Supporting Information

for

“Ruthenium(II) Porphyrin Catalyzed Amidation of Aromatic Heterocycles”

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General Experimental Section: All reactions were performed under a nitrogen atmosphere. $[\text{Ru}^{\text{II}}(\text{TTP})(\text{CO})]$ and $[\text{Ru}^{\text{II}}(\text{F}_{20}\text{-TPP})(\text{CO})]$ were prepared according to known literature procedures.^{S1} Unless specified, all reagents and starting materials were purchased from commercial sources and used as received. 4 Å Molecular sieves were dried at 300°C and cooled under reduced pressure prior to use. Solvents were purified following standard literature procedures.^{S2} ^1H and ^{13}C NMR spectra were measured at 400, 300, 100 and 75 MHz, respectively, with tetramethylsilane (TMS) as the internal standard and with chemical shifts (ppm) recorded relative to TMS. Mass spectra {including fast atom bombardment mass spectra (FAB)} were determined at an ionizing voltage of 20eV on a Finnigan MAT 95 mass spectrometer. UV-visible spectra (UV/vis) were recorded on a Hewlett-Packard HP8452A Diode Array spectrophotometer interfaced with IBM compatible PC or Perkin Elmer Lambda 19 spectrophotometer. Elemental analyses were carried out by the Institute of Chemistry, the Chinese Academy of Sciences (Beijing, P. R. China).

Typical Procedure for the Preparation of *N*-Alkyl and Aryl Substituted Pyrroles. Pyrrole (1 equiv), R-I (R = Me, C₆H₅, *o*-MeC₆H₄, *p*-MeC₆H₄, *p*-MeOC₆H₄, *p*-FC₆H₄, *p*-NO₂C₆H₄) (1 equiv), $^t\text{Bu}_4\text{NBr}$ (0.1 equiv), CuI (0.1 equiv) and K₂CO₃ (3 equiv) were reflux at 140°C in 10 mL of degassed toluene under an Ar atmosphere for 7 h. After cooling, the reaction mixture was diluted with a solution of NH₄Cl (sat.) followed by extraction with 150 mL of diethyl ether. The organic layer was concentrated to 2 mL and purification by column chromatography on silica gel (*n*-hexane as eluent) gave the title product. NMR spectra of corresponding arylated pyrroles obtained were consistent with literature data.^{S3}

Typical Procedure for Direct Amidation of Unfunctionalized Heteroarenes with $\text{PhI}=\text{NR}$ (R = Ts, Ns). To a dry Schlenk flask under an Ar atmosphere was added the heteroarene (1 equiv), $\text{PhI}=\text{NR}$ (1.5-5 equiv), catalyst (2-10 mol%), 4 Å molecular sieves (amount used equivalent by mass to amount of $\text{PhI}=\text{NTs}$) and CH₂Cl₂ (10 mL). The reaction mixture was placed in a sonicating bath at 40°C for 2 h. On cooling to room temperature, the mixture was filtered, concentrated *in situ* and purified by silica gel column chromatography (petroleum ether/EtOAc as eluent) to give the title compounds.

***N,N*-Di(toluenep-sulfonyl)-(furan-2-yl)-amine 1.** ^1H NMR (400 MHz, CD_3CN): δ 7.70 (d, 4H, $J = 8.4$ Hz), 7.51-7.50 (m, 1H), 7.43 (d, 4H, $J = 8.6$ Hz), 6.54-6.52 (m, 1H), 6.33-6.31 (m, 1H), 2.46 (s, 6H); ^{13}C NMR (75 MHz, CD_3CN): δ 146.8, 144.0, 130.0, 128.3, 128.2, 112.6, 112.1, 21.0; HRMS (EI): m/z calcd. for $\text{C}_{18}\text{H}_{17}\text{NO}_5\text{S}_2$: 391.0548, found: 391.0544.

***N,N*-Di(nitrobenzene-*p*-sulfonyl)-(furan-2-yl)-amine 2.** ^1H NMR (300 MHz, CDCl_3): δ 8.45 (d, 4H, $J = 8.9$ Hz), 8.23 (d, 4H, $J = 8.9$ Hz), 7.48-7.47 (m, 1H), 6.52-6.51 (m, 1H), 6.30-6.29 (m, 1H); ^{13}C NMR (75 MHz, CDCl_3): δ 150.0, 145.0, 130.5, 124.9, 116.0, 112.7; HRMS (EI): m/z calcd. for $\text{C}_{16}\text{H}_{11}\text{N}_3\text{O}_9\text{S}_2$: 452.9937, found: 452.9940.

5-(*N,N*-Di(toluenep-sulfonyl)amino)-furan-2-carboxylic acid methyl ester 3. ^1H NMR (400 MHz, CDCl_3): δ 7.91 (d, 2H, $J = 8.4$ Hz), 7.39 (d, 2H, $J = 8.1$ Hz), 7.18 (d, 1H, $J = 3.5$ Hz), 6.30 (d, 1H, $J = 3.5$ Hz), 3.90 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3): δ 158.7, 146.0, 136.0, 130.0, 129.2, 129.1, 119.0, 113.9, 52.5, 22.0; HRMS (EI): m/z calcd. for $\text{C}_{20}\text{H}_{19}\text{NO}_7\text{S}_2$: 449.0603, found: 449.0598.

***N,N*-Di(toluenep-sulfonyl)-(benzofuran-2-yl)-amine 4.** ^1H NMR (400 MHz, CDCl_3): δ 7.95 (d, 4H, $J = 8.4$ Hz), 7.58 (d, 1H, $J = 0.4$ Hz), 7.49 (d, 1H, $J = 0.7$ Hz), 7.40 (d, 4H, $J = 8.1$ Hz), 7.30-7.27 (m, 2H), 6.59 (s, 1H), 2.51 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3): δ 153.7, 145.5, 141.9, 136.0, 129.7, 128.8, 127.3, 126.1, 123.3, 121.8, 111.8, 108.8, 21.8; HRMS (EI): m/z calcd. for $\text{C}_{22}\text{H}_{19}\text{NO}_5\text{S}_2$: 441.0705, found: 441.0694.

4-Methyl-*N*-[1-(toluenep-sulfonyl)-1*H*-indol-2-yl]-benzenesulfonamide 5a and 4-Methyl-*N*-[1-(toluenep-sulfonyl)-1*H*-indol-3-yl]-benzenesulfonamide 5b. ^1H NMR (400 MHz, CDCl_3): δ 7.94 (d, 1H, $J = 7.1$ Hz), 7.76 (d, 1H, $J = 7.2$ Hz), 7.58-7.07 (m, 9H), 6.93-6.66 (m, 3H), 4.14 (d, 1H, $J = 6.9$ Hz), 2.44 (s, 3H, **5a** or **5b**); ^{13}C -NMR (75 MHz, CD_2Cl_2): δ 136.5, 130.2, 130.0, 129.9, 128.7, 128.3, 128.0, 127.8, 123.9, 121.5, 121.3, 110.9, 21.7; MS (FAB): m/z 362 [M^+].

***N,N*-Di(toluenep-sulfonyl)-(thiophen-2-yl)-amine 6.** ^1H NMR (400 MHz, CD_3CN): δ 6.86 (d, 4H, $J = 8.2$ Hz), 6.63 (d, 1H, $J = 5.6$ Hz), 6.55 (d, 4H, $J = 8.1$ Hz), 6.10 (t, 1H, $J = 4.8$ Hz), 5.89 (d, 1H, $J = 3.6$ Hz), 1.28 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3): δ 145.7, 135.4, 131.2, 130.3, 129.6, 128.8, 128.4, 125.6, 116.8, 20.2; HRMS (EI): m/z calcd. for $\text{C}_{18}\text{H}_{17}\text{NO}_4\text{S}_3$: 407.0319, found: 407.0322.

***N,N*-Di(toluenep-sulfonyl)-(N-[1-(toluenep-sulfonyl)-1*H*-pyrrol-2-yl])-amine 7.** ^1H NMR (400 MHz, CDCl_3): δ 7.88 (d, 6H, $J = 8.4$ Hz), 7.39-7.28 (m, 6H), 7.22-7.20 (m, 1H), 6.25 (t, 1H, $J = 3.7$ Hz), 6.04-6.03 (m, 1H), 2.48 (s, 6H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 145.7, 145.6, 136.5, 135.9, 130.1, 130.0, 129.7, 128.9, 124.8, 123.0, 117.6, 111.0, 22.2, 22.1; HRMS (EI): m/z calcd. for $\text{C}_{25}\text{H}_{24}\text{N}_2\text{O}_6\text{S}_3$: 544.0797, found: 544.0809.

Zwitterion 8. Anal. calcd. for $\text{C}_{16}\text{H}_{15}\text{N}_3\text{O}_2\text{S}$: C 61.32, H 4.82, N 13.41, found C 61.07, H 4.83, N 13.28; ^1H NMR (300 MHz, $\text{DMSO}-d_6$): δ 9.41 (t, 1H, $J = 1.6$ Hz), 8.04 (t, 1H, $J = 2.0$ Hz), 7.72 (d, 2H, $J = 8.0$ Hz), 7.62-7.57 (m, 2H), 7.54-7.50 (m, 3H), 7.34 (t, 1H, $J = 1.7$ Hz), 7.24 (d, 2H, $J = 7.9$ Hz), 2.34 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3): δ 141.8, 140.4, 135.4, 133.1, 131.0, 130.5,

129.5, 127.6, 126.2, 122.3, 117.9, 21.8; HRMS (EI): m/z calcd. for $C_{16}H_{15}N_3O_2S$: 313.0885, found: 313.0880.

3,4-Di(toluene-*p*-sulfonamido)-1-methylpyrrole 9. 1H NMR (400 MHz, $CDCl_3$): δ 7.87 (s, 2H), 7.84 (d, 4H, $J = 8.2$ Hz), 7.33 (d, 4H, $J = 8.1$ Hz), 3.07 (s, 3H), 2.43 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 126.1, 144.4, 137.0, 129.7, 129.4, 127.3, 26.9, 21.7; HRMS (EI): m/z calcd. for $C_{19}H_{21}N_3S_2O_4$: 419.0973, found: 419.0885.

3,4-Di(toluene-*p*-sulfonamido)-1-phenylpyrrole 10. 1H NMR (400 MHz, CD_2Cl_2): δ 8.05 (s, 2H), 7.75 (d, 4H, $J = 8.4$ Hz), 7.45-7.43 (m, 3H), 7.34 (d, 4H, $J = 8.0$ Hz), 7.17-7.14 (m, 2H), 2.45 (s, 6H); ^{13}C NMR (75 MHz, DMSO- d_6): δ 130.1, 129.7, 129.4, 128.5, 127.4, 21.7; HRMS (EI): m/z calcd. for $C_{24}H_{23}N_3O_4S_2$: 481.1130, found: 481.0973.

3,4-Di(toluene-*p*-sulfonamido)-1-(2-methylphenyl)pyrrole 11. 1H NMR (400 MHz, $CDCl_3$): δ 8.03 (s, 2H), 7.69 (d, 4H, $J = 8.3$ Hz), 7.23-7.28 (m, 5H), 7.19-7.16 (m, 2H), 6.94 (d, 1H, $J = 8.1$ Hz), 2.39 (s, 6H), 1.89 (s, 3H); ^{13}C NMR (400 MHz, $(CD_3)_2CO$): δ 162.8, 144.3, 137.3, 136.5, 131.4, 130.6, 129.7, 129.6, 129.5, 129.2, 126.9, 126.6, 20.5, 16.6; HRMS (EI): m/z calcd. for $C_{25}H_{25}N_3O_4S_2$: 495.1287, found: 495.1280.

3,4-Di(toluene-*p*-sulfonamido)-1-(4-methylphenyl)pyrrole 12. Anal. calcd. for $C_{25}H_{25}N_3O_4S_2 \cdot 0.75CH_2Cl_2$: C 55.37, H 4.65, N 7.52, found C 55.54, H 4.40, N 8.01; 1H -NMR (300 MHz, CD_2Cl_2): δ 8.04 (s, 2H), 7.76 (d, 4H, $J = 8.1$ Hz), 7.35 (d, 4H, $J = 8.0$ Hz), 7.25 (d, 2H, $J = 8.2$ Hz), 7.03 (d, 2H, $J = 8.3$ Hz), 2.46 (s, 6H), 2.41 (s, 3H); ^{13}C NMR (75 MHz, CD_2Cl_2): δ 145.0, 139.8, 139.0, 130.1, 130.0, 129.7, 128.2, 127.4, 21.7, 21.3; HRMS (EI): m/z calcd. for $C_{25}H_{25}N_3O_4S_2$: 495.1286, found: 495.1206.

3,4-Di(toluene-*p*-sulfonamido)-1-(4-methoxyphenyl)pyrrole 13. Anal. calcd. for $C_{25}H_{25}N_3O_5S_2$: C 58.01, H, 5.06, N 8.12, found C 58.03, H 4.54, N 8.12; 1H NMR (300 MHz, $CDCl_3$): δ 7.99 (s, 2H), 7.73 (d, 4H, $J = 8.3$ Hz), 7.26 (d, 4H, $J = 8.1$ Hz), 7.00 (d, 2H, $J = 9.0$ Hz), 6.84 (d, 2H, $J = 9.0$ Hz), 3.79 (s, 3H), 2.40 (s, 6H); ^{13}C NMR (75 MHz, DMSO- d_6): 142.8, 130.8, 130.6, 130.2, 127.6, 126.5, 115.0, 56.2, 21.9, 21.7; HRMS (EI): m/z calcd. for $C_{25}H_{25}N_3O_5S_2$: 511.1236, found: 511.1075.

3,4-Di(toluene-*p*-sulfonamido)-1-(4-fluorophenyl)pyrrole 14. 1H NMR (500 MHz, DMF- d_7): δ 8.10 (s, 2H), 7.80 (d, 4H, $J = 8.1$ Hz), 7.39-7.50 (m, 6H), 7.28 (t, 2H, $J = 8.7$ Hz), 2.42 (s, 6H); ^{13}C NMR (125 MHz, DMF- d_7): 144.8, 137.9, 131.5, 131.4, 130.1, 129.9, 129.0, 128.9, 127.3, 126.9, 116.2, 116.1, 21.0; HRMS(FAB): m/z 499 [M^+].

3,4-Di(toluene-*p*-sulfonamido)-1-(4-nitrophenyl)pyrrole 15. 1H -NMR (300 MHz, CD_2Cl_2): δ 8.24 (d, 2H, $J = 9.1$ Hz), 8.09 (s, 2H), 7.75 (d, 4H, $J = 8.3$ Hz), 7.39-7.33 (m, 6H), 2.43 (s, 6H); ^{13}C -NMR (75 MHz, CD_2Cl_2): δ 161.7, 145.4, 137.4, 136.9, 130.2, 129.9, 129.4, 127.6, 124.5, 21.7; HRMS (EI): m/z calcd. for $C_{24}H_{22}N_4O_6S_2$: 526.0981, found: 526.0762.

Typical Procedure for the Direct Amidation of Unfunctionalized Heteroarenes with $PhI(OAc)_2$ and NH_2 Ns. To a dry Schlenk flask under an Ar atmosphere was added the heteroarene (1 equiv), $PhI(OAc)_2$ (1.5-10 equiv), NH_2 Ns (1-10 equiv), catalyst (1.5-10 mol%), 4

Å molecular sieves (amount used equivalent by mass to amount of $\text{PhI}(\text{OAc})_2$) and dichloroethane (10 mL). The reaction mixture was stirred at 65°C. On cooling to room temperature, the mixture was filtered, concentrated *in situ* and purified by silica gel column chromatography (petroleum ether/EtOAc as eluent) to give the title compounds.

***N,N*-Di(nitrobenzene-*p*-sulfonyl)-(methyl 2-furoate)-amine 16.** ^1H NMR (300 MHz, CD_2Cl_2): δ 8.48 (d, 4H, $J = 9.1$ Hz), 8.25 (d, 4H, $J = 9.1$ Hz), 7.24 (d, 1H, $J = 3.6$ Hz), 6.45 (d, 1H, $J = 3.6$ Hz), 3.92 (s, 3H); ^{13}C NMR (75 MHz, CD_2Cl_2): δ 145.5, 139.0, 137.6, 124.4, 118.7, 112.8, 108.6, 23.8; HRMS (EI): m/z calcd. for $\text{C}_{18}\text{H}_{13}\text{N}_3\text{O}_{11}\text{S}_2$: 510.9992, found: 510.9995.

***N*-Benzofuran-2-yl-4-nitro-benzenesulfonamide 17.** ^1H NMR (400 MHz, CD_3CN): δ 8.47 (d, 2H, $J = 9.0$ Hz), 8.25 (d, 2H, $J = 9.1$ Hz), 7.72 (d, 1H, $J = 0.2$ Hz), 7.56 (d, 1H, $J = 0.2$ Hz), 7.51 (t, 1H, $J = 0.2$ Hz), 7.35 (t, 1H, $J = 0.2$ Hz), 6.95 (s, 1H); ^{13}C NMR (75 MHz, CD_3CN): δ 146.5, 130.4, 126.9, 124.1, 122.5, 117.6, 109.2, 99.2; HRMS (EI): m/z calcd. for $\text{C}_{14}\text{H}_{10}\text{N}_2\text{O}_5\text{S}$: 318.0310, found: 318.0302.

***N,N*-Di(nitrobenzene-*p*-sulfonyl)-(thiophene-2-yl)-amine 18.** ^1H NMR (400 MHz, CDCl_3): δ 8.45 (d, 4H, $J = 9.0$ Hz), 8.16 (d, 4H, $J = 9.1$ Hz), 7.65-7.63 (m, 1H), 7.07-7.06 (m, 1H), 6.92-6.91 (m, 1H); ^{13}C NMR (75 MHz, CD_3CN): δ 152.0, 151.0, 142.0; 132.0, 131.3, 130.0, 126.0, 125.0; HRMS (EI): m/z calcd. for $\text{C}_{16}\text{H}_{11}\text{O}_8\text{N}_3\text{S}_3$: 468.9708, found: 468.9709.

Attempted Amidation with $[\text{Ru}^{\text{VI}}(\text{TMP})(\text{NR})_2]$ ($\text{R} = \text{Ts}, \text{Ns}$).^{S4} To a solution of furan or *N*-phenylpyrrole (50 equiv) in CH_2Cl_2 (1 mL) was added $[\text{Ru}^{\text{VI}}(\text{TMP})(\text{NNs})_2]$ (1 equiv) and 4Å molecular sieves. The mixture was stirred for 3 h under argon. After removal of the solvent *in vacuo*, a solution of *n*-pentane and Et_2O (5:1 v/v) was added, resulting in formation of a reddish brown precipitate. The precipitate was collected by filtration and washed with *n*-pentane followed by column chromatography on aluminium oxide using *n*-hexane: $\text{CH}_2\text{Cl}_2 = 1: 1$ to elute the leading yellow pale orange band followed by $\text{CH}_2\text{Cl}_2: \text{CH}_3\text{Cl} = 1: 1$ to collect the red or orange band. The product was recovered by re-crystallization from a solution of CH_2Cl_2 and *n*-hexane, filtered and washed with *n*-hexane. The organic filtrate was evaporated to dryness and subjected to ^1H and ^{13}C NMR spectroscopy and TLC analysis which indicated no reaction. Similarly, the same reaction conducted with pyrazole (2% v/v) under ultrasound for 45 min. gave no reaction. With the more stable $[\text{Ru}^{\text{VI}}(\text{TMP})(\text{NTs})_2]$ complex (1 equiv), with and without pyrazole (2% v/v) under ultrasound for 3 h, no reaction was also observed. The addition of radical initiator benzyl peroxide and oxidant $\text{PhI}(\text{OAc})_2$ {5 equiv} in place of pyrazole under similar conditions faired no better. In every instance, reduction of the $\text{Ru}(\text{VI})$ species (416 (Soret), 535 (β) and 565 (α) nm for $\text{R} = \text{Ns}$; 421 (Soret), 536 (β) and 566 (α) nm for $\text{R} = \text{Ts}$) to a $\text{Ru}(\text{IV})$ [405-411 (Soret) and 525-529 nm] was observed by UV/vis spectroscopy.

X-Ray Crystal Structure Determination of Compounds 1 and 8. X-Ray diffraction data were collected on a MAR diffractometer using graphite monochromatized $\text{Mo-K}\alpha$ radiation ($\lambda = 0.71073$ Å) at 253 K. The images were interpreted and the intensities integrated by using the program DENZO.^{S5} The structures were solved by direct methods by employing SHELXS-97^{S6} program on a PC computer. Structure refinements were performed by the full-matrix least squares using the software package SHELXL-97^{S7} on a PC computer. The structures of **1** and **8** were established by X-ray crystallography; the crystal data, bond distances and angles are listed

in Tables S1-S10, respectively. Figures S1-S2 depict the corresponding ORTEP drawings with the atom-numbering schemes.^{S8}

References:

- S1. (a) Adler, A. D.; Longo, F. R.; Finarelli, J. D.; Goldmacher, J.; Assour, J.; Korsakoff, L. *J. Org. Chem.* **1967**, 32, 476. (b) Rillema, D. P.; Nagle, J. K.; Barringer, L. F., Jr.; Meyer, T. J. *J. Am. Chem. Soc.* **1981**, 103, 56. (c) Li, Z.-Y.; Huang, J.-S.; Che, C.-M.; Chang, C.-K. *Inorg. Chem.* **1992**, 31, 2670. (d) Falvo, R. E.; Mink, L.M. *J. Chem. Educ.* **1999**, 76, 237.
- S2. Armarego, W. L. F.; Perrin, D. D. *Purification of Laboratory Chemicals*, 4th ed.; Butterworth-Heinemann: Bath, 2000.
- S3. Pouchert, C. J.; Behnke, J. *The Aldrich Library of ¹³C and ¹H FT NMR Spectra*, Ed. 1, 1993.
- S4. Unpublished results, please contact corresponding author for preparative procedure.
- S5. Otwinowski, Z. and Minor, W., "Processing of X-ray Diffraction Data Collected in Oscillation Mode", *Methods in Enzymology*, Volume 276: Macromolecular Crystallography, part A, p. 307-326, 1997. Carter C. W., Sweet Jr. & R. M., Eds., Academic Press.
- S6. SHELXS97, Sheldrick, G. M. (1997). SHELX97. Programs for Crystal Structure Analysis (Release 97-2). University of Goettingen, Germany.
- S7. SHELXL97, Sheldrick, G. M. (1997). SHELX97. Programs for Crystal Structure Analysis (Release 97-2). University of Goettingen, Germany.
- S8. CCDC 219719-219720 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html (or from the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033; e-mail: deposit@ccdc.cam.ac.uk).

Table S1. Crystal Data and Structure Refinement for **1**

Identification code	mar1020	
Empirical formula	C ₁₈ H ₁₇ NO ₅ S ₂	
Formula weight	391.45	
Temperature	253(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P –1(Nr. 2)	
Unit cell dimensions	a = 9.058(2) Å	α = 76.41(3)°.
	b = 9.751(2) Å	β = 86.49(3)°.
	c = 10.809(2) Å	γ = 80.15(3)°.
Volume	914.1(3) Å ³	
Z	2	
Density (calculated)	1.422 Mg/m ³	
Absorption coefficient	0.320 mm ⁻¹	
F(000)	408	
Crystal size	0.40 x 0.30 x 0.25 mm ³	
Theta range for data collection	1.94 to 25.35°.	
Index ranges	-10 ≤ h ≤ 10, -10 ≤ k ≤ 10, -13 ≤ l ≤ 12	
Reflections collected	4719	
Independent reflections	2834 [R(int) = 0.0259]	
Completeness to theta = 25.35°	84.6 %	
Absorption correction	None	
Max. and min. transmission	0.9242 and 0.8826	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	2834 / 0 / 237	
Goodness-of-fit on F ²	1.082	
Final R indices [I > 2σ(I)]	R1 = 0.0477, wR2 = 0.1450	
R indices (all data)	R1 = 0.0554, wR2 = 0.1496	
Largest diff. peak and hole	0.253 and -0.319 e.Å ⁻³	

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	2533(1)	8419(1)	8109(1)	45(1)
S(2)	1868(1)	11487(1)	6764(1)	46(1)
O(1)	3901(2)	8898(2)	8236(2)	58(1)
O(2)	1802(2)	7679(2)	9196(2)	58(1)
O(3)	3188(2)	11186(2)	6031(2)	60(1)
O(4)	550(2)	12319(2)	6161(2)	61(1)
O(5)	-1038(2)	10130(2)	8580(2)	71(1)
N(1)	1310(2)	9904(2)	7497(2)	45(1)
C(1)	-226(3)	9822(3)	7565(2)	46(1)
C(2)	-1059(3)	9515(3)	6723(3)	64(1)
C(3)	-2541(4)	9620(4)	7310(5)	101(2)
C(4)	-2466(4)	9988(4)	8373(5)	91(1)
C(5)	2702(3)	7438(3)	6925(2)	45(1)
C(6)	1748(3)	6468(3)	6956(3)	54(1)
C(7)	1818(3)	5775(3)	5986(3)	60(1)
C(8)	2806(3)	6048(3)	4969(3)	60(1)
C(9)	3783(3)	6996(4)	4979(3)	66(1)
C(10)	3736(3)	7695(3)	5937(3)	58(1)
C(11)	2808(4)	5337(4)	3861(3)	88(1)
C(12)	2281(3)	12213(3)	8011(2)	44(1)
C(13)	1106(3)	12747(3)	8751(3)	53(1)
C(14)	1435(3)	13355(3)	9707(3)	59(1)
C(15)	2895(3)	13464(3)	9938(3)	55(1)
C(16)	4042(3)	12928(3)	9197(3)	57(1)
C(17)	3746(3)	12282(3)	8232(2)	50(1)
C(18)	3209(4)	14124(4)	11001(3)	79(1)

Table S3. Bond lengths [Å] and angles [°] for **1**.

S(1)-O(2)	1.417(2)	O(3)-S(2)-N(1)	108.16(11)
S(1)-O(1)	1.4214(19)	O(4)-S(2)-N(1)	103.58(11)
S(1)-N(1)	1.689(2)	O(3)-S(2)-C(12)	109.98(12)
S(1)-C(5)	1.754(2)	O(4)-S(2)-C(12)	108.96(12)
S(2)-O(3)	1.4201(19)	N(1)-S(2)-C(12)	104.67(11)
S(2)-O(4)	1.423(2)	C(1)-O(5)-C(4)	105.4(3)
S(2)-N(1)	1.706(2)	C(1)-N(1)-S(1)	118.67(16)
S(2)-C(12)	1.749(2)	C(1)-N(1)-S(2)	118.63(16)
O(5)-C(1)	1.347(3)	S(1)-N(1)-S(2)	122.68(12)
O(5)-C(4)	1.362(4)	C(2)-C(1)-O(5)	112.5(2)
N(1)-C(1)	1.404(3)	C(2)-C(1)-N(1)	128.9(3)
C(1)-C(2)	1.334(4)	O(5)-C(1)-N(1)	118.6(2)
C(2)-C(3)	1.447(5)	C(1)-C(2)-C(3)	103.1(3)
C(3)-C(4)	1.290(6)	C(4)-C(3)-C(2)	108.2(3)
C(5)-C(6)	1.380(3)	C(3)-C(4)-O(5)	110.8(3)
C(5)-C(10)	1.383(3)	C(6)-C(5)-C(10)	120.6(2)
C(6)-C(7)	1.368(4)	C(6)-C(5)-S(1)	119.48(19)
C(7)-C(8)	1.380(4)	C(10)-C(5)-S(1)	119.8(2)
C(8)-C(9)	1.386(4)	C(7)-C(6)-C(5)	119.3(2)
C(8)-C(11)	1.518(4)	C(6)-C(7)-C(8)	121.1(3)
C(9)-C(10)	1.362(4)	C(7)-C(8)-C(9)	118.5(2)
C(12)-C(17)	1.378(3)	C(7)-C(8)-C(11)	120.5(3)
C(12)-C(13)	1.394(3)	C(9)-C(8)-C(11)	121.0(3)
C(13)-C(14)	1.376(4)	C(10)-C(9)-C(8)	121.4(3)
C(14)-C(15)	1.387(4)	C(9)-C(10)-C(5)	119.1(3)
C(15)-C(16)	1.379(4)	C(17)-C(12)-C(13)	121.0(2)
C(15)-C(18)	1.506(4)	C(17)-C(12)-S(2)	119.98(19)
C(16)-C(17)	1.399(4)	C(13)-C(12)-S(2)	119.0(2)
		C(14)-C(13)-C(12)	118.7(3)
O(2)-S(1)-O(1)	120.19(12)	C(13)-C(14)-C(15)	121.7(2)
O(2)-S(1)-N(1)	105.91(11)	C(16)-C(15)-C(14)	118.8(2)
O(1)-S(1)-N(1)	105.83(11)	C(16)-C(15)-C(18)	121.2(3)
O(2)-S(1)-C(5)	109.00(12)	C(14)-C(15)-C(18)	120.0(3)
O(1)-S(1)-C(5)	110.91(12)	C(15)-C(16)-C(17)	120.9(3)
N(1)-S(1)-C(5)	103.54(11)	C(12)-C(17)-C(16)	118.9(2)
O(3)-S(2)-O(4)	120.24(12)		

Table S4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	40(1)	50(1)	45(1)	-13(1)	-6(1)	-2(1)
S(2)	48(1)	49(1)	43(1)	-11(1)	-4(1)	-11(1)
O(1)	42(1)	67(1)	70(1)	-23(1)	-16(1)	-5(1)
O(2)	63(1)	62(1)	43(1)	-7(1)	4(1)	-2(1)
O(3)	62(1)	76(1)	50(1)	-23(1)	12(1)	-24(1)
O(4)	64(1)	54(1)	61(1)	-3(1)	-25(1)	-6(1)
O(5)	59(1)	74(1)	72(1)	-13(1)	6(1)	1(1)
N(1)	36(1)	45(1)	55(1)	-13(1)	-6(1)	-6(1)
C(1)	38(1)	47(1)	54(2)	-12(1)	0(1)	-6(1)
C(2)	65(2)	60(2)	68(2)	-15(1)	-28(2)	-7(1)
C(3)	51(2)	74(2)	168(5)	14(3)	-49(2)	-24(2)
C(4)	40(2)	90(3)	117(3)	15(2)	7(2)	-1(2)
C(5)	41(1)	46(1)	45(1)	-9(1)	-1(1)	-3(1)
C(6)	58(2)	54(2)	50(2)	-9(1)	2(1)	-14(1)
C(7)	67(2)	50(2)	65(2)	-18(1)	-7(1)	-11(1)
C(8)	63(2)	58(2)	54(2)	-18(1)	-12(1)	12(1)
C(9)	66(2)	75(2)	58(2)	-22(1)	16(1)	-10(2)
C(10)	53(2)	65(2)	59(2)	-19(1)	11(1)	-15(1)
C(11)	107(3)	90(3)	74(2)	-46(2)	-18(2)	9(2)
C(12)	48(1)	43(2)	45(1)	-13(1)	-2(1)	-13(1)
C(13)	46(1)	54(2)	62(2)	-20(1)	4(1)	-10(1)
C(14)	68(2)	52(2)	58(2)	-19(1)	11(1)	-6(1)
C(15)	82(2)	38(2)	48(2)	-12(1)	-6(1)	-11(1)
C(16)	58(2)	59(2)	58(2)	-15(1)	-12(1)	-17(1)
C(17)	46(1)	58(2)	49(2)	-15(1)	0(1)	-10(1)
C(18)	114(3)	67(2)	64(2)	-29(2)	-16(2)	-14(2)

Table S5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **1**.

	x	y	z	U(eq)
H(2)	-761	9287	5946	76
H(3)	-3399	9452	6979	121
H(4)	-3278	10137	8923	109
H(6)	1065	6287	7630	65
H(7)	1189	5108	6012	72
H(9)	4484	7159	4318	80
H(10)	4390	8336	5927	69
H(11A)	2422	4455	4146	132
H(11B)	3813	5147	3536	132
H(11C)	2188	5960	3201	132
H(13)	119	12694	8601	63
H(14)	658	13701	10212	71
H(16)	5025	12997	9341	68
H(17)	4526	11905	7747	60
H(18A)	4272	14021	11093	118
H(18B)	2768	13651	11781	118
H(18C)	2786	15121	10808	118

Table S6. Crystal data and structure refinement for **8**.

Identification code	mar1068	
Empirical formula	C ₁₆ H ₁₆ N ₃ O ₂ S.0.5C ₄ H ₈ O ₂	
Formula weight	358.43	
Temperature	253(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2 ₁ /c	
Unit cell dimensions	a = 11.785(2) Å	α = 90°.
	b = 6.1130(12) Å	β = 101.95(3)°.
	c = 25.017(5) Å	γ = 90°.
Volume	1763.2(6) Å ³	
Z	4	
Density (calculated)	1.350 Mg/m ³	
Absorption coefficient	0.206 mm ⁻¹	
F(000)	756	
Crystal size	0.4 x 0.25 x 0.2 mm ³	
Theta range for data collection	2.16 to 25.41°.	
Index ranges	-12 ≤ h ≤ 12, -6 ≤ k ≤ 6, -30 ≤ l ≤ 30	
Reflections collected	9460	
Independent reflections	2740 [R(int) = 0.0362]	
Completeness to theta = 25.41°	84.1 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	2740 / 0 / 225	
Goodness-of-fit on F ²	1.121	
Final R indices [I > 2σ(I)]	R1 = 0.0546, wR2 = 0.1574	
R indices (all data)	R1 = 0.0681, wR2 = 0.1638	
Largest diff. peak and hole	0.365 and -0.420 e.Å ⁻³	

Table S7. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **8**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	3555(1)	5837(1)	3133(1)	42(1)
O(1)	4214(2)	6199(3)	3676(1)	62(1)
O(2)	3213(2)	7727(3)	2792(1)	61(1)
N(1)	4297(2)	4110(3)	2870(1)	44(1)
N(2)	3531(2)	4111(3)	1433(1)	42(1)
N(3)	3831(2)	3785(3)	2311(1)	39(1)
C(1)	4050(2)	5013(4)	1906(1)	42(1)
C(2)	3161(2)	2023(4)	2090(1)	46(1)
C(3)	2974(2)	2237(4)	1544(1)	47(1)
C(4)	2239(2)	4557(4)	3197(1)	44(1)
C(5)	2265(3)	2478(5)	3421(1)	55(1)
C(6)	1229(3)	1521(6)	3488(1)	66(1)
C(7)	171(3)	2601(6)	3337(1)	66(1)
C(8)	171(3)	4625(6)	3101(2)	70(1)
C(9)	1183(3)	5611(5)	3029(1)	59(1)
C(10)	-933(3)	1550(8)	3423(2)	99(1)
C(11)	3592(2)	4953(5)	904(1)	48(1)
C(12)	3205(3)	3656(6)	445(1)	70(1)
C(13)	3293(4)	4494(8)	-61(1)	90(1)
C(14)	3737(4)	6534(8)	-115(2)	88(1)
C(15)	4119(3)	7782(6)	344(2)	79(1)
C(16)	4052(3)	7008(5)	856(1)	60(1)
O(3)	900(11)	245(19)	464(5)	179(4)
O(4)	-1107(11)	1120(20)	502(5)	204(5)
C(17)	61(18)	220(40)	275(7)	158(6)
C(18)	-620(14)	2250(30)	324(6)	156(5)
C(19)	270(17)	1240(30)	-10(11)	188(7)
C(20)	-250(20)	4020(30)	185(9)	229(9)

Table S8. Bond lengths [Å] and angles [°] for **8**.

S(1)-O(1)	1.436(2)	C(18)-C(19)	1.59(3)
S(1)-O(2)	1.442(2)	C(19)-C(17)#1	1.134(18)
S(1)-N(1)	1.596(2)	C(19)-C(19)#1	1.65(4)
S(1)-C(4)	1.774(3)	C(19)-O(3)#1	1.83(3)
N(1)-N(3)	1.409(3)	C(19)-C(20)	1.90(3)
N(2)-C(1)	1.334(3)	C(20)-C(20)#2	1.69(4)
N(2)-C(3)	1.377(3)		
N(2)-C(11)	1.436(3)	O(1)-S(1)-O(2)	117.77(13)
N(3)-C(1)	1.328(3)	O(1)-S(1)-N(1)	104.82(13)
N(3)-C(2)	1.381(3)	O(2)-S(1)-N(1)	113.37(12)
C(2)-C(3)	1.343(4)	O(1)-S(1)-C(4)	107.10(13)
C(4)-C(9)	1.387(4)	O(2)-S(1)-C(4)	105.33(14)
C(4)-C(5)	1.387(4)	N(1)-S(1)-C(4)	108.01(12)
C(5)-C(6)	1.395(4)	N(3)-N(1)-S(1)	111.59(16)
C(6)-C(7)	1.393(5)	C(1)-N(2)-C(3)	108.3(2)
C(7)-C(8)	1.371(5)	C(1)-N(2)-C(11)	124.6(2)
C(7)-C(10)	1.506(5)	C(3)-N(2)-C(11)	127.0(2)
C(8)-C(9)	1.382(4)	C(1)-N(3)-C(2)	108.8(2)
C(11)-C(16)	1.383(4)	C(1)-N(3)-N(1)	125.5(2)
C(11)-C(12)	1.392(4)	C(2)-N(3)-N(1)	125.5(2)
C(12)-C(13)	1.390(5)	N(3)-C(1)-N(2)	108.5(2)
C(13)-C(14)	1.370(6)	C(3)-C(2)-N(3)	106.8(2)
C(14)-C(15)	1.374(5)	C(2)-C(3)-N(2)	107.6(2)
C(15)-C(16)	1.381(4)	C(9)-C(4)-C(5)	119.5(3)
O(3)-C(17)	1.004(18)	C(9)-C(4)-S(1)	120.9(2)
O(3)-C(19)	1.40(2)	C(5)-C(4)-S(1)	119.6(2)
O(3)-C(19)#1	1.83(3)	C(4)-C(5)-C(6)	119.1(3)
O(4)-C(18)	1.055(18)	C(7)-C(6)-C(5)	121.7(3)
O(4)-C(17)	1.69(2)	C(8)-C(7)-C(6)	117.7(3)
C(17)-C(19)	1.01(2)	C(8)-C(7)-C(10)	121.6(4)
C(17)-C(19)#1	1.134(18)	C(6)-C(7)-C(10)	120.7(4)
C(17)-C(17)#1	1.38(3)	C(7)-C(8)-C(9)	121.8(3)
C(17)-C(18)	1.49(2)	C(8)-C(9)-C(4)	120.2(3)
C(18)-C(20)	1.25(2)	C(16)-C(11)-C(12)	120.9(3)

C(16)-C(11)-N(2)	120.1(3)	C(17)#1-C(19)-C(18)	115(2)
C(12)-C(11)-N(2)	119.0(3)	O(3)-C(19)-C(18)	90.9(16)
C(13)-C(12)-C(11)	117.9(4)	C(17)-C(19)-C(19)#1	42.5(16)
C(14)-C(13)-C(12)	121.8(4)	C(17)#1-C(19)-C(19)#1	37.2(13)
C(13)-C(14)-C(15)	119.3(3)	O(3)-C(19)-C(19)#1	73.4(17)
C(14)-C(15)-C(16)	120.8(4)	C(18)-C(19)-C(19)#1	92.3(19)
C(15)-C(16)-C(11)	119.4(3)	C(17)-C(19)-O(3)#1	83(2)
C(17)-O(3)-C(19)	46.4(14)	C(17)#1-C(19)-O(3)#1	28.9(11)
C(17)-O(3)-C(19)#1	33.1(13)	O(3)-C(19)-O(3)#1	120.4(15)
C(19)-O(3)-C(19)#1	59.6(15)	C(18)-C(19)-O(3)#1	91.4(11)
C(18)-O(4)-C(17)	61.0(13)	C(19)#1-C(19)-O(3)#1	47.1(13)
O(3)-C(17)-C(19)	88(2)	C(17)-C(19)-C(20)	103(2)
O(3)-C(17)-C(19)#1	118(2)	C(17)#1-C(19)-C(20)	140.1(19)
C(19)-C(17)-C(19)#1	100(3)	O(3)-C(19)-C(20)	108.2(17)
O(3)-C(17)-C(17)#1	111(2)	C(18)-C(19)-C(20)	40.6(10)
C(19)-C(17)-C(17)#1	53.9(17)	C(19)#1-C(19)-C(20)	132(2)
C(19)#1-C(17)-C(17)#1	46.3(15)	O(3)#1-C(19)-C(20)	111.3(13)
O(3)-C(17)-C(18)	116(2)	C(18)-C(20)-C(20)#2	162(3)
C(19)-C(17)-C(18)	76(2)	C(18)-C(20)-C(19)	56.2(12)
C(19)#1-C(17)-C(18)	125(2)	C(20)#2-C(20)-C(19)	109.0(18)
C(17)#1-C(17)-C(18)	107(2)		
O(3)-C(17)-O(4)	129.1(18)		
C(19)-C(17)-O(4)	112(2)		
C(19)#1-C(17)-O(4)	104(2)		
C(17)#1-C(17)-O(4)	119(2)		
C(18)-C(17)-O(4)	38.2(8)		
O(4)-C(18)-C(20)	160(2)		
O(4)-C(18)-C(17)	80.8(15)		
C(20)-C(18)-C(17)	118(2)		
O(4)-C(18)-C(19)	116.3(18)		
C(20)-C(18)-C(19)	83.2(17)		
C(17)-C(18)-C(19)	38.2(9)		
C(17)-C(19)-C(17)#1	80(3)		
C(17)-C(19)-O(3)	45.7(15)		
C(17)#1-C(19)-O(3)	102(2)		
C(17)-C(19)-C(18)	65.6(18)		

Table S9. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **8**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	47(1)	39(1)	42(1)	-2(1)	15(1)	-5(1)
O(1)	61(1)	77(2)	51(1)	-17(1)	13(1)	-16(1)
O(2)	76(2)	41(1)	74(2)	12(1)	34(1)	3(1)
N(1)	45(1)	52(1)	35(1)	2(1)	8(1)	2(1)
N(2)	42(1)	46(1)	39(1)	1(1)	10(1)	4(1)
N(3)	38(1)	41(1)	40(1)	2(1)	9(1)	2(1)
C(1)	44(2)	43(2)	40(1)	1(1)	13(1)	-3(1)
C(2)	47(2)	41(2)	51(2)	1(1)	12(1)	-3(1)
C(3)	48(2)	44(2)	49(2)	-1(1)	7(1)	-4(1)
C(4)	48(2)	46(2)	40(1)	0(1)	15(1)	-2(1)
C(5)	54(2)	54(2)	57(2)	10(1)	14(2)	0(1)
C(6)	81(3)	58(2)	63(2)	6(2)	25(2)	-21(2)
C(7)	54(2)	91(2)	54(2)	-2(2)	13(2)	-21(2)
C(8)	45(2)	91(3)	76(2)	7(2)	16(2)	2(2)
C(9)	58(2)	56(2)	64(2)	10(1)	18(2)	8(1)
C(10)	67(3)	143(4)	88(3)	-1(3)	20(2)	-43(3)
C(11)	47(2)	59(2)	38(2)	5(1)	9(1)	8(1)
C(12)	77(3)	85(2)	46(2)	-4(2)	11(2)	-7(2)
C(13)	95(3)	132(4)	41(2)	-3(2)	11(2)	-3(3)
C(14)	92(3)	122(3)	53(2)	27(2)	22(2)	10(3)
C(15)	94(3)	86(3)	62(2)	22(2)	30(2)	4(2)
C(16)	71(2)	60(2)	53(2)	8(1)	22(2)	2(2)

Table S10. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **8**.

	x	y	z	U(eq)
H(1)	4491	6287	1946	50
H(2)	2891	903	2282	55
H(3)	2547	1292	1288	57
H(5)	2964	1732	3526	66
H(6)	1246	126	3638	79
H(8)	-530	5355	2987	84
H(9)	1157	6984	2867	70
H(10A)	-1059	1927	3779	148
H(10B)	-872	-10	3396	148
H(10C)	-1573	2064	3150	148
H(12)	2896	2273	476	83
H(13)	3044	3647	-372	107
H(14)	3780	7070	-458	105
H(15)	4426	9164	310	94
H(16)	4313	7861	1164	72

Figure S1. ORTEP drawing of **1** with atom-numbering scheme. Thermal ellipsoids are drawn on the 30% probability level.

Figure S2. ORTEP drawing of **8** with atom-numbering scheme. Thermal ellipsoids are drawn on the 30% probability level.

Figure S3. ^1H Spectrum of *N,N*-Di(toluen-*p*-sulfonyl)-(furan-2-yl)-amine **1**.

Figure S4. ^1H Spectrum of *N,N*-Di(nitrobenzene-*p*-sulfonyl)-(furan-2-yl)-amine **2**.

Figure S5. ^1H Spectrum of 5-(*N,N*-Di(toluene-4-sulfonyl)amino)-furan-2-carboxylic acid methyl ester **3**.

Figure S6. ^1H Spectrum of *N,N*-Di(toluen-*p*-sulfonyl)-(benzofuran-2-yl)-amine **4**.

Figure S7. ^1H Spectrum of 4-Methyl-*N*-[1-(toluene-*p*-sulfonyl)-1*H*-indol-2-yl]-benzenesulfonamide **5a** and 4-Methyl-*N*-[1-(toluene-*p*-sulfonyl)-1*H*-indol-3-yl]-benzenesulfonamide **5b**.

Figure S8. ^1H Spectrum of *N,N*-Di(toluen-*p*-sulfonyl)-(thiophen-2-yl)-amine **6**.

Figure S9. ^1H Spectrum of *N,N*-Di(toluen-*p*-sulfonyl)-(N-[1-(toluen-*p*-sulfonyl)-1*H*-pyrrol-2-yl])-amine **7**.

Figure S10. ^1H Spectrum of 3,4-Di(toluene-*p*-sulfonamido)-1-methylpyrrole **9**.

Figure S11. ^1H Spectrum of 3,4-Di(toluene-*p*-sulfonamido)-1-phenylpyrrole **10**.

Figure S12. ^1H Spectrum of 3,4-Di(toluene-*p*-sulfonamido)-1-(2-methylphenyl)pyrrole 11.

Figure S13. ^1H Spectrum of 3,4-Di(toluene-*p*-sulfonamido)-1-(4-fluorophenyl)pyrrole **14**.

Figure S14. ^1H Spectrum of 3,4-Di(toluene-*p*-sulfonamido)-1-(4-nitrophenyl)pyrrole **15**.

Figure S15. ^1H Spectrum of *N,N*-Di(nitrobenzene-*p*-sulfonyl)-(methyl 2-furoate)-amine **16**.

Figure S16. ^1H Spectrum of *N*-Benzofuran-2-yl-4-nitro-benzenesulfonamide **17**.

Figure S17. ^1H Spectrum of *N,N*-Di(nitrobenzene-*p*-sulfonyl)-(thiophene-2-yl)-amine **18**.