SUPPORTING INFORMATION

Palladium-Catalyzed α -Arylation of Sulfoximines

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TABLE OF CONTENTS

• Synthesis of N-benzoyl sulfoximine 7	S1
• Synthesis of N-benzoyl sulfoximine ethyl ester 3	S2
• General procedure for palladium-catalyzed α -arylation of N-benzoyl sulfoximine ethyl ester 3	S2
• Analytical data for compounds 8a-h	S2
• Hydrolysis of compound 8a to give 10	S5
• Removal of benzoyl protecting group to give 11	S5
• References	S5
• ^1H and ^{13}C NMR spectra of the reported compounds	S6

^1H and ^{13}C NMR (400 and 100 MHz, respectively) spectra were recorded in CDCl_3 using TMS as internal standard. Chemical shifts are given in ppm and spin-spin coupling constants, J , are given in Hz. IR spectra were recorded as KBr pellets. All reagents were purchased from commercial suppliers and used without further purification.

Synthesis of N-benzoyl sulfoximine 7 (Scheme 1): *rac*-Sulfoximine **1a**¹ (1.55 g, 10 mmol) and NaH (60% in mineral oil, 600 mg, 15 mmol) were dissolved in anhydrous dichloromethane (50 mL) under argon at room temperature. Benzoyl chloride (1.28 mL, 11 mmol) was then added and the reaction mixture was stirred for two hours at room temperature. Subsequently water (30 mL) was added and the resulting mixture was extracted with dichloromethane several times. The combined organic layers were dried over MgSO_4 and concentrated. Purification by crystallization (pentane and ethyl acetate) and column chromatography (SiO_2) gave 2.33 g (90%) of compound **7** as a white solid. Mp. 108-110 °C; ^1H NMR (CDCl_3): δ 8.17 (d, J = 7.2 Hz, 2H), 8.04 (d, J = 7.2 Hz, 2H), 7.69-7.38 (m, 6H), 3.45 (s, 3H); ^{13}C NMR (CDCl_3): δ 174.0, 138.8, 135.5, 133.7, 132.0, 129.6, 129.3, 127.9, 127.0, 44.2; IR (KBr): ν 3019, 1617, 1447, 1214 cm^{-1} ; MS (CI), m/z (relative intensity): 260 ($[\text{M}+1]^+$); Calcd. for $\text{C}_{14}\text{H}_{13}\text{NO}_2\text{S}$: C, 64.84; H, 5.05; N, 5.40; found C, 64.90; H, 5.11; N, 5.32.

Synthesis of N-benzoyl sulfoximine ethyl ester **3² (Scheme 1):** To a stirred solution of tetramethylpiperidine (2.4 mL, 14 mmol) in anhydrous THF (6 mL) was slowly added a solution of *n*-butyllithium (15% in hexane, 7.5 mL, 12 mmol) at 0 °C. After 10 min, the reaction mixture was cooled to –78 °C and a solution of compound **7** (1.55 g, 6 mmol) in THF (10 mL) was added slowly via syringe. After stirring for 30 min at this temperature, ethyl chloroform (1.4 mL, 12 mmol) was added dropwise at –78 °C and the stirring was continued for 2 hours without further control of temperature. The reaction mixture was quenched with saturated ammonium chloride (2 mL) and extracted with dichloromethane several times. The combined organic layers were dried over MgSO₄ and concentrated. Purification by column chromatography gave 1.76 g (89%) of compound **3** as a pale yellow solid. Mp. 88-89 °C; ¹H NMR (CDCl₃): δ 8.14-8.10 (m, 2H), 8.06-8.02 (m, 2H), 7.69-7.63 (m, 1H), 7.59-7.53 (m, 2H), 7.49-7.43 (m, 1H), 7.39-7.33 (m, 2H), 4.76 (d, *J* = 14.1 Hz, 1H), 4.56 (d, *J* = 14.1 Hz, 1H), 4.04-3.97 (m, 2H), 1.03 (t, *J* = 7.2 Hz, 3H); ¹³C NMR (CDCl₃): δ 174.3, 162.1, 136.9, 135.4, 134.4, 132.4, 129.6, 129.5, 128.6, 128.1, 62.5, 59.5, 13.8; IR (KBr): ν 3056, 2987, 2930, 1741 cm⁻¹; MS (CI), *m/z* (relative intensity): 332 ([M+1]⁺); Calcd. for C₁₇H₁₇NO₄S: C, 61.61; H, 5.17; N, 4.23; found C, 61.56; H, 4.94; N, 4.09.

General procedure for palladium-catalyzed α-arylation of N-benzoyl sulfoximine ethyl ester **3:** A solution of N-benzoyl sulfoximine ethyl ester **3** (70 mg, 0.21 mmol), Pd(OAc)₂ or Pd₂(dba)₃ (3 mol%), PCy₃ (9 mol%), sodium *tert*-butoxide (60 mg, 0.63 mmol), and aryl bromide (1.2 equiv) in anhydrous dioxane (2 mL) was heated to reflux under argon until the starting material completely disappeared (ca. in 1 hour) by TLC analysis. After cooling to room temperature, 10 % HCl (aq.) and ethyl acetate were added, and the organic layer was separated, dried (MgSO₄), and concentrated. The product was purified by column chromatography (SiO₂).

Compound **8a (entry 1, Table 1):** Following the general procedure using Pd(OAc)₂ and bromobenzene (0.026 mL, 0.24 mmol) gave 67.4 mg (79%) of compound **8a** as a white solid and as a mixture of diastereomers. ¹H NMR (CDCl₃): δ 8.21-8.18 (m, 1H), 8.16-8.13 (m, 1H), 7.69-7.67 (m, 1H), 7.63-7.61 (m, 2H), 7.53-7.50 (m, 1H), 7.45-7.25 (m, 7H), 7.20-7.18 (m, 2H), 6.27/6.17 due to diastereomers (s, ds, 1H), 4.39-4.07 (m, 2H), 1.33/1.13 (t, *J* = 7.14 Hz, 3H); ¹³C NMR (CDCl₃): δ 174.1/174.0, 164.8/164.5, 135.5, 135.5, 134.1, 134.0, 133.2, 133.0, 132.2, 132.1, 130.6, 130.4, 130.3, 130.1, 129.8, 129.4, 128.3, 128.3, 127.9, 127.3, 126.9, 74.5/72.7, 62.7/62.4, 14.0/13.9; IR (KBr): ν 3067, 2975, 1731, 1629, 1576 cm⁻¹; MS (CI), *m/z* (relative intensity): 408 ([M+1]⁺); Calcd. for C₂₃H₂₁NO₄S: C, 67.79; H, 5.19; N, 3.44; found C, 67.73; H, 5.27; N, 3.35.

Compound **8b (entry 2, Table 1):** Following the general procedure using Pd(OAc)₂ and 4-bromoanisole (0.032 mL, 0.25 mmol) gave 76.0 mg (83%) of compound **8b** as a white solid and as a mixture of diastereomers. ¹H NMR (CDCl₃): δ 8.20-8.18 (m, 1H), 8.16-8.14 (m, 1H), 7.71-7.68 (m, 1H), 7.65-7.61 (m, 2H), 7.54-7.49 (m, 1H), 7.46-7.39 (m, 4H), 7.22-7.18 (m, 1H), 7.13-7.09 (m, 1H), 6.79-6.75 (m, 1H), 6.72-6.68 (m, 1H), 6.12/6.11 (s, 1H), 4.40-4.05 (m, 2H), 3.79/3.74 (s, 3H), 1.32/1.12 (t, *J* = 7.14 Hz, 3H); ¹³C NMR (CDCl₃): δ 174.0/173.8, 164.9/164.7, 160.7/160.7, 135.5, 135.5, 134.0, 133.9, 133.3, 133.0, 132.1, 132.0, 131.6, 130.4, 130.1, 129.3, 128.3, 128.2, 127.9, 119.0, 118.5, 113.8, 113.7, 73.9/72.2, 62.6/62.3, 55.3/55.2, 14.0/13.9; IR (KBr): ν 3016, 1739, 1633, 1310, 1280 cm⁻¹; MS (CI), *m/z* (relative intensity): 438 ([M+1]⁺); Calcd. for C₂₄H₂₃NO₅S: C, 65.89; H, 5.30; N, 3.20; found C, 65.58; H, 5.34; N, 3.19.

Compound 8c (entry 3, Table 1): Following the general procedure using $\text{Pd}_2(\text{dba})_3$ and 4-bromobenzonitrile (45 mg, 0.25 mmol) gave 80.0 mg (88%) of compound **8c** as colorless oil and as a mixture of diastereomer. ^1H NMR (CDCl_3): δ 8.18-8.11 (m, 2H), 7.72-7.64 (m, 3H), 7.59-7.34 (m, 9H), 6.50/6.29 (s, 1H), 4.42-4.09 (m, 2H), 1.34/1.10 (t, $J = 7.17$ Hz, 3H); ^{13}C NMR (CDCl_3): δ 174.0, 164.1, 135.2, 134.7, 132.9, 132.6, 132.5, 132.3, 132.0, 131.5, 131.1, 130.3, 130.2, 129.5, 128.8, 128.7, 128.2, 128.1, 118.0, 113.8, 73.4/71.9, 63.2/62.9, 13.9/13.7; IR (KBr): ν 3260, 3019, 2231, 1740, 1634 cm^{-1} ; MS (CI), m/z (relative intensity): 433 ($[\text{M}+1]^+$); HRMS of $[\text{M}]^+$: Calcd. 432.1144; found 432.1143.

Compound 8d (entry 4, Table 1): Following the general procedure using $\text{Pd}(\text{OAc})_2$ and 4-bromo nitrobenzene (51 mg, 0.25 mmol) gave 69.6 mg (73%) of compound **8d** as yellow oil and as a mixture of diastereomers. ^1H NMR (CDCl_3): δ 8.19-8.12 (m, 3H), 8.05-8.03 (m, 1H), 7.74-7.66 (m, 3H), 7.57-7.41 (m, 7H), 6.49/6.37 (s, 1H), 4.42-4.07 (m, 2H), 1.35/1.10 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (CDCl_3): δ 174.0/173.8, 164.0/163.9, 148.5, 135.1, 135.0, 134.7, 134.4, 134.1, 132.7, 132.6, 132.5, 131.8, 131.4, 130.2, 130.1, 129.4, 128.7, 128.7, 128.1, 128.1, 123.3, 73.1/71.6, 63.3/63.0, 14.0/13.8; IR (KBr): ν 2934, 1740, 1635, 1526, 1348, 1278 cm^{-1} ; MS (CI), m/z (relative intensity): 453 ($[\text{M}+1]^+$); Calcd. for $\text{C}_{18}\text{H}_{14}\text{N}_2\text{O}_5\text{S}_2$: C, 61.05; H, 4.46; N, 6.19; found C, 61.24; H, 4.46; N, 6.18.

Compound 8e (entry 5, Table 1): Following the general procedure using $\text{Pd}_2(\text{dba})_3$ and 4-bromo chlorobenzene (48 mg, 0.25 mmol) gave 62.5 mg (68%) of compound **8e** as a white solid and as a mixture of diastereomers. ^1H NMR (CDCl_3): δ 8.19-8.13 (m, 2H), 7.72-7.64 (m, 3H), 7.53-7.40 (m, 5H), 7.26-7.25 (m, 2H), 7.16-7.13 (m, 2H), 6.29/6.17 (s, 1H), 4.39-4.09 (m, 2H), 1.33/1.11 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (CDCl_3): δ 174.0/173.8, 164.5/164.3, 136.2, 135.3, 134.3, 133.0, 132.9, 132.3, 132.3, 132.0, 131.6, 130.6, 130.4, 130.1, 129.4, 128.6, 128.5, 128.4, 128.0, 128.0, 125.9, 125.5, 73.5/71.8, 62.9/62.6, 14.0/13.8; IR (KBr): ν 3018, 1739, 1634, 1491, 1279 cm^{-1} ; MS (CI), m/z (relative intensity): 442 ($[\text{M}+1]^+$); HRMS of $[\text{M}]^+$: Calcd. 441.0802; found 441.0802.

Compound 8f (entry 6, Table 1): Following general procedure using $\text{Pd}(\text{OAc})_2$ and 4-bromothioanisole (51 mg, 0.25 mmol) gave 80.6 mg (85%) of compound **8f** as colorless oil and as a mixture of diastereomers. ^1H NMR (CDCl_3): δ 8.20-8.13 (m, 2H), 7.73-7.61 (m, 3H), 7.53-7.39 (m, 5H), 7.21-7.18 (m, 1H), 7.12-7.18 (m, 1H), 7.03-7.01 (m, 1H), 6.26/6.14 (s, 1H), 4.35-4.08 (m, 2H), 2.46/2.42 (s, 3H), 1.32/1.12 (t, $J = 7.2$ Hz, 3H); ^{13}C NMR (CDCl_3): δ 174.1, 164.9/164.7, 141.6, 135.6, 134.2, 133.3, 133.1, 132.3, 132.2, 131.0, 130.6, 130.5, 130.3, 129.5, 128.5, 128.4, 128.0, 125.6, 125.4, 123.5, 123.1, 74.0/72.3, 62.7/62.4, 15.1/15.0, 13.9/13.8; IR (KBr): ν 3681, 3434, 3064, 2924, 2365, 1737, 1633 cm^{-1} ; MS (CI), m/z (relative intensity): 454 ($[\text{M}+1]^+$); Calcd. for $\text{C}_{24}\text{H}_{23}\text{NO}_4\text{S}_2$: C, 63.55; H, 5.11; N, 3.09; found C, 63.48; H, 5.46; N, 2.94.

Compound 8g (entry 7, Table 1): Following the general procedure using $\text{Pd}(\text{OAc})_2$ and 4-bromodiphenyl (59 mg, 0.25 mmol) gave 87.1 mg (86%) of compound **8g** as a white solid and as a mixture of diastereomers. ^1H NMR (CDCl_3): δ 8.22-8.17 (m, 2H), 7.76-7.74 (m, 1H), 7.69-7.62 (m, 2H), 7.58-7.36 (m, 13H), 7.28-7.26 (m, 1H), 6.35/6.25 (s, 1H), 4.19-4.12 (m, 2H), 1.35/1.15 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (CDCl_3): δ 174.0/173.9, 164.8/164.6, 142.6/142.6, 139.8/129.6, 135.5/135.5, 134.1, 134.1, 133.3, 133.0, 132.2, 132.2, 131.0, 130.7, 130.5, 130.2, 129.4, 128.8, 128.8, 128.4, 128.3, 128.0, 127.9, 127.8, 127.8, 127.0, 126.9, 126.9, 126.2, 125.8, 74.2, 72.5,

62.8, 62.5, 14.0, 13.9; IR (KBr): ν 3067, 2973, 1738, 1633, 1578, 1312, 1283 cm^{-1} ; MS (EI), m/z (relative intensity): 483 ($[\text{M}]^+$); HRMS of $[\text{M}]^+$: Calcd. 483.1504; found 483.1503.

Compound 8h (entry 8, Table 1): Following the general procedure using $\text{Pd}(\text{OAc})_2$ and 3-bromoanisole (0.032 mL, 0.25 mmol) gave 72.3 mg (79%) of compound **8h** as colorless oil and as a mixture of diastereomers. ^1H NMR (CDCl_3): δ 8.21–8.18 (m, 1H), 8.16–8.14 (m, 1H), 7.73–7.71 (m, 1H), 7.67–7.62 (m, 2H), 7.53–7.50 (m, 1H), 7.47–7.39 (m, 4H), 7.19–7.05 (m, 1H), 6.93–6.80 (m, 2H), 6.74–6.72 (m, 1H), 4.36–4.10 (m, 2H), 1.33/1.13 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (CDCl_3): δ 174.1/173.9, 164.8/164.5, 159.2/159.2, 135.5, 135.5, 134.1, 133.0, 132.2, 132.2, 130.5, 130.3, 129.4, 129.4, 129.3, 129.2, 128.9, 128.6, 128.5, 128.3, 128.1, 127.9, 127.9, 123.2, 122.6, 116.6, 116.4, 115.2, 114.6, 74.4/72.2, 62.7/62.4, 55.2/55.0, 14.0/13.9; IR (KBr): ν 3065, 3011, 2963, 2838, 1739, 1449, 1281 cm^{-1} ; MS (CI), m/z (relative intensity): 438 ($[\text{M}+1]^+$); Calcd. for $\text{C}_{24}\text{H}_{23}\text{NO}_5\text{S}$: C, 65.89; H, 5.30; N, 3.20; found C, 65.89; H, 5.58; N, 3.12.

Compound 8i (entry 9, Table 1): Following the general procedure using $\text{Pd}_2(\text{dba})_3$ and 3-bromonitrobenzene (50.5 mg, 0.25 mmol) gave 48.6 mg (51%) of compound **8i** as yellow oil and as a mixture of diastereomers. ^1H NMR (CDCl_3): δ 8.26–8.06 (m, 4H), 7.79–7.64 (m, 4H), 7.55–7.41 (m, 6H), 6.39/6.30 (s, 1H), 4.39–4.11 (m, 2H), 1.34/1.11 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (CDCl_3): δ 174.0/174.0, 164.1/163.9, 147.9/147.8, 137.1, 136.4, 136.4, 135.2, 135.1, 134.8, 132.7, 132.6, 132.5, 130.2, 130.1, 129.7, 129.5, 129.3, 128.9, 128.8, 128.1, 125.6, 125.4, 124.7, 73.0/71.8, 63.3/63.0, 13.9/13.7; IR (KBr): ν 3068, 3019, 1740, 1635, 1533, 1448, 1278 cm^{-1} ; MS (CI), m/z (relative intensity): 453 ($[\text{M}+1]^+$); Calcd. for $\text{C}_{23}\text{H}_{20}\text{N}_2\text{O}_6\text{S}$: C, 61.05; H, 4.46; N, 6.19; found C, 61.32; H, 4.62; N, 6.22.

Compound 8j (entry 10, Table 2): Following the general procedure using compound **4** (119 mg, 0.36 mmol), 1,3-dibromobenzene (0.02 mL, 0.17 mmol), $\text{Pd}(\text{OAc})_2$ (2.2 mg, 0.01 mmol), PCy_3 (8.4 mg, 0.03 mmol) and sodium *tert*-butoxide (103 mg, 1.1 mmol) gave 33.4 mg (41%) of monocoupled compound **8j-A** and 50.4 mg (41%) of dicoupled compound **8j-B** as a white solid each as a mixture of diastereomers.

Compound 8j-A: ^1H NMR (CDCl_3): 8.20–8.13 (m, 2H), 7.70–7.18 (m, 12H), 6.27/6.26/6.17/6.13 (s, 1H), 4.43–4.03 (m, 2H), 1.36–1.31/1.16–1.10 (m, 3H); ^{13}C NMR (CDCl_3): δ 175.1/174.0, 164.9, 164.6, 164.5, 135.6, 135.4, 134.5, 134.1, 133.5, 133.3, 133.1, 133.0, 132.3, 132.2, 130.7, 130.5, 130.4, 130.3, 130.2, 129.9, 129.9, 129.6, 129.5, 129.2, 129.1, 128.5, 128.5, 128.4, 128.3, 128.0, 128.0, 127.4, 127.0, 122.3, 74.4, 73.6, 72.7, 71.9, 62.9, 62.7, 62.6, 62.4, 13.9, 13.8; IR (KBr): ν 3016, 2966, 1739, 1312, 1279 cm^{-1} ; MS (CI), m/z (relative intensity): 486/488 ($[\text{M}+1]^+$); HRMS of $[\text{M}-\text{C}_{10}\text{H}_{10}\text{O}_2\text{Br}]^+$: Calcd. 244.0432; found 244.0432.

Compound 8j-B: ^1H NMR (CDCl_3): δ 8.18–8.11 (m, 4H), 7.72–7.31 (m, 18H), 7.23–7.10 (m, 2H), 6.14/6.06/5.95/5.93/5.84 (s, 2H), 4.40–3.85 (m, 4H), 1.37–1.27/1.15–1.04 (m, 3H); ^{13}C NMR (CDCl_3): δ 173.5, 163.8, 134.9, 133.9, 133.8, 132.7, 131.9, 131.6, 131.5, 131.4, 129.9, 129.8, 129.7, 129.3, 129.1, 129.1, 129.1, 128.4, 128.3, 128.2, 128.1, 127.6, 127.3, 73.4, 73.2, 72.4, 65.4, 62.5, 62.1, 62.0, 13.5, 13.3; IR (KBr): ν 3438, 3066, 2973, 1736, 1635, 1449, 1279 cm^{-1} ; MS (CI), m/z (relative intensity): 737 ($[\text{M}+1]^+$); Calcd. for $\text{C}_{40}\text{H}_{36}\text{N}_2\text{O}_8\text{S}_2$: C, 65.20; H, 4.92; N, 3.80; found C, 65.08; H, 5.16; N, 3.58.

Compound 8k (entry 11, Table 1): Following the general procedure using $\text{Pd}(\text{OAc})_2$ and 2-bromotoluene (0.03 mL, 0.25 mmol) gave 64.4 mg (73%) of compound **8k** as a white solid and as a mixture of diastereomers. ^1H NMR (CDCl_3): δ 8.22–8.14 (m, 2H), 7.77–7.39 (m, 8H), 7.30–7.22 (m, 2H), 7.16–7.00 (m, 1H), 6.91–6.90 (m, 1H), 6.70/6.06 (s, 1H), 4.37–4.02 (m, 2H),

2.66/2.05 (s, 1H), 1.35-1.30/1.14-1.09 (m, 3H); ^{13}C NMR (CDCl_3): δ 174.1/173.6, 165.1/164.4, 139.8, 138.4, 135.5, 134.1, 133.9, 133.0, 132.1, 132.1, 130.9, 130.7, 130.4, 130.4, 129.8, 129.7, 129.5, 129.4, 129.4, 128.8, 128.2, 127.9, 126.0, 125.7, 125.4, 125.2, 69.6/69.5, 62.7/62.3, 20.4/19.5, 14.0/13.8; IR (KBr): ν 2968, 1734, 1630, 1312, 1276, 1229 cm^{-1} ; MS (CI), m/z (relative intensity): 422.0 ($[\text{M}+1]^+$); Calcd. for $\text{C}_{24}\text{H}_{23}\text{NO}_4\text{S}$: C, 68.39; H, 5.50; N, 3.32; found C, 68.16; H, 5.81; N, 3.23.

Hydrolysis of compound 8a (Scheme 2) to give 10: To a solution of 1 N NaOH (aq, 3 mL) and methanol (6 mL) was added compound **8a** at room temperature and the reaction mixture was stirred for 2 hours. 10 % HOAc was added to the reaction mixture and the product was extracted with dichloromethane. The combined organic layers were dried over MgSO_4 and concentrated. Purification by column chromatography (SiO_2) gave 75.5 mg (98%) of N-benzoyl benzylphenyl sulfoximine (**10**) as a white solid. Mp. 132-133 $^\circ\text{C}$; ^1H NMR (CDCl_3): 8.20-8.17 (m, 2H), 7.72-7.69 (m, 2H), 7.65-7.59 (m, 1H), 7.55-7.40 (m, 5H), 7.32-7.17 (m, 3H), 7.02-7.00 (m, 2H), 4.95 (d, J = 13.6 Hz, 1H), 4.87 (d, J = 13.6 Hz, 1H); ^{13}C NMR (CDCl_3): δ 174.3, 135.7, 135.4, 133.7, 132.0, 131.1, 129.3, 129.0, 128.9, 128.4, 127.9, 127.2, 62.1; IR (KBr): ν 3455, 3060, 1627, 1447, 1279 cm^{-1} ; MS (CI), m/z (relative intensity): 336.0 ($[\text{M}+1]^+$); Calcd. for $\text{C}_{20}\text{H}_{17}\text{NO}_2\text{S}$: C, 71.62; H, 5.11; N, 4.18; found C, 71.33; H, 5.45; N, 4.04.

Removal of benzoyl protecting group to give 11³: BH_3 -THF (1.0 M in THF, 0.3 mL, 0.3 mmol) was slowly added to a solution of N-benzoyl benzylphenyl sulfoximine (32 mg, 0.1 mmol) at 0 $^\circ\text{C}$. After stirring for 3 hours at this temperature, the reaction mixture was quenched carefully with MeOH- H_2O (1:1, 3 mL), extracted with dichloromethane, dried over MgSO_4 and concentrated. Purification by column chromatography (SiO_2) gave 13.7 mg (62%) of NH-free benzylphenyl sulfoximine (**11**) as a white solid. Mp. 112-113 $^\circ\text{C}$; ^1H NMR (CDCl_3): 7.77-7.75 (m, 2H), 7.60-7.53 (m, 1H), 7.47-7.41 (m, 2H), 7.34-7.23 (m, 3H), 7.12-7.09 (m, 2H), 4.39 (d, J = 13.4 Hz, 1H), 4.30 (d, J = 13.4 Hz, 1H), 2.75 (bs, 1H); ^{13}C NMR (CDCl_3): δ 140.3, 133.0, 129.9, 128.7, 128.6, 128.5, 128.4, 64.5; IR (KBr): ν 3972, 3317, 3056, 2923, 1445, 1217, 1110 cm^{-1} ; MS (CI), m/z (relative intensity): 232.0 ($[\text{M}+1]^+$); Calcd. for $\text{C}_{13}\text{H}_{13}\text{NOS}$: C, 67.50; H, 5.66; N, 6.06; found C, 67.33; H, 5.91; N, 6.06.

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Plot at 160 Hz/cm : 0.40 ppm/cm

CHO 57 inova400/b/a4110930 h : Nov 10 2004 (CDCl3)

12.6 12.0 11.4 10.8 ppm

plot at 604 Hz/cm :

8.00 ppm/cm

CHO 75 mercury/300/b/a4111053 c : Nov 11 2004 (CDCI3)

plot at 160 Hz/cm : 0.40 ppm/cm

CHO 77 inova400/b/a4120316 h : Dec 6 2004 (CDCl3)

12.6 12.0 11.4 10.8 ppm

plot at 604 Hz/cm ; 8.00 ppm/cm

CHO VII-77 mercury300/b/a5010565 c : Jan 7 2005 (CDCI3)

at 120 Hz/cm : 0.40 ppm/cm

12.6 12.0 11.4 10.8 ppm

CHO 26A mercury300/b/a4120631 h : Dec 7 2004 (CDCl3)

plot at 604 Hz/cm : 8.00 ppm/cm

CHO 8-36 A mercury300/b/a5010566 c : Jan 7 2005 (CDCl3)

plot at 604 Hz/cm : 8.00 ppm/cm

CHO 8-268 mercury300/b/a4112988 c : Dec 1 2004 (CDCI3)

plot at 120 Hz/cm : 0.40 ppm/cm

12.6 12.0 11.4 10.8 ppm

CHO 86 mercury300/b/a4120665 h : Dec 8 2004 (CDCl3)

plot at 805 Hz/cm : 8.00 ppm/cm

CHO VII-53 inova400/b/a4113004 c : Nov 30 2004 (CDCl3)

CHO V56 mercury300/b/a5010556 h : Jan 7 2005 (CDCI3)

12.6 12.0 11.4 10.8 ppm

plot at 805 Hz/cm : 8.00 ppm/cm

CHO V-56 inova400/b/a5010623 c : Jan 7 2005 (CDCl3)

plot at 120 MHz/cm : 0.40 ppm/cm

12.6 12.0 11.4 10.8 ppm

CHO 8-50 mercury300/b/a5011059 h : Jan 11 2005 (CDCl3)

Plot at 604 Hz/cm : 8.00 ppm/cm

CHO 8-50 mercury300/b/a5011059 c : Jan 11 2005 (CDCl3)