\(^+\) = 322.2. Calculated at 322.0.

Table 2, entry 10

4-methyl-N-[4-nitro-2-(trifluoromethyl)phenyl]benzenesulfonamide (10a) and
4-methyl-N-[2-nitro-6-(trifluoromethyl)phenyl]benzenesulfonamide (10b)

10a: Yellow solid. \( R_f = 0.31, 30\% \) ethyl acetate/hexanes. \(^1\)H NMR (500 MHz, CDCl\textsubscript{3}) \( \delta = 8.41 \) (d, \( J = 2.8 \) Hz, 1H), 8.35 (dd, \( J = 9.2 \), 2.8 Hz, 1H), 7.97 (d, \( J = 9.2 \) Hz, 1H), 7.76 (d, \( J = 8.5 \) Hz, 2H), 7.32 – 7.27 (m, 3H), 2.41 (s, 3H). \(^{13}\)C NMR (125 MHz, CDCl\textsubscript{3}) \( \delta = 145.5 \) (C\textsubscript{4}), 143.0 (C\textsubscript{4}), 140.4 (q, \( ^{3}\)J\textsubscript{C-F} = 1.8 Hz, C\textsubscript{4}), 134.8 (C\textsubscript{4}), 130.1 (CH), 128.3 (CH), 127.4 (CH), 122.9 (q, \( ^{3}\)J\textsubscript{C-F} = 6.4 Hz, CH), 122.5 (q, \( ^{1}\)J\textsubscript{C-F} = 274.0 Hz, C\textsubscript{4}), 120.7 (CH), 119.3 (q, \( ^{2}\)J\textsubscript{C-F} = 31.8 Hz, C\textsubscript{4}), 21.6 (CH\textsubscript{3}). MS (ESI\textsuperscript{-}): M-H\(^+\) = 359.0. Calculated at 359.0

10b: White solid. \( R_f = 0.16, 30\% \) ethyl acetate/hexanes. \(^1\)H NMR (500 MHz, CDCl\textsubscript{3}) \( \delta = 8.06 \) (dd, \( J = 8.0 \) Hz, 1H), 7.97 (dd, \( J = 8.0 \), 1.4 Hz, 1H), 7.62 (dd, \( J = 8.01 \), 0.81 Hz, 1H), 7.55 (d, \( J = 8.5 \) Hz, 2H), 7.28 (d, \( J = 8.5 \) Hz, 2H), 2.46 (s, 3H). \(^{13}\)C NMR (125 MHz, CDCl\textsubscript{3}) \( \delta = 148.1 \) (C\textsubscript{4}), 144.9 (C\textsubscript{4}), 135.4 (C\textsubscript{4}), 132.3 (q, \( ^{3}\)J\textsubscript{C-F} = 4.5 Hz, CH), 131.1 (q, \( ^{2}\)J\textsubscript{C-F} = 30.9 Hz, C\textsubscript{4}), 129.9 (CH), 128.6 (CH), 128.4 (CH),
127.9 (C₄), 127.3 (CH), 122.4 (q, \(^{1}J_{CF} = 275.2\), CF₃), 21.6 (CH₃). MS (ESI): M-H⁺ = 359.0. Calculated at 359.0.

Table 2, entry 11

4-methyl-N-[4-nitro-3-(trifluoromethyl)phenyl]benzenesulfonamide (11a) and
4-methyl-N-[2-nitro-3-(trifluoromethyl)phenyl]benzenesulfonamide (11b) and
4-methyl-N-[2-nitro-5-(trifluoromethyl)phenyl]benzenesulfonamide (11c)

11a: White solid. \(R_f = 0.12\), dichloromethane. \(^{1}H\) NMR (500 MHz, d₆-DMSO) \(\delta = 11.48\) (s, 1H), 8.12 (d, \(J = 8.7\) Hz, 1H), 7.77 (d, \(J = 8.5\) Hz, 2H), 7.60 – 7.54 (m, 2H), 7.41 (d, \(J = 8.5\) Hz, 2H), 2.35 (s, 3H). \(^{13}C\) NMR (125 MHz, d₆-DMSO) \(\delta = 144.4\) (C₄), 142.8 (C₄), 141.5 (q, \(^{3}J_{CF} = 1.8\) Hz, C₄), 135.7 (C₄), 130.1 (CH), 128.3 (CH), 126.8 (CH), 123.4 (q, \(^{2}J_{CF} = 33.6\) Hz, C₄), 121.7 (q, \(^{1}J_{CF} = 273.4\) Hz, CF₃), 121.1 (CH), 116.3 (q, \(^{3}J_{CF} = 6.4\) Hz, CH), 21.0 (CH₃). MS (ESI): M-H⁺ = 359.0 Calculated at 359.0.

11b: White solid. \(R_f = 0.23\), dichloromethane. \(^{1}H\) NMR (500 MHz, CDCl₃) \(\delta = 8.05\) (dd, \(J = 8.24, 0.8\) Hz, 1H), 7.67 – 7.62 (m, 1H), 7.60 (d, \(J = 8.5\) Hz, 2H), 7.56 (dd, \(J = 8.0\) Hz, 0.8 Hz, 1H), 7.49 (s, 1H), 7.27 (d, \(J = 8.5\) Hz, 2H) 2.42 (s, 3H). \(^{13}C\) NMR (125 MHz, CDCl₃) \(\delta = 145.2\) (C₄), 135.1 (C₄), 132.1 (CH), 130.6 (C₄), 130.2 (CH), 128.5 (CH), 127.0 (CH), 124.4 (q, \(^{3}J_{CF} = 34.5\) Hz, C₄), 124.1 (q, \(^{1}J_{CF} = 5.5\) Hz, CH), 121.5 (q, \(^{1}J_{CF} = 274.3\) Hz, CF₃), 21.6 (CH₃). MS (ESI): M-H⁺ = 359.0 Calculated at 359.0.

11c: Yellow-brown solid. \(R_f = 0.56\), 30% ethyl acetate/hexanes. \(^{1}H\) NMR (500 MHz, CDCl₃) \(\delta = 9.89\) (s, 1H), 8.24 (d, \(J = 8.7\) Hz, 1H), 8.15 (d, \(J = 1.4\) Hz, 1H), 7.77 (d, \(J = 8.5\) Hz, 2H), 7.38 (dd, \(J = 8.7, 1.6\) Hz, 1H), 7.31 (d, \(J = 8.5\) Hz, 2H), 2.41 (s, 3H). \(^{13}C\) NMR (125 MHz, CDCl₃) \(\delta = 145.4\) (C₄), 137.0 (q, \(^{3}J_{CF} = 33.6\) Hz, C₄), 135.1 (C₄), 134.6 (C₄), 130.2 (CH), 127.4 (CH), 127.1 (CH), 122.4 (q, \(^{1}J_{CF} = 273.4\) Hz, CF₃), 119.9 (q, \(^{3}J_{CF} = 3.6\) Hz, CH), 117.8 (q, \(^{3}J_{CF} = 3.6\) Hz, CH), 21.6 (CH₃). MS (ESI): M-H⁺ = 359.0 Calculated at 359.0.

Competition experiment #3 products

4-[[(4-methylphenyl)sulfonyl]methyl]-2-nitrophenol and
4-[[(4-methylphenyl)sulfonyl]methyl]-2,6-dinitrophenol
Yellow solid. Rf = 0.70, 10% Methanol/dichloromethane. \(^1\)H NMR (500 MHz, d<sub>6</sub>-DMSO) δ = 10.85 (s, 1H), 10.19 (s, 1H), 7.59 (d, J = 8.6 Hz, 2H), 7.55 (d, J = 2.7 Hz, 1H) 7.35 (d, J = 8.6 Hz, 2H), 7.24 (dd, J = 9.0, 2.7 Hz, 1H), 7.02 (d, J = 9.0 Hz, 1H), 2.34 (s, 3H).

\(^1\)C NMR (125 MHz, CDCl<sub>3</sub>) δ = 149.5 (C<sub>4</sub>), 143.5 (C<sub>4</sub>), 136.2 (C<sub>4</sub>), 136.0 (C<sub>4</sub>), 129.8 (CH), 129.2 (C<sub>4</sub>), 129.0 (CH), 126.8 (CH), 120.2 (CH), 117.3 (CH), 21.0 (CH<sub>3</sub>).

MS (ESI\(-\))\textsuperscript{+}: M-H\(^+\) = 307.2 Calculated at 307.3.

Orange solid. Rf = 0.1, 10% Methanol/dichloromethane. \(^1\)H NMR (500 MHz, d<sub>6</sub>-DMSO) δ = 10.18 (s, 1H), 7.69 (s, 2H), 7.62 (d, J = 8.2 Hz, 2H) 7.37 (d, J = 8.2 Hz, 2H), 2.35 (s, 3H). \(^1\)C NMR (125 MHz, CDCl<sub>3</sub>) δ = 149.1 (C<sub>4</sub>), 143.7 (C<sub>4</sub>), 140.9 (C<sub>4</sub>), 136.0 (C<sub>4</sub>), 129.9 (C<sub>4</sub>), 126.9 (CH), 123.9 (CH), 122.9(CH), 21.0 (CH<sub>3</sub>). MS (ESI\(-\))\textsuperscript{+}: M-H\(^+\) = 352.2 Calculated at 352.3

\(^1\)H, \(^13\)C, and \(^15\)N NMR assignment of N-(4-methoxy-2-nitrophenyl)-4-methylbenzenesulfonamide (Table 2, entry 1) and N-(4-chloro-2-nitrophenyl)-4-methylbenzenesulfonamide (Table 2, entry 3)

The \(^1\)H, \(^13\)C, and \(^15\)N chemical shifts for N-(4-chloro-2-nitrophenyl)-4-methylbenzenesulfonamide and N-(4-methoxy-2-nitrophenyl)-4-methylbenzenesulfonamide were obtained on a Bruker AVIII NMR Spectrometer at a magnetic field strength of 9.4 T (\(^1\)H frequency of 400 MHz) using a combination of 1D and 2D NMR experiments: \(^1\)H and \(^13\)C 1D, \(^1\)H,\(^13\)C-HSQC (heteronuclear single quantum correlation), \(^1\)H,\(^13\)C-HMBC (heteronuclear multiple bond correlation) optimized for long-range coupling constants of 7.7 Hz, \(^1\)H,\(^15\)N-HSQC, and \(^1\)H,\(^15\)N-HMBC optimized for 10 Hz couplings. In addition, 1D selective NOE experiments with mixing times of 300 ms were recorded (see below for details). \(^1\)H and \(^13\)C chemical shifts were referenced to the residual solvent signal (CDCl<sub>3</sub>).

The regiochemistry (the position of the nitro group) for N-(4-chloro-2-nitrophenyl)-4-methylbenzenesulfonamide and N-(4-methoxy-2-nitrophenyl)-4-methylbenzenesulfonamide was confirmed using correlations from H3 and H6 to the nitro-nitrogen (see figure A). For N-(4-methoxy-2-nitrophenyl)-4-methylbenzenesulfonamide, an NOE was observed between the methyl protons of the methoxy group and H3 (see figure B).
Figure A: Correlations observed in a $^1$H,$^{15}$N-HMBC experiment for $N$-(4-chloro-2-nitrophenyl)-4-methylbenzenesulfonamide, indicated by arrows.

Table A: Chemical shifts for $N$-(4-chloro-2-nitrophenyl)-4-methylbenzenesulfonamide

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Figure B: Correlations observed in a $^1$H, $^{15}$N-HMBC experiment (black arrows) and in 1D selective NOE experiments (red arrows) for N-(4-methoxy-2-nitrophenyl)-4-methylbenzenesulfonamide.

Table B: Chemical shifts for N-(4-methoxy-2-nitrophenyl)-4-methylbenzenesulfonamide

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Compound 1
d$_6$-DMSO, $^1$H NMR, 400 MHz
Compound 1

d$_6$-DMSO, $^{13}$C NMR, 150 MHz
Compound 3
d$_6$-DMSO, $^1$H NMR, 400 MHz
Compound 3
d$_6$-DMSO, $^{13}$C NMR, 150 MHz
Compound 4
d$_6$-DMSO, $^1$H NMR, 400 MHz
Compound 5a

d$_5$-DMSO, $^1$H NMR, 400 MHz
Compound 5a

d$_6$-DMSO, $^{13}$C APT, 100 MHz
Compound 5b

d$_6$-DMSO, $^1$H NMR, 400 MHz
Compound 5b

d$_6$-DMSO, $^{13}$C APT, $^{100}$ MHz
Competition experiment #3 starting material
d$_6$-DMSO $^1$HNMR, 500 MHz

![NMR spectrum image]
Competition experiment #3 starting material

d$_6$-DMSO $^{13}$CNMR, 125 MHz
Table 2, entry 1

CDCl₃, $^1$H NMR 500 MHz

![NMR Spectrum](00215-25.001.esp)
Table 2, entry 1:

CDCl$_3$, $^{13}$C NMR 125 MHz

![NMR spectrum image]
Table 2, entry 2

CDCl₃, ^1^H NMR 500 MHz

![Chemical Shift Chart]

Chemical Shift (ppm)

Normalized Intensity

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Table 2, entry 2

CDCl$_3$, $^{13}$C NMR 125 MHz

[NMR spectrum image]

Chemical Shift (ppm)

Normalized Intensity

[SI unit and standard deviation]
Table 2, entry 3:

CDCl₃, ¹H NMR 500MHz
Table 2, entry 3:

CDCl$_3$, $^{13}$C NMR 125 MHz

![Chemical Shift vs Normalized Intensity Graph](00215-26.002.esp)
Table 2, entry 4:

CDCl₃, $^1$H NMR 500 MHz

[Chemical structure image]

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Table 2, entry 4:

CDCl$_3$, $^{13}$C NMR 125 MHz

![NMR spectrum image]

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Table 2, entry 5:

CDCl$_3$, $^1$H NMR 500 MHz

[Chemical structure image]

Normalized Intensity vs. Chemical Shift (ppm)
Table 2, entry 5:

CDCl₃, ¹³C NMR 125 MHz

- Chemical Shift (ppm)
- Normalized Intensity
Table 2, entry 6:

$\text{d}_6$-DMSO, $^1$H NMR 500 MHz

![NMR spectrum of $\text{d}_6$-DMSO with chemical shifts and normalized intensity]
Table 2, entry 6:

$^{d_6}$DMSO, $^{13}$C NMR 125 MHz

![Chemical Shift Chart](image-url)
Table 2, entry 7:
d$_6$-DMSO, $^1$H NMR 500 MHz

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Table 2, entry 7:

$d_6$-DMSO, $^{13}$C NMR 125 MHz
Table 2, entry 8a:

d$_6$-DMSO, $^1$H NMR 500 MHz

![Chemical Shift (ppm)](00215-67-BOTTOM.001.esp)
Table 2, entry 8a:

$\text{d}_6$-DMSO, $^{13}$C NMR 125 MHz

![NMR Spectrum](image-url)
Table 2, entry 8b:

CDCl₃, ¹H NMR 500 MHz
Table 2, entry 8b:

CDCl$_3$, $^{13}$C NMR 125 MHz

[Chemical structure image]

[Graph image]
Table 2, entry 9a:
d$_6$-DMSO, $^1$H NMR 500 MHz

---

Chemical Shift (ppm)

Normalized Intensity

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Table 2, entry 9a:

$d_6$-DMSO, $^{13}$C NMR 125 MHz

\[
\begin{align*}
\text{NHs} \\
\text{O}_2\text{N}
\end{align*}
\]

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Table 2, entry 9b:

CDCl₃, ¹H NMR 500 MHz

Chemical Shift (ppm)
Table 2, entry 9b:

CDCl₃, $^{13}$C NMR 125 MHz
Table 2: entry 10 starting material:

CDCl₃, ¹H NMR 500 MHz

Chemical Shift (ppm)

Normalized Intensity
Table 2: entry 10 starting material:

CDCl₃, $^{13}$C NMR 150 MHz

![NMR Spectrum]

Chemical Shift (ppm)
Table 2, entry 10a:

CDCl$_3$, $^1$H NMR 500 MHz

![NMR spectrum](00215-098-1.001.esp)
Table 2, entry 10a:

**CDCl₃, $^{13}$C NMR 125 MHz**

![Chemical Structure](00215-098-1.002.esp)
Table 2, entry 10b:

CDCl₃, ¹H NMR 500 MHz

![NMR Spectrum Image](00215-098-2.001.esp)
Table 2, entry 10b:

CDCl₃, $^{13}$C NMR 125 MHz

![Chemical Structure Image]

Electronic Supplementary Material (ESI) for Chemical Communications
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Table 2, entry 11 starting material:

CDCl₃, \(^{1}\text{H} \text{NMR} \ 500 \text{ MHz}\)

![NMR Spectrum](792x612)
Table 2, entry 11 starting material:

CDCl₃, ¹³C NMR 125 MHz

\[
\text{NHTs}\quad \text{CF}_3
\]
Table 2, entry 11a:

d$_6$-DMSO, $^1$H NMR 500 MHz

![NMR spectrum graph]
Table 2, entry 11a:

d$_6$-DMSO, $^{13}$C NMR 125 MHz

![NMR Spectrum](image-url)
Table 2, entry 11b:

CDCl₃, ¹H NMR 500 MHz

![NMR Spectrum](00215-126-3.001.esp)
Table 2, entry 11b:

CDCl₃, $^{13}$C NMR 125 MHz

![Chemical Shift Chart]
Table 2, entry 11c:

**CDCl₃, $^1$H NMR 500 MHz**

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Diagram: Chemical structure and NMR spectrum
Table 2, entry 11c:

CDCl$_3$, $^{13}$C NMR 125 MHz

Chemical Species: NO$_2$-NHTs-CF$_3$
Competition experiment #3 product a

d$_6$-DMSO, $^1$HNMR, 500 MHz

![NMR spectrum diagram]

Electronic Supplementary Material (ESI) for Chemical Communications
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Competition experiment #3 product a
d$_6$-DMSO, $^{13}$CNMR, 150 MHz
Competition experiment #3 product b

d$_6$-DMSO, $^1$HNMR, 500 MHz

![Chemical Structure Diagram]
Competition experiment #3 product b

d$_6$-DMSO, $^{13}$C NMR, 150 MHz

![Chemical structure](BK00215-154-4.006.esp)

![NMR spectrum](BK00215-154-4.006.esp)
References


