Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information – Table of Contents

Synthesis of SFs and Related Probe Compounds

General Experimental Considerations: All reagents and solvents used were purchased from commercial sources and used without further purification unless otherwise. All reactions were performed under an atmosphere of dry nitrogen unless otherwise noted. *N*-arylacrylamides **10a** – **10e**[1] were prepared according to literature procedures. ^{1}H NMR spectra were obtained using a Bruker 300 MHz, 400 MHz or 500 MHz spectrometer at 27 °C unless otherwise noted; chemical shifts are expressed in parts per million (ppm, δ units) and are referenced to the residual mono-^{1}H isotopomer of the solvent ($CHCl_3$: 7.24 ppm; $CHDCl_2$: 5.32 ppm; $CD_3S(=O)CD_2H$: 2.49 ppm). Coupling constants are given in units of hertz (Hz). Splitting patterns describe apparent multiplicities and are designated as s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet) and br s (broad singlet). ^{13}C NMR was obtained using a Bruker 125 MHz spectrometer at 27 °C unless otherwise noted; chemical shifts are expressed in ppm (δ) and are referenced to the perdeuterated NMR solvent ($CHCl_3$: 77.0 ppm; $CHDCl_2$: 54.0 ppm; CD3S(=O)CD_2H: 39.50 ppm). ^{19}F NMR was obtained using a Bruker 282 or 470 MHz spectrometer at 27 °C unless otherwise noted; chemical shifts are expressed in ppm (δ). ^{19}F chemical shifts were automatically referenced in Topspin (Bruker Instruments) according to the resonance frequency of the perdeuterated lock solvent using the IUPAC Xi (Ξ) ratios. LC-MS was carried out using a Waters UPLC fitted with a Waters SQD mass spectrometer (Column temperature = 30 °C, UV = 210 - 400 nm; electrospray ionization with positive/negative switching) at a flow rate of 1 mL/min using a solvent system of 98% A + 2% B to 2% A + 98% B over 1.5 min, where A = 0.1% formic acid in water (for acidic work) or 0.1% ammonium hydroxide in water (for basic work) and B = 0.1% formic acid in acetonitrile (for acidic work) or acetonitrile (for basic work). For acidic analysis the column used was a Waters Acquity HSS T3 (1.8 μm, 2.1 x 30 mm), for basic analysis the column used was a Waters Acquity BEH C18 (1.7 μm, 2.1 x 30 mm). Reported molecular ions correspond to

[M+H]+ unless otherwise noted; for molecules with multiple isotopic patterns (Br, Cl, etc.) the reported value is the one obtained for the lowest isotope mass unless otherwise specified. Thin layer chromatography (TLC) was performed using EMD silica gel 60 F_{254} plates, which were visualized using either UV light, reversibly stained with iodine (I_2 absorbed on silica) or a stain prepared by dissolving 2 g $KMnO_4$ and 12 g Na_2CO_3 in 200 mL H_2O. Column chromatography was performed using RediSep R_f preloaded silica gel cartridges on Teledyne ISCO CombiFlash Companion automated purification systems. Reproduced NMR spectra for all new compounds are included as a separate file. **Note:** For clarity, all compounds which do not appear in the main text have been assigned numbers within the Supporting Information, beginning with **24**.

General Synthesis of Arylsulfonyl Fluorides (1a – 3f): To a stirring solution of arylsulfonyl chloride (1.0 mmol) in CH_3CN (5.5 mL) at room temperature was added a 2.0 M solution of KHF_2 in water (5.5 mL, 11.0 mmol, 11.0 eq.). The resulting biphasic mixture was stirred vigorously at room temperature until LC-MS indicated complete consumption of the starting sulfonyl chloride (typically 0.5 – 2 h). The reaction mixture was then diluted with water (15 mL) and ethyl acetate (15 mL) the layers separated. The aqueous phase was extracted with 2 x 15 mL portions of ethyl acetate, then the combined extracts were washed once with 20 mL saturated aqueous NaCl solution. The product solution was dried over $MgSO_4$, the solids filtered, then the filtrate was concentrated to afford the sulfonyl fluorides as either colorless oils or white/colorless solids. The sulfonyl fluorides were typically used without further purification. ^{1}H NMR spectra for all previously reported compounds matched previously reported data. Additionally, the following arylsulfonyl fluorides are commercially available: **1a, 1d, 1f, 1k, 1l, 1m, 2a, 2b, 3a, 3b, 3c, 3e, 3f, 4,** and **5** (Sigma-Aldrich); **1b, 1c, 1e, 1g, 1j,** and **6** (Enamine).

Benzenesulfonyl fluoride (1a)[2]: Isolated in 68% yield as a colorless oil. ^{1}H NMR (300 MHz, CD_2Cl_2): δ 7.95 - 8.07 (m, 2 H), 7.77 - 7.87 (m, 1 H), 7.62 - 7.72 (m, 2 H). ^{19}F NMR (282 MHz, CD_2Cl_2): δ 65.24.

4-Nitrobenzenesulfonyl fluoride (1b)[3]: Isolated in 77% yield as a white solid. ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.51 (d, *J* = 8.3 Hz, 2 H), 8.36 - 8.20 (m, 2 H). ^{19}F NMR (282 MHz, CD_2Cl_2): δ 65.47.

4-(Trifluoromethoxy)benzenesulfonyl fluoride (1c)[4]: Isolated in 86% yield as a light brown oil. ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.11 (d, *J* = 8.7 Hz, 2 H), 7.47 (d, *J* = 9.0 Hz, 2 H). ^{19}F NMR (282 MHz, CD_2Cl_2)**: δ** 65.86 (s, 1 F), -58.10 (s, 3 F).

4-Methoxybenzenesulfonyl fluoride (1d)[5]: Isolated in 54% yield as a light brown oil. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.96 (d, *J* = 9.0 Hz, 2 H), 7.09 (d, *J* = 9.0 Hz, 2 H), 3.93 (s, 3 H). ^{19}F NMR (282 MHz, CD_3CN): δ 65.96.

4-Aminobenzenesulfonyl fluoride (1e)[6]: Isolated in 73% yield as a white solid. ^{1}H NMR (300 MHz, CD_2Cl_2): δ 7.62 – 7.82 (m, 2 H), 6.61 – 6.83 (m , 2 H), 4.51 (br s, 2 H). ^{19}F NMR (282 MHz, CD_2Cl_2): δ 67.87.

4-Cyanobenzenesulfonyl fluoride (1f)[5]: Isolated in 76% yield as an off-white solid. ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.16 (d, *J* = 7.9 Hz, 2 H), 7.95 (d, *J* = 7.9 Hz, 2 H). ^{19}F NMR (282 MHz, CD_2Cl_2): δ 65.23.

4-(Trifluoromethyl)benzenesulfonyl fluoride (1g)[3]: Isolated in 78% yield as a white solid. ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.18 (d, *J* = 8.3 Hz, 2 H), 7.93 (d, *J* = 8.7 Hz, 2 H). ^{19}F NMR (282 MHz, CD_2Cl_2): δ 65.20 (s, 1 F), -63.89 (s, 3 F).

4-Carbamoylbenzenesulfonyl fluoride (1h): ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.36 (br s, 1 H), 8.26 (d, *J* = 8.5 Hz, 2 H), 8.20 (d, *J* = 8.2 Hz, 2 H), 7.83 (br s, 1 H). ^{13}C NMR (125 MHz, DMSO-d_6): δ 166.0, 141.4, 133.5 (d, *J* = 23.8 Hz) 129.3 (2 C),128.6 (2 C). ^{19}F NMR (471 MHz, DMSO-d_6): δ 66.14 (s, 1 F). MS: Calc. for $[M-H]^-$ m/z 202.0; Obs. 202.0. HRMS calculated for $[C_7H_6FNO_3S+H]^+$: 204.0125; found: 204.0125.

4-(2,2,2,-Trifluoroacetamido)benzenesulfonyl fluoride (1i)[7]: Isolated in 56% yield as a white solid. ^{1}H NMR (300 MHz, CD_2Cl_2): δ 8.19 (br s, 1 H), 8.07 (d, *J* = 9.0 Hz, 2 H), 7.90 (d, *J* = 9.0 Hz, 2 H). ^{19}F NMR (282 MHz, CD_2Cl_2): δ 65.92 (s, 1 H), -76.11 (s, 3 H).

4-Fluorobenzenesulfonyl fluoride (1j)[8]: Isolated in 77% yield as a slightly yellow oil. ^{1}H NMR (300 MHz, CD_2Cl_2): δ 7.88 - 8.15 (m, 2 H) 7.35 (app t, *J* = 8.7 Hz, 2 H). ^{19}F NMR (282 MHz, CD_2Cl_2): δ 66.09 (s, 1 F), -100.15 (s, 1 F).

4-Carboxybenzenesulfonyl fluoride (1k)[9]: Isolated in 82% yield as a white solid. ^{1}H NMR (300 MHz, DMSO-d_6): δ 13.77 (br s, 1 H), 8.25 (s, 4 H). ^{19}F NMR (282 MHz, CD_2Cl_2): δ 65.96.

4-Acetamidobenzenesulfonyl fluoride (1l)[4]: Isolated in 57% yield as a white solid. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.99 (d, *J* = 9.0 Hz, 2 H), 7.80 (d, *J* = 8.7 Hz, 2 H), 7.38 (br s, 1 H), 2.28 (s, 3 H). ^{19}F NMR (282 MHz, CD_2Cl_2): δ 66.16.

4-Methylbenzenesulfonyl fluoride (1m)[5]: Isolated in 74% yield as a colorless solid. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.92 (d, *J* = 8.3 Hz, 2 H), 7.44 (d, *J* = 8.7 Hz, 2 H), 2.52 (s, 3 H). ^{19}F NMR (282 MHz, CD_2Cl_2): δ 65.67.

3-Methoxybenzenesulfonyl fluoride (2a)[5]: Isolated in 54% yield as a clear, colorless oil. ^{1}H NMR (300 MHz, CD_2Cl_2): δ 7.55 - 7.68 (m, 2H), 7.51 - 7.54 (m, 1H), 7.29 - 7.41 (m, 1H), 3.93 (s, 3H). ^{19}F NMR (282 MHz, CD_2Cl_2): δ 64.94.

3-Carboxybenzenesulfonyl fluoride (2b)[10]: Isolated in 97% yield as a white solid. ^{1}H NMR (300 MHz, CD_2Cl_2): δ 8.70 - 8.74 (m, 1 H), 8.50 (d, *J* = 7.9 Hz, 1 H), 8.27 (dd, *J* = 6.4, 1.5 Hz, 1 H), 7.82 (app t, *J* = 7.9 Hz). ^{19}F NMR (282 MHz, CD_2Cl_2): δ 65.36.

2-Nitrobenzenesulfonyl fluoride (3a)[3]: Isolated in 90% yield as a white solid. ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.27 (dd, *J* = 7.5, 1.5 Hz 1 H), 8.02 - 8.13 (m, 1 H), 7.81 – 8.01 (m, 2 H). ^{19}F NMR (282 MHz, CD_2Cl_2): δ 64.49.

2-Cyanobenzenesulfonyl fluoride (3b)[11]: Isolated in 88% yield as a white solid. ^{1}H NMR (300 MHz, CD_2Cl_2): δ 8.18 - 8.27 (m, 1 H), 7.98 - 8.06 (m, 1 H), 7.86 - 7.97 (m, 2 H). ^{19}F NMR (282 MHz, CD_2Cl_2): δ 63.94.

2-(Trifluoromethyl)benzenesulfonyl fluoride (3c): Isolated in 98% yield as a light brown oil. ^{1}H NMR (300 MHz, CD_2Cl_2): δ 8.33 (d, *J* = 7.9 Hz, 1 H), 7.99 - 8.09 (m, 1 H), 7.82 - 7.98 (m, 2 H). ^{13}C NMR (125 MHz, CD_2Cl_2): δ 136.5, 133.7, 133.2, 131.6 (app d, *J* = 28.4 Hz), 129.6 (q, *J* = 5.5 Hz), 129.5 (q, *J* = 33.9 Hz), 122.6 (q, *J* = 274 Hz). ^{19}F NMR (471 MHz, CD_2Cl_2): δ 65.17 (q, *J* = 13.7 Hz, 1F), -59.22 (d, *J* = 13.7 Hz, 3 F). IR: 1414.07, 1314.99, 1212.54, 1166.62, 1127.21, 1110.33, 1098.64, 1060.67, 1020.66, 841.79, 794.78, 759.47, 731.38, 710.89, 608.68, 598.80, 528.17, 429.21 cm^{-1}

2-(Trifluoromethoxy)benzenesulfonyl fluoride (3d): Isolated in 78% yield as a light yellow oil. ^{1}H NMR (300 MHz, CD_2Cl_2): δ 8.10 (dd, *J* = 8.1, 1.3 Hz, 1 H), 7.86 (td, *J* = 8.0, 1.7 Hz, 1 H), 7.52 - 7.59 (m, 2 H). ^{13}C NMR (125 MHz, CD_2Cl_2): δ 147.4, 138.2, 132.2, 127.8, 126.4, 121.8, 120.8 (q, *J* = 261.7 Hz). ^{19}F NMR (471 MHz, CD_2Cl_2): δ 62.35 (br q, *J* = 2.3 Hz, 1F), -57.19 (d, *J* = 2.3 Hz, 3 F). IR: 1413.95, 1321.62, 1212.66, 1174.7, 1162.4, 1136.37, 1110.45, 1064.17, 793.46, 762.36, 713.06, 610.73, 588.79, 528.65, 494.9, 430.42 cm^{-1}

2-Methoxybenzenesulfonyl fluoride (3f)[5]: Isolated in 93% yield as a white solid. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.95 (d, *J* = 7.9 Hz 1 H), 7.71 (t, *J* = 7.9 Hz, 1 H), 7.05 – 7.21 (m, 2 H), 4.02 (s, 3 H). ^{19}F NMR (282 MHz, CD_2Cl_2): δ 58.19.

Synthesis of 4-Ureidobenzenesulfonyl fluoride (1n): To a stirring solution of 4-(fluorosulfonyl)benzoic acid (**1k**, 145 mg, 0.7 mmol, 1 eq.) in 1,4-dioxane (5.7 mL) at room temperature was added DMF (2.7 µL, 0.04 mmol, 0.05 eq.) and a 2.0 M solution of oxalyl chloride in CH_2Cl_2 (408 µL, 0.82 mmol, 1.15 eq.). The resulting clear, colorless mixture was allowed to stir at room temperature for 1 h. After 1 h the solution of crude acid chloride was

treated with a 0.5 M solution of NH_3 in 1,4-dioxane (5.7 mL, 2.8 mmol, 4.0 eq.). The resulting milky white suspension was stirred vigorously at room temperature for 5 min, then was diluted with CH_2Cl_2 (10 mL). The reaction mixture was filtered, then the filtrate was concentrated under reduced pressure to afford the crude product as a colorless oil. The crude product was purified by flash column chromatography (SiO_2, eluting with 0-50% EtOAc in CH_2Cl_2) to afford sulfonyl fluoride **1n** as a white solid (41 mg, 28% yield). ^{1}H NMR (500 MHz, DMSO-d_6): δ 9.38 (s, 1 H), 7.94 (d, J = 8.1 Hz, 2 H), 7.74 (d, J = 9.1 Hz, 2 H), 6.25 (br s, 2 H). ^{13}C NMR (125 MHz, DMSO-d_6): δ 155.2, 148.2, 130.0 (2 C), 121.5 (d, J = 22.9 Hz), 117.6 (2 C). ^{19}F NMR (471 MHz, DMSO-d_6): δ 68.09 (s, 1 F). MS: Calc. for $[M-H]^-$ 207.0; Obs. 207.0. HRMS calculated for $[C_7H_7FN_2O_3S+H]^+$: 219.0234; found: 219.0233.

Synthesis of 4-(Dimethylamino)benzenesulfonyl fluoride (1o)[12]: To a stirring solution of 4-fluorobenzenesulfonyl fluoride (300 mg, 1.7 mmol, 1 eq.) in THF (7.1 mL) at room temperature was added, in sequence, a 2.0 M solution of dimethylamine in THF (1.10 mL, 2.2 mmol, 1.3 eq.) and N,N-diisopropylethylamine (440 µL, 2.5 mmol, 1.7 eq.). The resulting clear, colorless mixture was allowed to stir at room temperature for 16 h. The mixture was diluted with 20 mL water, then was extracted with 3 x 25 mL portions of ethyl acetate. The combined extracts were washed with sequential 40 mL portions of saturated aqueous $NaHCO_3$ solution and saturated aqueous NaCl solution. The product solution was dried over $MgSO_4$, the solids filtered, and the filtrate concentrated to afford the crude product as a white solid. The product was purified by flash column chromatography over silica gel (20 g silica gel, eluting with 0-30% ethyl acetate in hexanes) to afford 4-(dimethylamino)benzenesulfonyl flouride as a white solid (240 mg, 70% yield). ^{1}H NMR (300 MHz, CD_2Cl_2): δ 7.78 (d, J = 9.4 Hz, 2 H) 6.74 (d, J = 9.0 Hz, 2 H) 3.09 (s, 6 H). ^{19}F NMR (282 MHz): δ 67.87 (s). MS: Calc. for $[M+H]^+$ m/z 204.0; Obs. 204.0.

Synthesis of 4-(Fluorosulfonyloxy)benzoic acid (7)[13]: Ethyl 4-((fluorosulfonyl)oxy)benzoate (170 mg, 0.68 mmol) (Sigma-Aldrich) was suspended 1M HCl aq. (7 mL, 7.00 mmol) and sealed in a microwave tube. The resultant reaction was heated to 100 °C overnight. The following morning, the reaction was cooled to room temp and a white solid precipitated out. Solid collected by filtration, and dissolved ethyl acetate, dried over sodium sulfate, filtered and evaporated to yield 4-((fluorosulfonyl)oxy)benzoic acid (137 mg, 91 %) as a white solid. ^{1}H NMR (300 MHz, CD_2Cl_2): 8.20 (d, J = 8.0 Hz, 2H), 7.46 (d, J = 8.1 Hz, 2H). ^{19}F NMR (282 MHz, CD_2Cl_2): δ ppm 38.18.

Synthesis of 3-(Fluorosulfonyloxy)benzoic acid (8)[13]: To a stirring solution of 3-hydroxybenzoic acid (1.00 g, 7.24 mmol, 1 eq.) in ether (26.6 mL) and pyridine (1.18 mL, 14.5 mmol, 2.00 eq.) at -78 °C was added, dropwise via syringe, sulfuryl chloride (1.18 mL, 14.5 mmol, 2.00 eq.). The resulting suspension was maintained at -78 °C for 1 h, then was allowed to warm to room temperature overnight. The reaction mixture was then diluted with 1.0 M HCl (50 mL), then was extracted with 2 x 50 mL portions of ethyl acetate. The combined extracts were dried over $MgSO_4$, the solidsfiltered, and the filtrate concentrated under reduced pressure. The crude chlorosulfate was dissolved in CH_3CN (25 mL), then was treated with solid AgF (2.76 g, 21.7 mmol, 3.00 eq.). The resulting supension was stirred vigorously at room temperature for 5 h, then was filtered and the filtrate concentrated under reduced pressure. The crude product was purified by reverse-phase flash column chromatography (C_{18}-capped SiO_2, 0 – 60% CH_3CN + 0.1% TFA in H_2O + 0.1% TFA). Fractions containing the desired fluorosulfate were partially evaporated under reduced pressure to remove CH_3CN, then residue was frozen at -78 °C and lyophilized to afford the title compound as a white powder (0.996 g, 62% yield). ^{1}H NMR (300 MHz, CD_2Cl_2): 13.58 (br. S., 1H), 8.01-8.20 (m, 1H), 7.83 – 7.93 (m, 1H), 7.65 – 7.81 (m, 1H) . ^{19}F NMR (282 MHz, MeOH-d_4): δ ppm 38.07.

Synthesis of *N*-Acetylbenzenesulfinamide (24a)[14]: To a suspension of benzenesulfinamide (200 mg, 1.42 mmol, 1 eq.) in THF at -78 °C was added, dropwise via syringe, a 2.5 M solution of *n*-butyllithium in hexanes (1.19 mL, 2.97 mmol, 2.1 eq.). The resulting suspension was warmed to 0 °C by means of an ice/water bath and was maintained at this temperature for 15 minutes, then was cooled to -78 °C. Acetic anhydride (160 µL, 1.70 mmol, 1.2 eq.) was added and the resulting suspension was allowed to warm to room temperature overnight. The reaction mixture was then diluted with a saturated aqueous solution of NH_4Cl (20 mL) and ethyl acetate (20 mL) and the layers separated. The aqueous phase was extracted with 2 x 25 mL portions of ethyl acetate, then the combined extracts were washed with sequential 20 mL portions of water and saturated aqueous NaCl solution. The product solution was dried over $MgSO_4$, the solids filtered, then the filtrate was concentrated to afford crude *N*-acetylbenzenesulfinamide as a waxy solid (254 mg, 98% yield). The crude sulfinamide was used without further purification. ^{1}H NMR (d^6-DMSO): δ 11.03 (s, 1 H), 7.68 – 7.72 (m, 2 H), 7.58 – 7.61 (m, 3H), 1.99 (s, 3 H).

General Synthesis of Arylsulfinamides – Procedure A: To a suspension of amide or carbamate (3.95 mmol, 1 eq.) in THF (5.5 mL) at -78 °C was added, dropwise via syringe, a 1.0 M solution of lithium bis(trimethylsilyl)amide in THF (4.35 mL, 4.35 mmol, 1.1 eq.). The resulting suspension was warmed to 0 °C by means of an ice/water bath and was maintained at this temperature for 15 minutes. The solution was then cooled to -78 °C before addition of the sulfinyl chloride. Meanwhile, a separate flask was charged with sodium phenylsulfinate (850 mg, 5.2 mmol), DMF (20 µL, 0.26 mmol, 0.05 eq. relative to sulfinate) and CH_2Cl_2 (23 mL) at room temperature. A 2.0 M solution of oxalyl chloride in CH_2Cl_2 (3.1 mL, 6.2 mmol, 1.2 eq. relative to sulfinate) was added and the resulting suspension was stirred vigorously at room

temperature for 1 h. The solution was then filtered through a 0.2 μM filter to remove NaCl and the filtrate was concentrated to afford the crude benzenesulfinyl chloride as a yellow oil. The crude sulfinyl chloride was dried by concentration from toluene (2 x 5 mL), then was used without further purification. The crude, dried sulfinyl chloride (762 mg, 4.7 mmol, 1.2 eq. relative to amide) was dissolved in THF (23 mL), then was added to the cold anion solution. The resulting suspension was allowed to warm to room temperature overnight. The reaction mixture was then diluted with a saturated aqueous solution of NH_4Cl (20 mL) and ethyl acetate (20 mL) and the layers separated. The aqueous phase was extracted with 2 x 25 mL portions of ethyl acetate, then the combined extracts were washed with sequential 20 mL portions of water and saturated aqueous NaCl solution. The product solution was dried over $MgSO_4$, the solids filtered, then the filtrate was concentrated to afford the crude sulfinamides. The crude sulfinamides were purified by flash column chromatography over silica gel to afford the pure sulfinamides. 1H NMR spectra for all previously reported compounds matched literature data.

General Synthesis of Arylsulfinamides – Procedure B: To a stirring suspension of sodium phenylsulfinate (1.0 g, 6.1 mmol, 1 eq.) and DMF (24 μL, 0.3 mmol, 0.05 eq.) in CH_2Cl_2 (26 mL) at room temperature was added, dropwise via syringe, a 2.0 M solution of oxalyl chloride in CH_2Cl_2 (3.2 mL, 6.4 mmol, 1.05 eq.). The resulting suspension was stirred vigorously at room temperature for 1 h. The corresponding amine (7.0 mmol, 1.15 eq.) and N.N-diisopropylethylamine (1.6 mL, 9.1 mmol, 1.5 eq.) were added, and the resulting suspension was maintained at room temperature overnight. The reaction mixture was then diluted with water (20 mL) and ethyl acetate (20 mL) and the layers separated. The aqueous phase was extracted with 2 x 15 mL portions of ethyl acetate, then the combined extracts were washed with sequential 20 mL portions of water and saturated aqueous NaCl solution. The product solution was dried over Na_2SO4, the solids filtered, then the filtrate was concentrated to afford

the crude sulfinamides. The crude sulfinamides were purified by flash column chromatography over silica gel to afford the pure sulfinamides. ^{1}H NMR spectra for all previously reported compounds matched literature data.

***N*-pivaloylbenzenesulfinamide (24b)[15]:** Prepared according to general procedure A above. Isolated in 29% yield as a white solid. ^{1}H NMR (300 MHz, CD_2Cl_2): δ 11.03 (s, 1 H) 7.70 – 7.75 (m, 2 H), 7.57 – 7.60 (m, 3H), 1.21 (s, 9 H).

***N*-(*tert*-butoxycarbonyl)benzenesulfinamide (24c)[16]:** Prepared according to general procedure A above. Isolated in 50% yield as a white solid. ^{1}H NMR (500 MHz, CD_2Cl_2): δ 11.03 (s, 1 H) 7.700 – 7.76 (m, 2 H), 7.55 – 7.58 (m, 3H), 1.42 (s, 9 H).

***N*-(4-(trifluoromethyl)phenyl)benzenesulfinamide (24d)[17]:** Prepared according to general procedure B above. Isolated in 35% yield as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6): δ 9.87 (s, 1 H), 7.76 (d, J = 6.9 Hz, 2 H), 7.55 – 7.63 (m, 5 H), 7.26 (d, J = 8.5 Hz, 2 H). ^{13}C NMR (125 MHz, DMSO-d_6): δ 145.8, 144.0, 131.3, 129.2, 126.5 (q, J = 3.7 Hz), 125.5, 123.9 (q, J = 136.9 Hz), 122.0 (q, J = 32.4 Hz), 116.9, 113.2. ^{19}F NMR (471 MHz, DMSO-d_6): δ -60.19. Calc. for $[M-H]^-$ m/z 284.0; Obs. 284.0.

***N*-(4-methylphenyl)benzenesulfinamide (24f)[18]:** Prepared according to general procedure B above. Isolated in 48% yield as an off-white solid. ^{1}H NMR (500 MHz, DMSO-d_6): δ 9.17 (s, 1 H), 7.72 (dd, J = 8.0, 1.5 Hz, 2 H), 7.51 – 7.60 (m, 3 H), 6.93 – 7.07 (m, 4 H), 2.19 (s, 3 H). ^{13}C NMR (125 MHz, DMSO-d_6): δ 144.7, 139.1, 131.1, 130.9, 129.5, 129.0, 125.6, 118.3, 20.2. Calc. for $[M-H]^-$ m/z 230.1; Obs. 230.1.

***N*-methylbenzenesulfinamide (24g)[19]:** Prepared according to general procedure B above. Isolated in 35% yield as a clear, colorless oil. ^{1}H NMR (300 MHz, CD_2Cl_2): δ 7.67 – 7.70 (m, 2 H), 7.48 – 7.55 (m, 3 H), 4.15 (br s, 1 H), 2.50 (d, J = 5.7 Hz, 3 H).

***N-tert*-butylbenzenesulfinamide (24h)[20]:** Prepared according to general procedure B above. Isolated in 68% yield as a clear, colorless oil. ^{1}H NMR (300 MHz, CD_2Cl_2): δ 7.63 – 7.72 (m, 2 H), 7.44 – 7.55 (m, 3 H), 5.13 (br s, 1 H), 1.39 (s, 9 H).

General Procedure of the Synthesis of Benzenesulfonimidoyl Fluorides – Procedure A: To a stirring solution of sulfinamide (0.55 mmol) in CH_3CN (2.7 mL) at room temperature was added, in one portion, *t*-butyl hypochloride (71 µL, 0.63 mmol, 1.15 eq.). The resulting solution was maintained at room temperature for 1 h, followed by the addition of a 2.0 M solution of KHF_2 in water (2.7 mL, 5.5 mmol, 10 eq.). The biphasic mixture was stirred vigorously until LC-MS analysis indicated complete disappearance of the intermediate sulfonimidoyl chloride (typically 2-6 h)[21]. The reaction mixture was then diluted with water (15 mL) and ethyl acetate (15 mL) the layers separated. The aqueous phase was extracted with 2 x 15 mL portions of ethyl acetate, then the combined extracts were washed once with 20 mL saturated aqueous NaCl solution. The product solution was dried over $MgSO_4$, the solids filtered, then the filtrate was concentrated to afford the sulfonimidoyl fluorides as either colorless oils or white/colorless solids. The sulfonimidoyl fluorides were typically obtained in >95% purity and were used without further purification.

General Procedure of the Synthesis of Benzenesulfonimidoyl Fluorides – Procedure B: To a stirring solution of sulfinamide (0.35 mmol) in CH_3CN (1.7 mL) at room temperature was added, in one portion, *t*-butyl hypochlorite (43 µL, 0.39 mmol, 1.1 eq.). The resulting solution was maintained at room temperature for 1 h, then was concentrated under reduced pressure. The crude sulfonimidoyl chloride was then dissolved in dry CH_3CN (3.5 mL) followed by the addition of solid AgF (53 mg, 0.42 mmol, 1.2 eq.). The resulting suspension was stirred vigorously at room temperature until LC-MS analysis indicated the reaction was complete

(typically 4 – 24 h) . The reaction mixture was then diluted with water (15 mL) and ethyl acetate (15 mL) the layers separated. The aqueous phase was extracted with 2 x 15 mL portions of ethyl acetate, then the combined extracts were washed once with 20 mL saturated aqueous NaCl solution. The product solution was dried over $MgSO_4$, the solids filtered, then the filtrate was concentrated to afford the sulfonimidoyl fluorides as either colorless oils or white/colorless solids. The sulfonimidoyl fluorides were typically obtained in >95% purity and were used without further purification.

***N*-Acetylbenzenesulfonimidoyl Fluoride (9a)**: Prepared according to Procedure A above. Isolated in 43% yield as a clear, colorless oil. ^{1}H NMR (500 MHz, CD_2Cl_2): δ 8.10 (dd, *J* = 8.4, 0.9 Hz, 2 H), 7.74 - 7.87 (m, 1 H), 7.61-7.71 (m, 1 H), 2.23 (s, 3 H). ^{13}C NMR (125 MHz, CD_2Cl_2): δ 175.5, 136.2, 134.5 (d, *J* = 20.3 Hz), 130.2 (2 C), 128.5 (2 C), 27.6. ^{19}F NMR (471 MHz, CD_2Cl_2): δ 66.05. MS: Calc. for $[M+H]^+$ m/z 202.0; Obs. 202.0.

***N*-Pivaloylbenzenesulfonimidoyl Fluoride (9b):** Prepared according to Procedure A above. Isolated in 55% yield as a clear, colorless oil. ^{1}H NMR (CD_2Cl_2): δ 8.00- 8.16 (m, 2 H), 7.76 – 7.83 (m, *J* = 7.2 Hz, 1 H), 7.60 - 7.71 (m, 2 H), 1.23 (s, 9 H). ^{13}C NMR (CD_2Cl_2): δ 184.0, 136.1, 135.0 (d, *J* = 20.3 Hz), 130.2 (2 C), 128.4 (2 C), 42.7, 27.4. ^{19}F NMR (CD_2Cl_2): δ 65.88. MS: Calc. for $[M+H]^+$ m/z 244.1; Obs. 244.1. HRMS calculated for $[C_{11}H_{14}FNO_2S+H]^+$: 244.0802; found: 244.0813.

***N*-(Tert-butoxycarbonyl)benzenesulfonimidoyl Fluoride (9c):** Prepared according to Procedure A above. Isolated in 44% yield as a clear, colorless oil. ^{1}H NMR (CD_2Cl_2): δ 8.09 (dd, *J* = 8.7, 1.1 Hz, 2 H), 7.75 - 7.88 (m, 1 H), 7.58 - 7.72 (m, 2 H), 1.50 (s, 9 H). ^{13}C NMR (CD_2Cl_2): δ 152.7, 136.2, 134.2 (d, *J* = 20.3 Hz), 130.2 (2 C), 128.5 (2 C), 83.0, 28.1. ^{19}F NMR (CD_2Cl_2): δ 67.86. MS: Calc. for $[M+H]^+$ m/z 260.1; Obs. 260.1. HRMS calculated for $[C_{11}H_{14}FNO_3S+H]^+$: 260.0751; found: 260.076.

***N*-((4-Trifluoromethyl)phenyl)benzenesulfonimidoyl Fluoride (9d):** Prepared according to Procedure B above. Isolated in 96% yield as a red-purple solid. ^{1}H NMR (CD_2Cl_2): δ 8.15 - 8.25 (m, 2 H), 7.76 - 7.88 (m, 1 H), 7.57 - 7.73 (m, 4 H), 7.35-7.41 (m, 2 H). ^{13}C NMR (CD_2Cl_2): δ 143.7, 143.6, 136.6 (2C), 135.3 (d, J = 20.3 Hz), 130.9 (2 C), 128.5 (2 C), 127.1, 124.6 (2C), 123.8. ^{19}F NMR (CD_2Cl_2): δ 80.66 (1 F), -62.39 (3 F). MS: Calc. for $[M+H]^+$ m/z 304.0; Obs. 304.0.

***N*-(phenyl)benzenesulfonimidoyl Fluoride (9e)**[22]: Prepared according to Procedure B above. Isolated in 6.5% yield as an orange oil. ^{1}H NMR (CD_2Cl_2): δ 8.23 (d, J = 7.9 Hz, 2H), 7.78-7.86 (m, 1H), 7.70 (s, 2H), 7.38 (d, J = 7.6 Hz, 2H), 7.30 (s, 2H), 7.16-7.22 (m, 1H). ^{19}F NMR (CD_2Cl_2): δ 81.57 (1 F). MS: Calc. for $[M+H]^+$ m/z 236.0; Obs. 236.1.

***N*-((4-Methyl)phenyl)benzenesulfonimidoyl Fluoride (9f):** Prepared according to Procedure B above. Isolated in 45% yield as a yellow solid. ^{1}H NMR (CD_2Cl_2): δ 8.14 – 8.21 (m, 2 H), 7.73 - 7.80 (m, 1 H), 7.61 - 7.68 (m, 2 H), 7.15 (app s, 4 H), 2.33 (s, 3 H). ^{13}C NMR (CD_2Cl_2): δ 138.5, 136.4 (d, J = 20.3 Hz), 135.1, 133.2, 130.4 (2 C), 129.9 (2 C), 128.2 (2C), 124.1 (2C), 21.1. ^{19}F NMR (CD_2Cl_2): δ 81.74. MS: Calc. for $[M+H]^+$ m/z 250.1; Obs. 250.1. HRMS calculated for $[C_{13}H_{12}FNOS+H]^+$: 250.0696; found: 250.0708.

***N*-Methylbenzenesulfonimidoyl Fluoride (9g)**[20]: Prepared according to Procedure B above. Isolated in 43% yield as a clear, colorless oil. ^{1}H NMR (CD_2Cl_2): δ 7.72 – 7.83 (m,, 2 H), 7.41 – 7.47 (m, 1 H) 7.32 – 7.41 (m, 2 H), 2.65 (s, 3 H). ^{13}C NMR (CD_2Cl_2): δ 139.3, 133.2, 129.7 (2 C), 127.6 (2 C), 29.8. ^{19}F NMR (CD_2Cl_2): δ 65.33. MS: Calc. for $[M+H]^+$ m/z 174.0; Obs. 174.0.

***N*-*t*-butylbenzenesulfonimidoyl Fluoride (9h):** Prepared according to Procedure B above. Isolated in 51% yield as a clear, colorless oil (1 : 1 mixture of confomers). ^{1}H NMR (CD_2Cl_2): δ 8.15 - 8.25 (m, 2 H), 7.76 - 7.88 (m, 1 H), 7.57 - 7.73 (m, 4 H), 7.35-7.41 (m, 2 H) 1.29 (d, J

= 7.6 Hz, 9 H). ^{13}C NMR (CD_2Cl_2): δ 144.1, 132.7, 129.5 (2 C) 127.4 (2 C), 55.0, 30.4 (3 C). ^{19}F NMR (CD_2Cl_2): 76.7 (d, *J* = 7.6 Hz, 1 F), 74.2 (d, *J* = 7.6 Hz, 1 F). MS: Calc. for $[M+H]^+$ m/z 216.1; Obs. 216.1.

General Procedure for the Synthesis of 5'-*O*-(3-(Fluorosulfonyl)benzoyl)adenosine (m-FSBA) Analogs: To a stirring solution of benzoic acid (0.92 mmol, 1 eq.) in 1,4-dioxane (4.3 mL) at room temperature was added, in sequence, *N*,*N*-dimethylformamide (3.6 μL, 0.05 mmol, 0.05 eq.) and a 2.0 M solution of oxalyl chloride in CH_2Cl_2 (0.55 mL, 1.10 mmol, 1.2 eq.). The resulting clear reaction mixture was allowed to stir at room temperature for 45 minutes, then adenosine (282 mg, 1.05 mmol, 1.15 eq.) and 1,3-dimethyltetrahydropyrimidin-2(1*H*)-one (DMPU, 4.3 mL) were added and the resulting suspension was allowed to stir at room temperature for 16 h. The reaction mixture was diluted with 10 mL water and 5 mL saturated aqueous NaCl solution, then was extracted with 3 x 25 mL portions of EtOAc. The combined extracts were washed with 2 x 20 mL portions of 50% saturated aqueous NaCl solution and 20 mL saturated aqueous NaCl solution. The product solution was dried over $MgSO_4$, the solids filtered, and the filtrate concentrated to afford the crude product as a viscous oil. The FSBA analogs were purified by reverse-phase HPLC to afford the desired compounds as colorless gums (typically as 1 : 1 trifluoroacetate salts). For ease of handling, the purified products were dissolved in 10-30% CH_3CN in water, rapidly frozen by immersion in a -78 °C bath (2-propanol/CO_2), then were lyophilized to afford the FSBA analogs as white powders. The parent compound p-FSBA (**18**, as the DMF-solvated HCl salt) was purchased from Sigma-Aldrich.

5'-*O*-(3-(Fluorosulfonyl)benzoyl)adenosine (m-FSBA, 19a)[23]: Isolated as the trifluoroacetate salt in 14% yield as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.39-8.52 (m, 2 H), 8.07-8.29 (m, 1H), 7.95 (t, *J* = 7.7 Hz, 1 H), 7.07 (t, *J* = 51 Hz, 1 H), 5.95 (d, *J* = 4.4

Hz, 1 H), 4.71 (t, *J* = 3.8 Hz, 1 H), 4.68 (dd, *J* = 12.0, 3.5 Hz, 1 H), 4.55 (dd, *J* = 11.7, 6.0 Hz, 1 H), 4.42 (t, *J* = 6.0 Hz, 1 H), 4.27 (br dd, *J* = 9.1, 5.7 Hz, 1 H).

5'-*O*-(4-Nitro-3-(fluorosulfonyl)benzoyl)adenosine (NO_2-m-FSBA, 19b): Isolated as the trifluoroacetate salt in 9% yield as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.58 - 8.66 (m, 2 H), 8.45 (d, *J* = 8.2 Hz, 1 H), 8.34 (s, 1 H), 8.05 (s, 1 H), 7.11 (t, *J* = 51 Hz, 1 H), 5.93 (d, *J* = 5.0 Hz, 1 H), 4.63-4.77 (m, 2 H), 4.50 - 4.61 (m, 2 H), 4.42 - 4.48 (m, 1 H), 4.21 - 4.29 (m, 1 H). ^{13}C NMR (125 MHz, DMSO-d_6): δ 162.8, 158.1 (q, *J* = 30.2 Hz), 149.8, 149.5, 149.1, 140.6, 138.9, 134.4, 132.6, 127.6, 118.8, 116.3, 90.2, 88.5, 84.0, 81.6, 73.0. ^{19}F NMR (470 MHz, DMSO-d_6): δ 66.48 (s, 1 F), -73.54 (s, 3 F). MS: Calc. for $[M+H]^+$ m/z 499.4; Obs. 499.4. HRMS calculated for $[C_{17}H_{15}FN_6O_9S+H]^+$: 499.0678; found: 499.0671.

5'-*O*-(4-Cyano-3-(fluorosulfonyl)benzoyl)adenosine (CN-m-FSBA, 19c): Isolated as the trifluoroacetate salt in 35% yield as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.49-8.63 (m, 4 H), 8.29 (s, 1 H), 5.97 (d, *J* = 4.7 Hz, 1 H), 4.64-4.76 (m, 2 H), 4.59 (dd, *J* = 12.0, 6.3 Hz, 1 H), 4.41 (t, *J* = 5.2 Hz, 1 H), 4.23-4.35 (m, 1 H)**.** ^{13}C NMR (125 MHz, DMSO-d_6): δ 162.6, 158.4 (q, *J* = 35.7 Hz), 152.3, 148.5, 147.8, 141.8, 137.6, 136.7, 134.4, 133.9, 133.6, 130.9, 119.0, 117.0, 114.7, 114.0, 113.7, 88.4, 81.4, 73.0, 70.1, 65.8. ^{19}F NMR (470 MHz, DMSO-d_6): δ 65.23 (s, 1 F), -74.60 (s, 3 F). MS: Calc. for $[M+H]^+$ m/z 479.1; Obs. 479.1. HRMS calculated for $[C_{18}H_{15}FN_6O_7S+H]^+$: 479.0780; found: 479.0770.

5'-*O*-(4-Bromo-3-(fluorosulfonyl)benzoyl)adenosine (Br-m-FSBA, 19e): Isolated as the trifluoroacetate salt in 11% yield as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6): 8.49 (d, *J* = 6.0 Hz, 2 H), 8.16-8.32 (m, 3 H), 7.14 (t, *J* = 51.1 Hz, 1 H), 5.96 (d, *J* = 4.7 Hz, 1 H), 4.69 (t, *J* = 4.7 Hz, 1 H), 4.66 (dd, *J* = 11.7, 3.5 Hz, 1 H), 4.55 (dd, *J* = 12.0, 6.3 Hz, 1 H), 4.40 (t, *J* = 5.2 Hz, 1 H), 4.23-4.30 (m, 1 H). ^{13}C NMR (125 MHz, DMSO-d_6): δ 163.2, 158.5 (q, *J* = 33.9 Hz), 153.0, 148.6, 141.4, 137.2, 137.0, 133.0, 132.8, 132.3, 132.2, 129.9, 129.7, 125.6, 119.1, 117.4, 115.1, 88.3, 81.4, 73.0, 70.1, 65.4. ^{19}F NMR (470 MHz, DMSO-d_6): δ 58.58 (s,

1 F), -74.32 (s, 3 F). MS: Calc. for $[M+H]^+$ m/z 533.3; Obs. 533.3. HRMS calculated for $[C_{17}H_{15}BrFN_5O_7S+H]^+$: 531.9932; found: 531.9943.

5'-*O*-(4-Fluoro-3-(fluorosulfonyl)benzoyl)adenosine (F-m-FSBA, 19f): Isolated as the formate salt in 36% yield as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.44-8.53 (m, 2 H), 8.40 (dd, *J* = 6.5, 2.0 Hz, 1 H), 8.22 (br s, 2 H), 7.86 (t, *J* = 9.3 Hz, 1 H), 5.95 (d, *J* = 4.7 Hz, 1 H), 4.71 (t, *J* = 5.0 Hz, 1 H), 4.66 (dd, *J* = 12.0, 6.3 Hz, 1 H), 4.54 (dd, *J* = 11.8, 6.1 Hz, 1 H), 4.41 (t, *J* = 5.2 Hz, 1 H), 4.22-4.33 (m, 1 H). ^{13}C NMR (125 MHz, DMSO-d_6): δ 162.8, 161.2 (d, *J* = 265 Hz), 153.0, 148.6, 141.5, 140.3 (d, *J* = 11.0 Hz), 140.2, 131.9, 127.2, 127.2, 120.5 (dd, *J* = 27.0, 15.1 Hz), 119.2 (d, *J* = 21.1 Hz), 119.0, 88.3, 81.5, 73.0, 70.1, 65.4. ^{19}F NMR (470 MHz, DMSO-d_6): δ 65.29 (d, $_J$ = 10.7 Hz, 1 F), -101.87 (d, *J* = 10.7 Hz, 1 F). MS: Calc. for $[M+H]^+$ m/z 472.4; Obs. 472.4. HRMS calculated for $[C_{17}H_{15}F_2N_5O7S+H]^+$: 472.0733; found: 472.0746.

5'-*O*-(3-(Fluorosulfonyl)-4-methylbenzoyl)adenosine (CH_3-m-FSBA, 19g): Isolated as the trifluoroacetate salt in 8% yield as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.55 (s, 1 H), 8.41 (d, *J* = 1.6 Hz, 1 H), 8.31 (s, 1 H), 8.26 (d, *J* = 8.0 Hz, 1 H), 7.79 (d, *J* = 7.9 Hz, 1 H), 5.97 (d, *J* = 4.4 Hz, 1 H), 4.69 (t, *J* = 5.0 Hz, 1 H), 4.66 (dd, *J* = 12.0, 3.5 Hz, 1 H), 4.53 (dd, *J* = 12.0, 6.0 Hz, 1 H), 4.40 (t, *J* = 5.2 Hz, 1 H), 4.27 (br dd, *J* = 9.1, 5.4 Hz, 1 H), 2.69 (s, 3 H). ^{13}C NMR (125 MHz, DMSO-d_6): δ 163.6, 158.7 (q, *J* = 34.8 Hz), 152.2, 148.5, 147.6, 143.9, 141.8, 136.3, 134.2, 131.6, 131.4, 130.2, 128.5, 119.0, 117.3, 114.9, 88.4, 81.6, 73.1, 70.1, 65.1, 19.8. ^{19}F NMR (470 MHz, DMSO-d_6): δ 61.33 (s, 1 F), -74.50 (s, 3 F). MS: Calc. for $[M+H]^+$ m/z 468.1; Obs. 468.1. HRMS calculated for $[C_{18}H_{18}FN_5O_7S+H]^+$: 468.0984; found: 468.0997.

5'-*O*-(4-Ethyl-3-(fluorosulfonyl)benzoyl)adenosine (Et-m-FSBA, 19h): Isolated as the trifluoroacetate salt in 27% yield as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.55 (s, 1 H), 8.42 (d, *J* = 1.6 Hz, H), 8.26-8.35 (m, 2 H), 7.84 (d, *J* = 7.9 Hz, 1 H), 5.97 (d, *J* = 4.7 Hz,

1 H), 4.70 (t, *J* = Hz 1 H), 4.66 (dd, *J* = 12.0, 3.5 Hz, 1 H), 4.54 (dd, *J* = 12.0, 6.0 Hz, 1 H), 4.40 (t, *J* = 5.2 Hz, 1 H), 4.28 (br dd, *J* = 9.5, 5.4 Hz, 1 H), 3.04 (q, *J* = 7.6 Hz, 2 H), 1.26 (t, *J* = 7.6 Hz, 3 H). ^{13}C NMR (125 MHz, DMSO-d_6): δ ^{13}C NMR (DMSO-d_6) δ: 162.4, 157.6 (q, *J* = 34.8 Hz), 151.2, 148.6, 147.4, 146.5, 140.7, 135.3, 131.6, 129.9, 129.7, 129.3, 127.4, 117.9, 116.1, 113.8, 87.2, 80.5, 72.0, 69.0, 64.0, 24.7, 13.7. ^{19}F NMR (470 MHz, DMSO-d_6): δ 63.73 (s, 1 F), -74.52 (s, 3 F). MS: Calc. for $[M+H]^+$ m/z 482.1; Obs. 482.1. HRMS calculated for $[C_{19}H_{20}FN_5O_7S+H]^+$: 482.1140; found: 482.1152.

5'-*O*-(3-(Fluorosulfonyl)-4-isopropylbenzoyl)adenosine (^{i}Pr-m-FSBA, 19i): Isolated as the formate salt in 40% yield as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6): 8.43 (d, *J* = 1.6 Hz, 1 H), 8.27-8.34 (m, 2 H), 8.01 (s, 1 H), 7.97 (d, *J* = 8.2 Hz, 1 H), 7.29 (s, 2 H), 5.92 (d, *J* = 4.7 Hz, 1 H), 5.59 (br d, *J* = 5.7 Hz, 1 H), 5.43 (br d, *J* = 5.0 Hz, 1 H), 4.77 (br d, *J* = 5.0 Hz, 1 H), 4.66 (dd, *J* = 11.8, 3.6 Hz, 1 H), 4.52 (dd, *J* = 12.0, 6.0 Hz, 1 H), 4.43 (br d, *J* = 4.7 Hz, 1 H), 4.17-4.29 (m, 1 H), 3.56-3.65 (septet, *J* = 6.9 Hz, 1H), 1.29 (d, *J* = 6.9 Hz, 6 H). ^{13}C NMR (125 MHz, DMSO-d_6): δ 163.5, 156.0, 154.4, 152.5, 149.2, 140.1, 136.5, 130.6, 130.4, 130.2, 130.0, 128.5, 119.2, 88.1, 81.3, 72.6, 70.2, 65.2, 30.1, 23.2. ^{19}F NMR (470 MHz, DMSO-d_6): δ 64.00 (s, 1 F). MS: Calc. for $[M+H]^+$ m/z 496.1; Obs. 496.1. HRMS calculated for $[C_{20}H_{22}FN_5O_7S+H]^+$: 496.1297; found: 496.1309.

5'-*O*-(3-(Fluorosulfonyl)-4-methoxybenzoyl)adenosine (OCH_3-m-FSBA, 19j): Isolated as the trifluoroacetate salt in 27% yield as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.68 (s, 1 H), 8.44-8.51 (m, 2 H), 7.68 (d, *J* = 9.5 Hz, 1 H), 6.11 (d, *J* = 4.7 Hz, 1 H), 4.83 (t, *J* = 4.7 Hz, 1 H), 4.77 (dd, *J* = 12.0, 3.5 Hz, 1 H), 4.65 (dd, *J* = 12.1, 6.1 Hz, 1 H), 4.53 (t, *J* = 5.2 Hz, 1 H), 4.40 (br dd, *J* = 9.5, 5.7 Hz, 1 H), 4.23 (s, 3 H), 2.98 (br s, 1H). ^{13}C NMR (125 MHz, DMSO-d_6): δ 162.3, 159.9, 157.5 (q, *J* = 35.1 Hz), 151.2, 147.4, 146.5, 140.6, 138.0, 130.6, 120.8, 118.8, 118.6, 117.9, 116.1, 113.8, 113.5, 87.2, 80.5, 72.0, 69.0, 63.8, 56.7. ^{19}F NMR

(470 MHz, DMSO-d_6): δ 59.34 (s, 1 F), -74.49 (s, 3 F). MS: Calc. for $[M+H]^+$ m/z 484.1; Obs. 484.1. HRMS calculated for $[C_{18}H_{19}FN_5O_8S+H]^+$: 484.0933; found: 484.0941.

5'-*O*-(4-((Fluorosulfonyl)oxy)benzoyl)adenosine (20): Isolated as the trifluoroacetate salt in 25% yield as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.40 (s, 1 H), 8.15 (s, 1 H), 8.12 (d, *J* = 8.8 Hz, 1H), 7.55 (app d, *J* = 8.8 Hz, 3 H), 5.93 (d, *J* = 4.7 Hz, 1 H), 4.75 (t, *J* = 5.0 Hz, 1 H), 4.68 (dd, *J* = 12.0, 3.5 Hz, 1 H), 4.48 (dd, *J* = 12.0, 5.8 Hz, 1 H), 4.41 (t, *J* = 5.0 Hz, 1 H), 4.23 (br dd, *J* = 8.8, 5.0 Hz, 1 H). ^{13}C NMR (150 MHz, DMSO-d_6): δ 164.2, 157 .9 (q, *J* = 33.0 Hz), 152.5, 149.0, 140.7, 132.0 (2 C), 130.2, 121.7 (2 C), 119.1, 117.9, 115.5, 88.1, 81.5, 72.9, 70.1, 64.8. ^{19}F NMR (471 MHz, DMSO-d_6): δ 39.74 (s, 1 F), -73.96 (s, 3 F). MS: Calc. for $[M+H]^+$ m/z 470.1; Obs. 470.1. HRMS calculated for $[C_{17}H_{16}FN_5O_8S+H]^+$: 470.0776; found: 470.0788.

5'-*O*-(3-((Fluorosulfonyl)oxy)benzoyl)adenosine (21): Isolated as the trifluoroacetate salt in 28% yield as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.61 (s, 1 H), 8.29 (s, 1 H), 8.07 (s, 1H), 7.94 (d, *J* = 7.9 Hz, 1 H), 7.75 (app t, *J* = 7.9 Hz, 1 H), 5.97 (d, *J* = 3.8 Hz, 1 H), 4.59 – 4.73 (m, 2 H), 4.52 (dd, *J* = 11.8, 5.8 Hz, 1 H), 4.40 (br s, 1 H), 4.27 (br s, 1 H). ^{13}C NMR (125 MHz, DMSO-d_6): δ 164.1, 158 .6 (q, *J* = 34.8 Hz), 152.6, 149.7, 148.8, 148.1, 141.8, 132.2, 131.8, 130.1, 126.4, 121.9, 119.2, 117.3, 114.9, 88.4, 81.8, 73.3, 70.3, 65.2. ^{19}F NMR (DMSO-d_6): δ 39.18 (s, 1 F), -74.54 (s, 3 F). MS: Calc. for $[M+H]^+$ m/z 470.1; Obs. 470.1. HRMS calculated for $[C_{17}H_{16}FN_5O_8S+H]^+$: 470.0776; found: 470.0789.

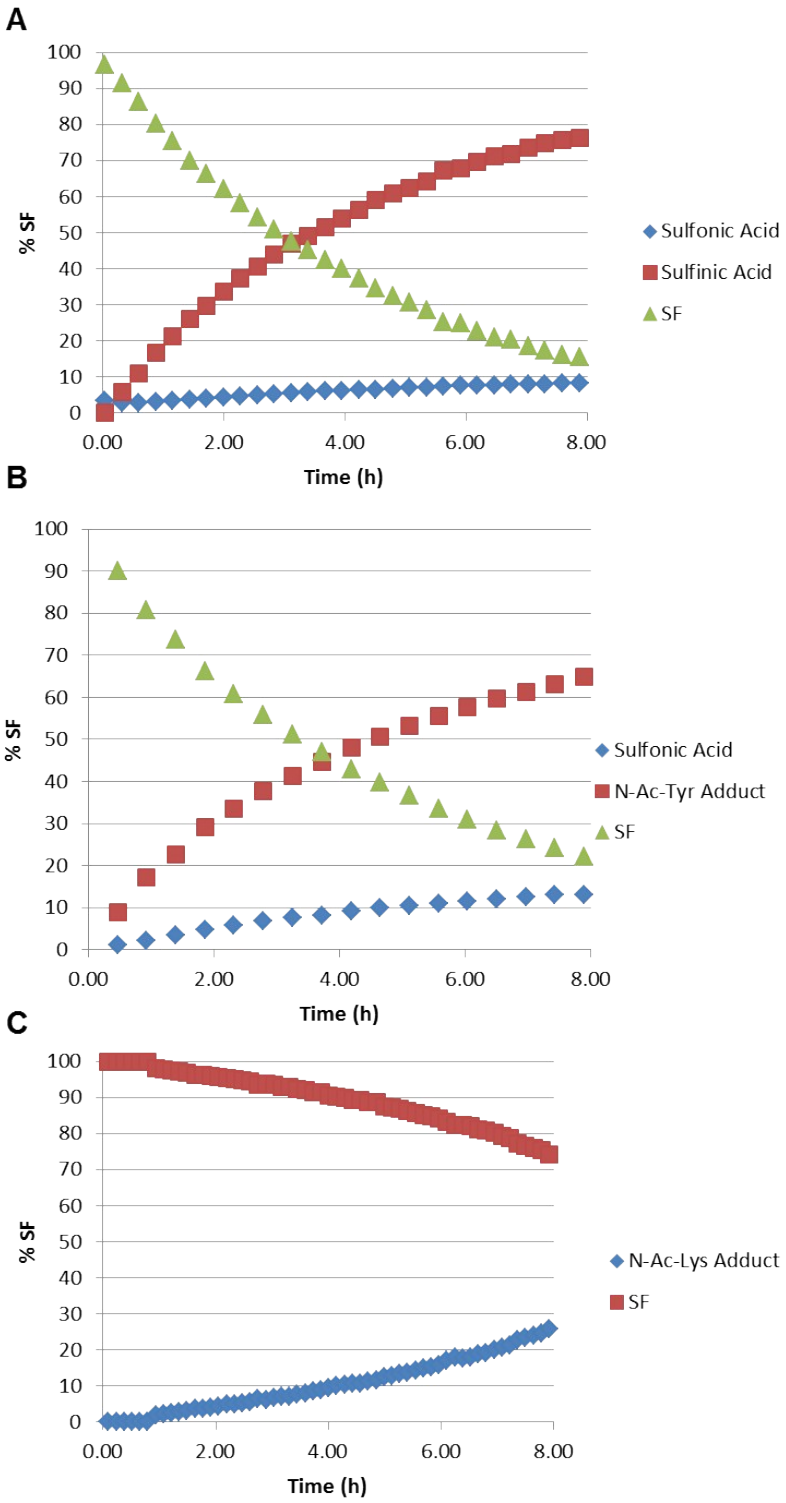

Figure S1. A. Plot depicting the progress of the reaction of sulfonyl fluoride **1a** with *N*-acetylcysteine (for experimental conditions, please refer to the text). Relative reaction rates were obtained by determining the slope of the sulfinic acid concentration (red squares) over time within the first 1 h of reaction; these rates were used to complete the Hammett analysis

reported in the text. B. Plot depicting the progress of the reaction of sulfonyl fluoride **1a** with N-acetyltyrosine. Relative reaction rates were obtained as in A, with the exception that in this case the initial adduct (red squares) could be directly observed. C. Plot depicting the progress of the reaction of sulfonyl fluoride **1m** with *N*-acetyllysine. Relative reaction rates were obtained as in A, with the exception that in this case the initial adduct (blue diamonds squares) could be directly observed. Note that in this case the hydrolysis product could not be observed by MS due to rapid elusion under LCMS conditions.

Effects of Buffer Concentration on Sulfonyl Fluoride Reactivity: In order to probe the effects of general acid/base catalysis on the reactivity of sulfonyl fluorides towards *N*-acetyltyrosine, we repeated the profiling experiments described above with varying buffer concentrations or identities. In all cases, the concentration of NaCl in the reaction mixture was modified to maintain a constant $[Na^+]$ = 1.18 M across all reactions. These experiments revealed that the reactivity of sulfonyl fluorides towards *N*-acetyltyrosine is susceptible to general acid/base catalysis, and thus both the concentration of reaction buffer and its identity influence the observed rates of reaction (**Figure S2**). Specifically, our data indicate that at our standard buffer concentration of 100 mM, buffer catalysis contributes ~40% of the observed reaction rate.

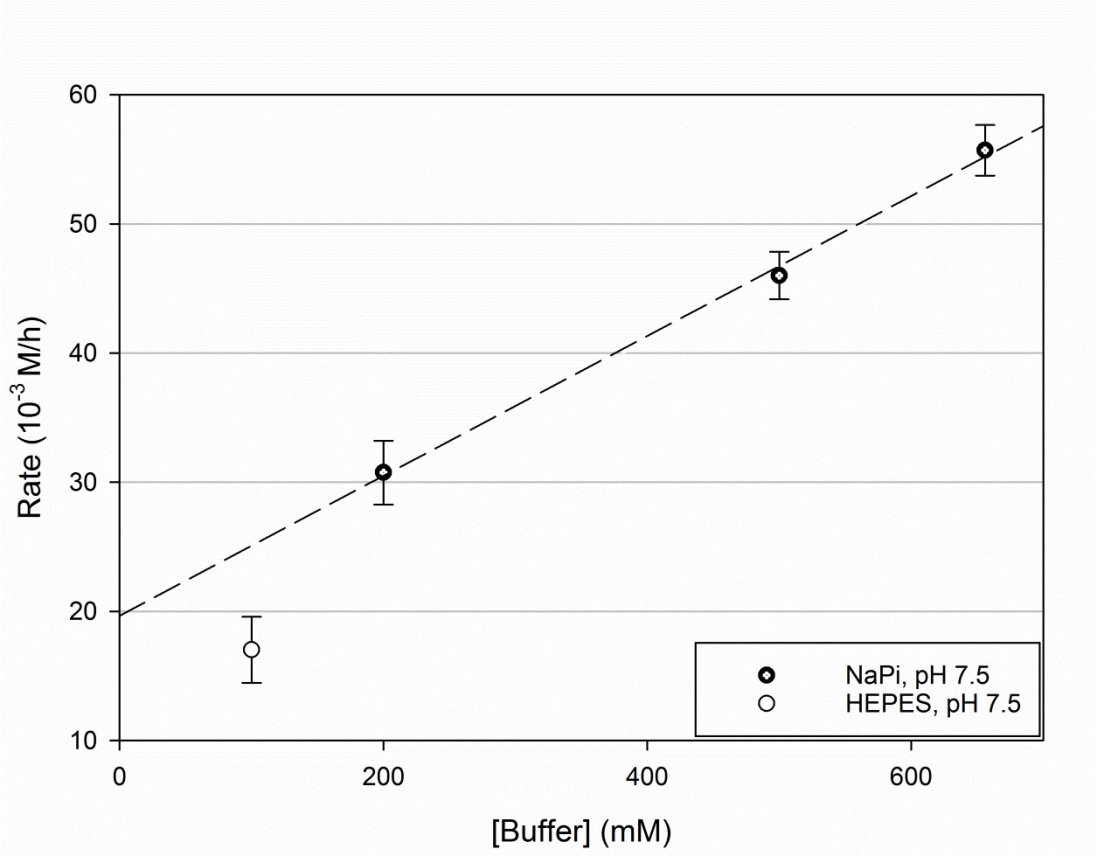

Figure S2. Effects of buffer identity and concentration on the rate of reaction of benzenesulfonyl fluoride (**1a**) with *N*-acetyltyrosine. The dashed line indicates the linear fit of the sodium phosphate buffer experiments extrapolated a buffer concentration of 0.

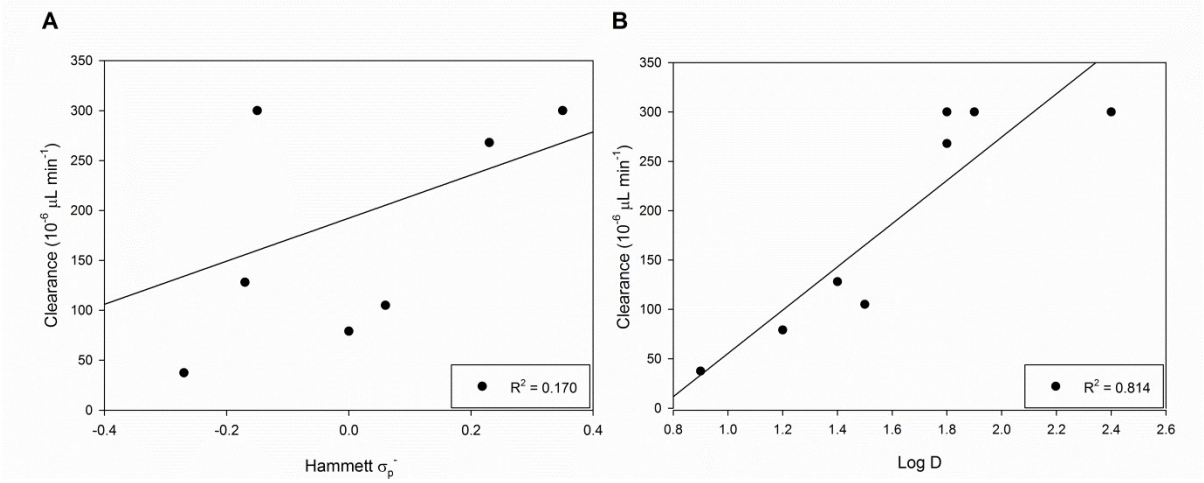

Figure S3. **A**. Relationship between metabolic clearance measured in rat hepatocytes and Hammett σ_p^- value for m-FSBA analogs **19b - i**. **B**. Relationship between metabolic clearance measured in rat hepatocytes and log D for m-FSBA analogs **19b - i**.

Preparation of the FGFR1 Construct for MS Analysis: Briefly, a TEV-FGFR1(468-765) gene was inserted into a pT7#3.3-6His vector. BL21 cells were transformed with the vector, then the cells were treated with IPTG (0.1 mM) for 24 h to induce protein synthesis. The cells were then pelleted and resuspended in lysis buffer (20 mM Tris-HCl, pH 7.8; 10 mM imidazole; 300 mM NaCl; 2 mM TCEP; 0.02% benzonase; 1 x EDTA-free protease cocktail (Roche)). The cells were homogenized using a ConstantSystems Z Plus Series 11 kW Cell Disrupted (25 kpsi, 30 s) and the resulting lysates were pelleted by centrifugation (23 500 x *g*, 45 min). The supernants were removed and filtered through a 0.45 μm membrane to afford the clarified lysate. The clarified lysate was loaded onto a Ni-NTA column that was pre-equilibrated with > 10 column volumes of wash buffer (20 mM Tris-HCl, pH 7.8; 10 mM imidazole; 300 mM NaCl; 2 mM TCEP); the column was then washed with > 5 column volumes of wash buffer. The target protein was eluted with > 2 column volumes elution buffer (20 mM Tris-HCl, pH 7.8; 250 mM imidazole; 300 mM NaCl). Fractions were analyzed for purity by SDS-PAGE; fractions containing the FGFR1 construct were pooled and concentrated usig a size exclusion spin column. The concentrated protein sample was exchanged into reaction buffer (20 mM Tris, pH 7.5; 150 mM NaCl; 2 mM TCEP) using a gel filtration column (HiPrep Sephacryl S-200). Protein concentrations were estimated by UV absorbance at 280 nm; purity was assessed by LC-MS and SDS-PAGE and was typically > 95%.

Structure Determination of the FGFR1-m-FSBA Covalent Complex

X-ray diffraction data were collected at cryogenic temperatures (100 K) at the Diamond Light Source beamiles I03 (**19a**) and I04-1 (**19h**). Data were processed using the progams XDS[24] and Aimless.[25] The structures were solved using molecular replacement as implemented in Phaser,[26] using in-house structures as search models. The models were built manually with Coot[27] and refined with BUSTER.[28] Data collection and processing statistics are summarised in Table S1.

	19a	19h
PDB accession code		
Data collection		
Space group	C2	C2
Cell dimensions		
a, *b*, *c* (Å)	209.55, 57.59, 65.52	211.14, 57.27, 66.80
β (°)	107.64	107.57
Resolution (Å)	1.91-49.92 (1.91-1.96)	2.01-63.68 (2.06-2.01)
Number of reflections	183275 (11705)	167464 (12626)
Number of unique reflections	57008 (4147)	50255 (3721)
R_{merge}	0.036 (0.735)	0.030 (0.858)
CC(1/2)	0.998 (0.548)	0.999 (0.683)
$I / \sigma I$	13.9 (1.5)	15.1 (1.4)
Completeness (%)	98.2 (97.8)	98.9 (99.7)
Redundancy	3.2 (2.8)	3.3 (3.4)
Refinement		
Resolution (Å)	1.91-49.92 (1.91-1.96)	2.01-63.68 (2.01-2.06)
No. reflections	57050 (4138)	14863 (868)
R_{work} / R_{free}	0.200/0.220	0.217/0.225
No. atoms		
Protein	4308	4428
Heteroatoms	75	86
Solvent	131	190
B-factors		
Protein	53.73	62.35
Heteroatoms	60.29	89.98
Water	67.59	83.62
R.m.s. deviations		
Bond lengths (Å)	0.018	0.011
Bond angles (°)	1.540	1.260

Table S1. X-ray crystallography data collection and refinement statistics. Values in parentheses are for highest-resolution shell.

Appendix I: Tabulated Second Order Rate Data

#	R	σ^-	Relative Rate (Tyrosine)	Second Order Rate Constant (Tyrosine) $M^{-1}\ h^{-1}$	Relative Rate (Hydrolysis)	Second Order Rate Constant (Hydrolysis) $M^{-1}\ h^{-1}$	Ratio (Tyrosine/hydrolysis)
1a	H	0.00	**1.00**[a]	**164**	**1.00**[a]	**0.044**	**3727**
1b	4-NO_2	0.78	10.6 ± 1.7	1738.4 ± 278.8	9.5 ± 0.7	0.418 ± 0.0308	4158.9
1c	4-OCF_3	0.35	1.6 ± 0.3	262.4 ± 49.2	3.3 ± 0.8	0.145 ± 0.035	1807.2
1d	4-OCH_3	-0.27	0.11 ± 0.01	18.04 ± 1.64	0.28 ± 0.03	0.0123 ± 0.001	1464.3
1e	4-NH_2	-0.66	0.08 ± 0.01	13.12 ± 1.64	0.10 ± 0.04	0.004 ± 0.0017	2981.8
1f	4-CN	0.66	8.7 ± 1.9	1426.8 ± 311.6	7.7 ± 1.1	0.339 ± 0.048	4211.3
1g	4-CF_3	0.54	6.3 ± 0.7	1033.2 ± 114.8	5.0 ± 1.2	0.220 ± 0.053	4696.4
1h	4-$CONH_2$	0.36	2.0 ± 0.4	328 ± 65.6	5.8 ± 2.5	0.255 ± 0.11	1285.3
1i	4-$NHCOCF_3$	0.12	1.3 ± 0.3	213.2 ± 49.2	2.7 ± 0.7	0.119 ± 0.031	1794.6
1j	4-F	0.06	ND[c]		ND[c]		-
1k	4-CO_2H	0.00[b]	0.94 ± 0.04	154.16 ± 6.56	0.92 ± 0.12	0.041 ± 0.005	3808.3
1l	4-$NHCOCH_3$	-0.15	0.36 ± 0.05	59.04 ± 8.2	0.42 ± 0.06	0.018 ± 0.003	3194.8
1m	4-CH_3	-0.17	0.35 ± 0.03	57.4 ± 4.92	0.57 ± 0.23	0.025 ± 0.010	2288.7
1n	4-$NHCONH_2$	-0.24	0.20 ± 0.06	32.8 ± 9.84	0.26 ± 0.08	0.011 ± 0.003	2867.1
1o	4-$N(CH_3)_2$	-0.83	ND[c]		ND[c]		-
2a	3-OCH_3	0.12	1.1 ± 0.03	180.4 ± 4.92	2.3 ± 0.4	0.101 ± 0.017	1782.6
2b	3-CO_2H	-0.10[b]	0.72 ± 0.14	118.08 ± 22.96	0.88 ± 0.10	0.0387 ± 0.004	3049.6
3a	2-NO_2	0.78	4.4 ± 1.0	721.6 ± 164	5.6 ± 1.1	0.246 ± 0.048	2928.6
3b	2-CN	0.66	11.6 ± 7.0	1902.4 ± 1148	13.5 ± 3.0	0.594 ± 0.132	3202.7
3c	2-CF_3	0.54	2.8 ± 0.4	459.2 ± 65.6	3.8 ± 0.5	0.167 ± 0.022	2746.4
3d	2-OCF_3	0.35	2.2 ± 0.4	360.8 ± 65.6	3.3 ± 0.9	0.145 ± 0.040	2484.8
3e	2-CH_3	-0.17	0.47 ± 0.03	77.08 ± 4.92	0.77 ± 0.20	0.033 ± 0.009	2275.1
3f	2-OCH_3	-0.27	0.12 ± 0.02	19.68 ± 3.28	0.14 ± 0.06	0.00616 ± 0.003	3194.8

[a]: By definition.
[b]: Hammett value for the CO_2^- group since the acid was assumed to be fully deprotonated at pH 7.5.
[c]: The solubilities of **1f** and **1o** were too low to obtain rate data under our assay conditions.

Table S2: Relative rate data for the modification of *N*-acetyltyrosine by arylsulfonyl fluorides **1a – 3f**. Reactions were performed at pH 7.5 and 37 °C; all rates are relative to that of sulfonyl fluoride **1a**.

N-Ac-Cys	pH 5.0	pH 7.5	pH 10.0
1a	ND[a]	310	ND[b]
1b	241.8	ND[b]	ND[b]
1c	18.6	384.4	ND[b]
1d	ND[a]	68.2	ND[b]
1e	ND[a]	ND[a]	ND[b]
N-Ac-Tyr			
1a	ND[a]	164	ND[b]
1b	67.24	2853.6	ND[b]
1c	13.12	264.04	ND[b]
1d	ND[a]	32.8	1412.04
1e	ND[a]	13.12	644.52
N-Ac-Lys			
1a	ND[a]	61	ND[b]
1b	5.49	381.25	ND[b]
1c	ND[a]	89.67	ND[b]
1d	ND[a]	9.15	1427.4
1e	ND[a]	2.44	495.32

ND = Not determined

[a]: Complete loss of SF within 1 h.

[b]: Less than 1% loss of SF within 1h.

Table S3. Effects of pH on the second-order rate constants of modification of *N*-acetylcysteine, *N*-acetyltyrosine, and *N*-acetyllysine by sulfonyl fluorides **1a – e**. All reactions were performed at 37 °C; data represent the average of three experiments.

Rate (M^{-1} h^{-1})[a]	pH 5.0	pH 7.5	pH 10.0
1a	0.0012 (0.40)[b]	0.029 (**1.0**)	(>100)[c]
1b	0.070 (2.4)	0.27 (9.4)	(>100)[c]
1c	0.026 (0.88)	0.096 (3.3)	(>100)[c]
1d	(<0.01)[d]	0.0081 (0.28)	0.19 (6.4)
1e	(<0.01)[d]	0.0029 (0.10)	0.058 (2.1)

[a]: Second order rate constants for reactions conducted at 37 °C.

[b]: Values in parentheses indicate rates relative to the rate of hydrolysis of **1a** at pH 7.5.

[c]: Corresponds to complete loss of SF within 1 h.

[d]: Corresponds to less than 1% loss of SF within 1h.

Table S4. Effects of pH on hydrolytic stability of **1a** – **1e**. All reactions were performed at 37 °C; data represent the average of three experiments.

#	R	Second Order Rate Constant (M^{-1} h^{-1}, Tyrosine)	Second Order Rate Constant (M^{-1} h^{-1}, Hydrolysis)	Ratio (Tyrosine/ hydrolysis)
1a	Ph-	164	0.044	3727.27
4	PhCHCH-	18.04	0.0035	5125.28
5	$PhCH_2$-	-[a]	0.426	NA
6	$PhCH_2CH_2$-	-[a]	0.033	NA
7	p-(CO_2H)PhO-	ND[b]	ND[b]	NA
8	m-(CO_2H)PhO-	ND[b]	ND[b]	NA

ND = Not determined

[a]: Adduct not observed.

[b]: Less than 1% loss of SF within 1h.

Table S5. Relative rates of modification of *N*-acetyltyrosine by vinylsulfonyl fluoride **4**, alkylsulfonyl fluorides **5** and **6**, and arylfluorosulfonates 7 and **8**. All reactions were performed at pH 7.5 and at 37 °C; data represent the average of three experiments.

#	=*N*-**R**	**Second Order Rate Constant (M^{-1} h^{-1}, Tyrosine)**	**Second Order Rate Constant (M^{-1} h^{-1}, Hydrolysis)**	**Ratio (Tyrosine/ hydrolysis)**
1a	-	164	0.044	3727.27
9a	Ac	410	0.0804	5148.17
9b	Piv	200.08	0.004	41338.84
9c	Boc	160.72	0.017	9365.97
9d	4-CF_3Ph	8.2	0.003	2662.34
9e	Ph	-[b]	0.290	-[b]
9f	4-CH_3Ph	-[b]	0.233	-[b]
9g	CH_3	-[b]	<0.03	-[b]
9h	*t*-Bu	-[b]	<0.03	-[b]

[a]: By definition.

[b]: Adduct not observed.

Table S6. Relative rates of modification of *N*-acetyltyrosine by *N*-substituted benzenesulfonimidoyl fluorides. All reactions were performed at pH 7.5 and at 37 °C; data represent the average of three experiments.

Supporting References

[1] Cee, V. J.; Volak, L. P.; Chen, Y.; Bartberger, M. D.; Tegley, C.; Arvedson, T.; McCarter, J.; Tasker, A. S.; Fotsch, C. *J. Med. Chem.* **2015**, *58*, 9171–9178.
[2] Meanwell, M.; Nodwell, M. B.; Martin, R. E.; Britton, R. *Angew. Chem., Int. Edition*, **2016**, *55*, 13244-13248.
[3] Barrow, A. S.; Moses, J. E. *Synlett*. **2016**, *27*, 1840-1843
[4] Faming, Z. S. **2015**, *CN* 105198683 A 20151230.
[5] Tribby, A. L.; Rodriguez, I.; Shariffudin, S.; Ball, N. D. *J. Org. Chem*. **2017**, *82*, 2294-2299
[6] Li, S.; Wu, P.; Moses, J. E.; Sharpless, K. B. *Angew. Chem., Int. Ed.* **2017**, *56,* 2903-2908
[7] Yoshimura, T., Barker, L. N., Powers, J. C. *J. Biol. Chem.* **1982**, *257*, 5077–5084.
[8] Guo, S.; Cong, F.; Guo, R.; Wang, L.; Tang, P. *Nat. Chem*. **2017**, *9*, 546-551.
[9] Jorg, M.; Glukhova, A.; Abdul-Ridha, A.; Vecchio, E. A.; Nguyen, A. T. N.; Sexton, P. M.; White, P. J.; May, L. T.; Christopoulos, A.; Scammells, P. J. *J. Med. Chem.* **2016**, *59*, 11182-11194.
[10] Santiago, C. B.; Milo, A.; Sigman, M. S. *J. Am. Chem. Soc.* **2016**, *138*, 13424-13430
[11] Dong, J.; Sharpless, K. B. *PCT Int. Appl.* **2015**, WO 2015188120 A1 20151210
[12] Lindner, E., Weber, H. *Chem. Ber.* **1968**, *101*, 2832–2836.
[13] Baranczak, A.; Liu, Y.; Connelly, S.; Du, W-G. H.; Greiner, E. R.; Genereux, J. C.; Wiseman, R. L.; Eisele, Y. S.; Bradbury, N. C.; Dong, J.; Noodleman, L.; Sharpless, K. B.; Wilson, I. A.; Encalada, S. E.; Kelley, J. W. *J. Am. Chem. Soc.* **2015**, *137*, 7404–7414.
[14] Harpp, D. N.; Mullins, D. F.; Steliou, K.; Triassi, I. *J. Org. Chem.* **1979**, *44*, 4196–4197.
[15] Gaillard, S.; Papamicaël, C.; Dupas, G.; Marsais, F.; Levacher, V. *Tetrahedron.* **2005**, *61*, 8138–8147.
[16] Maldonado, M. F.; Sehgelmeble, F.; Bjarnemark, F.; Svensson, M.; Åhman, J.; Arvidsson, P. I. *Tetrahedron*. **2012**, *68*, 7456–7462.
[17] Reves, M.; Achard, T.; Sola, J.; Riera, A.; Verdaguer, X. *J. Org. Chem.* **2008**, *73*, 7080-7087.
[18] Clarke, V.; Cole, E. *Phosphorus, Sulfur and Silicon and the Related Elements*, **1989**, *45*, 243-8.
[19] Piggot, A. M.; Karuso, P. *Tet. Lett.* **2007**, *48*, 7452–7455.
[20] Harmata, M.; Zheng, P.; Huang, C.; Gomes, M. G.; Ying, W.; Ranyanil, K.-O.; Balan, G.; Calkins, N. L. *J. Org. Chem.* **2007**, *72*, 683–685.
[21] In some cases, the intermediate sulfonimidoyl chloride completely hydrolyzed to the corresponding sulfonamide during the LC-MS run. The product sulfonimidoyl fluorides, however, were stable towards LC-MS analysis under acidic conditions.
[22] Johnson, C. R.; Bis, K. G.; Cantillo, J. H.; Meanwell, N. A.; Reinhard, M. F. D.; Zeller, J. R.; Vonk, G. P. *J. Org. Chem.* **1983**, *48*, 1-3.
[23] Hsu, Y.-L.; Yang, C.-C.; Lan, C.-Y.; Lin, J.-J.; Lo, L.-C.; *J. Chin. Chem. Soc.*, **2013**, *60*, 846–854.
[24] Kabsch, W. *Acta Cryst.* **2010**, *D66*, 125–132.
[25] Evans, P.R.; Murshudov, G.N. *Acta Cryst.* **2013**, *D69*, 1204–1214.
[26] McCoy, A. J.; Grosse-Kunstleve, R. W.; Adams, P. D.; Winn, M. D.; Storoni, L. C.; Read, R. J. *J. Appl. Cryst.* **2007**, *40*, 658–674.
[27] Emsley, P.; Lohkamp, P.; Scott, W.; Cowtan, K. *Acta Cryst.* **2010**, *D66*, 486–501.
[28] Bricogne, G.; Blanc, E.; Brandl, M.; Flensburg, C.; Keller, P.; Paciorek, W.; Roversi, P.; Sharff, A.; Smart, O. S.; Vonrhein, C. BUSTER v. 2.11.6. Global Phasing Ltd., Cambridge, United Kingdom.