Supporting Information

"Branch-Selective Reductive Coupling of 2-Vinyl Pyridines and Imines via Rhodium Catalyzed C-C Bond Forming Hydrogenation"

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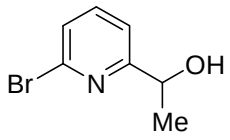
I. Experimental Section

General: All reactions were run under an atmosphere of argon, unless otherwise indicated. Anhydrous solvents were transferred by an oven-dried syringe. Flasks were flame-dried and cooled under a stream of nitrogen. Dichloromethane (DCM) was distilled from calcium hydride. $Rh(cod)_2BARF$ was donated by *Umicore Chemicals* and tri-2-trifurylphosphine was purchased from *Aldrich Chemicals.* The imines were prepared in accordance with literature procedures.[1, 2] All hydrogen-mediated reductive coupling reactions were carried out in 13 x 100 mm test tubes. Analytical thin-layer chromatography (TLC) was carried out using 0.2 mm commercial silica gel plates (DC-Fertigplatten Kieselgel 60 F_{254}). Preparative column chromatography employing silica gel was performed according to the method of Still.[3] Solvents for chromatography are listed as volume/volume ratios. Infrared spectra were recorded on a Perkin-Elmer 1600 spectrometer. High-resolution mass spectra (HRMS, CI method) were obtained on a Karatos MS9 and are reported as m/z (relative intensity). Accurate masses are reported for the molecular ion [M] or [M+1] or a suitable fragment ion. Proton nuclear magnetic resonance (^{1}H-NMR) spectra were recorded with a Varian Gemini (400 MHz) spectrometer. Chemical shifts are reported in delta (δ) units, parts per million (ppm) downfield from trimethylsilane. Coupling constants are reported in Hertz (Hz). Carbon-13 nuclear magnetic resonance (^{13}C-NMR) spectra were recorded with a Varian Gemini 400 (100 MHz) spectrometer. Chemical shifts are reported in delta (δ) units, ppm relative to the center of the triplet at 77.0 ppm for deuteriochloroform. ^{13}C NMR spectra were routinely run with broadband decoupling.

II. Full Characterization Data

1-(6-Bromo-pyridin-2-yl)-ethanol



4a

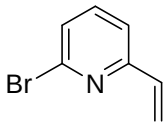
The following procedure is an adaptation of a known protocol.[4] To a flame dried 500 mL round bottom flask equipped with a stir bar was added 2,6-dibromopyridine (19.0 g, 80 mmol, 100 mol%). An addition funnel was attached and the vessel was purged with argon. Dry DCM (250 mL) was added and the reaction vessel was cooled to -78 ^{o}C using a dry ice/acetone bath. A solution of *n*-BuLi in hexanes (35.5 mL, 2.5 M, 88 mmol, 110 mol%) was added dropwise via addition funnel over a period of 15 minutes. The solution became forest green and was allowed to stir for 1 hour at this temperature. Acetaldehyde (6.7 mL, 120 mmol, 150 mol%) was added

(1) Stalick, W. E. *et. al*. *Synth. Commun*., **2003**, *33*, 341.
(2) Li, Z. *et. al*. *Green chem.,* **2006,** *8*, 433.
(3) Still, W. C.; Kahn, M.; Mitra, A. *J. Org. Chem.*, **1978**, *43*, 2923.
(4) Peterson, M. A.; Mitchell, J. R. *J. Org. Chem.,* **1997**, *62*, 8237.

dropwise over a period of 5 minutes and the reaction was allowed to stir for 30 minutes at -78 ^{o}C before it was warmed to room temperature. The color changed from green to brown. Saturated aqueous NH_4Cl (50 mL) was added and the mixture was extracted with DCM (3 x 50 mL). The combined organic phases were washed with brine (2 x 50 mL), dried ($MgSO_4$) and filtered. The solvent was removed *in vacuo* and the resulting residue was purified by flash silica gel column chromatography (R_f = 0.20, 30% EtOAc/hexanes, gradient: 10 - 30% EtOAc/hexanes) to furnish the title compound (11.4 g, 56.40 mmol) as a brown syrup in 72% yield.

^{1}H NMR ($CDCl_3$): δ 7.55 (t, *J* = 7.5 Hz, 1H), 7.38 (d, *J* = 7.5 Hz 1 H), 4.87-4.97 (m, 1H), 3.35 (br s, 1H), 1.50 (d, *J* = 6.8 Hz, 3H).
^{13}C NMR ($CDCl_3$): δ 165.4, 141.2, 139.4, 126.8, 118.7, 69.3, 24.2.
HRMS Cald. for C_7H_8BrNO (M+1): 200.9764, Found: 202.9768.

6-Bromo-2-vinyl-pyridine

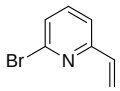


1a

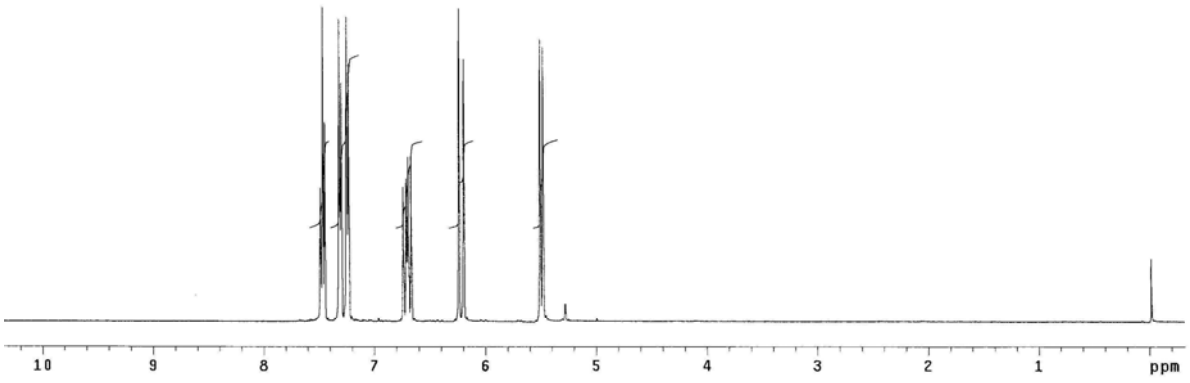
This following procedure is an adaptation of a known protocol.[5] Compound **4a** (11.5 g, 56.90 mmol, 100 mol%) was added to a 250 mL round bottom flask equipped with a stir bar. The flask was cooled to 0 ^{o}C and concentrated H_2SO_4 (70 mL, 1260 mmol, 220 mol%) was added slowly. The reaction mixture became black immediately. The flask was fitted with a reflux condenser and purged with argon and then placed in a 110 ^{o}C oil bath for 16 hours. The reaction mixture was allowed to reach room temperature and was transferred to a 1 L Erlenmeyer flask containing a large stir bar with the aid of water (approximately 150 mL). The mixture was cooled to 0 ^{o}C. Solid NaOH was added in portions until the solution was neutral. At this point, the solution became light brown in color. Any solid materials were removed by filtration and the aqueous solution was extracted with diethyl ether (3 x 50 mL). The combined organic extracts were washed with brine (2 x 50 mL), dried ($MgSO_4$) and filtered. The solvent was removed in vacuo and the resulting residue was purified by flash silica gel column chromatography to provide the title compound (10.8 g, 58.10 mmol) as a light yellow oil in 74% yield, (R_f = 0.30, 5% EtOAc/hexanes). **1a** was stored at -10 ^{o}C. Spectral data is consistent with prior reports.[6]

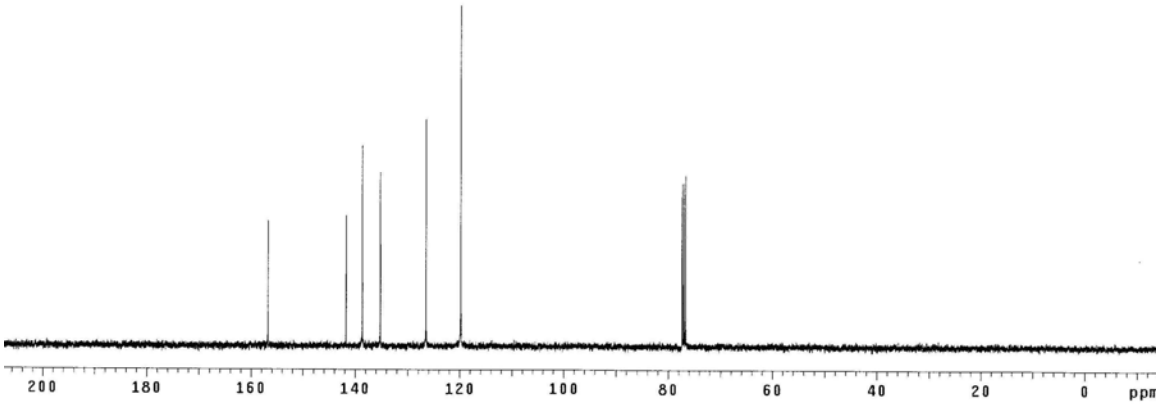
^{1}H NMR ($CDCl_3$): δ 7.43 (dd, *J* = 7.7, 7.7 Hz, 1H), 7.27 (d, *J* = 7.7 Hz, 1H), 7.20 (d, *J* = 7.7 Hz, 1H), 6.66 (dd, *J* = 17.3, 10.5 Hz, 1H), 6.17 (dd, *J* = 17.3, 1.1 Hz, 1H), 5.46 (dd, *J* = 10.5, 1.1 Hz, 1H).
^{13}C NMR ($CDCl_3$): δ 157.4, 142.4, 139.1, 135.8, 127, 120.4, 120.3.
HRMS Cald. for C_7H_6BrN (M+1): 184.9671, Found: 184.9660.

(5) Chelucci, G. *et. al. Synth. Commun.*, **1992**, *22*, 2645.
(6) Abarca, B.; Ballesteros, R.; Blanco, F. *ARKIVOC*, **2007**, iv, 297.

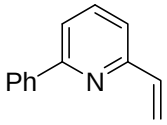


1a





6-Phenyl-2-vinylpyridine

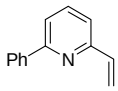


1c

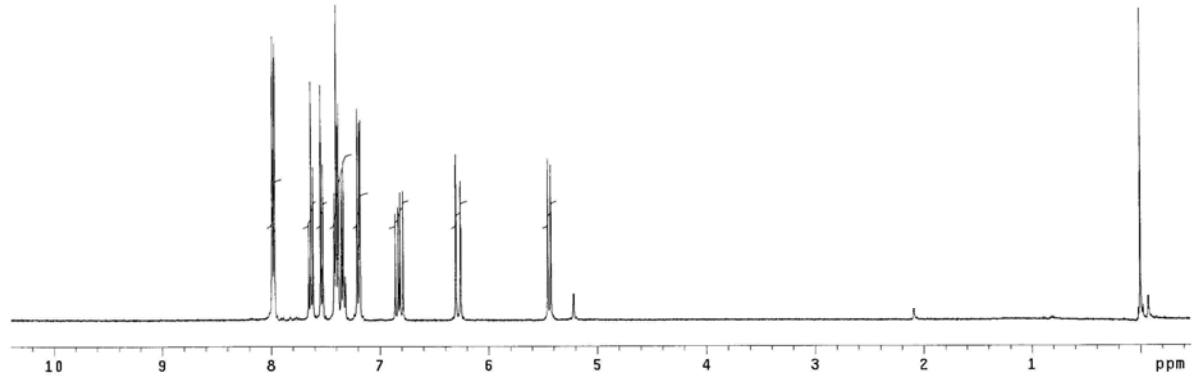
To a degassed solution of 6-bromo-2-vinylpyridine (300 mg, 1.62 mmol, 100 mol%) in toluene (5 mL) in a 50 mL round bottom flask, [$(Ph_3P)_4Pd$] (94 mg, 0.08 mmol, 5 mol%) was added and stirred for 20 minutes at ambient temperature. A degassed suspension of freshly recrystallized phenylboronic acid (300 mg, 1.95 mmol, 120 mol%) in methanol (3 mL) and an aqueous solution of Na_2CO_3 (3 mL, 2 M) were added in succession. The reaction vessel was placed in a 100 $^{\circ}$C oil bath and was allowed to stir under an argon atmosphere for 16 hours.[7] The crude reaction mixture was cooled to ambient temperature and extracted with diethyl ether (2 x 20 mL). The combined organic layers were washed with water (20 mL) followed by brine (20 mL), dried (Na_2SO_4) and filtered. The solvent was removed *in vacuo* and the residue was purified by flash silica gel column chromatography (R_f = 0.25, 2% EtOAc/hexanes) to furnish the title compound (152 mg, 0.61 mmol) as a colorless oil in 52% yield.

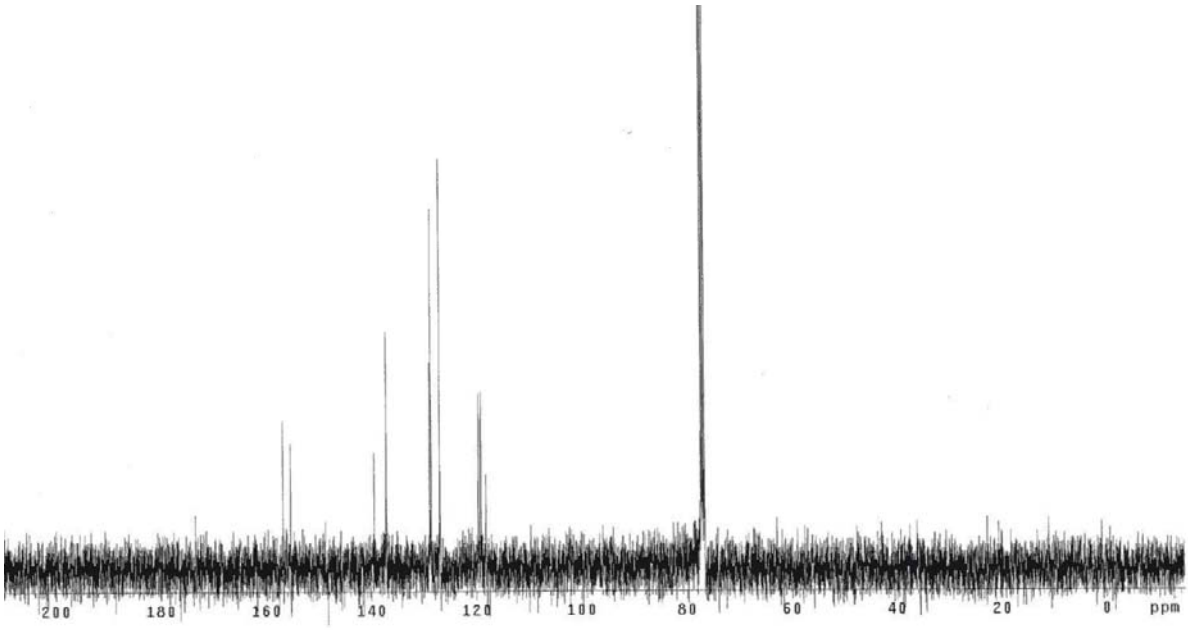
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.98 (d, *J* = 8.4 Hz, 2H), 7.63 (t, *J* = 7.6 Hz, 1H), 7.53 (d, *J* = 7.6 Hz, 1H), 7.41-7.38 (m, 2H), 7.34 (d, *J* = 7.6 Hz, 1H), 7.20 (dd, *J* = 7.6, 3.2 Hz, 1H), 6.85-6.78 (m, 1H), 6.28 (dd, *J* = 17.2, 1.2 Hz, 1H), 5.44 (dd, *J* = 11.2, 1.6 Hz, 1H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 156.8, 155.4, 139.4, 137.1, 128.8, 128.6, 126.5, 126.9, 119.6, 119.1, 118.2.
HRMS Calcd. for $C_{13}H_{11}N$ (M+1): 181.0189, Found: 181.0186.
FTIR (NaCl Film): 3058, 1586, 1564, 1456, 1444, 1202, 1160, 922, 821, 764, 690 cm^{-1}.

(7) Chuang C-I. *et. al. Inorg. Chem.*, **1995,** *34***,** 2562.

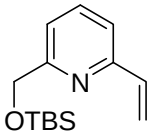


1c





6-((*tert*-butyldimethylsilyloxy) methyl)-2-vinylpyridine



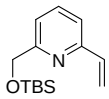
1d

A stirred solution of 6-vinylpicolinaldehyde[8] (540 mg, 4.06 mmol, 100 mol%) in THF (5 mL) in a 50 mL round bottomed flask was cooled to 0 °C and sodium borohydride (75 mg, 2.02 mmol, 50 mol%) was added and stirring was continued for 15 minutes at 0 °C. The reaction mixture was quenched with aqueous HCl (0.5 mL, 0.1 M), diluted with water (20 mL) and the resulting mixture was extracted with EtOAc (2 x 15 mL). The combined organic layers were washed with water (20 mL) and brine (20 mL), dried (Na_2SO_4) and filtered. The solvent was removed *in vacuo* and the crude alcohol (480 mg) was used directly in the subsequent next step.

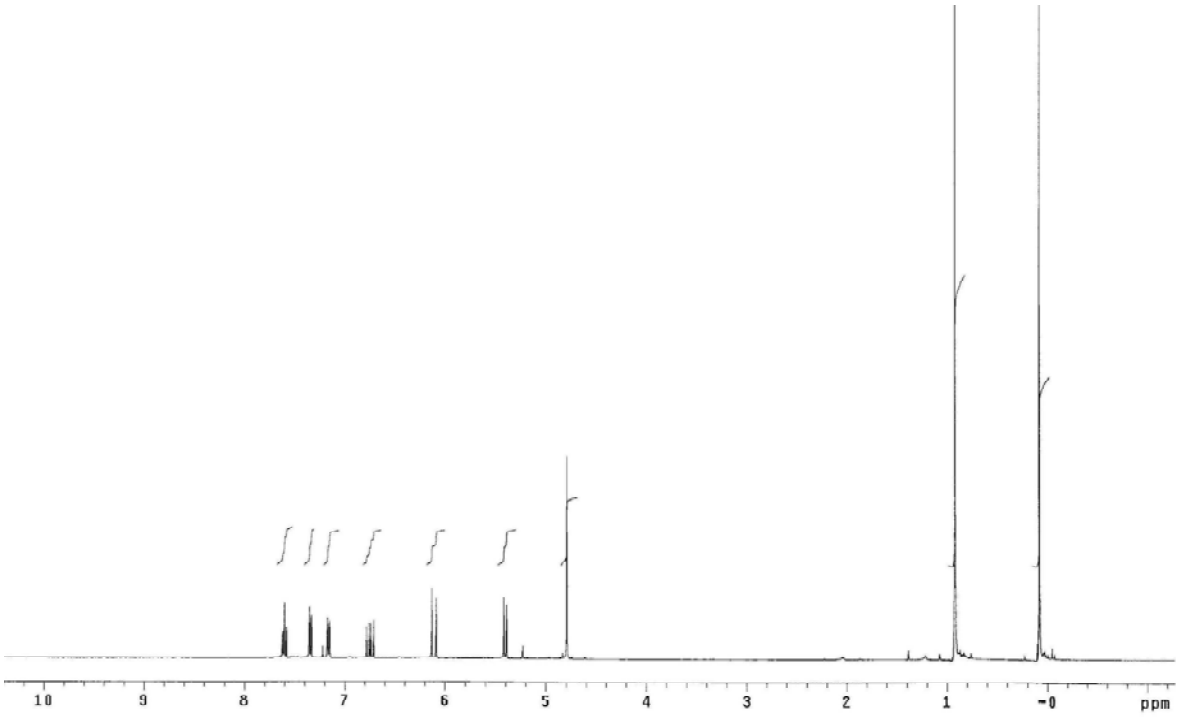
The crude alcohol (480 mg, 3.55 mmol, 100 mol%) was dissolved in DMF (6 mL) in a 50 mL round bottom flask and cooled to 0 °C. Imidazole (360 mg, 5.33 mmol, 150 mol%) and *tert*-butyldimethylsilyl chloride (800 mg, 5.33 mmol, 150 mol%) were added and the reaction was allowed to warm to ambient temperature and stirring was continued for 5 hours under an argon atmosphere. Once the reaction was complete it was diluted with water (20 mL) and extracted with diethyl ether (2 x 20 mL). The organic layer was separated, washed with brine (20 mL), dried (anhydrous Na_2SO_4) and filtered. The solvent was removed *in vacuo* and the residue was purified by flash silica gel column chromatography (R_f = 0.23, 5% diethyl ether/hexanes) to furnish the title compound (620 mg, 2.47 mmol) as a colorless oil in 62% yield over two steps.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.60 (t, *J* = 7.6 Hz, 1H), 7.34 (d, *J* = 8.0 Hz, 1H), 7.16 (d, *J* = 8.0 Hz, 1H), 6.74 (ddd, *J* = 17.6, 10.8, 1.2 Hz, 1H), 6.10 (dd, *J* = 17.6, 1.2, 1H), 5.40 (dd, *J* = 11.2, 1.6 Hz, 1H), 4.74 (s, 2H), 0.92 (s, 9H), 0.08 (s, 6H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 161.1, 154.6, 137.0, 136.9, 119.0, 118.6, 117.9, 66.1, 25.8, 18.3, -5.4.
HRMS Calcd. for $C_{14}H_{23}NOSi$ (M+1): 250.1627, Found: 250.1632.
FTIR (NaCl Film): 2954, 2928, 2885, 2856, 1582, 1471, 1450, 1254, 1152, 1113, 989, 929, 835, 808, 775, 749 cm^{-1}.

(8) He, W. *et. al. Bioorg. Med. Chem. Lett.*, **2006,** *16,* 2109.


N
OTBS

1d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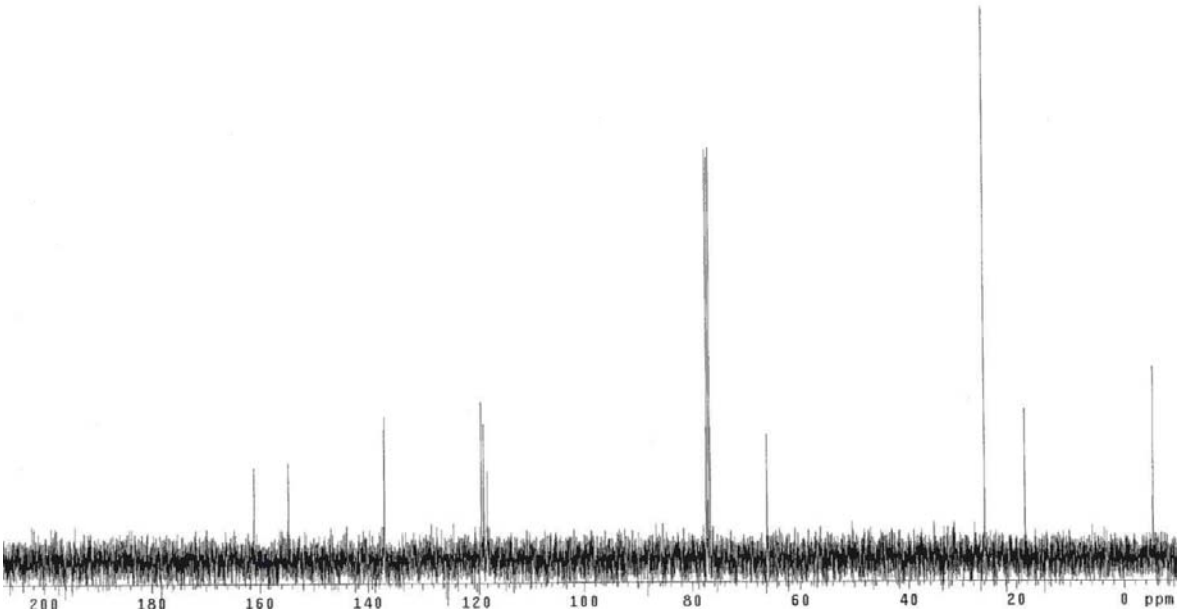
200
180
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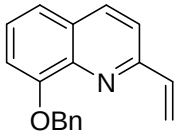
8-(benzoloxy)-2-vinylquinoline

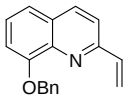


1e

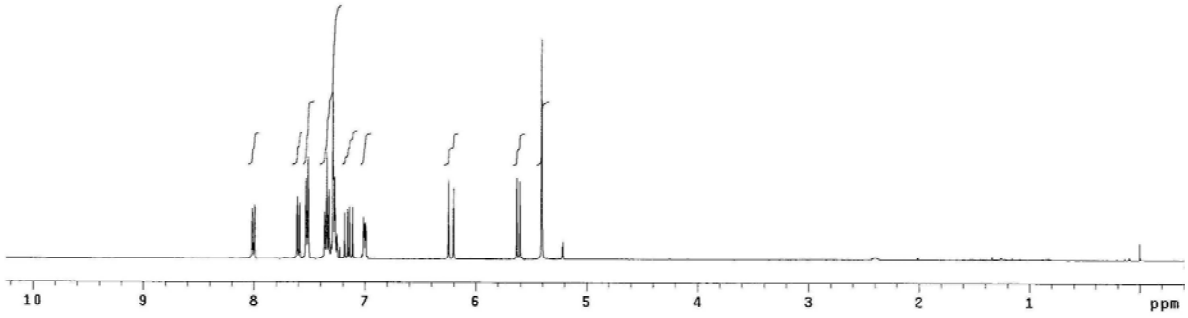
To a stirred suspension of methyltriphenylphosphonium bromide (4.46 g, 12.5 mmol, 110 mol%) in THF (20 mL) at 0 °C in a 100 mL round bottom flask was added a THF solution (1 M) of LHMDS (12.5 mL, 12.5 mmol, 110 mol%). The mixture was allowed to stir under an argon atmosphere for 45 minutes, at which point a THF solution (12 mL) of 8-(benzyloxy)quinoline-2-carbaldehyde[9] (3.01 g, 11.35 mmol, 100 mol%) at 0 °C was added. The reaction mixture was allowed to warm to ambient temperature and was allowed to stir for 30 minutes. Saturated aqueous NH_4Cl (15 mL) was added and the resulting mixture was extracted with diethyl ether (2 x 50 mL). The organic layer was separated, washed with brine solution (20 mL) dried (Na_2SO_4), and filtered. The solvent was removed *in vacuo* and the title compound was purified by flash silica gel column chromatography (R_f = 0.30, 5% EtOAc /hexanes) to furnish the title compound (2.11 g, 8.05 mmol) as a thick brown oil in 68% yield.

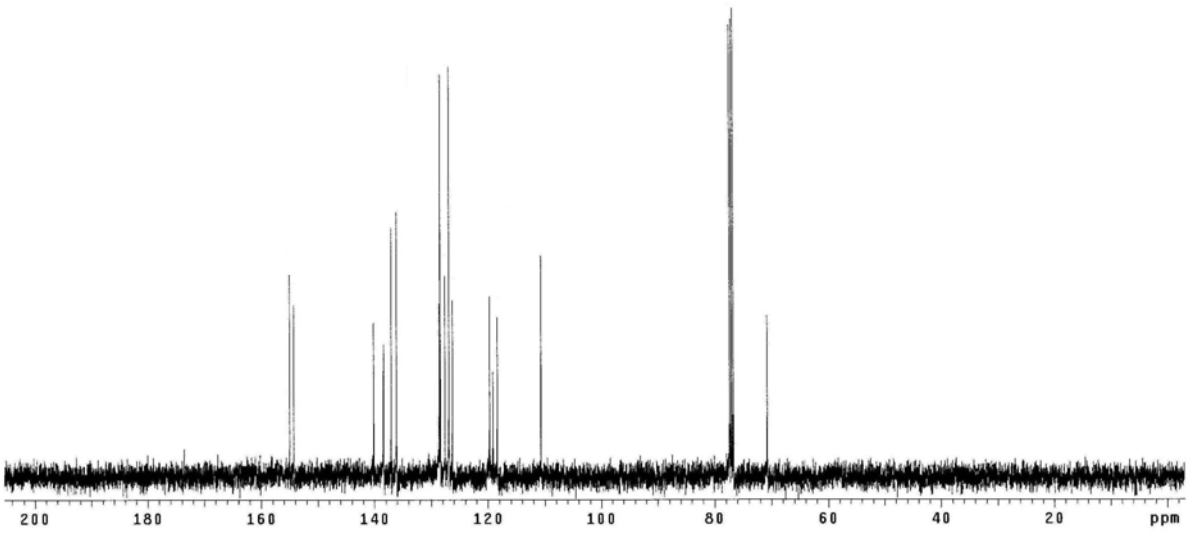
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.00 (dd, *J* = 8.8, 1.6 Hz, 1H), 7.60 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.52 (d, *J* = 7.2 Hz, 1H), 7.34 (t, *J* = 7.6 Hz, 1H), 7.29-7.26 (m, 5H), 7.18-7.11 (m, 1H), 6.98 (dd, *J* = 6.8, 2.8 Hz, 1H), 6.22 (d, *J* = 18.0 Hz, 1H), 5.62 (d, *J* = 10.8 Hz, 1H), 5.40 (s, 2H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 154.9, 154.2, 140.0, 138.3, 137.0, 136.0, 128.5, 128.3, 127.5, 126.8, 126.2, 119.7, 119.1, 118.3, 110.6, 70.7.
HRMS Calcd. for $C_{16}H_{16}NO$ (M+1): 262.1232, Found: 262.1235.
FTIR (NaCl Film): 3059, 2968, 1598, 1610, 1503, 1458, 1431, 1328, 1263, 1092, 1076, 1015, 931, 878, 860, 754, 730, 694 cm^{-1}.

(9) Petkova, E. G. *et. al.*, *Polyhedron*, 2001, *20*, 747.

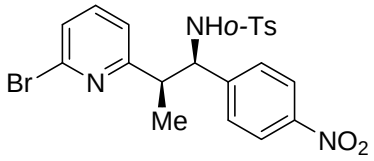


1e





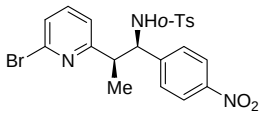
General Procedure for Hydrogenative Reductive Coupling, Preparation of *N*-((1*R*, 2*R*)-2-(6-bromopyridin-2-yl)-1-(4-nitrophenyl) propyl)-2-methylbenzenesulfonamide



3a

An oven dried test tube (13 x 100 mm) was charged with a stir bar, imine **2a** (80 mg, 0.26 mmol, 100 mol%), [Rh(cod)$_2$BARF] (15.6 mg, 13.20 μmol, 5 mol%), tri(2-furyl)phosphine (7.4 mg, 31.70 μmol, 12 mol%), and anhydrous sodium sulfate (75 mg, 0.53 mmol, 200 mol%). The vessel was sealed with a rubber septum, evacuated and placed under an argon atmosphere. A degassed solution of 6-bromo-2-vinylpyridine **1a** (144 mg, 0.79 mmol) in DCM (0.9 mL) was added to the reaction vessel via syringe and the solution was sparged with argon for 5 seconds. The solution was stirred until homogeneous, at which point hydrogen gas was bubbled directly into the solution for 5 seconds with the aid of a balloon using an 11½ inch 21 gauge needle. The needle was pulled above the solution and the reaction mixture was allowed to stir under a hydrogen atmosphere for 72 hr. The reaction mixture was concentrated and the title compound (128 mg, 0.196 mmol) was isolated as a pale yellow solid in 97% yield after purification by flash silica gel column chromatography (separable mixture of diastereomers in 3:1 ratio, $R_{f\ major}$ = 0.23, $R_{f\ minor}$ = 0.27, 25% EtOAc/hexanes, gradient: 10 - 25% EtOAc/hexanes).

^{1}H NMR (400 MHz, $CDCl_3$, Major Isomer): δ 7.76 (d, *J* = 8.4 Hz, 2H), 7.55 (d, *J* = 7.6 Hz, 1H), 7.30-7.19 (m, 3H), 6.98-7.12 (m, 2H), 6.91 (d, *J* = 8.8 Hz, 2H), 6.78 (d, *J* = 6.8 Hz, 1H), 6.67 (d, *J* = 6.8 Hz, 1H), 4.69 (t, *J* = 6.4 Hz, 1H), 3.22 (quintet, *J* = 6.8 Hz, 1H), 2.49 (s, 3H), 1.20 (d, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 162.1, 146.8, 146.0, 141.2, 139.0, 137.9, 136.5, 132.6, 132.2, 129.0, 128.2, 126.6, 126.1, 125.9, 122.8, 121.1, 61.6, 45.3, 20.4, 15.7.
HRMS Cald. for $C_{21}H_{20}BrN_3O_4S$ (M+1): 490.0358, Found: 490.0331.
FTIR (NaCl Film): 3286, 2952, 2850, 1606, 1581, 1519, 1434, 1346, 1159, 131, 1066, 910, 853, 760, 733 cm^{-1}.
MP = 143-145 0 ^oC.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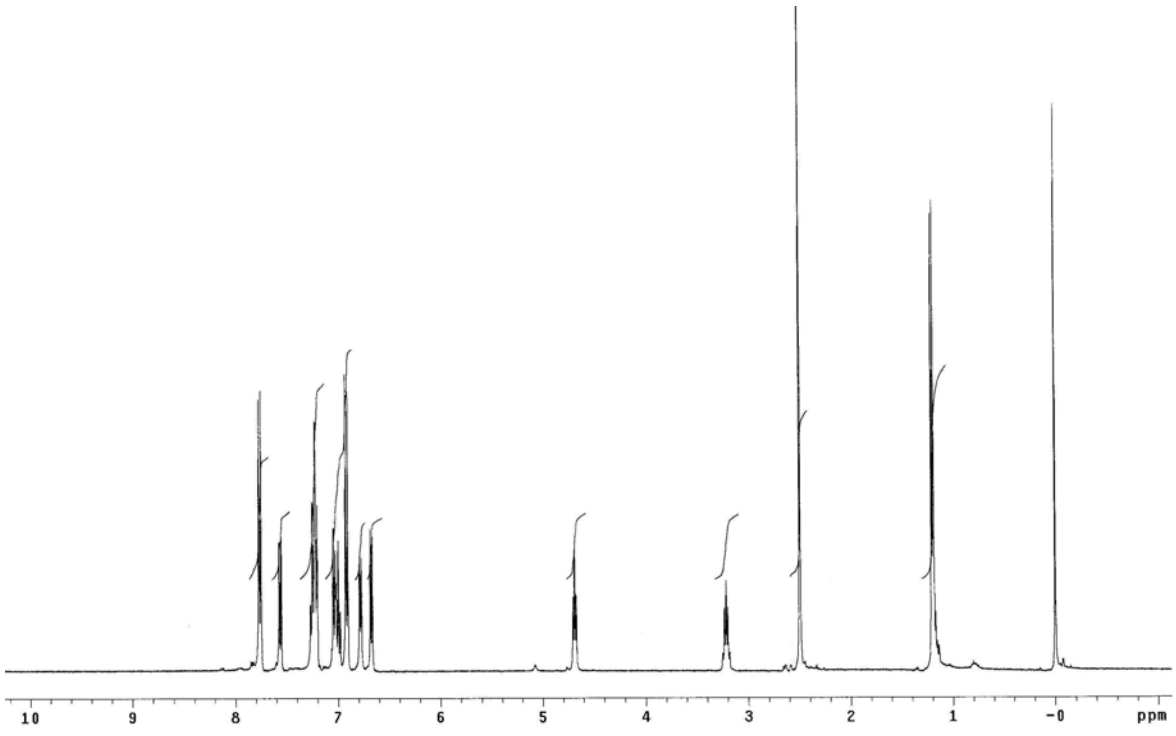
NO2

3a, major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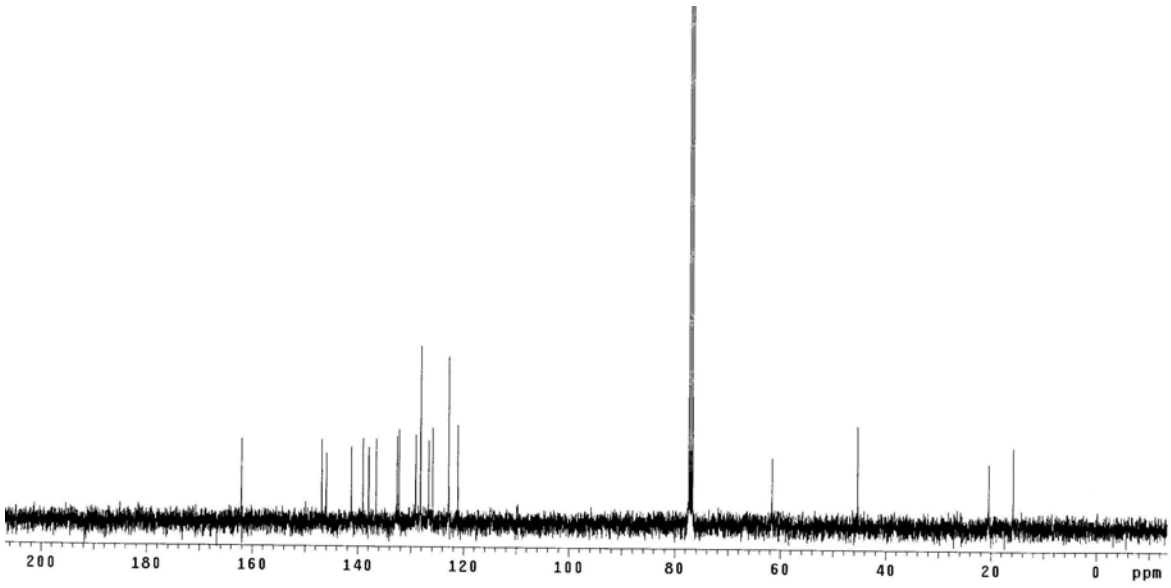
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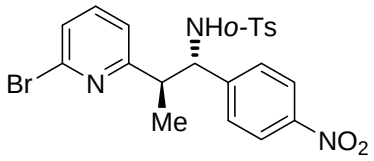
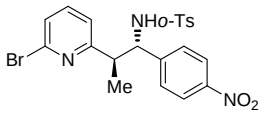
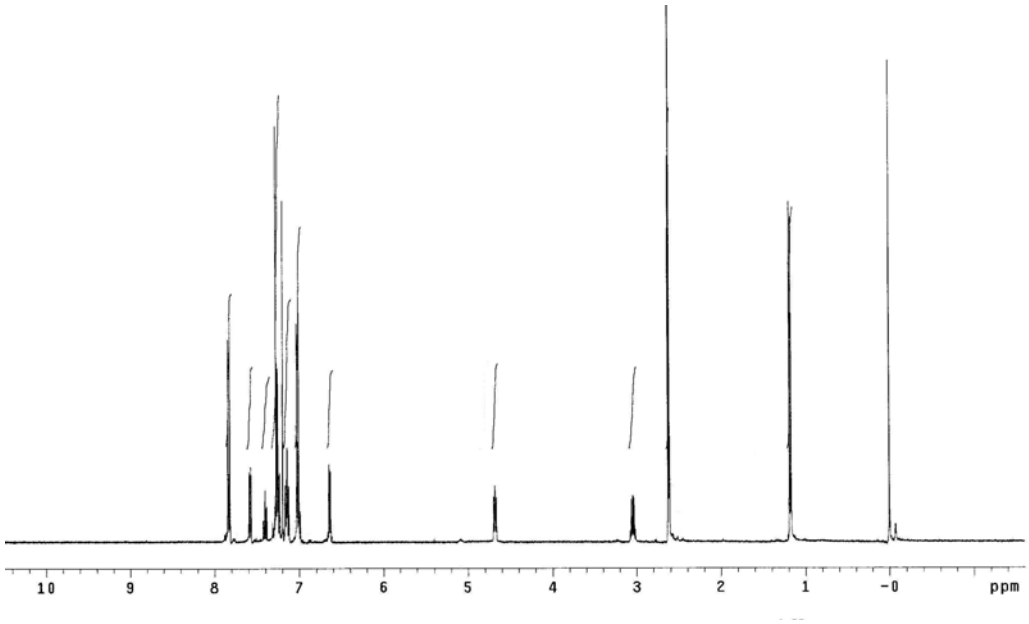


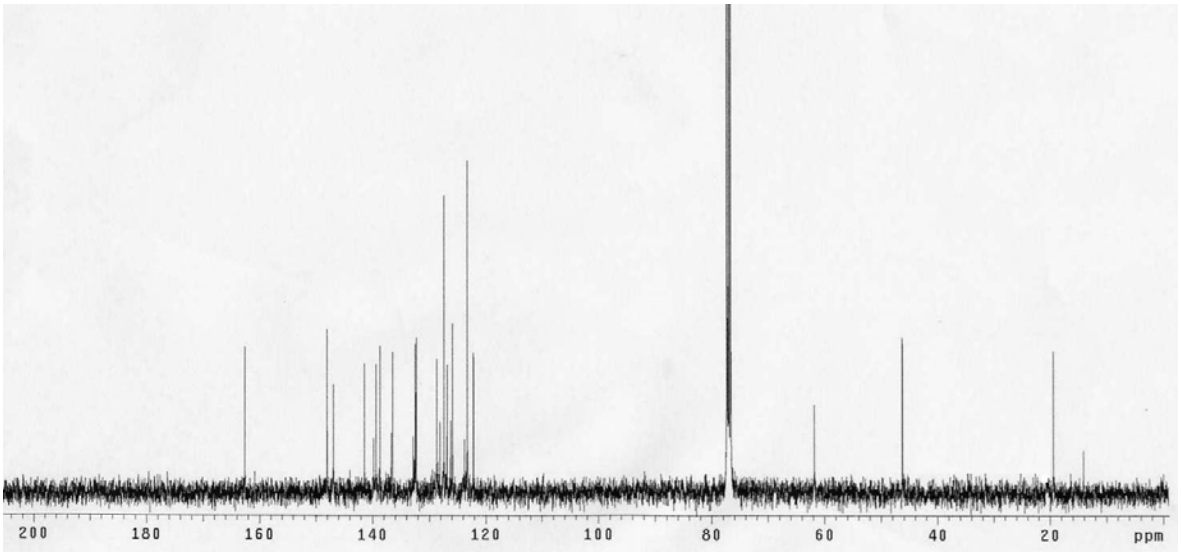
3a

^{1}H NMR (400 MHz, $CDCl_3$, Minor Isomer): δ 7.91 (d, *J* = 8.4 Hz, 2H), 7.66 (d, *J* = 7.6 Hz, 1H), 7.34-7.24 (m, 5H), 7.21 (t, *J* = 9.6 Hz, 1H), 7.10 (d, *J* = 9.2 Hz, 2H), 6.73-6.70 (m, 1H), 4.75 (t, *J* = 5.6 Hz, 1H), 3.15-3.08 (m, 1H), 2.67 (s, 3H), 1.24 (d, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 162.6, 147.9, 146.8, 146.1, 141.4, 139.3, 138.6, 136.4, 132.4, 132.3, 128.6, 127.3, 126.8, 126.1, 125.8, 123.2, 122.1, 61.8, 46.2, 20.4, 14.8.
HRMS Calcd. for $C_{21}H_{20}BrN_3O_4S$ (M+1): 490.0358, Found: 490.0329.
FTIR (NaCl Film): 3286, 2952, 2850, 1606, 1581, 1519, 1434, 1346, 1159, 131, 1066, 910, 853, 760, 733 cm^{-1}.
MP = 124-128 0 ^{o}C.

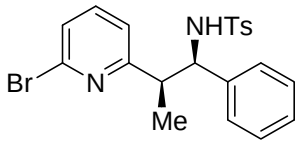

NHo-Ts
Br
N
Me
NO2

3a, minor


10
9
8
7
6
5
4
3
2
1
-0
ppm


200
180
160
140
120
100
80
60
40
20
ppm

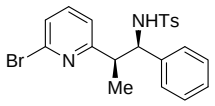
***N*-[2-(6-Bromo-pyridin-2-yl)-1-phenyl-propyl]-4-methyl-benzenesulfonamide**



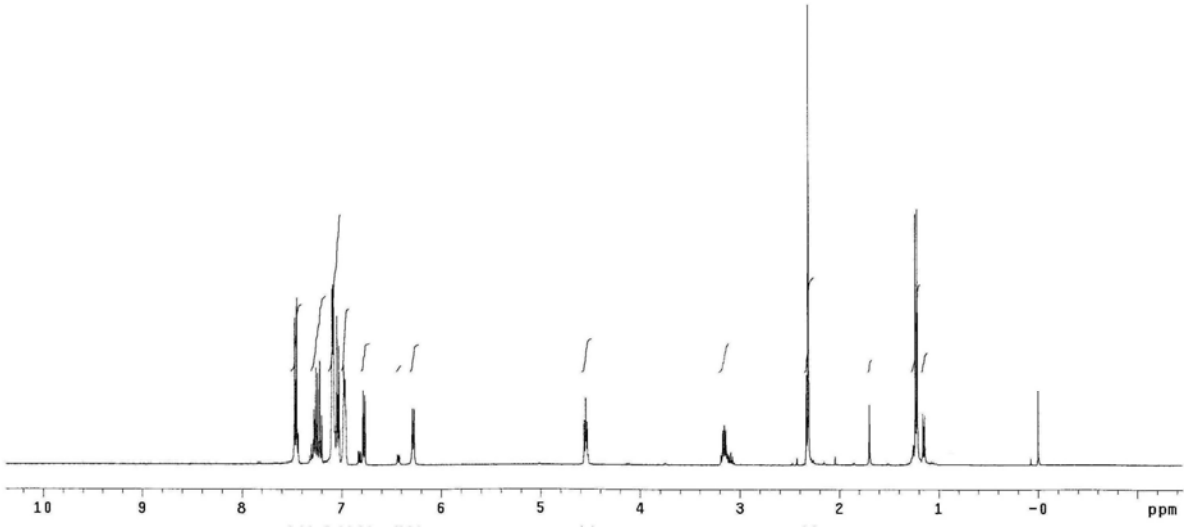
3b

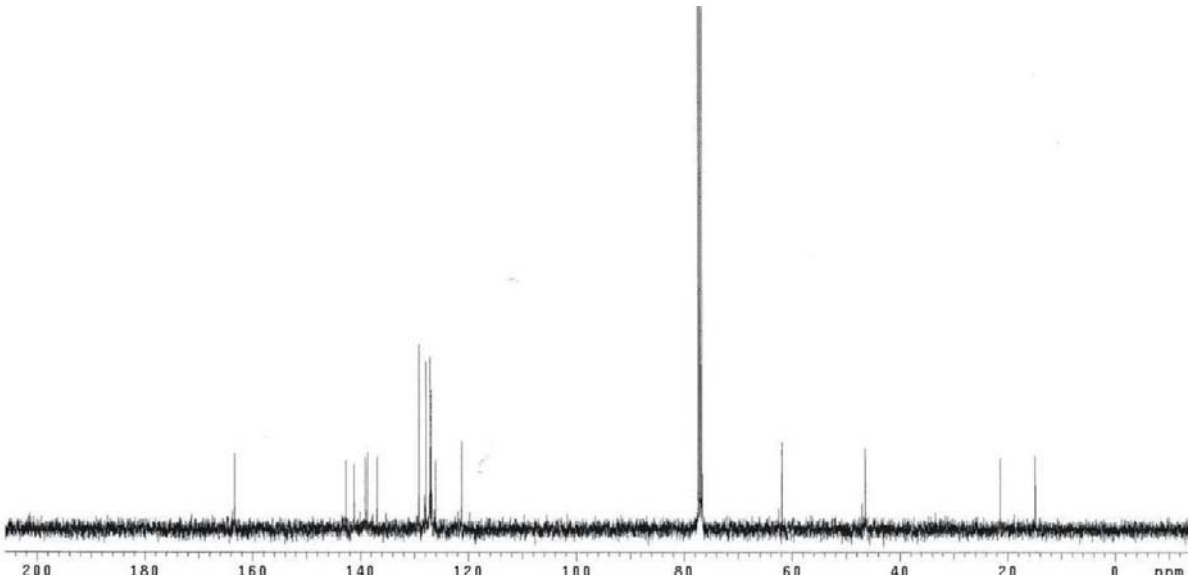
In accordance with the general procedure, 6-bromo-2-vinylpyridine **1a** (144 mg, 0.79 mmol, 300 mol%) was coupled to imine **2b** (68 mg, 0.26 mmol, 100 mol%) to provide the title compound (93 mg, 0.21 mmol) as a colorless liquid in 80% yield after purification by flash silica gel column chromatography (Inseparable mixture of diastereomers in 3:1 ratio, R_f = 0.22, 20% EtOAc/hexanes, gradient: 10 - 20% EtOAc/hexanes). *Spectral data is reported for the major isomer.*

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.43 (d, *J* = 8.0 Hz, 2H), 7.28-7.20 (m, 3H), 7.10-7.08 (m, 2H), 7.04 (d, *J* = 7.6 Hz, 2H), 6.98-6.95 (m, 2H), 6.77 (dd, *J* = 7.6 Hz, 1.2 Hz, 1H), 6.26 (d, *J* = 6.4 Hz, 1H), 4.54 (t, *J* = 6.4 Hz, 1H), 3.19-3.12 (m, 1H), 2.31 (s, 3H), 1.22 (d, *J* = 6.8 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 163.3, 142.7, 141.2, 139.1, 138.7, 136.9, 129.1, 127.9, 127.1, 127.08, 126.9, 126.1, 121.2, 61.9, 46.4, 21.4, 14.9.
HRMS Calcd. for $C_{21}H_{21}BrN_2O_2S$ (M+1): 444.0507, Found: 445.0580.
FTIR (NaCl Film): 3276, 2980, 2895, 1581, 1598, 1454, 1432, 1322, 1155, 1123, 1091, 1155, 1123, 811, 678 cm^{-1}.

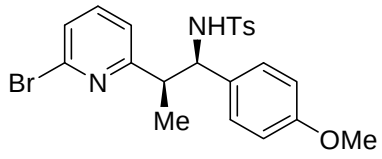

NHTs
Br
N
Me

3b


10
9
8
7
6
5
4
3
2
1
-0
ppm


200
180
160
140
120
100
80
60
40
20
0
ppm

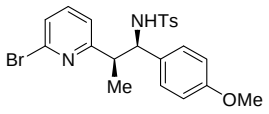
***N*-[2-(6-Bromo-pyridin-2-yl)-1-(4-methoxy-phenyl)-propyl]-4-methyl-benzenesulfonamide**



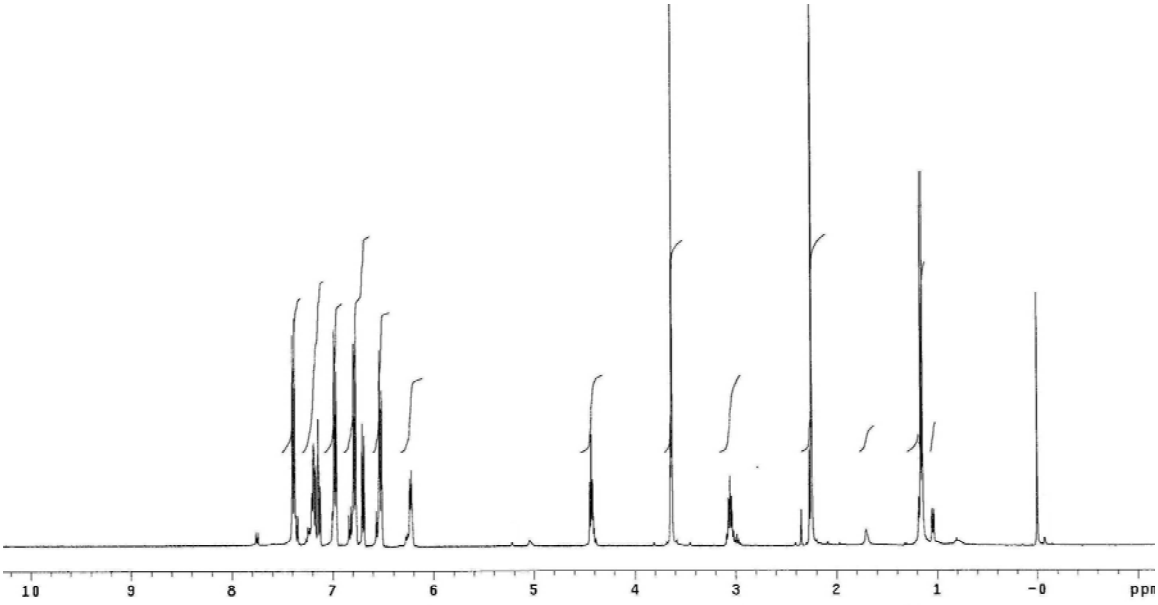
3c

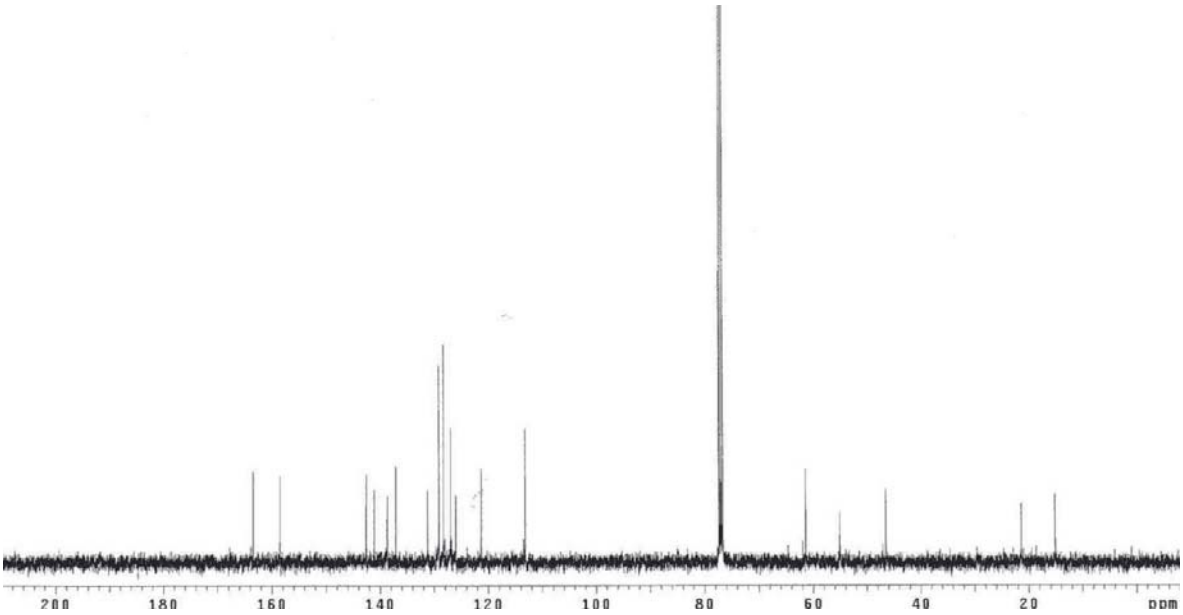
In accordance with the general procedure, 6-bromo-2-vinylpyridine **1a** (144 mg, 0.79 mmol, 300 mol%) was coupled to imine **2c** (76 mg, 0.26 mmol, 100 mol%) to provide the title compound (88 mg, 0.18 mmol) as a colorless liquid in 72% yield after purification by flash silica gel column chromatography (Inseparable mixture of diastereomers in 5:1 ratio, R_f = 0.25, 30% EtOAc/hexanes, gradient: 10 - 30% EtOAc/hexanes). *Spectral data is reported for the major isomer.*

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38 (d, *J* = 8.0 Hz, 2H), 7.20-7.12 (m, 2H), 6.97 (d, *J* = 8.0 Hz, 2H), 6.78 (d, *J* = 8.8 Hz, 2H), 6.69 (d, *J* = 7.6 Hz, 1H), 6.52 (dd, *J* = 8.4, 0.8 Hz, 2H), 6.46 (d, *J* = 6.4 Hz, 1H), 4.43 (t, *J* = 6.4 Hz, 1H), 3.63 (s, 3H), 3.06 (quintet, *J* = 6.4 Hz, 1H), 2.25 (s, 3H), 1.15 (d, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 163.3, 142.7, 141.2, 139.1, 138.7, 136.9, 129.1, 127.9, 127.1, 127.08, 126.9, 126.1, 121.2, 61.9, 55.1, 46.4, 21.4, 14.9.
HRMS Calcd. for $C_{21}H_{21}BrN_2O_2S$ (M+1): 444.0507, Found: 445.0580.
FTIR (NaCl Film): 3275, 2918, 1581, 1553, 1433, 1409, 1321, 1304, 1248, 1156, 1124, 1032, 833, 705, 666 cm^{-1}.

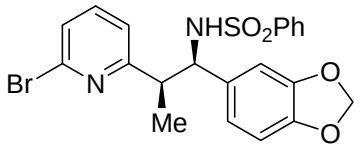

NHTs
Br
N
Me
OMe

3c


10
9
8
7
6
5
4
3
2
1
-0
ppm


200
180
160
140
120
100
80
60
40
20
ppm

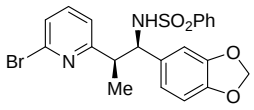
***N*-[1-Benzo [1,3]dioxol-5-yl-2-(6-bromo-pyridin-2-yl)-propyl]-benzenesulfonamide**



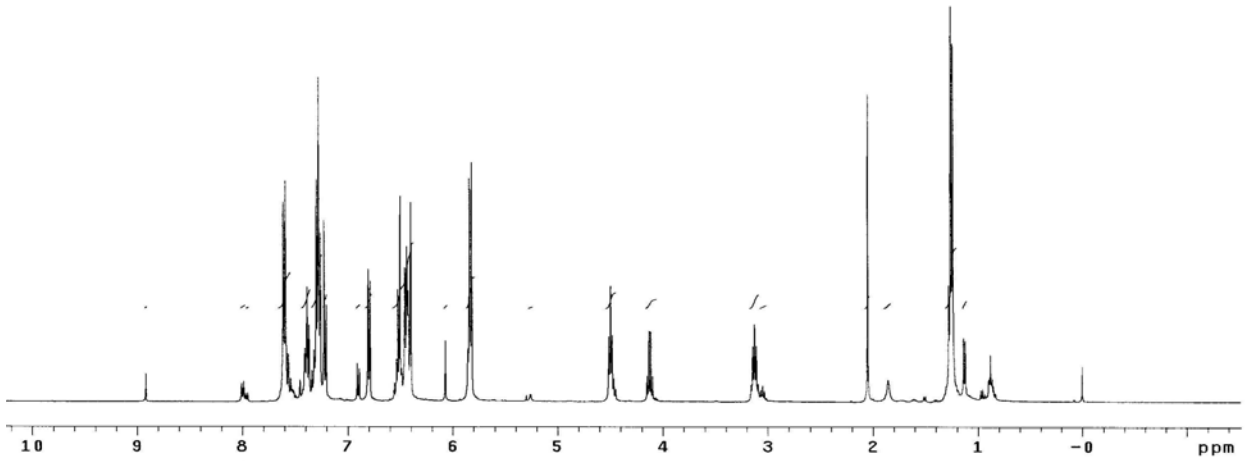
3d

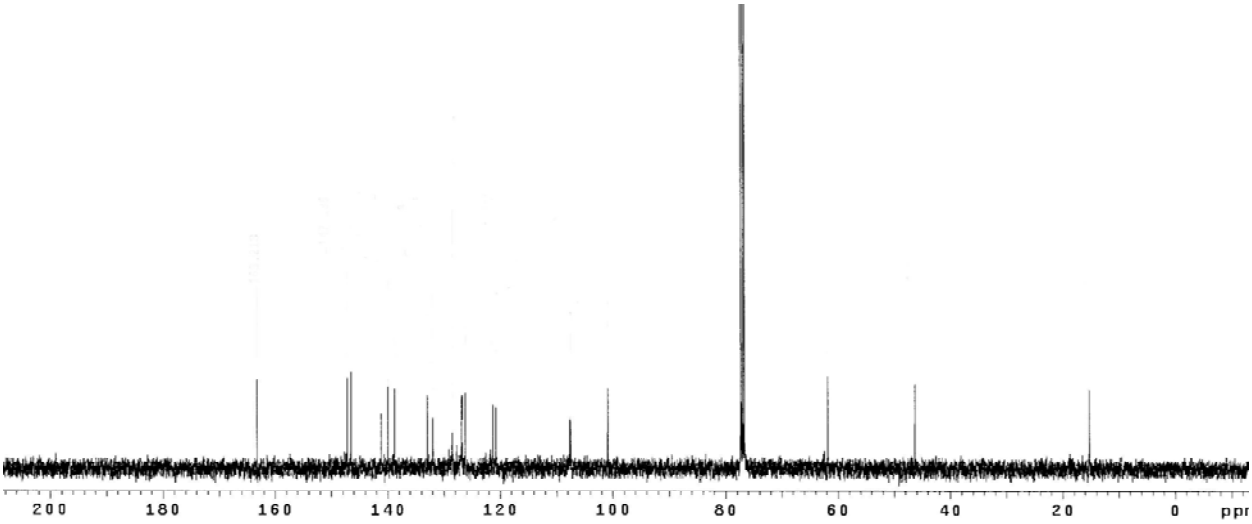
In accordance with the general procedure, 6-bromo-2-vinylpyridine **1a** (144 mg, 0.79 mmol, 300 mol%) was coupled to imine **2d** (76 mg, 0.26 mmol, 100 mol%) to provide the title compound (117 mg, 0.24 mmol) as a white solid in 91% yield after purification by flash silica gel column chromatography (Inseparable mixture of diastereomers in 5:1 ratio, R_f = 0.45, 50% EtOAc, gradient: 10 - 50% EtOAc/hexanes). *Spectral data is reported for the major isomer.*

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.60 (d, *J* = 7.6 Hz, 2H), 7.43-7.21 (m, 6H), 6.8 (d, *J* = 7.6 Hz, 1H), 6.56- 6.40 (m, 4H), 5.84 (d, *J* = 1.6 Hz, 1H), 5.82 (d, *J* = 8.0 Hz, 1H), 4.51-4.48 (m, 1H), 3.16-3.09 (m, 1H), 1.24 (d, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 163.2, 147.1, 146.5, 141.1, 139.9, 138.8, 132.9, 132.0, 128.5, 126.9, 126.7, 126.2, 121.3, 120.8, 107.6, 107.5, 100.8, 61.8, 46.3, 15.2.
HMRS: Cald. for $C_{21}H_{19}BrN_2O_4S$ (M+1): 475.0200, Found: 475.0327.
FTIR (NaCl film): 3274, 2893, 1581, 1554, 1503, 1489, 1446, 1433, 1371, 1345, 1239, 1157, 1125, 1092, 1037 cm^{-1}.

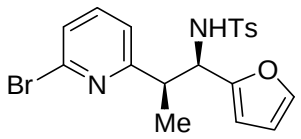

NHSO2Ph
Br
N
Me
O
O

3d


10
9
8
7
6
5
4
3
2
1
−0
ppm


200
180
160
140
120
100
80
60
40
20
0
ppr

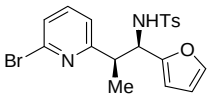
***N*-[2-(6-Bromo-pyridin-2-yl)-1-furan-2-yl-propyl]-4-methyl-benzenesulfonamide**



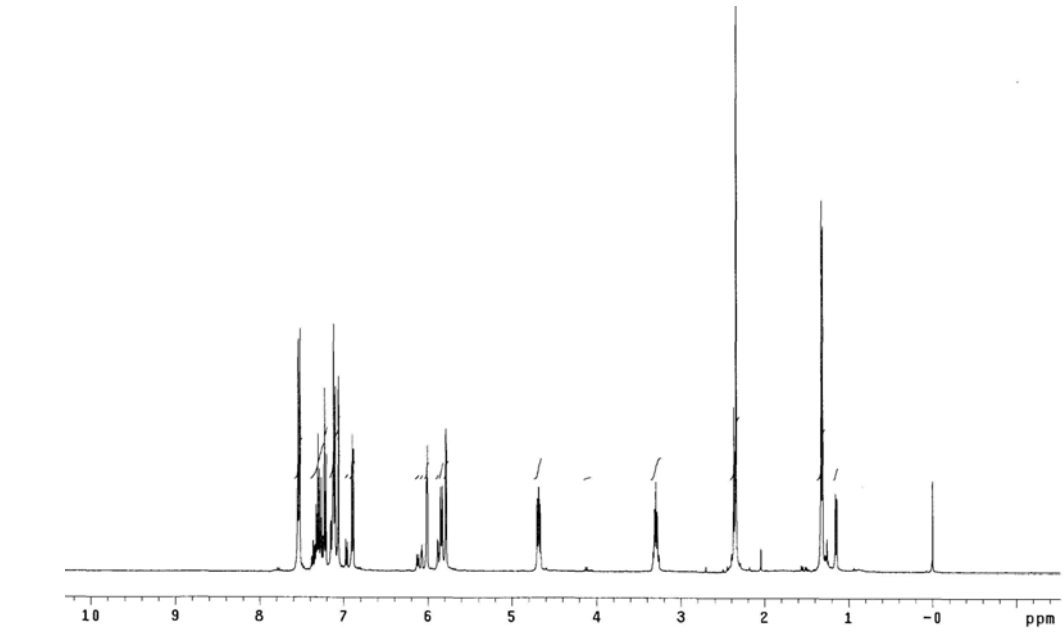
3e

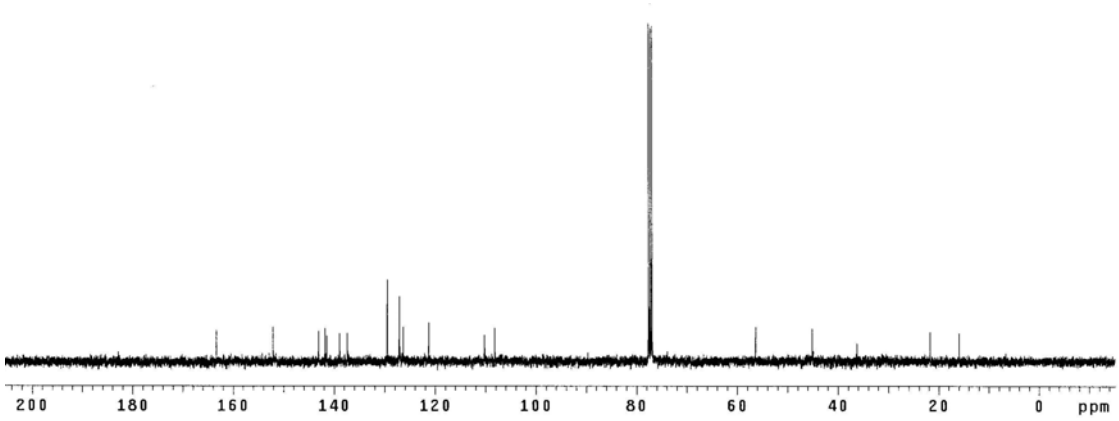
In accordance with the general procedure, 6-bromo-2-vinylpyridine **1a** (144 mg, 0.79 mmol, 300 mol%) was coupled to imine **2e** (66 mg, 0.26 mmol, 100 mol%) to provide the title compound (114 mg, 0.26 mmol) as a colorless oil in 99% yield after purification by flash silica gel column chromatography (Inseparable mixture of diastereomers in 4:1 ratio, R_f = 0.45, 20% EtOAc, gradient: 10 - 20% EtOAc/hexanes). *Spectral data is reported for the major isomer.*

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.54 (d, *J* = 8.0 Hz, 2H), 7.39-7.21 (m, 3H), 7.16-7.06 (m, 3H), 6.90 (d, *J* = 7.6 Hz, 1H), 6.02-6.01 (m, 1H), 5.81 (d, *J* = 8.8 Hz, 1H), 5.79 (d, *J* = 2.8 Hz, 1H), 4.68 (dd, *J* = 6.4, 2.0 Hz, 1H), 3.33-3.26 (m, 1H), 3.34 (s, 3H), 1.33 (d, *J* = 7.4 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 163.4, 152, 143.1, 141.8, 141.4, 138.9, 137.3, 129.5, 127.1, 126.3, 121.3, 110.2, 108.2, 56.4, 45.1, 44.8, 36.2, 21.7, 15.9.
HMRS: Cald. for $C_{19}H_{19}BrN_2O_3S$ (M+1): 435.0368, Found: 435.0373.
FTIR (NaCl film): 3271, 2920, 1581, 1554, 1496, 1433, 1410, 1328, 1231, 1156, 1124, 1092, 1048, 1011 cm^{-1}.

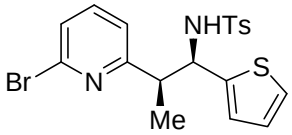

NHTs
Br
N
O
Me

3e


10
9
8
7
6
5
4
3
2
1
-0
ppm


200
180
160
140
120
100
80
60
40
20
0
ppm

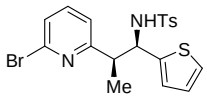
***N*-((1*R*, 2*R*)-2-(6-bromopyridin-2-yl)-1-(thiophen-2-yl)propyl)-4-methylbenzenesulfonamide**



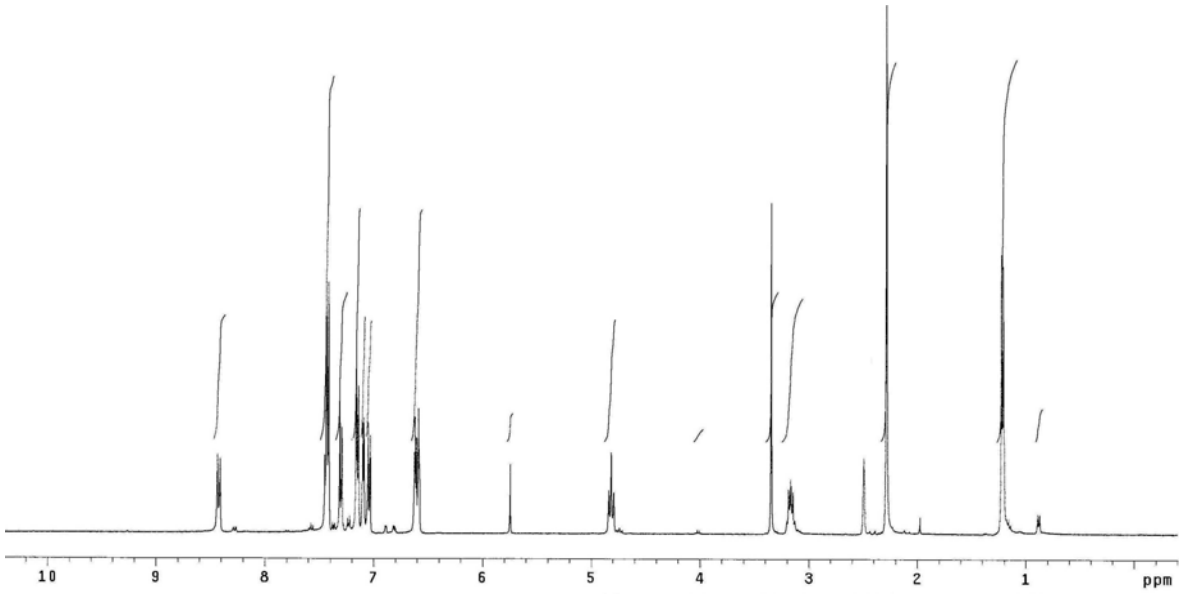
3f

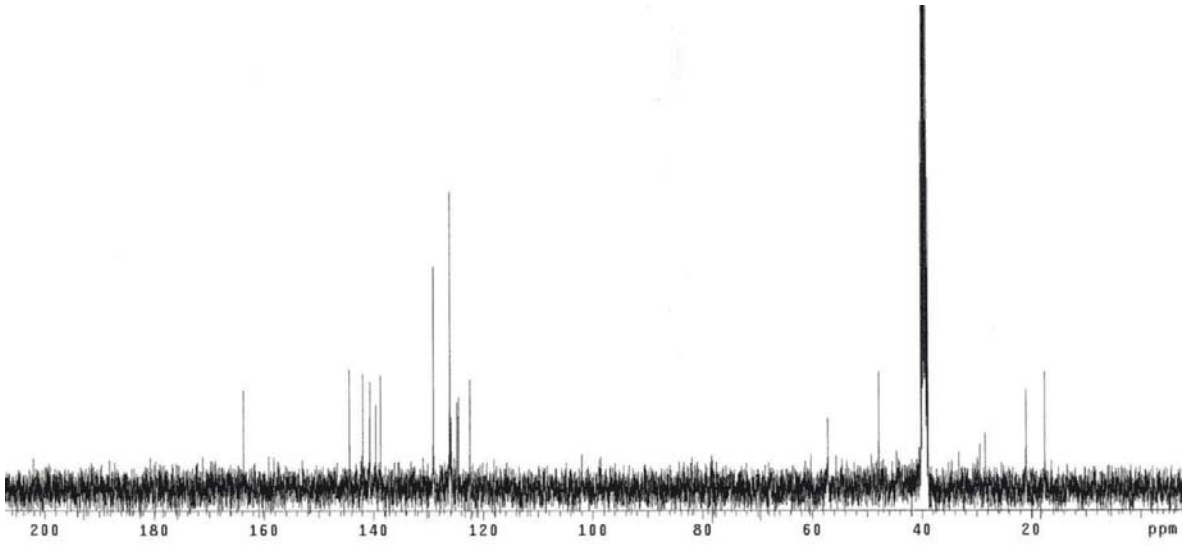
In accordance with the general procedure, 6-bromo-2-vinylpyridine **1a** (73 mg, 0.79 mmol, 300 mol%) was coupled to imine **2f** (70 mg, 0.26 mmol, 100 mol%) to provide the title compound (87 mg, 0.19 mmol) as a white solid in 72% yield after purification by flash silica gel column chromatography (Inseparable mixture of diastereomers in 7:1 ratio, R_f = 0.25, 20% EtOAc/hexanes, gradient: 10 - 20% EtOAc/hexanes). *Spectral data is reported for the major isomer*.

^{1}H NMR (400 MHz, CD_3SOCD_3): δ 8.43 (d, *J* = 9.2 Hz, 1H), 7.43 (d, *J* = 8.4 Hz, 2H), 7.31 (d, *J* = 7.6 Hz, 1H), 7.15 (d, *J* = 8.4 Hz, 2H), 7.10 (dd, *J* = 4.8, 1.6 Hz, 1H), 7.04 (d, *J* = 7.2 Hz, 1H), 6.62-6.57 (m, 2H), 4.81 (t, *J* = 9.2 Hz, 1H), 3.34 (s, 1H), 3.20-3.12 (m, 1H), 2.27 (s, 3H), 1.27 (d, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, CD_3SOCD_3): δ 163.7, 144.3, 141.9, 140.6, 139.5, 138.7, 129.0, 126.0, 125.8, 124.7, 124.5, 122.4, 57.1, 47.8, 20.9, 17.4.
HRMS Calcd. for $C_{21}H_{19}BrN_2O_2S_2$ (M+1): 451.0071, Found: 451.0075.
FTIR (NaCl Film): 3273, 2973, 2925, 1586, 1434, 1356, 1328, 1264, 1161, 1091, 895, 814, 733, 703 cm^{-1}.

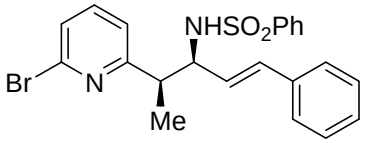

NHTs
Br
N
S
Me

3f


10
9
8
7
6
5
4
3
2
1
ppm


200
180
160
140
120
100
80
60
40
20
ppm

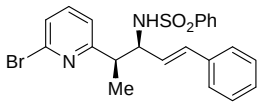
***N*-{1-[1-(6-Bromo-pyridin-2-yl)-ethyl]-3-phenyl-allyl}-4-methyl-benzenesulfonamide**



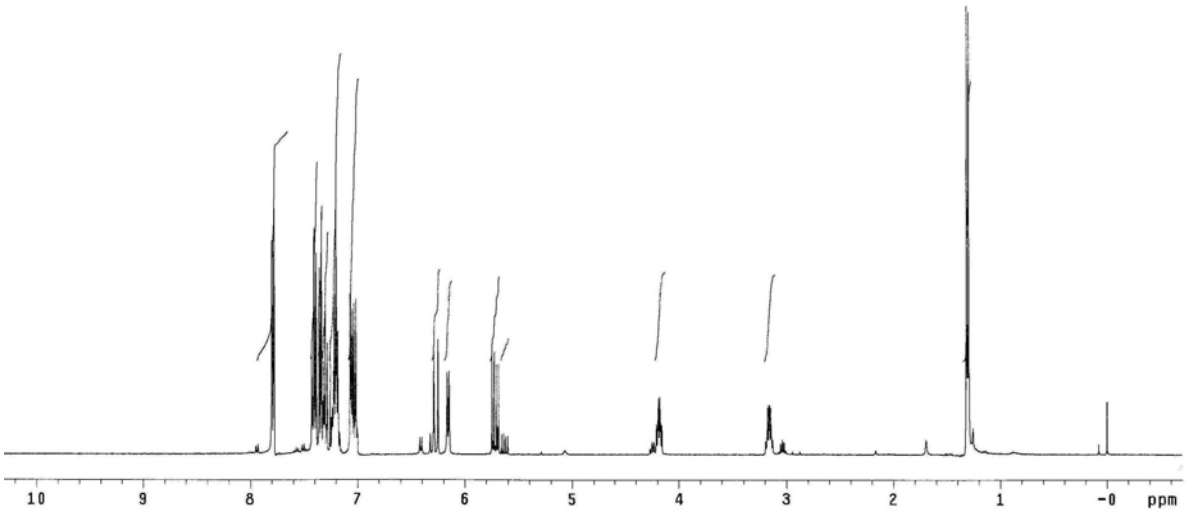
3g

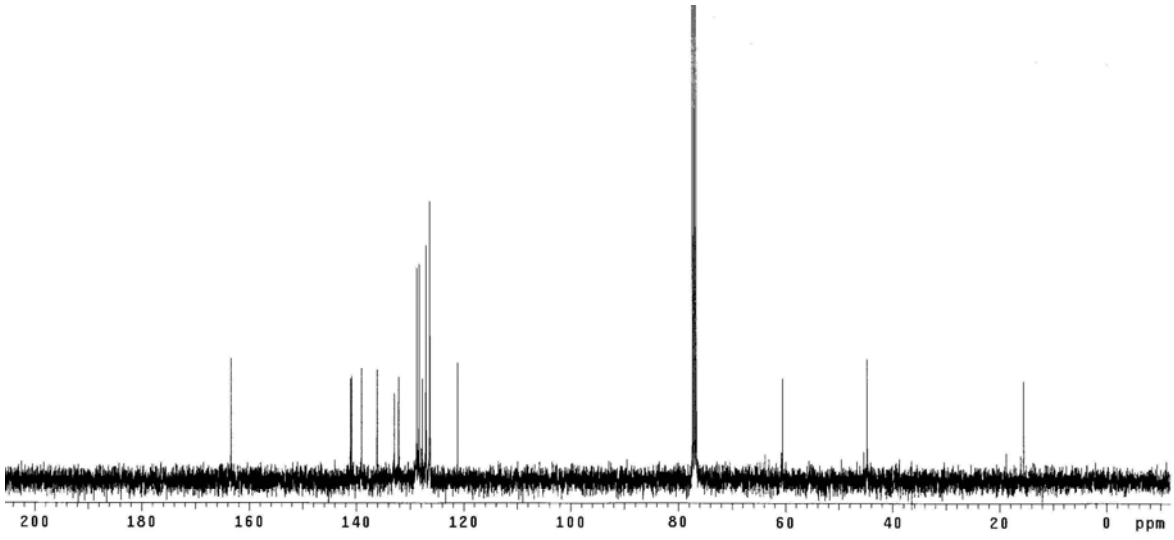
In accordance with the general procedure, 6-bromo-2-vinylpyridine **1a** (144 mg, 0.79 mmol, 300 mol%) was coupled to imine **2g** (72 mg, 0.26 mmol, 100 mol%) to provide the title compound (79 mg, 0.17 mmol) as a white solid in 67% yield after purification by flash silica gel column chromatography (Inseparable mixture of diastereomers in 4:1 ratio, R_f = 0.25, 25% EtOAc/hexanes, gradient: 10 - 25% EtOAc/hexanes). *Spectral data is reported for the major isomer.*

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.29 (dd, *J* = 8.0, 0.8 Hz, 2H), 7.39 (d, *J* = 7.2 Hz, 2H), 7.34 (d, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 5.6 Hz, 1H), 7.22-7.18 (m, 3H), 7.07-7.01 (m, 3H), 6.27 (d, *J* = 15.6 Hz, 1H), 6.15 (d, *J* = 7.2 Hz, 1H), 5.71 (dd, *J* = 16.0, 7.6 Hz, 1H), 4.18 (ddd, *J* = 8.0, 4.4, 1. 2 Hz, 1H), 3.19-3.12 (m, 1H), 1.30 (d, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 163.4, 141.0, 140.9, 139.0, 136.1, 133.0, 132.1, 128.8, 128.3, 127.7, 127.2, 126.4, 126.3, 126.3, 126.26, 121.13, 60.5, 44.7, 15.5.
HRMS Calcd. for $C_{23}H_{23}BrN_2O_2S$ (M+1): 457.0507, Found: 457.0586.
FTIR (NaCl Film): 3269, 3058, 2916, 1580, 1553, 1446, 1433, 1324, 1157, 1125, 1092, 984, 833, 721, 688 cm^{-1}.

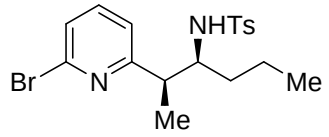

NHSO2Ph
Br
N
Me

3g


10
9
8
7
6
5
4
3
2
1
-0
ppm


200
180
160
140
120
100
80
60
40
20
0
ppm

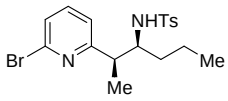
***N*-{1-[1-(6-Bromo-pyridin-2-yl)-ethyl]-butyl}-4-methyl-benzenesulfonamide**



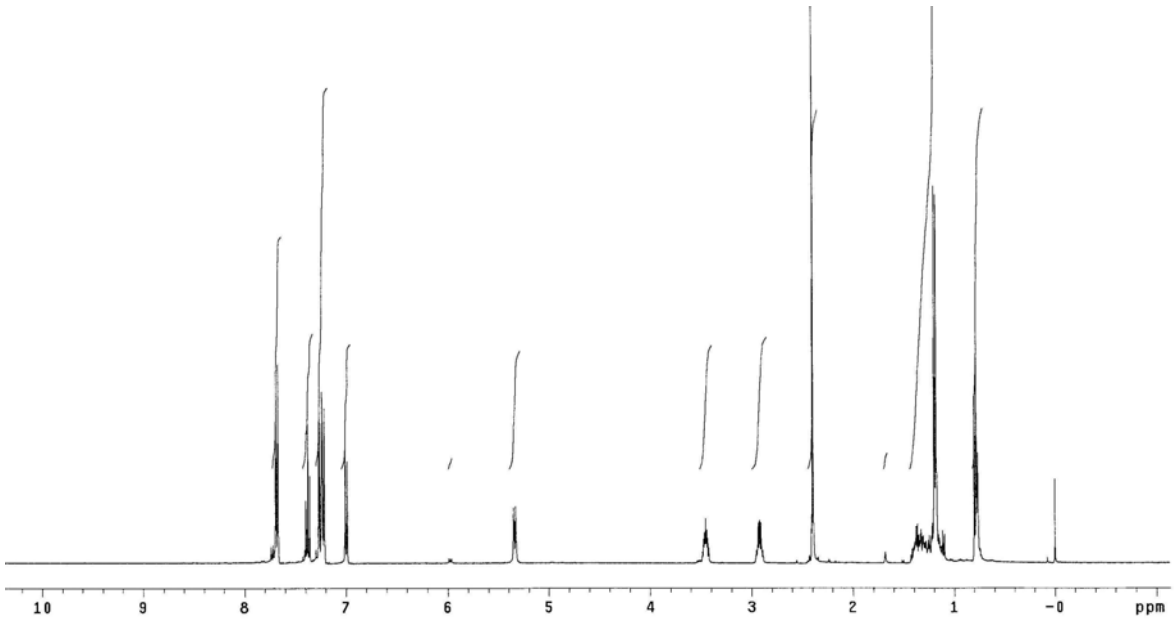
3h

In accordance with the general procedure, 6-bromo-2-vinylpyridine **1a** (144 mg, 0.79 mmol, 300 mol%) was coupled to imine **2h** (62 mg, 0.26 mmol, 100 mol%) to provide the title compound (71 mg, 0.17 mmol) as a colorless liquid in 63% yield after purification by flash silica gel column chromatography (Inseparable mixture of diastereomers in 8:1 ratio, R_f = 0.28, 15% EtOAc/hexanes, gradient: 10 - 15% EtOAc/hexanes). *Spectral data is reported for the major isomer.*

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.88 (d, *J* = 10.4 Hz, 2H), 7.35 (t, *J* = 8.0 Hz, 1H), 7.26-7.21 (m, 3H), 6.92 (d, *J* = 7.6 Hz, 1H), 5.34 (d, *J* = 8.4 Hz, 1H), 3.48-3.42 (m, 1H), 2.92 (ddd, *J* = 14.4, 7.2, 4.8 Hz, 1H), 2.41 (s, 3H), 1.42-1.16 (m, 4H), 1.21 (d, *J* = 7.2 Hz, 3H), 0.78 (t, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 164.2, 142.9, 141.2, 138.6, 137.9, 129.4, 126.9, 125.9, 121.1, 58.2, 43.1, 34.2, 21.5, 18.9, 14.7, 13.7.
HRMS Calcd. for $C_{18}H_{23}BrN_2O_2S$ (M+1): 411.0664, Found: 411.0736.
FTIR (NaCl Film): 3280, 2959, 2872, 1579, 1553, 1433, 1408, 1323, 1156, 1120, 1092, 812, 706, 664 cm^{-1}.


NHTs
Br
N
Me
Me

3h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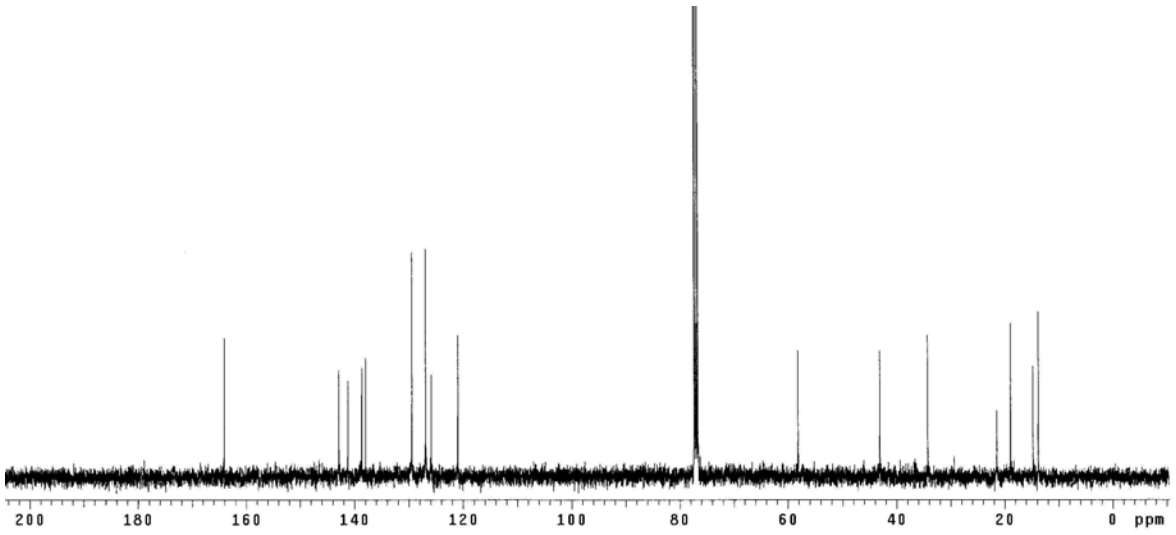
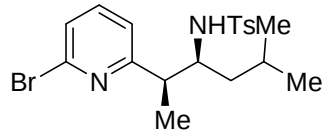
-0
ppm


200
180
160
140
120
100
80
60
40
20
0
ppm

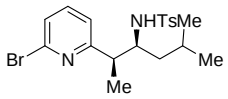
***N*-((2*R*, 3*S*)-2-(6-bromopyridin-2-yl)-5-methylhexan-3-yl)-4-methylbenzenesulfonamide**



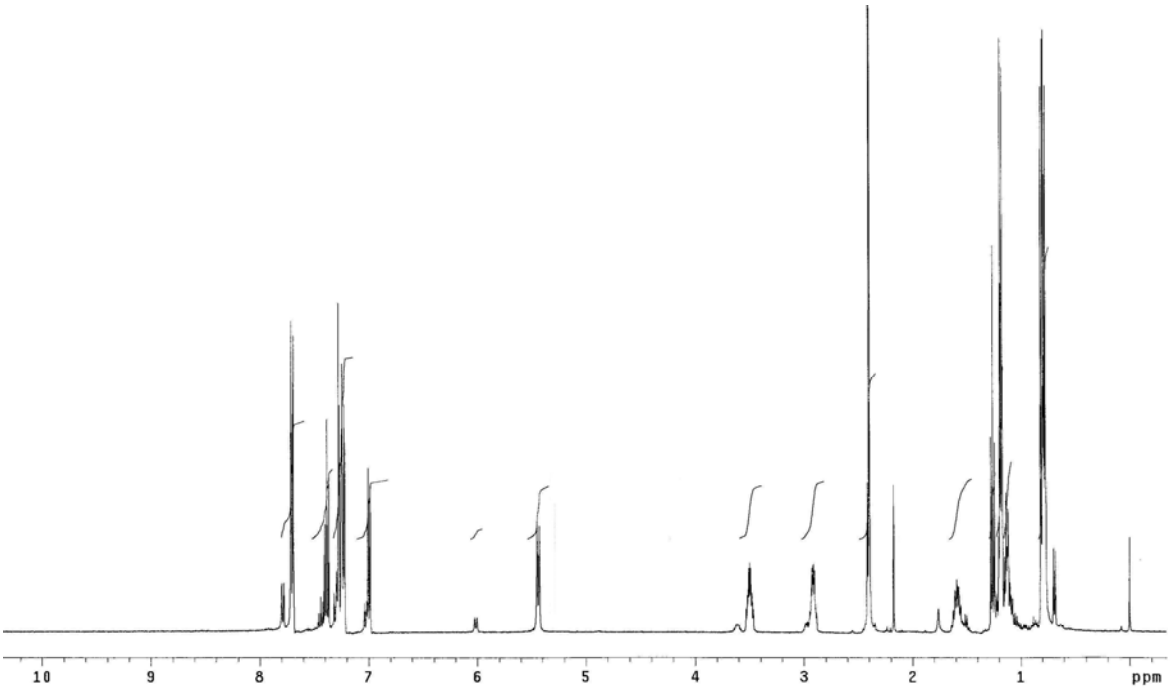
3i

In accordance with the general procedure, 6-bromo-2-vinylpyridine **1a** (144 mg, 0.79 mmol, 300 mol%) was coupled to imine **2i** (63 mg, 0.26 mmol, 100 mol%) to provide the title compound (82 mg, 0.19 mmol) as a colorless liquid in 74% yield after purification by flash silica gel column chromatography (Inseparable mixture of diastereomers in 6:1 ratio, R_f = 0.25, 20% EtOAc/hexanes, gradient: 10 - 20% EtOAc/hexanes). *Spectral data is reported for the major isomer*.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.70 (d, *J* = 8.4 Hz, 2H), 7.38 (t, *J* = 7.6 Hz, 1H), 7.27-7.22 (m, 3H), 6.95 (d, *J* = 7.2 Hz, 1H), 5.43 (dd, *J* = 8.4, 1.6 Hz, 1H), 3.53-3.46 (m, 1H), 2.91 (ddd, *J* = 14.4, 6.8, 4.0 Hz, 1H), 2.35 (s, 3H), 1.58-1.42 (m, 2H), 1.17 (d, *J* = 7.2 Hz, 3H), 1.15-1.10 (m, 1H), 0.80 (d, *J* = 6.8 Hz, 3H), 0.77 (d, *J* = 6.4 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 163.9, 142.5, 141.0, 138.6, 137.9, 129.4, 126.9, 125.8, 120.9, 56.4, 42.8, 41.1, 24.1, 22.9, 21.7, 21.4, 14.5.
HRMS Calcd. for $C_{19}H_{25}BrN_2O_2S$ (M+1): 425.0820, Found: 425.0818.
FTIR (NaCl Film): 3275, 2948, 2876, 1578, 1543, 1433, 1408, 1320, 1159, 1123, 1090, 812, 702, 664 cm^{-1}.


NHTsMe
Br
N
Me
Me

3i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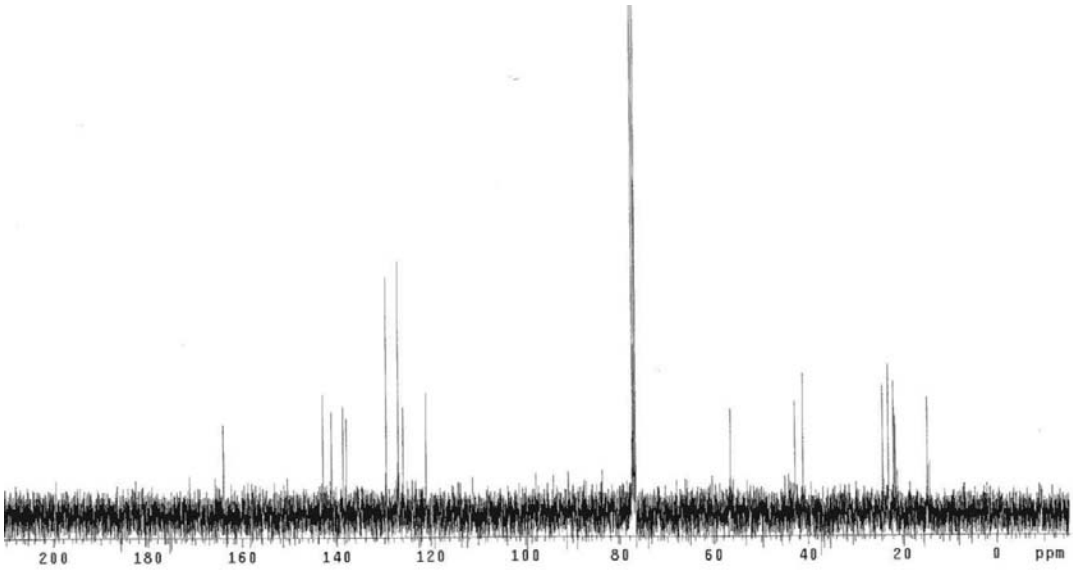
2
1
ppm


200
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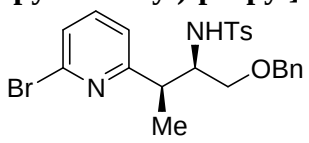
140
120
100
80
60
40
20
0
ppm

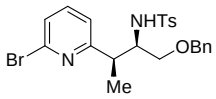
***N*-[1-Benzyloxymethyl-2-(6-bromo-pyridin-2-yl)-propyl]-4-methyl-benzenesulfonamide**



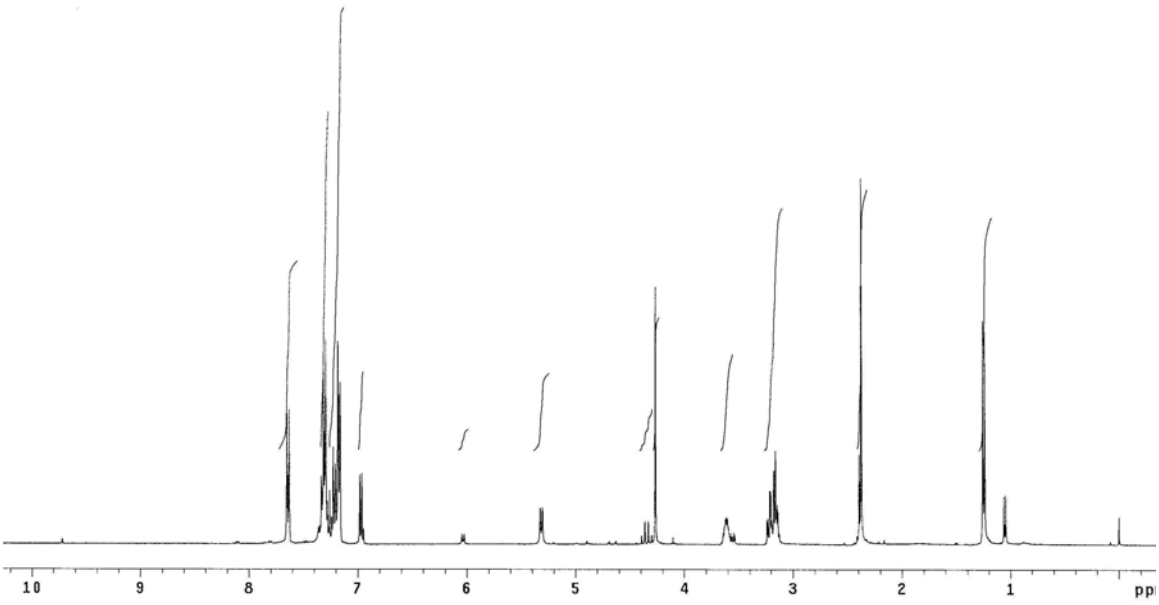
3j

In accordance with the general procedure, 6-bromo-2-vinylpyridine **1a** (144 mg, 0.79 mmol, 300 mol%) was coupled to imine **2j** (80 mg, 0.26 mmol, 100 mol%) to provide the title compound (89 mg, 0.18 mmol) as a colorless liquid in 69% yield after purification by flash silica gel column chromatography (Inseparable mixture of diastereomers in 5:1 ratio, R_f = 0.30, 15% EtOAc/hexanes, gradient: 10 - 15% EtOAc/hexanes). *Spectral data is reported for the major isomer.*

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.64 (d, *J* = 8.4 Hz, 2H), 7.33-7.25 (m, 4H), 7.23-7.16 (m, 5H) 6.97 (d, *J* = 6.8 Hz, 1H), 5.31 (d, *J* = 8.0 Hz, 1H), 4.26 (s, 2H), 3.61 (ddd, *J* = 11.6, 5.2 , 3.2 Hz, 1H), 3.23-3.13 (m, 3H), 2.37 (s, 3H), 1.25 (d, *J* = 6.8 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 164.2, 143.0, 141.5, 138.6, 137.6, 137.3, 129.5, 128.3, 127.7, 126.9, 126.8, 125.9, 121.6, 73.1, 69.3, 57.2, 42.1, 21.4, 16.0.
HRMS Calcd. for $C_{23}H_{25}BrN_2O_3S$ (M+1): 489.0769, Found: 489.0842.
FTIR (NaCl Film): 3279, 3001, 1866, 1580, 1553, 1453, 1432, 1328, 1117, 1087, 1022, 812, 794, 736, 664 cm^{-1}.


NHTs
Br
N
OBn
Me

3j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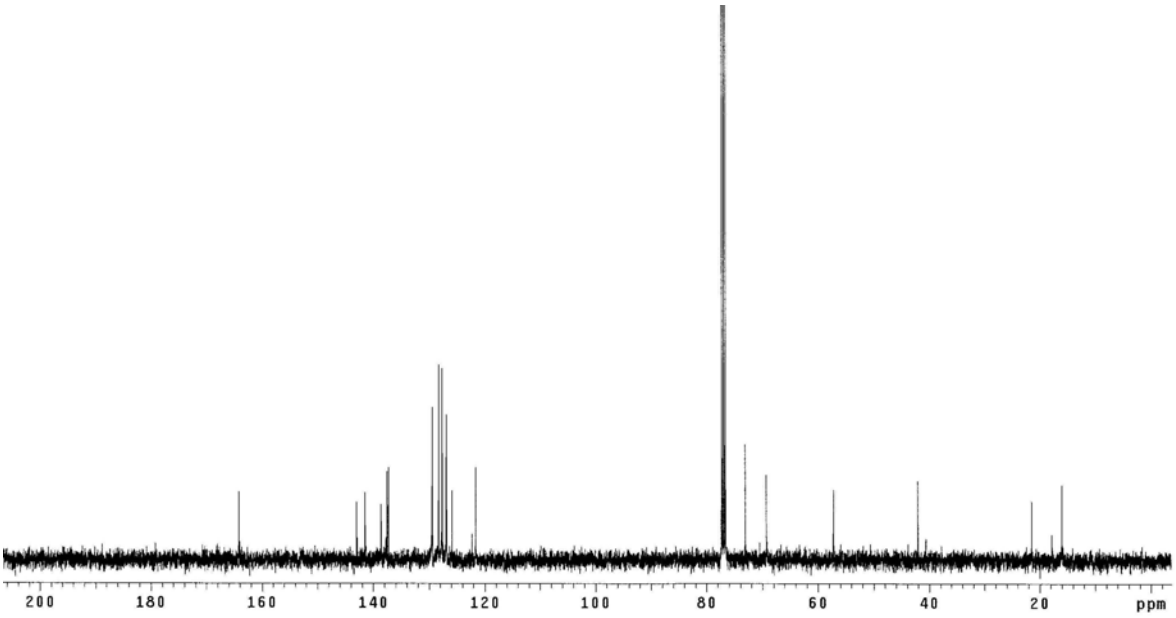
2
1


200
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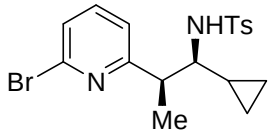
120
100
80
60
40
20
ppm

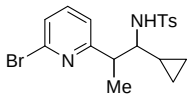
***N*-((1*S*, 2*R*)-2-(6-bromopyridin-2-yl)-1-cyclopropyl)-4-methylbenzenesulfonamide**



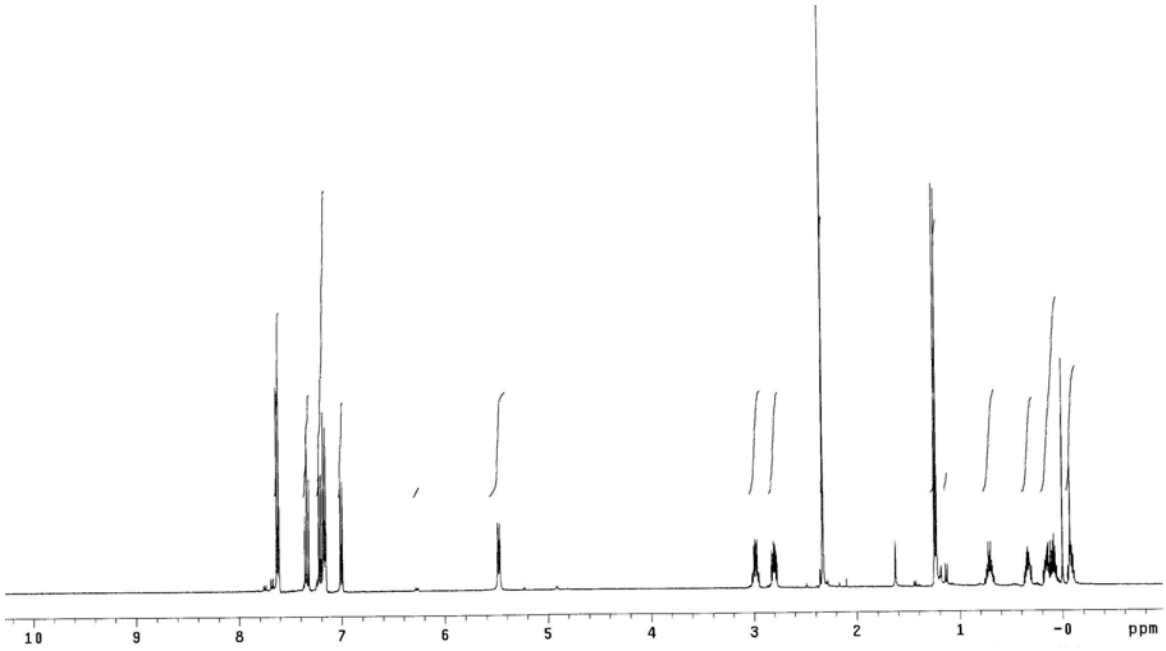
3k

In accordance with the general procedure, 6-bromo-2-vinylpyridine **1a** (144 mg, 0.79 mmol, 300 mol%) was coupled to imine **2k** (60 mg, 0.26 mmol, 100 mol%) to provide the title compound (79 mg, 0.19 mmol) as a colorless liquid in 72% yield after purification by flash silica gel column chromatography (Inseparable mixture of diastereomers in 9:1 ratio, R_f = 0.30, 15% EtOAc/hexanes, gradient: 10 - 15% EtOAc/hexanes). *Spectral data is reported for the major isomer.*

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.62 (d, *J* = 8.8 Hz, 2H), 7.33 (t, *J* = 7.6 Hz, 1H), 7.21 (d, *J* = 8.0 Hz, 1H), 7.18 (d, *J* = 8.0 Hz, 2H), 7.01 (d, *J* = 7.6 Hz, 1H), 5.47 (d, *J* = 7.6 Hz, 1H), 3.01-2.95 (m, 1H), 2.80 (ddd, *J* = 12.4, 7.6, 4.8 Hz, 1H), 2.33 (s, 3H), 1.24 (d, *J* = 7.2 Hz, 3H), 0.75-0.67 (m, 1H), 0.37-0.30 (m, 1H), 0.18-0.05 (m, 2H), -0.05- -0.11 (m, 1H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 164.1, 142.8, 141.0, 138.6, 138.1, 129.4, 126.9, 125.9, 121.3, 62.5, 45.1, 21.4, 15.3, 13.9, 4.5, 3.2.
HRMS Calcd. for $C_{18}H_{21}BrN_2O_2S$ (M+1): 408.0507, Found: 408.0509.
FTIR (NaCl Film): 3276, 2973, 2322, 2050, 1581, 1553, 1434, 1326, 1157, 1093, 814, 706, 666 cm^{-1}.


NHTs
Br
N
Me

3k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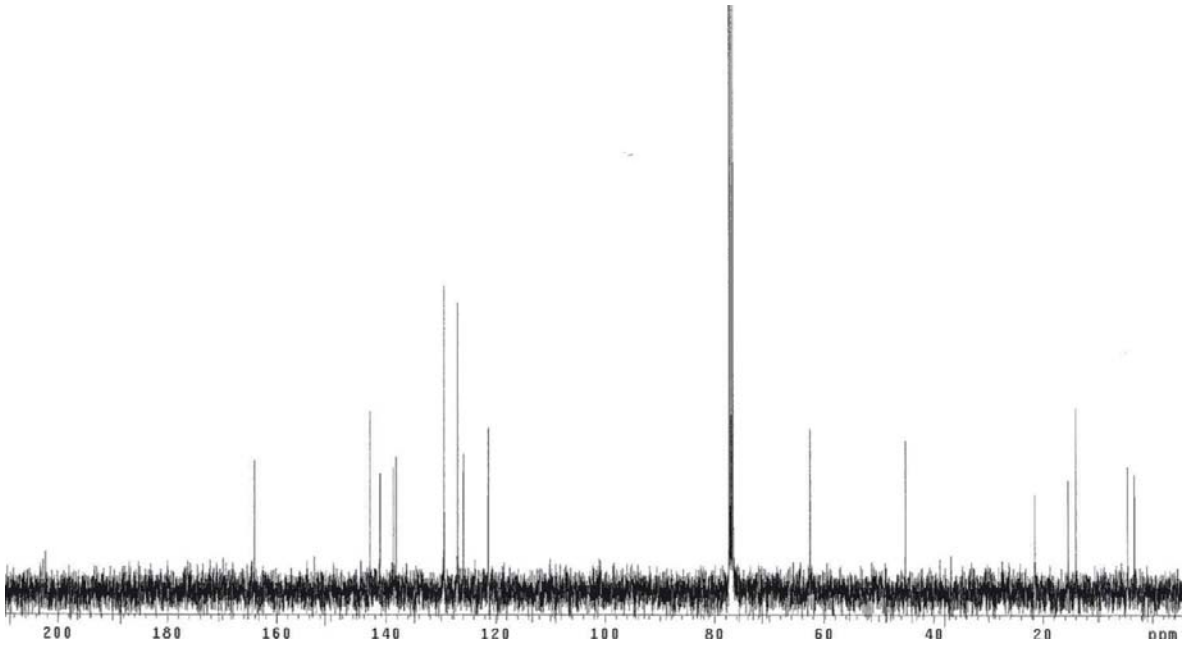
200
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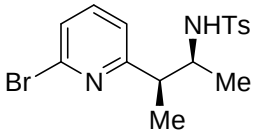
140
120
100
80
60
40
20
ppm

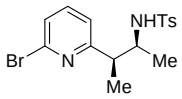
***N*-((2*S*, 1*R*)-3-(6-bromopyridin-2-yl) butan-2-yl)-4-methylbenzenesulfonamide**



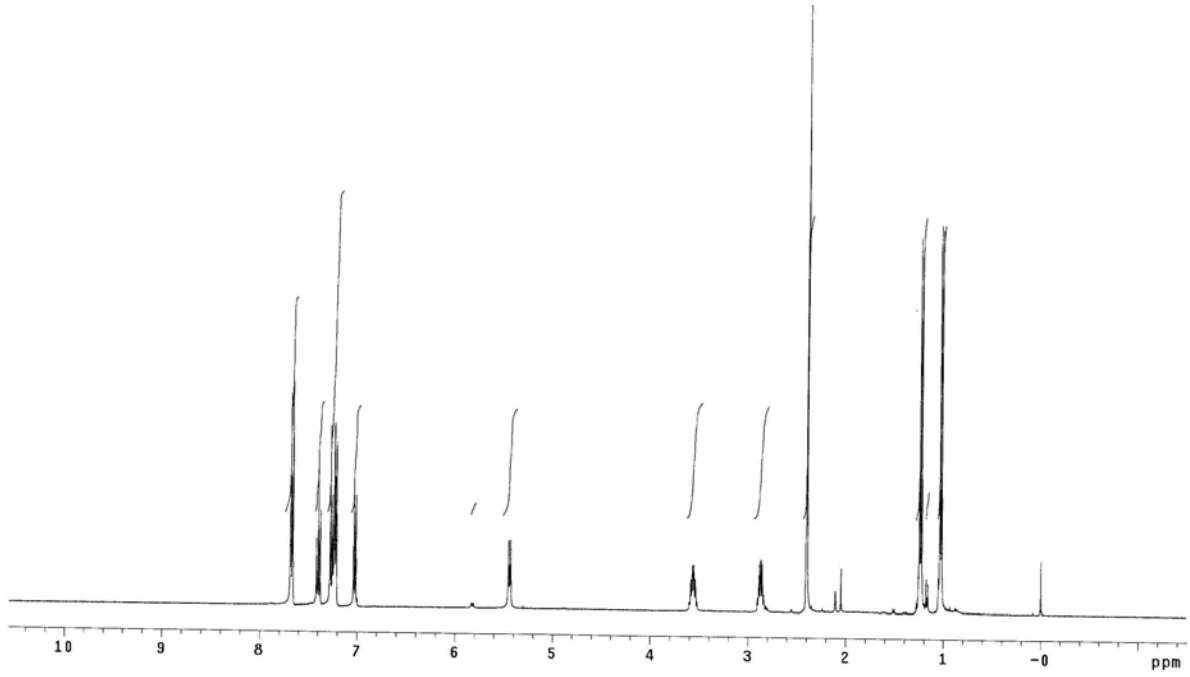
3l

In accordance with the general procedure, 6-bromo-2-vinylpyridine **1a** (144 mg, 0.79 mmol, 300 mol%) was coupled to imine **2l** (52 mg, 0.26 mmol, 100 mol%) to provide the title compound (64 mg, 0.17 mmol) as a colorless liquid in 64% yield after purification by flash silica gel column chromatography (Inseparable mixture of diastereomers in 13:1 ratio, R_f = 0.25, 15% EtOAc/hexanes. *Spectral data is reported for the major isomer.*

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.67 (d, *J* = 8.4 Hz, 2H), 7.40 (t, *J* = 7.2 Hz, 1H), 7.26 (d, *J* = 8.0 Hz, 1H), 7.22 (d, *J* = 8.0 Hz, 2H), 7.02 (d, *J* = 7.6 Hz, 1H), 5.44 (d, *J* = 7.6 Hz, 1H), 3.60-3.52 (m, 1H), 2.87 (quintet, *J* = 6.4 Hz, 1H), 2.39 (s, 3H), 1.23 (d, *J* = 7.2 Hz, 3H), 1.04 (d, *J* = 6.4 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 164.0, 142.9, 141.2, 138.7, 137.4, 129.4, 126.8, 125.9, 121.0, 53.7, 45.4, 21.4, 19.1, 14.8.
HRMS Calcd. for $C_{16}H_{19}BrN_2O_2S$ (M+1): 383.0429, Found: 383.0435.
FTIR (NaCl Film): 3275, 2971, 2322, 1581, 1552, 1430, 1380, 1324, 1126, 1089, 958, 911, 813, 705, 667 cm^{-1}.


NHTs
Br
N
Me
Me

3l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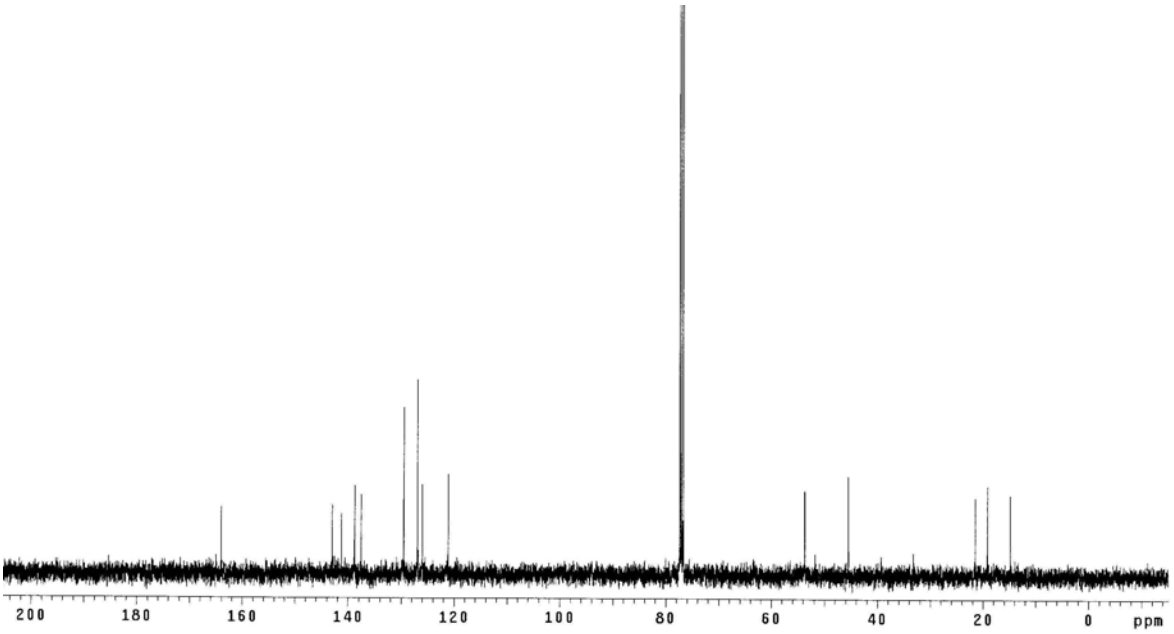
ppm


200
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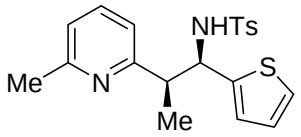
80
60
40
20
0
ppm

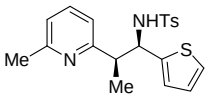
4-methyl-*N*-((1*R*, 2*R*)-2-(6-methylpyridin-2-yl)-1-(thiophen-2-yl) propyl) benzenesulfonamide



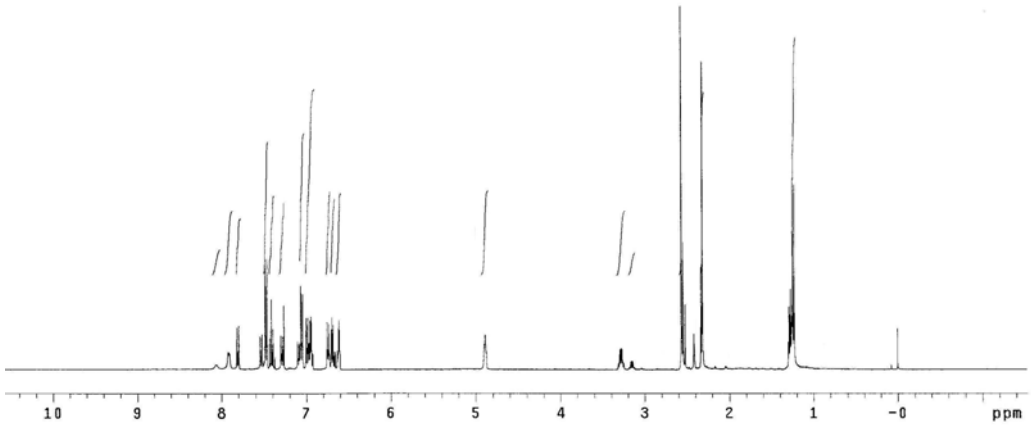
3m

In accordance with the general procedure, commercially available 6-methyl-2-vinylpyridine **1b** (95 mg, 0.79 mmol, 300 mol%) was coupled to imine **2f** (70 mg, 0.26 mmol, 100 mol%) to provide the title compound (71 mg, 0.18 mmol) as an yellow thick syrup in 70% yield after purification by flash silica gel column chromatography (Inseparable mixture of diastereomers in 5:1 ratio, R_f = 0.25, 20% EtOAc/hexanes, gradient: 10 - 20% EtOAc/hexanes). *Spectral data is reported for the major isomer*.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.81 (d, *J* = 8.0 Hz, 1H), 7.47 (d, *J* = 8.0 Hz, 2H), 7.41 (t, *J* = 8.0 Hz, 1H), 7.29 (d, *J* = 7.6 Hz, 1H), 7.05 (d, *J* = 8.0 Hz, 2H), 6.99 (d, *J* = 7.6 Hz, 1H), 6.95 (dd, *J* = 4.8, 0.8 Hz, 1H), 6.74 (d, *J* = 8.0 Hz, 1H), 6.69 (dd, *J* = 4.8, 3.6 Hz, 1H), 6.61 (d, *J* = 4.0 Hz, 1H), 4.88 (dd, *J* = 5.2, 4.4 Hz, 1H), 3.31-3.25 (m, 1H), 2.56 (s, 3H), 2.32 (s, 3H), 1.24 (d, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 160.8, 157.0, 142.4, 137.7, 137.0, 129.6, 129.0, 126.7, 126.1, 125.7, 124.6, 121.5, 119.3, 58.4, 44.7, 24.3, 21.3, 15.6.
HRMS Calcd. for $C_{20}H_{23}N_2O_2S_2$ (M+1): 387.1201, Found: 387.1201.
FTIR (NaCl Film): 3268, 2924, 1594, 1460, 1376, 1327, 1156, 1092, 812, 749, 666 cm^{-1}.


NHTs
Me
N
S
Me

3m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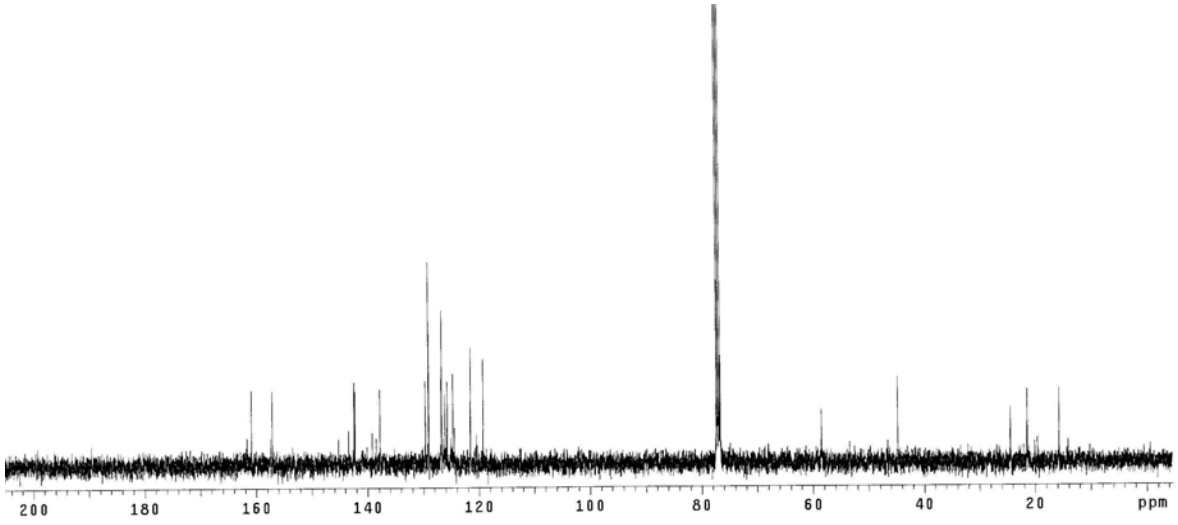
200
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60
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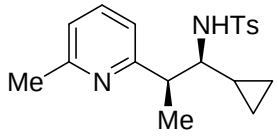
ppm

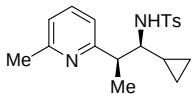
***N*-((1*S*, 2*R*)-1-cyclopropyl-2-(6-methylpyridin-2-yl) propyl)-4-methylbenzenesulfonamide**



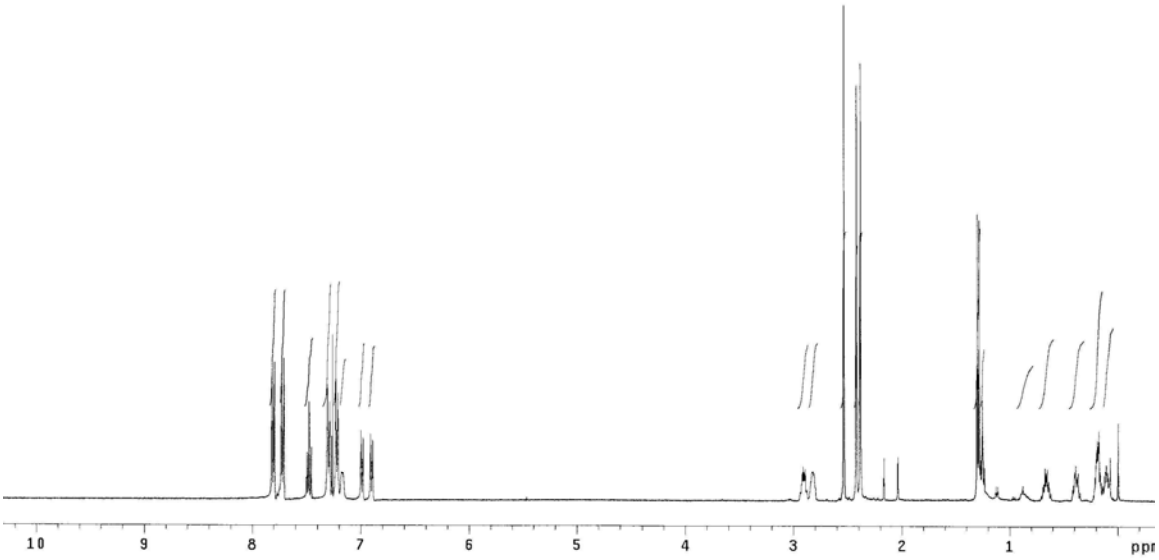
3n

In accordance with the general procedure, commercially available 6-methyl-2-vinylpyridine **1b** (95 mg, 0.79 mmol, 300 mol%) was coupled to imine **2k** (60 mg, 0.26 mmol, 100 mol%) to provide the title compound (51 mg, 0.15 mmol) as a colorless liquid in 56% yield after purification by flash silica gel column chromatography (Inseparable mixture of diastereomers in 10:1 ratio, R_f = 0.23, 25% EtOAc/hexanes, gradient: 10 - 25% EtOAc/hexanes). *Spectral data is reported for the major isomer*.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.72 (d, *J* = 8.0 Hz, 2H), 7.47 (t, *J* = 7.6 Hz, 1H), 7.22 (d, *J* = 8.0 Hz, 2H), 7.19-7.14 (m, 1H), 6.99 (d, *J* = 8.0 Hz, 1H), 6.90 (d, *J* = 7.6 Hz, 1H), 2.95-2.87 (m, 1H), 2.85-2.79 (m, 1H), 2.42 (s, 3H), 2.38 (s, 3H), 1.29 (d, *J* = 7.2 Hz, 3H), 0.68-0.63 (m, 1H), 0.40-0.36 (m, 1H), 0.20-0.17 (m, 2H), 0.15-0.07 (m, 1H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 161.9, 157.2, 143.4, 139.1, 138.5, 126.9, 126.3, 121.2, 118.9, 62.3, 43.8, 24.4, 21.4, 15.6, 13.1, 3.8, 3.3.
HRMS Calcd. for $C_{19}H_{25}N_2O_2S_2$ (M+1): 345.1637, Found: 345.1639.
FTIR (NaCl Film): 3272, 2924, 1595, 1458, 1327, 1158, 1094, 1041, 814, 669 cm^{-1}.


NHTs
Me
N
Me

3n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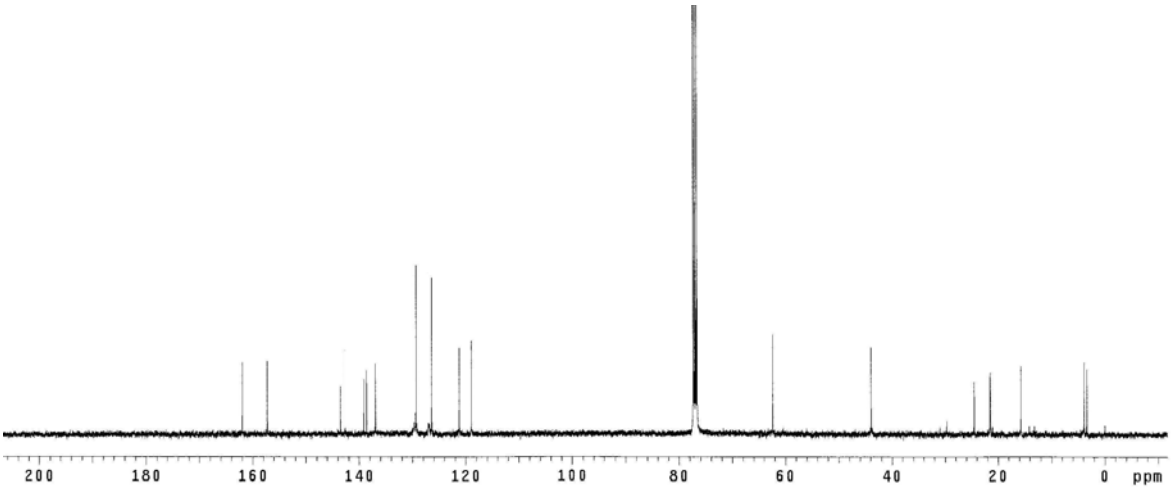
1
ppm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60
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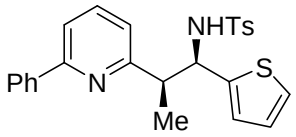
ppm

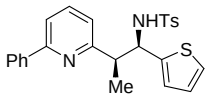
4-methyl-*N*-((1*R*, 2*R*)-2-(6-phenylpyridin-2-yl)-1-(thiophen-2-yl) propyl)benzenesulfonamide



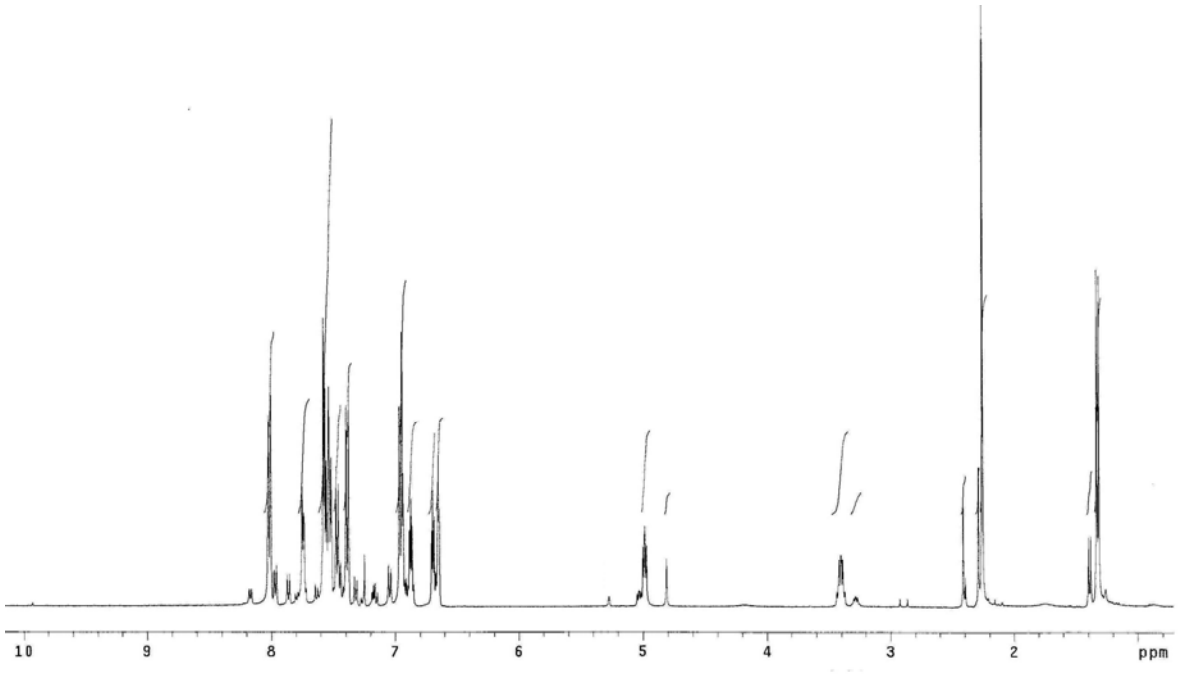
3o

In accordance with the general procedure, 6-phenyl-2-vinylpyridine **1c** (141 mg, 0.79 mmol, 300 mol%) was coupled to imine **2f** (70 mg, 0.26 mmol, 100 mol%) to provide the title compound (90 mg, 0.20 mmol) as a white solid in 77% yield after purification by flash silica gel column chromatography (Inseparable mixture of diastereomers in 5:1 ratio, R_f = 0.30, 20% EtOAc/hexanes, gradient: 10 - 20% EtOAc/hexanes). *Spectral data is reported for the major isomer*.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01 (dd, *J* = 8.8, 1.6 Hz, 1H), 7.75-7.73 (m, 1H), 7.47 (d, *J* = 8.4 Hz, 2H), 7.58-7.51 (m, 4H), 7.46 (d, *J* = 6.8 Hz, 1H), 7.38 (d, *J* = 8.4 Hz, 2H), 6.96-6.93 (m, 2H), 6.87 (t, *J* = 4.0 Hz, 1H), 6.69 (t, *J* = 3.6 Hz, 1H) 5.64 (d, *J* = 3.6 Hz, 1H), 4.99 (dd, *J* = 6.0, 5.2 Hz, 1H), 3.46-3.37 (m, 1H), 2.25 (s, 3H), 1.32 (d, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 161.2, 155.9, 142.4, 142.3, 138.6, 137.6, 137.5, 129.2, 128.9, 128.8, 126.7, 126.6, 126.0, 125.8, 124.6, 120.8, 118.7, 58.4, 45.3, 21.3, 15.6.
HRMS Calcd. for $C_{25}H_{24}N_2O_2S_2$ (M+1): 449.1357, Found: 449.1360.
FTIR (NaCl Film): 3270, 3064, 1591, 1569, 1447, 1327, 1155, 1091, 908, 853, 761, 694, 666 cm^{-1}.


NHTs
Ph
N
S
Me

3o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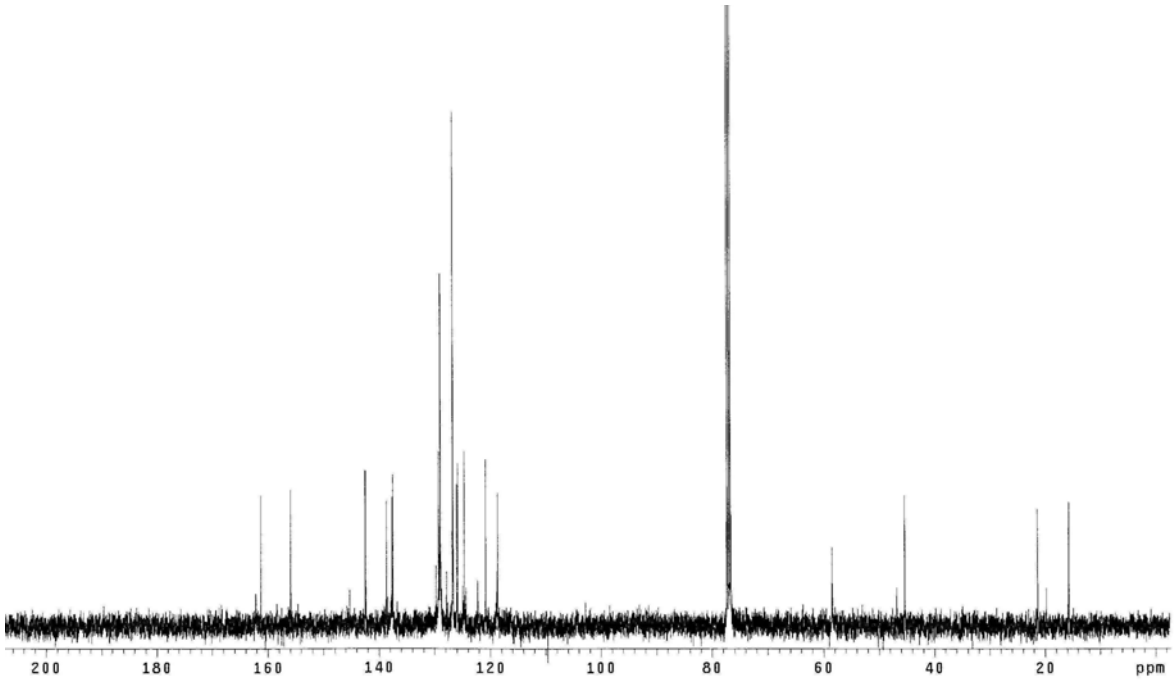
7
6
5
4
3
2
ppm


200
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80
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40
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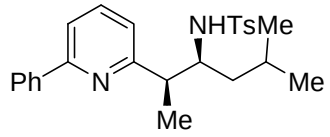
ppm

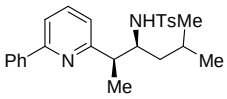
4-methyl-*N*-((2*R*, 3*S*)-5-methyl-2-(6-phenylpyridin-2-yl) hexan-3-yl) benzenesulfonamide



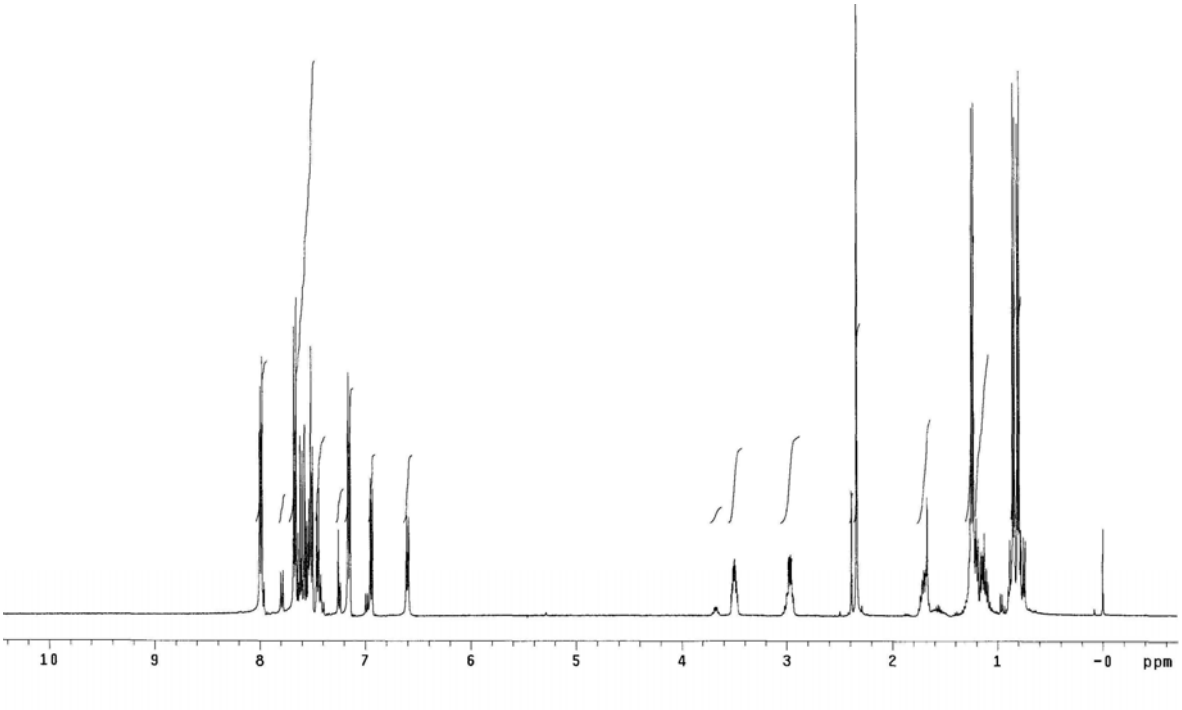
3p

In accordance with the general procedure, 6-phenyl-2-vinylpyridine **1c** (144 mg, 0.79 mmol, 300 mol%) was coupled to imine **2i** (63 mg, 0.26 mmol, 100 mol%) to provide the title compound (88 mg, 0.20 mmol) as a colorless liquid in 80% yield after purification by flash silica gel column chromatography (Inseparable mixture of diastereomers in 4:1 ratio, R_f = 0.30, 20% EtOAc/hexanes, gradient: 10 - 20% EtOAc/hexanes). *Spectral data is reported for the major isomer*.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.00-7.98 (m, 2H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.66 (d, *J* = 8.4 Hz, 2H), 7.62-7.56 (m, 2H), 7.51 (dd, *J* = 8.0, 1.6 Hz, 2H), 7.44 (dd, *J* = 7.6, 2.0 Hz, 1H), 7.14 (d, *J* = 8.0 Hz, 2H), 6.93 (d, *J* = 8.4 Hz, 1H), 6.62 (d, *J* = 7.6 Hz, 1H) 3.53-3.47 (m, 1H), 2.97 (ddd, *J* = 14.8, 7.2, 3.6 Hz, 1H), 2.32 (s, 3H), 1.73-1.66 (m, 1H), 1.23 (d, *J* = 7.2 Hz, 3H), 1.18-1.05 (m, 1H), 0.84 (d, *J* = 6.4 Hz, 3H), 0.84 (d, *J* = 6.8 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 162.0, 155.9, 142.6, 139.4, 138.0, 137.4, 129.3, 129.2, 129.1, 126.8, 126.7, 120.2, 118.1, 56.5, 44.5, 40.4, 23.9, 23.0, 22.2, 21.8, 14.9.
HRMS Calcd. for $C_{25}H_{31}N_2O_2S$ (M+1): 423.2106, Found: 423.2111.
FTIR (NaCl Film): 3278, 2955, 2866, 1590, 1569, 1495, 1447, 1385, 1367, 1325, 1155, 1092, 960, 763, 731, 693, 662 cm^{-1}.


NHTsMe
Ph
N
Me
Me

3p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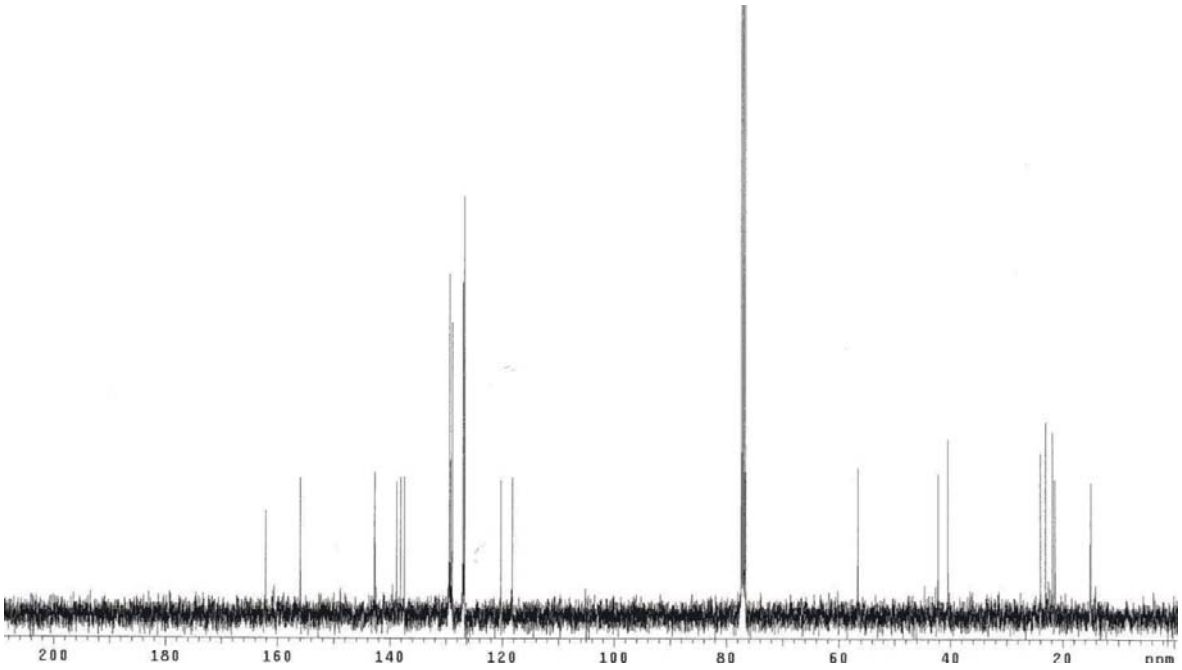
ppm


200
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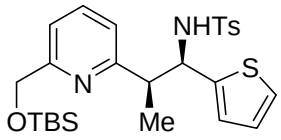
120
100
80
60
40
20
ppm

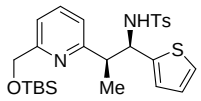
***N*-((1*R*, 2*R*)-2-(6-((*tert*-butyldimethylsilyloxy) methyl) pyridine-2-yl)-1-(thiophen-2-yl) propyl)-4-methanebenzenesulfonamide**



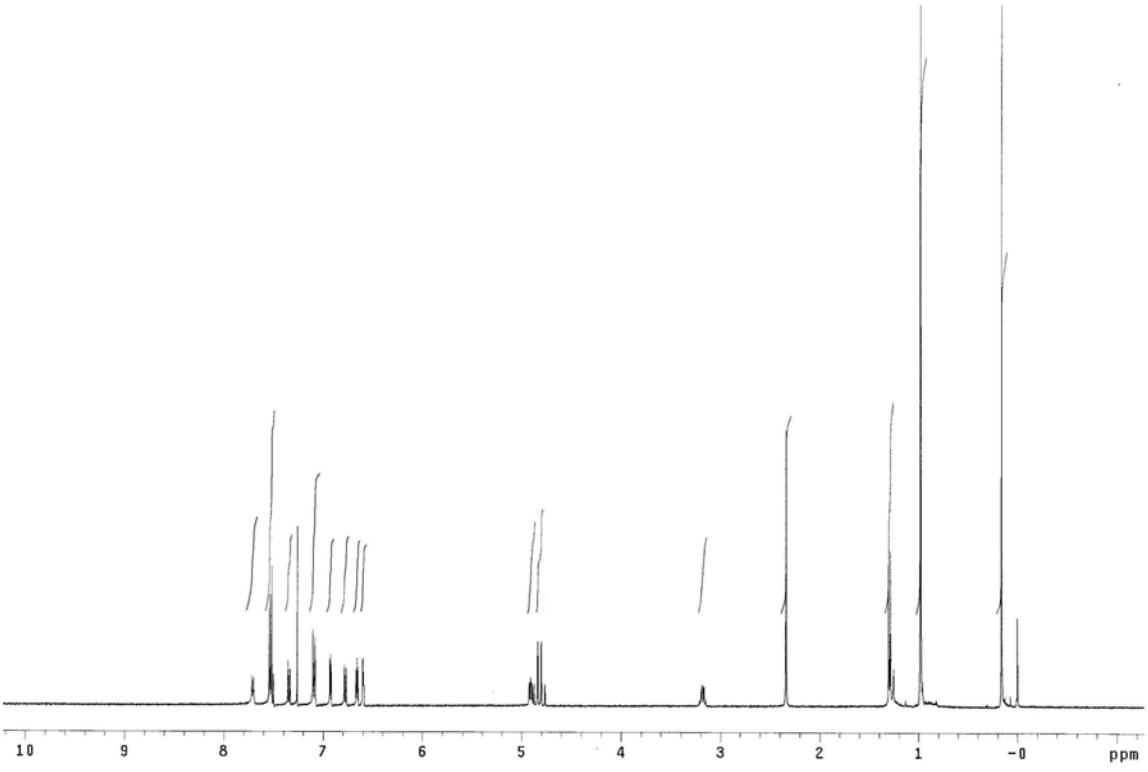
3q

In accordance with the general procedure, 6-silyloxymethyl-2-vinylpyridine **1d** (197 mg, 0.79 mmol, 300 mol%) was coupled to imine **2f** (70 mg, 0.26 mmol, 100 mol%) to provide the title compound (96 mg, 0.18 mmol) as a colorless liquid in 71% yield after purification by flash silica gel column chromatography (separable mixture of diastereomers in 5:1 ratio, $R_{f,\ major}$ = 0.30, $R_{f,\ minor}$ = 0.25, 15% EtOAc/hexanes, gradient: 10 - 15% EtOAc/hexanes).

^{1}H NMR (400 MHz, $CDCl_3$, Major Isomer): δ 7.71 (d, *J* = 7.2 Hz, 1H), 7.53 (d, *J* = 8.0 Hz, 2H), 7.34 (d, *J* = 7.6 Hz, 1H), 7.09 (d, *J* = 8.0 Hz, 2H), 7.14 (d, *J* = 8.0 Hz, 2H), 6.93 (dd, *J* = 5.2, 1.6 Hz, 1H), 6.77 (d, *J* = 7.6 Hz, 1H), 6.67-6.64 (m, 1H), 6.60 (d, *J* = 3.2 Hz, 1H), 4.91 (dd, *J* = 7.2, 5.2 Hz, 1H), 4.82 (q, *J* = 14.8 Hz, 2H), 3.21-3.14 (m, 1H), 2.38 (s, 3H), 1.29 (d, *J* = 6.8 Hz, 3H) 0.98 (s, 9H), 0.16 (s, 6H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 161.2, 160.5, 145.1, 142.3, 138.4, 137.5, 129.0, 121.7, 125.9, 125.0, 124.3, 121.8, 118.3, 65.9, 59.5, 46.7, 25.9, 21.4, 19.5, 18.3, -5.2.
HRMS Calcd. for $C_{26}H_{37}N_2O_3Si\ S_2$ (M+1): 517.2015, Found: 517.2015.
FTIR (NaCl Film): 3273, 2953, 2928, 2855, 1594, 1462, 1449, 1361, 1158, 1117, 1093, 837, 778, 696, 668 cm^{-1}.


NHTs
N
S
OTBS
Me

3q, Major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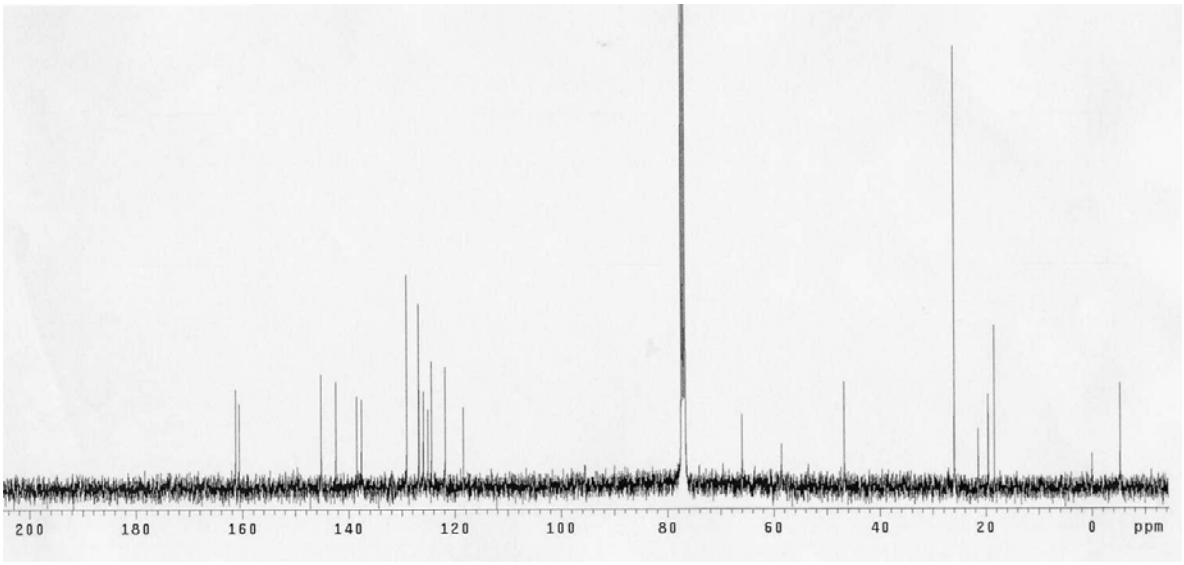
ppm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100
80
60
40
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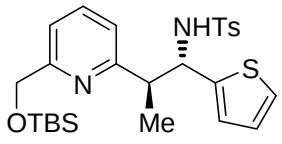
0
ppm



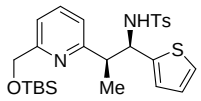
3q

^{1}H NMR (400 MHz, $CDCl_3$, Minor Isomer): 7.53 (d, *J* = 7.6 Hz, 1H), 7.45 (d, *J* = 8.0 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 1H), 7.04 (d, *J* = 8.0 Hz, 2H), 7.14 (d, *J* = 8.0 Hz, 2H), 6.95 (dd, *J* = 4.8, 2.0 Hz, 1H), 6.80 (d, *J* = 8.0 Hz, 1H), 6.69-6.74 (m, 1H), 6.58 (d, *J* = 2.8 Hz, 1H), 4.88 (dd, *J* = 6.8, 4.4 Hz, 1H), 4.83-4.82 (m, 2H), 3.34-3.27 (m, 1H), 2.32 (s, 3H), 1.28 (d, *J* = 6.8 Hz, 3H) 0.99 (s, 9H), 0.18 (s, 6H).

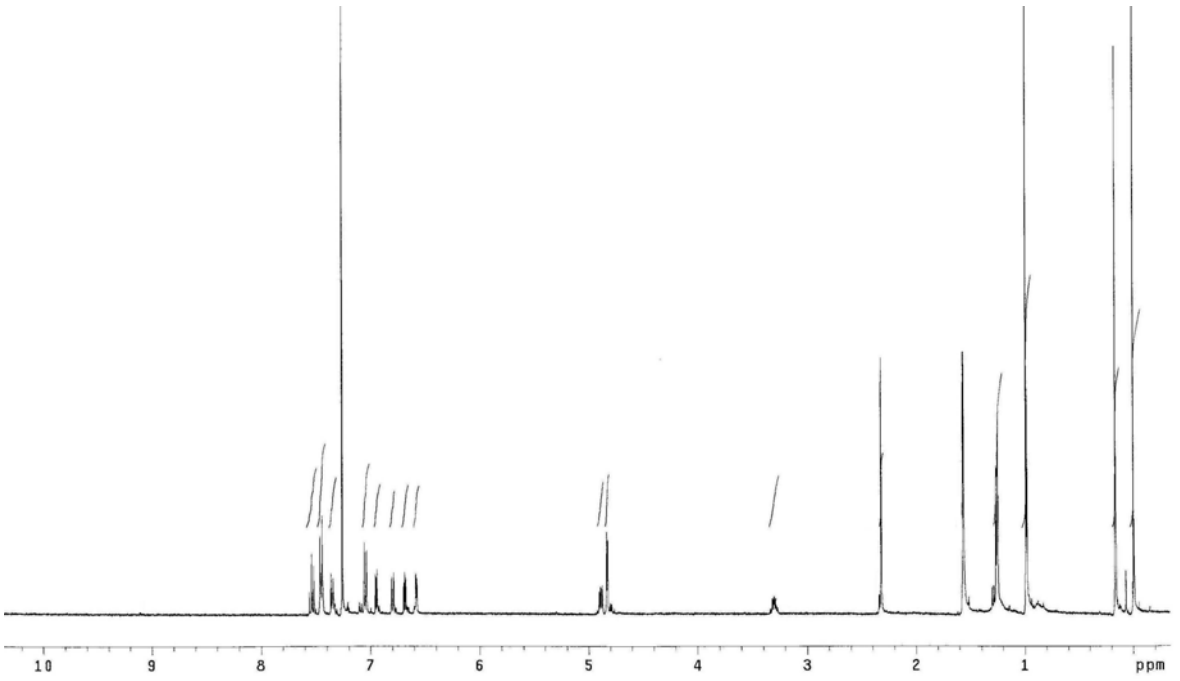
^{13}C NMR (100 MHz, $CDCl_3$): 165.3, 160.3, 142.4, 142.2, 137.7, 137.4, 129.1, 126.7, 126.1, 125.7, 124.7, 120.5, 118.3, 65.9, 58.4, 45.0, 29.6, 25.9, 21.4, 15.8, -0.01, -5.3.

HRMS Calcd. for $C_{26}H_{37}N_2O_3Si\,S_2$ (M+1):517.2015, Found:517.2017.

FTIR (NaCl Film): 3270, 2957, 2929, 2850, 1589, 1460, 1441, 1360, 1156, 1116, 1093, 837, 771, 692, 666 cm^{-1}.


NHTs
S
N
OTBS
Me

3q, Minor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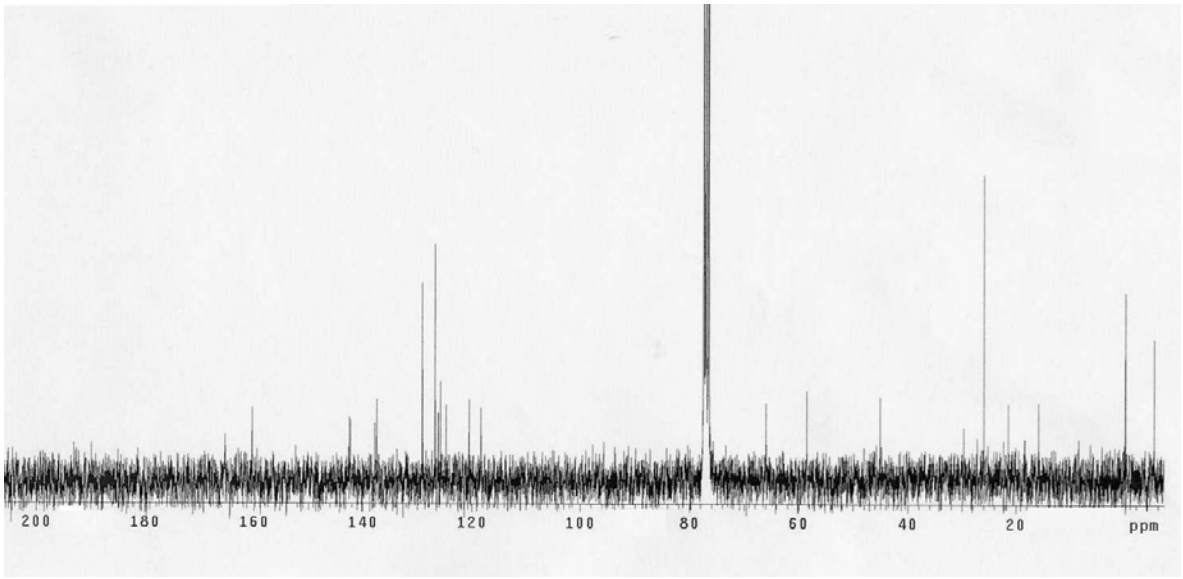
ppm


200
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120
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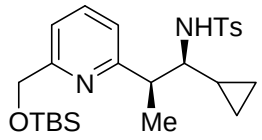
80
60
40
20
ppm

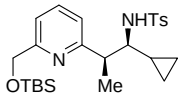
***N*-((1*S*, 2*R*)-2-(6-((tert-butyldimethylsilyloxy) methyl) pyridin-2-yl)-1-cyclopropylpropyl)-4-methylbenzenesulfonamide**



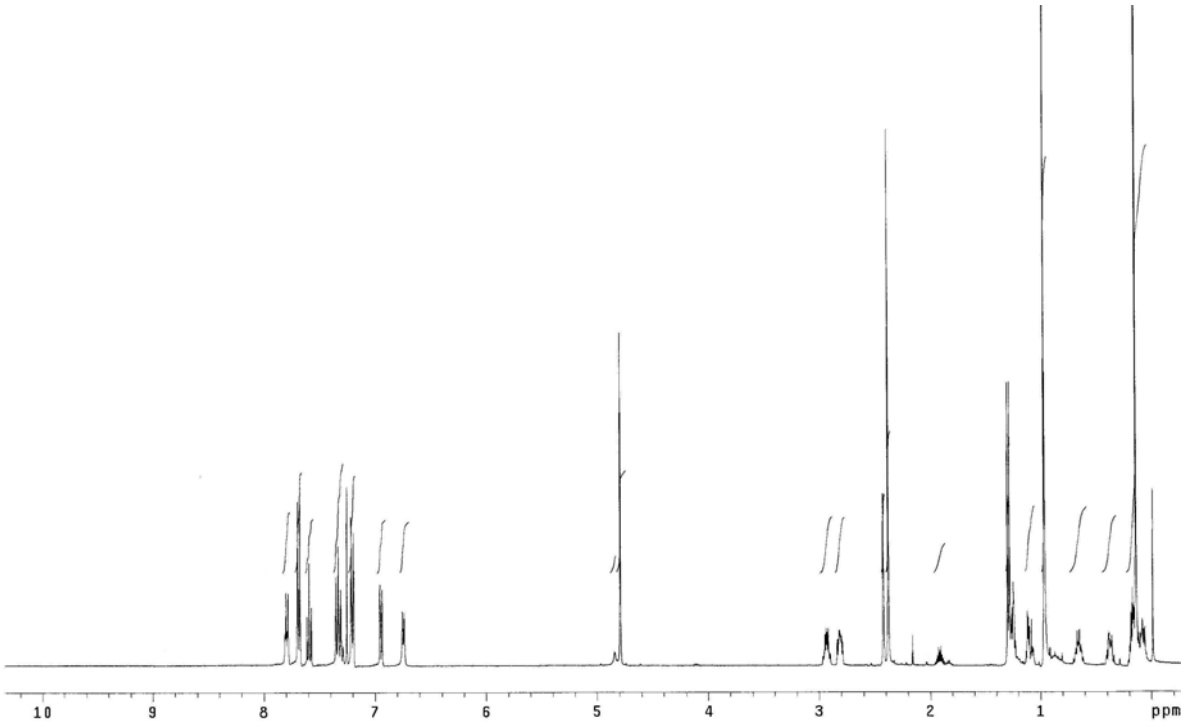
3r

In accordance with the general procedure, 6-silyloxymethyl-2-vinylpyridine **1d** (197 mg, 0.79 mmol, 300 mol%) was coupled to imine **2k** (60 mg, 0.26 mmol, 100 mol%) to provide the title compound (85 mg, 0.18 mmol) as colorless liquid in 67% yield after purification by flash silica gel column chromatography (Inseparable mixture of diastereomers in 6:1 ratio, R_f = 0.25, 15% EtOAc/hexanes, gradient: 10 - 15% EtOAc/hexanes). *Spectral data is reported for the major isomer*.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.80 (d, *J* = 8.4 Hz, 1H), 7.68 (d, *J* = 8.0 Hz, 2H), 7.59 (t, *J* = 7.6 Hz, 1H), 7.43-7.30 (m, 1H), 7.20 (d, *J* = 8.0 Hz, 2H), 6.94 (d, *J* = 8.0 Hz, 1H), 4.79 (s, 2H), 2.97-2.90 (m, 1H), 2.81 (ddd, *J* = 8.0, 6.4, 3.6 Hz, 1H), 2.33 (s, 3H), 1.29 (d, *J* = 7.2 Hz, 3H), 1.11-1.09 (m, 1H), 0.96 (s, 9H), 0.70-0.61 (m, 1H), 0.40-0.35 (m, 1H), 0.18-0.08 (m, 2H), 0.13 (s, 6H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 161.5, 160.3, 142.6, 138.5, 137.3, 129.6, 127.8, 120.2, 118.0, 66.0, 62.4, 44.1, 25.9, 21.4, 18.3, 15.7, 13.1, 10.6, 3.9, 3.2, -5.3.
HRMS Calcd. for $C_{25}H_{39}N_2O_3SiS$ (M+1): 475.2451, Found: 475.2453.
FTIR (NaCl Film): 3285, 2953, 2928, 2855, 1595, 1461, 1326, 1158, 1117, 1093, 1042, 837, 813, 706, 669 cm^{-1}.


NHTs
N
OTBS
Me

3r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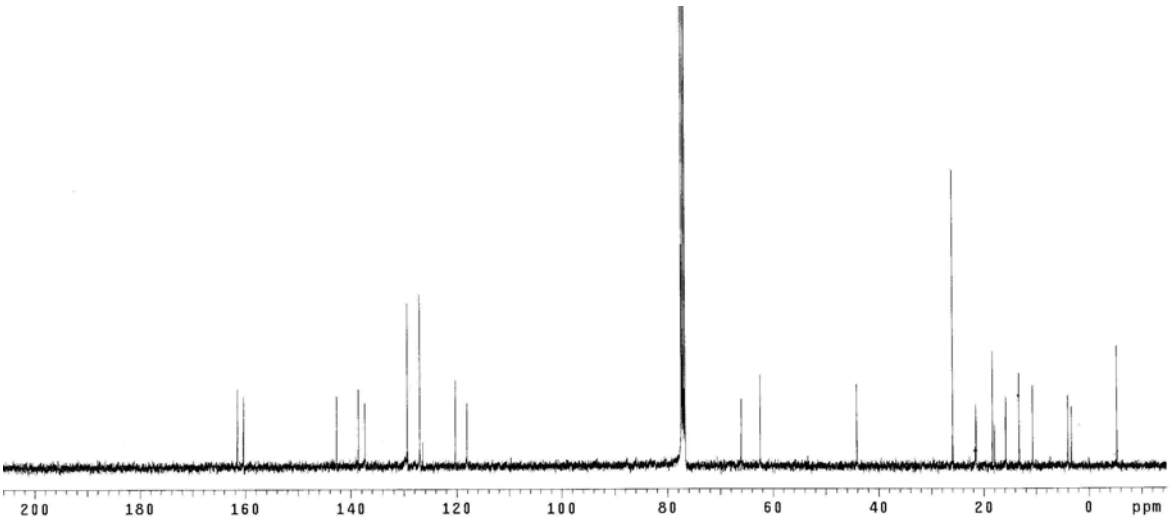
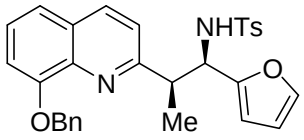
ppm


200
180
160
140
120
100
80
60
40
20
0
ppm

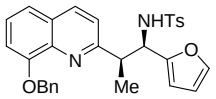
***N*-((1*R*, 2*R*)-2-(8-(benzyloxy) quinolin-2-yl)-1-(furan-2-yl)propyl)-4-methylbenzenesulfonamide**



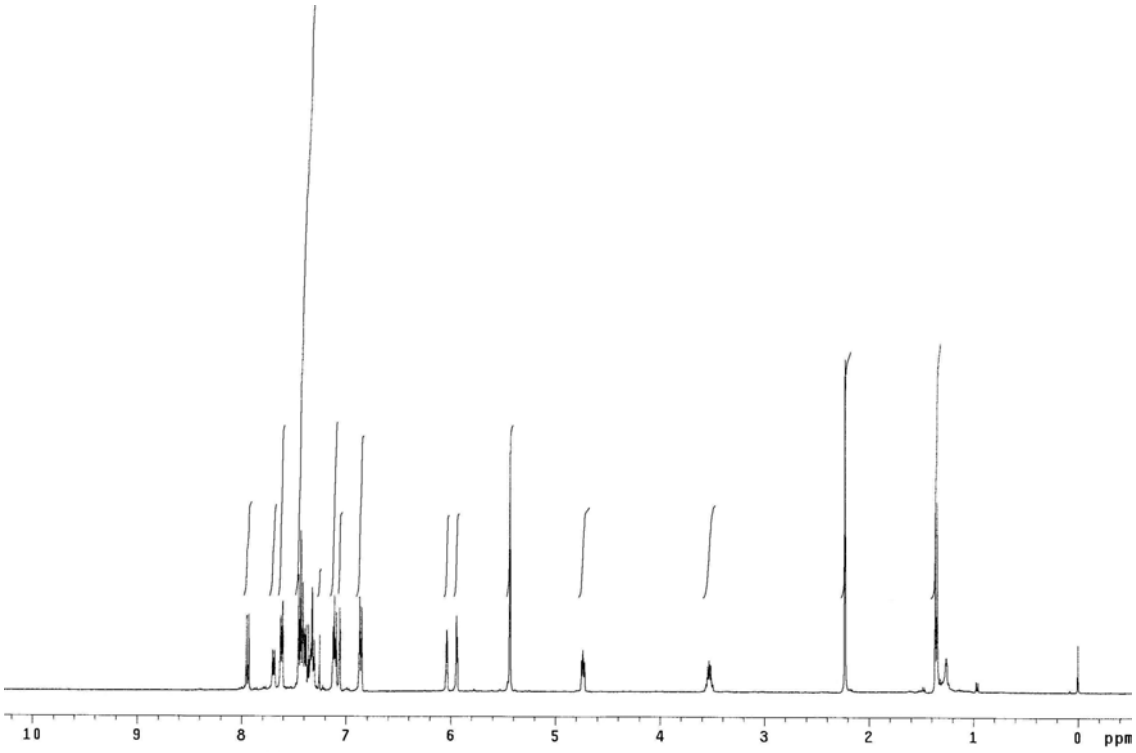
3s

In accordance with the general procedure, 6-benzyloxy-2-vinylquinoline **1e** (207 mg, 0.79 mmol, 300 mol%) was coupled to imine **2e** (66 mg, 0.26 mmol, 100 mol%) to provide the title compound (125 mg, 0.24 mmol) as an yellow liquid in 94% yield after purification by flash silica gel column chromatography (separable mixture of diastereomers in 3:1 ratio, $R_{f\ major}$ = 0.25, $R_{f\ major}$ = 0.30, 25% EtOAc/hexanes, gradient: 10 - 25 % EtOAc/hexanes).

^{1}H NMR (400 MHz, $CDCl_3$, Major Isomer): δ 7.94 (d, *J* = 8.8 Hz, 1H), 7.67 (d, *J* = 6.8 Hz, 1H), 7.61 (d, *J* = 8.0 Hz, 2H) 7.45-7.30 (m, 7H), 7.12-7.09 (m, 3H), 7.06 (d, *J* = 1.6 Hz, 1H), 6.85 (d, *J* = 7.6 Hz, 1H), 6.04-6.03 (m, 1H), 5.94 (dd, *J* = 3.2 Hz, 1H), 5.43 (m, 2H), 4.78 (dd, *J* = 8.4, 4.8 Hz, 1H), 3.56-3.49 (m, 1H), 2.22 (s, 3H), 1.35 (d, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 160.6, 154.0, 152.5, 142.1, 141.1, 139.1, 137.4, 136.8, 136.4, 128.9, 128.6, 128.0, 127.8, 127.5, 126.7, 126.3, 120.3, 119.4, 110.3, 110.0, 108.3, 70.8, 56.1, 44.0, 21.3, 15.6 .
HRMS Calcd. for $C_{30}H_{29}N_2O_4S$ (M+1): 513.1848, Found: 513.1851.
FTIR (NaCl Film): 3271, 3061, 2927, 1599, 1503, 1452, 1324, 1159, 1094, 883, 733, 696 cm^{-1}.


NHTs
N
O
OBn
Me

3s, major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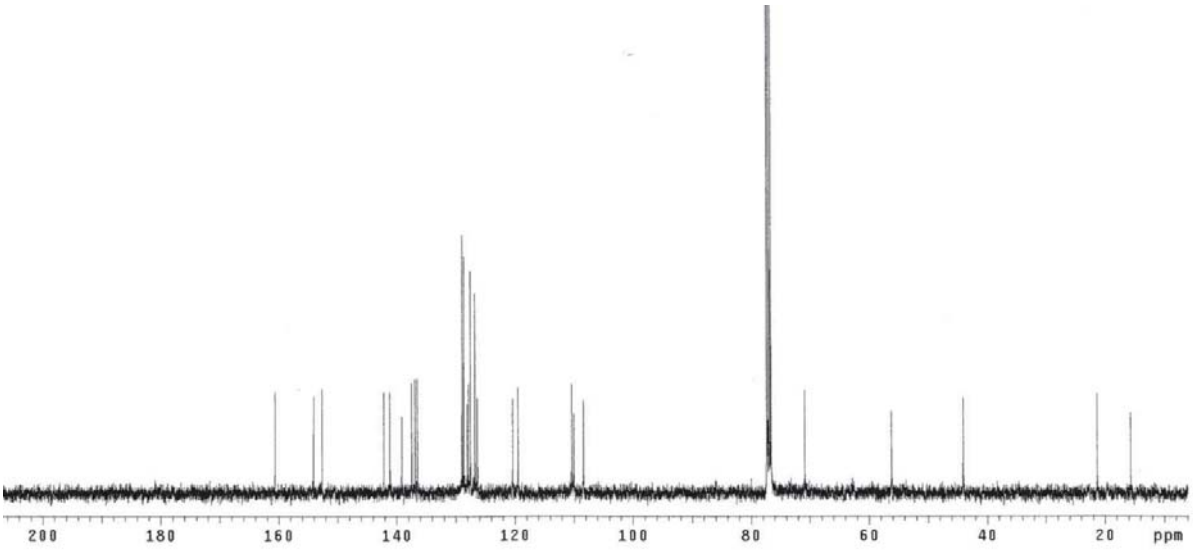
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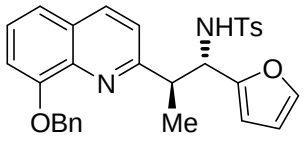
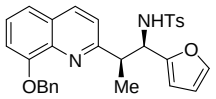
ppm

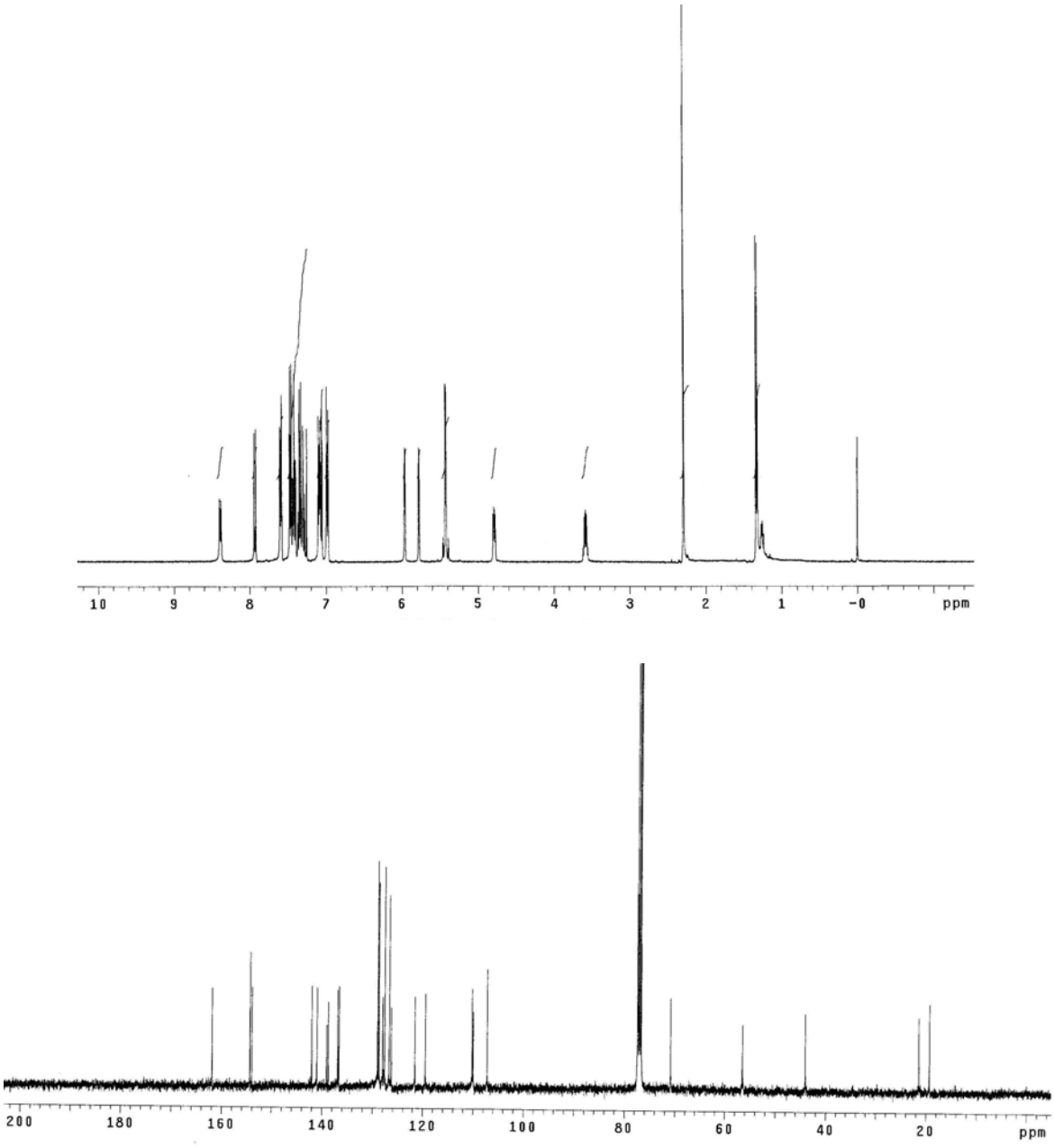


3s

^{1}H NMR (400 MHz, $CDCl_3$, Minor Isomer): δ 8.39 (d, *J* = 8.0 Hz, 1H), 7.93 (d, *J* = 8.4 Hz, 1H), 7.60 (d, *J* = 8.4 Hz, 2H), 7.47-7.28 (m, 7H), 7.10-7.05 (m, 3H), 6.98 (d, *J* = 8.0 Hz, 2H), 5.94 (dd, *J* = 3.2, 1.6 Hz, 1H), 5.77 (d, *J* = 3.2 Hz, 1H), 5.42 (m, 2H), 4.79 (dd, *J* = 8.4, 4.8 Hz, 1H), 3.61-3.55 (m, 1H), 2.29 (s, 3H), 1.33 (d, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 161.8, 154.3, 153.9, 142.0, 140.9, 139.0, 138.7, 136.8, 136.6, 128.9, 128.6, 128.0, 127.9, 127.5, 126.6, 126.2, 121.5, 119.5, 110.1, 109.9, 107.1, 70.7, 56.4, 44.0, 21.3, 19.2 .
HRMS Calcd. for $C_{30}H_{29}N_2O_4S$ (M+1): 513.1848, Found: 513.1854.
FTIR (NaCl Film): 3269, 3063, 2925, 1593, 1500, 1458, 1329, 1200, 1094, 881, 733, 696 cm^{-1}.


NHTs
N
O
OBn
Me

3s, Minor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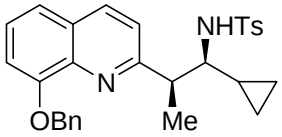
8
7
6
5
4
3
2
1
-0
ppm
200
180
160
140
120
100
80
60
40
20
ppm

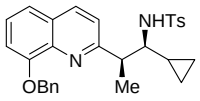
***N*-((1*R*, 2*R*)-2-(8-(benzyloxy) quinolin-2-yl)-1-(cyclopropyl-4-methylbenzenesulfonamide)**



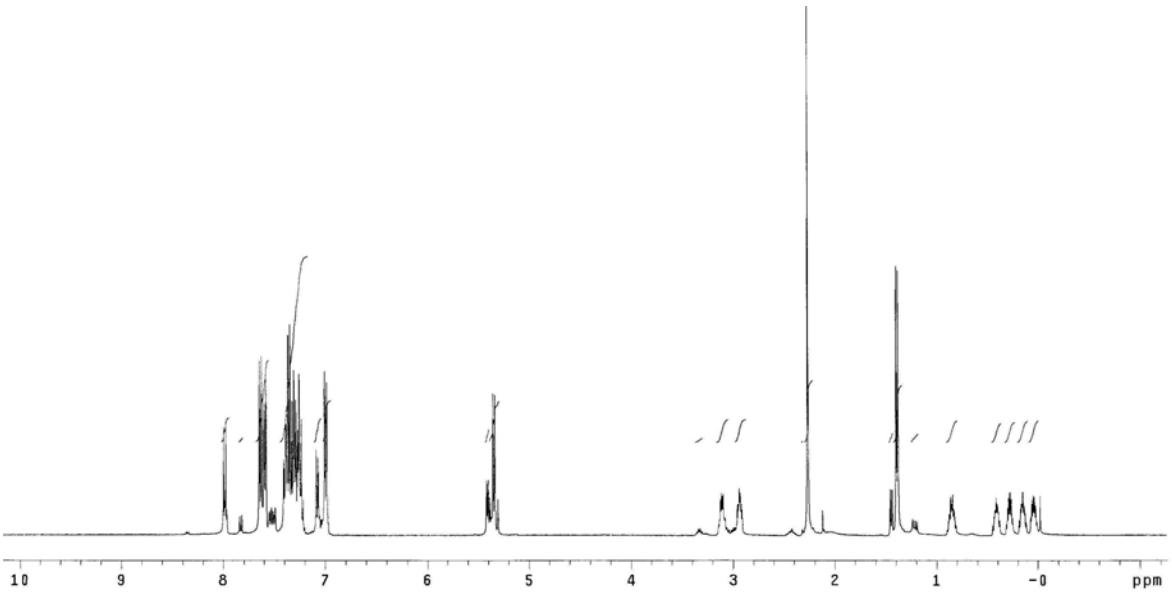
3t

In accordance with the general procedure, 6-benzyloxy-2-vinylquinoline **1e** (207 mg, 0.79 mmol, 300 mol%) was coupled to imine **2k** (60 mg, 0.26 mmol, 100 mol%) to provide the title compound (107 mg, 0.22 mmol) as a pale yellow thick syrup in 81% yield after purification by flash silica gel column chromatography (Inseparable mixture of diastereomers in 6:1 ratio, R_f = 0.32, 15% EtOAc/hexanes, gradient: 10 - 15 % EtOAc/hexanes). *Spectral data is reported for the major isomer*.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.98 (d, *J* = 8.4 Hz, 1H), 7.63 (d, *J* = 8.0 Hz, 2H), 7.59 (d, *J* = 7.6 Hz, 1H) 7.40-7.23 (m, 7H), 7.06 (d, *J* = 7.2 Hz, 1H), 6.98 (d, *J* = 8.0 Hz, 2H), 5.41 (d, *J* = 6.4 Hz, 1H), 5.34 (dd, *J* = 19.6, 12.0 Hz, 2H), 3.12-3.09 (m, 1H), 2.93 (ddd, *J* = 10.8, 7.6, 3.6 Hz, 1H), 2.26 (s, 3H), 1.38 (d, *J* = 7.6 Hz, 3H), 0.89-0.81 (m, 1H), 0.44-0.38 (m, 1H), 0.31-0.25 (m, 1H), 0.18-0.11 (m, 1H), 0.07-0.01 (m, 1H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 161.5, 154.0, 142.2, 139.0, 138.6, 136.7, 136.4, 129.0, 128.5, 128.3, 127.8, 127.7, 127.6, 126.8, 120.5, 119.3, 109.9, 70.6, 62.0, 44.3, 21.3, 15.9, 12.6, 4.1, 2.8.
HRMS Calcd. for $C_{29}H_{31}N_2O_3S$ (M+1): 487.2055, Found: 487.2066.
FTIR (NaCl Film): 3210, 3063, 2954, 1599, 1562, 1452, 1322, 1261, 1157, 1098, 834, 730, 669, 663 cm^{-1}.


NHTs
N
OBn
Me

3t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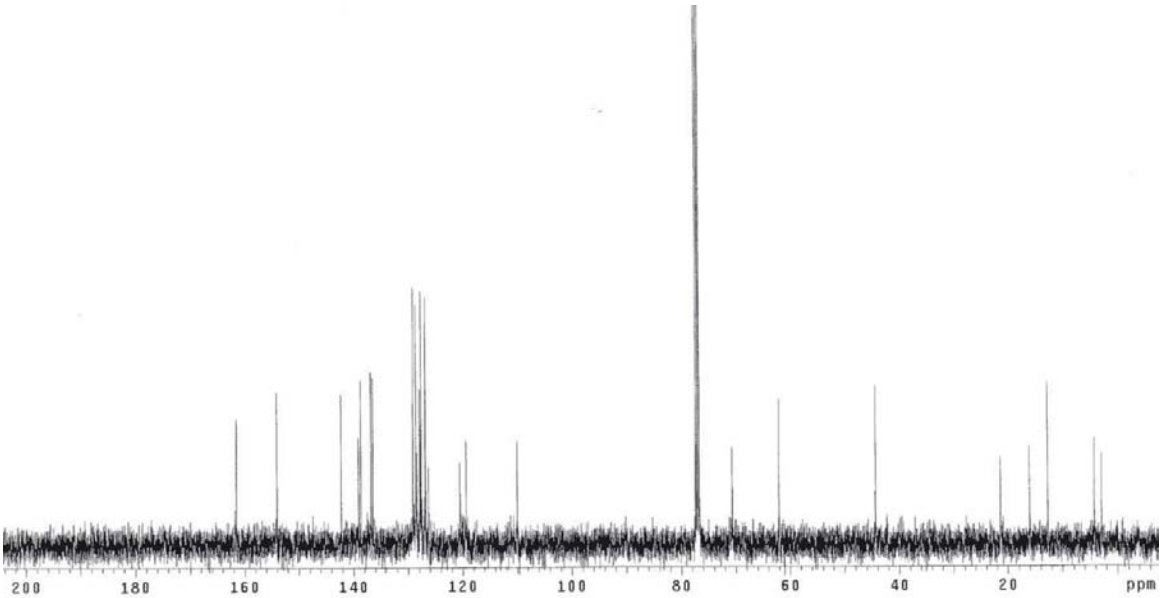
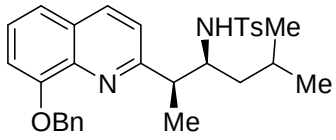
6
5
4
3
2
1
-0
ppm


200
180
160
140
120
100
80
60
40
20
ppm

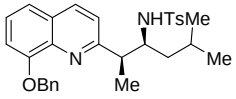
***N*-((1*R*, 2*R*)-2-(8-(benzyloxy) quinolin-2-yl)-5methylhexan-3-yl)-4-methylbenzenesulfonamide**



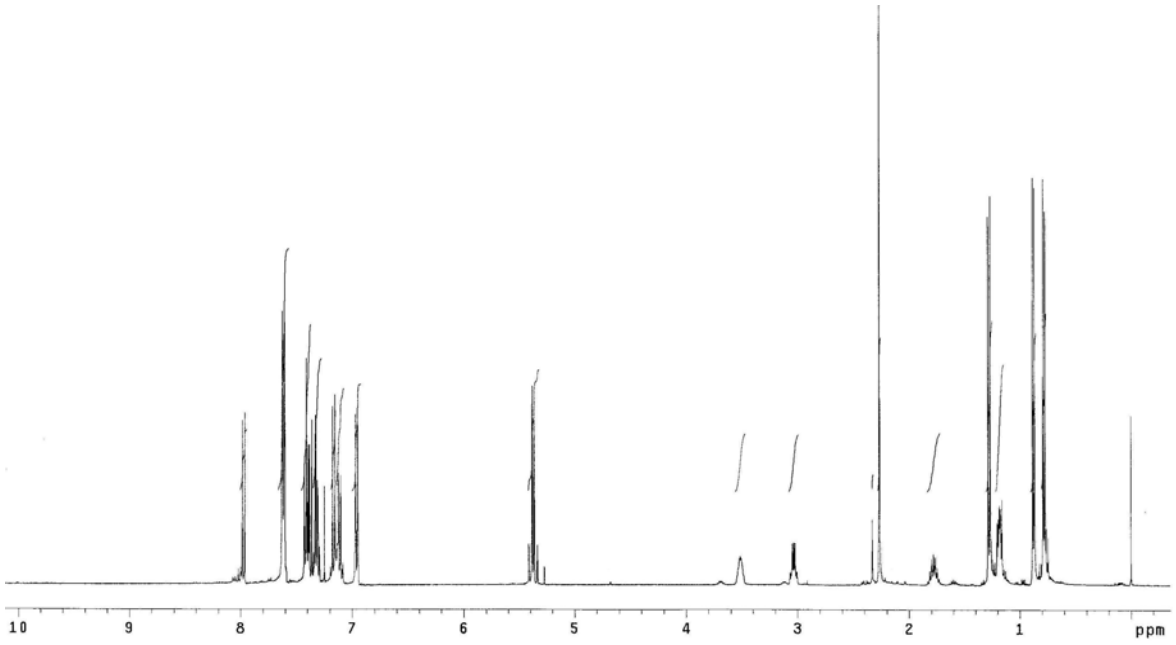
3u

In accordance with the general procedure, 6-benzyloxy-2-vinylquinoline **1e** (207 mg, 0.79 mmol, 300 mol%) was coupled to imine **2i** (63 mg, 0.26 mmol, 100 mol%) to provide the title compound (90 mg, 0.18 mmol) as a pale yellow thick syrup in 68% yield after purification by flash silica gel column chromatography (Inseparable mixture of diastereomers in 8:1 ratio, R_f = 0.30, 25% EtOAc/hexanes, gradient: 10 - 25 % EtOAc/hexanes). *Spectral data is reported for the major isomer*.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.97 (d, *J* = 8.8 Hz, 1H), 7.63-7.60 (m, 5H), 7.42-7.37 (m, 3H), 7.32-7.30 (m, 2H), 7.16 (d, *J* = 8.8 Hz, 1H), 7.11 (dd, *J* = 7.6, 1.2 Hz, 1H), 6.95 (d, *J* = 8.4 Hz, 2H), 5.37 (dd, *J* = 18.8, 11.6 Hz, 2H), 3.55-3.48 (m, 1H), 3.03 (ddd, *J* = 14.8, 7.2, 4.0 Hz, 1H), 2.26 (s, 3H), 1.83-1.73 (m, 1H), 1.27 (d, *J* = 7.2 Hz, 3H), 1.20-1.16 (m, 2H), 0.87 (d, *J* = 6.4 Hz, 3H), 0.77 (d, *J* = 6.4 Hz, 3H) .
^{13}C NMR (100 MHz, $CDCl_3$): δ 161.3, 154.0, 142.2, 139.1, 138.4, 136.7, 136.4, 129.0, 128.6, 128.5, 127.9, 127.8, 127.6, 126.7, 126.2, 120.1, 119.3, 109.8, 70.6, 56.6, 42.1, 40.2, 23.9, 23.1, 21.7, 15.1.
HRMS Calcd. for $C_{30}H_{35}N_2O_3S$ (M+1): 503.2368, Found: 503.2372.
FTIR (NaCl Film): 3200, 3063, 2954, 2868, 1599, 1503, 1453, 1324, 1262, 1160, 1094, 837, 735, 696, 665 cm^{-1}.


NHTsMe
N
Me
OBn
Me

3u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7
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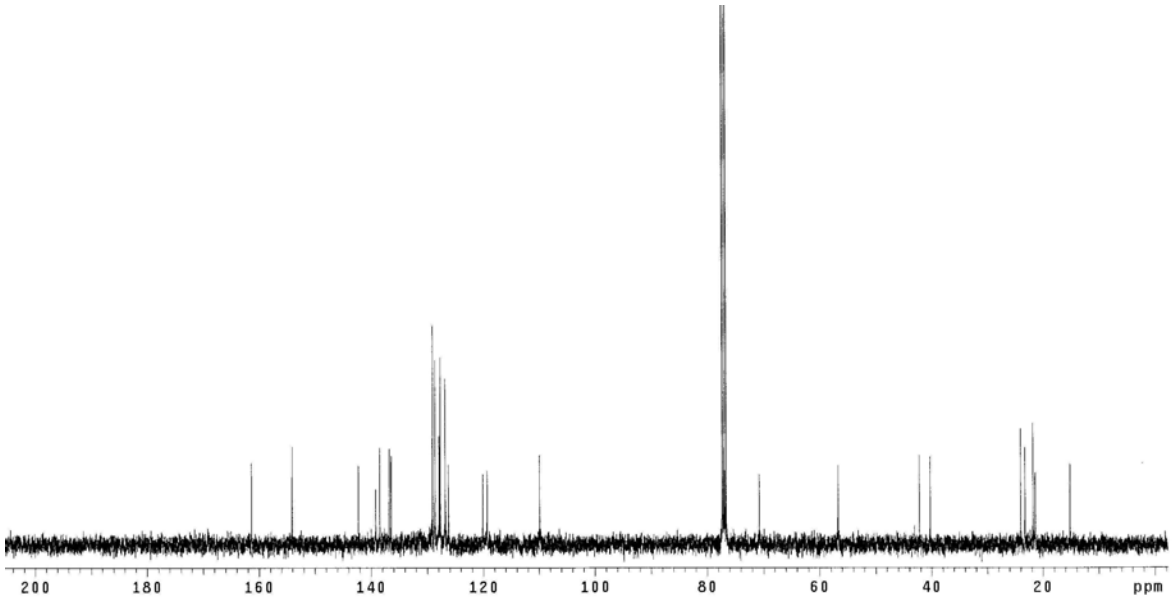
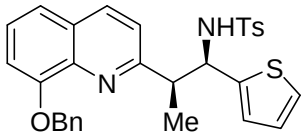
5
4
3
2
1
ppm


200
180
160
140
120
100
80
60
40
20
ppm

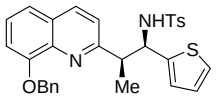
***N*-((1*R*, 2*R*)-2-(8-(benzyloxy) quinolin-2-yl)-1-(thiophen-2-yl) propyl)-4-methylbenzenesulfonamide**



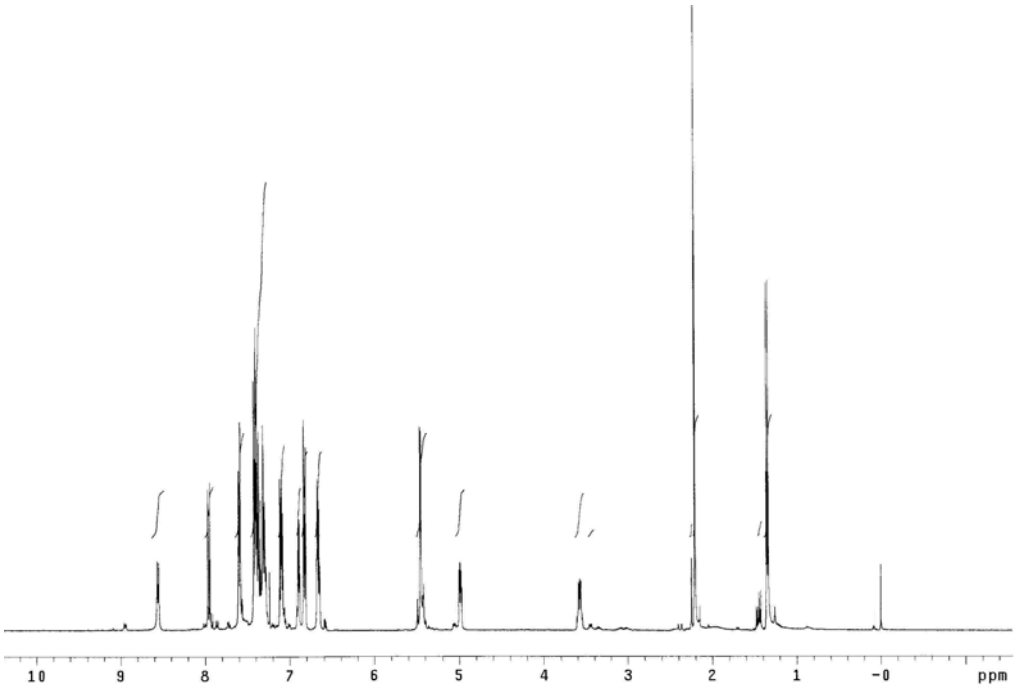
3v

In accordance with the general procedure, 6-benzyloxy-2-vinylquinoline **1e** (207 mg, 0.79 mmol, 300 mol%) was coupled to imine **2f** (70 mg, 0.26 mmol, 100 mol%) to provide the title compound (112 mg, 0.21 mmol) as a pale brown liquid in 79% yield after purification by flash silica gel column chromatography (Inseparable mixture of diastereomers in 6:1 ratio, R_f = 0.27, 25% EtOAc/hexanes, gradient: 10 - 25 % EtOAc/hexanes). *Spectral data is reported for the major isomer*.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.55 (d, *J* = 7.2 Hz, 1H), 7.95 (d, *J* = 8.4 Hz, 1H), 7.59 (d, *J* = 7.6 Hz, 2H), 7.42-7.28 (m, 7H), 7.11-7.08 (m, 2H), 6.89 (d, *J* = 4.0 Hz, 1H), 6.82 (d, *J* = 8.0 Hz, 2H), 6.68-6.64 (m, 2H), 5.45 (dd, *J* = 18.8, 11.6 Hz, 2H), 4.94 (dd, *J* = 8.0, 4.0 Hz, 1H), 3.60-3.54 (m, 1H), 2.21 (s, 3H), 1.34 (d, *J* = 7.6 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 160.4, 153.8, 142.0, 141.9, 138.7, 137.9, 136.8, 136.6, 128.7, 128.6, 128.0, 127.8, 127.3, 126.6, 126.5, 126.4, 125.6, 124.7, 120.5, 129.3, 110.2, 70.6, 58.5, 44.8, 21.2, 15.9.
HRMS Calcd. for $C_{30}H_{29}N_2O_3S_2$ (M+1): 529.1620, Found: 529.1620.
FTIR (NaCl Film): 3063, 2926, 1564, 1503, 1452, 1430, 1324, 1261, 1157, 1094, 836, 696, 665 cm^{-1}.


NHTs
N
S
OBn
Me

3v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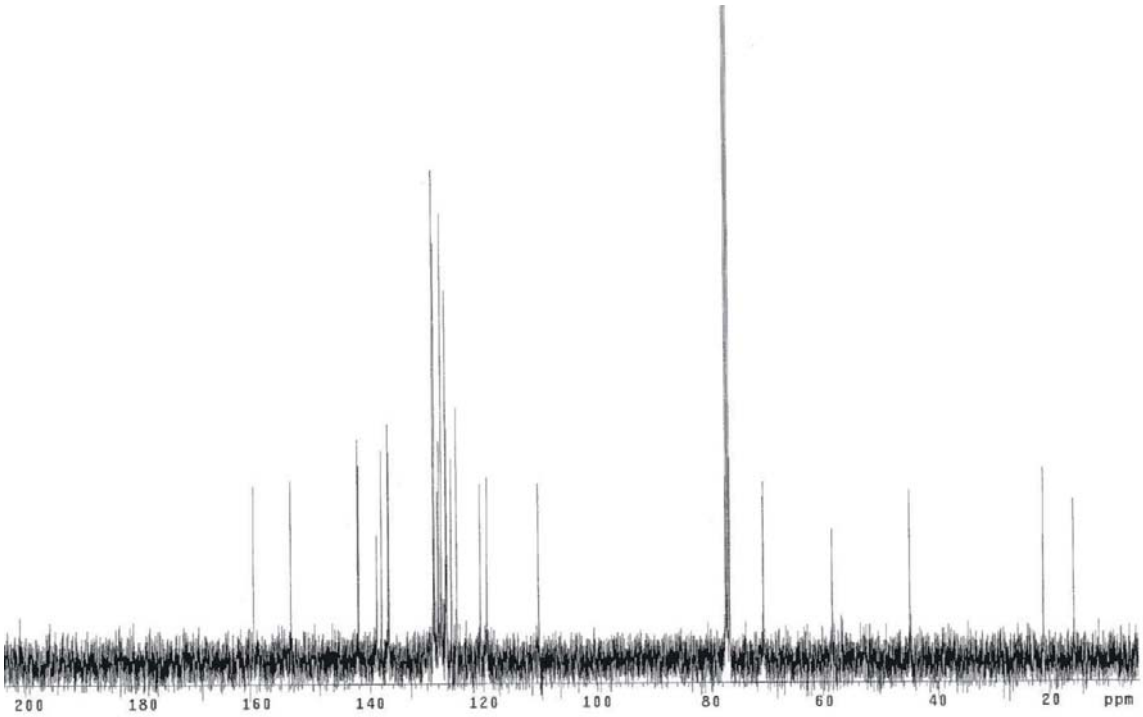
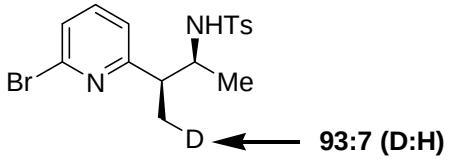
-0
ppm


200
180
160
140
120
100
80
60
40
20
ppm

III. Deuterium Labeling Experiment

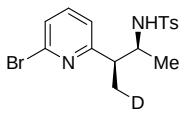
N-((2*S*, 1*R*)-3-(6-bromopyridin-2-yl) butan-2-yl)-4-methylbenzenesulfonamide (Deuterio)

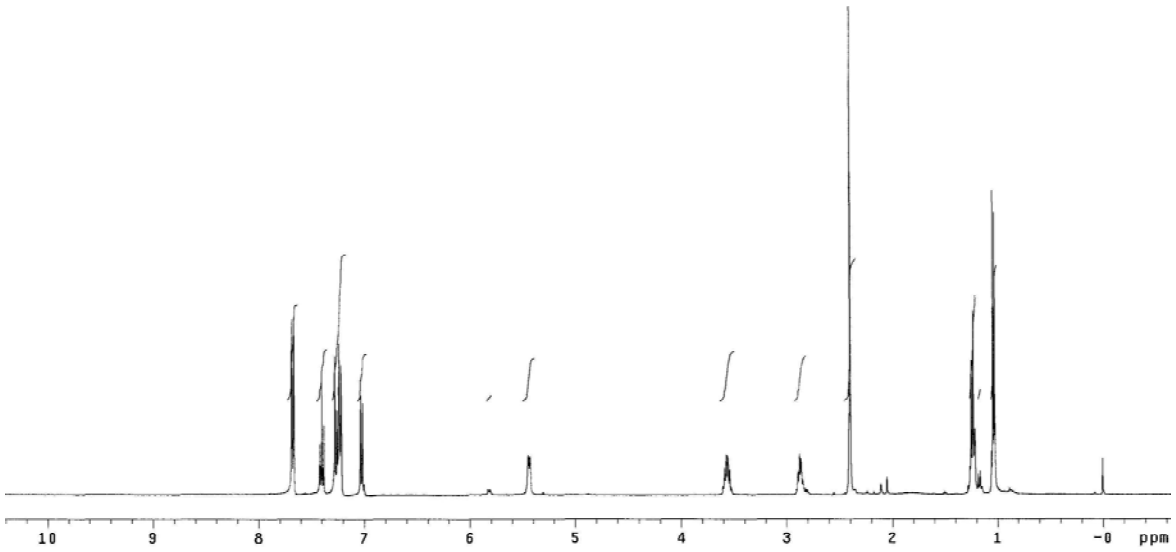


Deuterio 3l

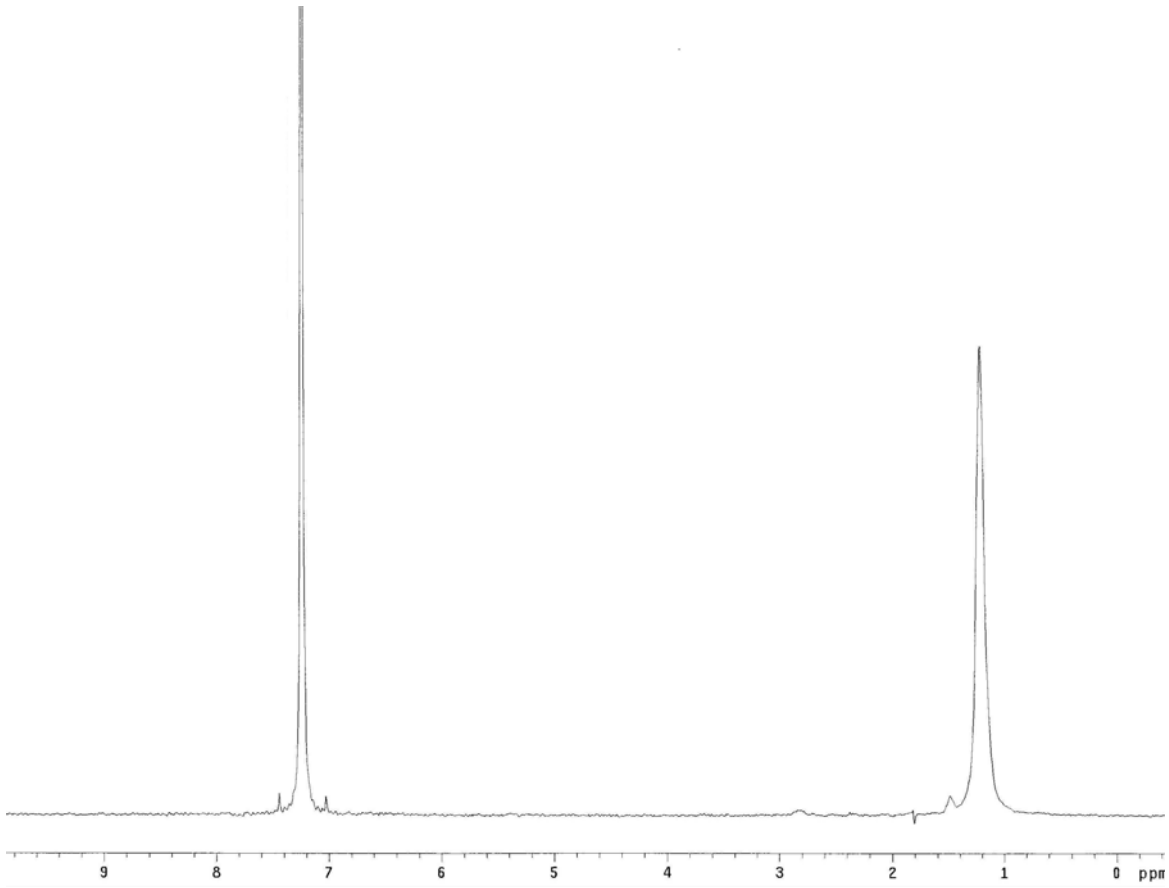
In accordance with the general procedure, 6-bromo-2-vinylpyridine **1a** (144 mg, 0.79 mmol, 300 mol%) was coupled to imine **2l** (52 mg, 0.26 mmol, 100 mol%) under deuterium gas (99.6% pure) atmosphere to provide the title compound (66 mg, 0.17 mmol) as a colorless liquid in 65% yield after purification by flash silica gel column chromatography (Inseparable mixture of diastereomers in 11:1 ratio, R_f = 0.25, 15% EtOAc/hexanes. *Spectral data is reported for the major isomer.*

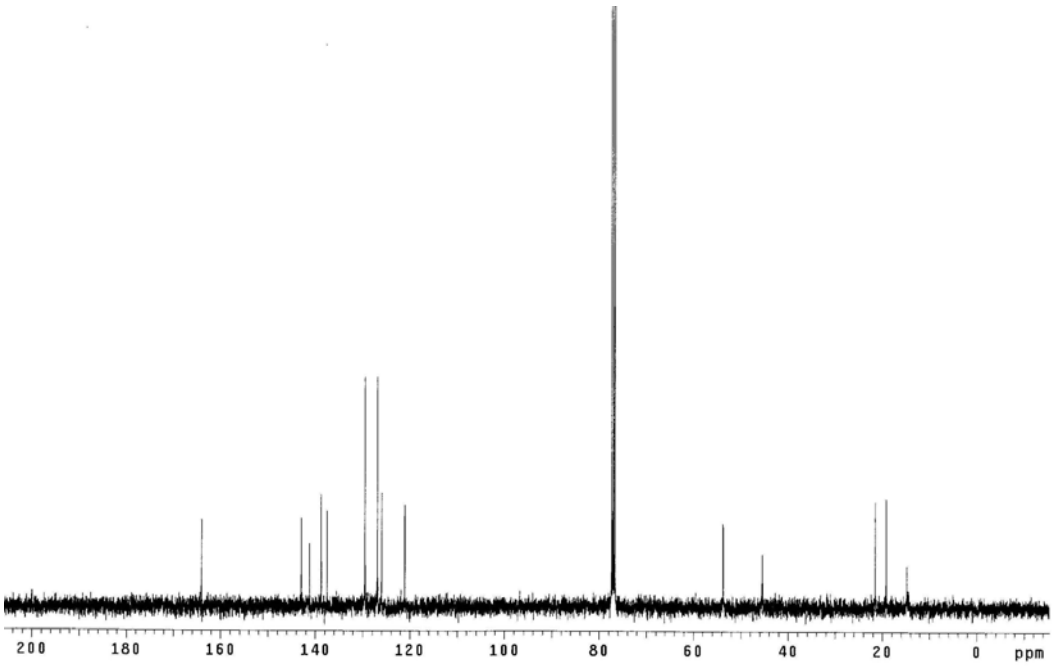
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.67 (d, *J* = 8.0 Hz, 2H), 7.40 (t, *J* = 7.6 Hz, 1H), 7.26 (d, *J* = 8.0 Hz, 1H), 7.22 (d, *J* = 8.0 Hz, 2H), 7.02 (d, *J* = 7.2 Hz, 1H), 5.44 (d, *J* = 7.6 Hz, 1H), 3.61-3.52 (m, 1H), 2.91-2.82 (m, 1H), 2.39 (s, 3H), 1.25-1.21 (m, 2H), 1.03 (d, *J* = 6.4 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 164.0, 142.9, 141.2, 138.7, 137.4, 129.5, 126.9, 125.9, 121.0, 53.7, 45.4, 45.3, 21.4, 19.1, 14.8.
HRMS Calcd. for $C_{16}H_{18}DBrN_2O_2S$ (M+1): 384.0413, Found: 384.0413.
FTIR (NaCl Film): 3272, 2975, 2322, 1580, 1553, 1433, 1380, 1324, 1126, 1089, 959, 911, 813, 706, 663 cm^{-1}.





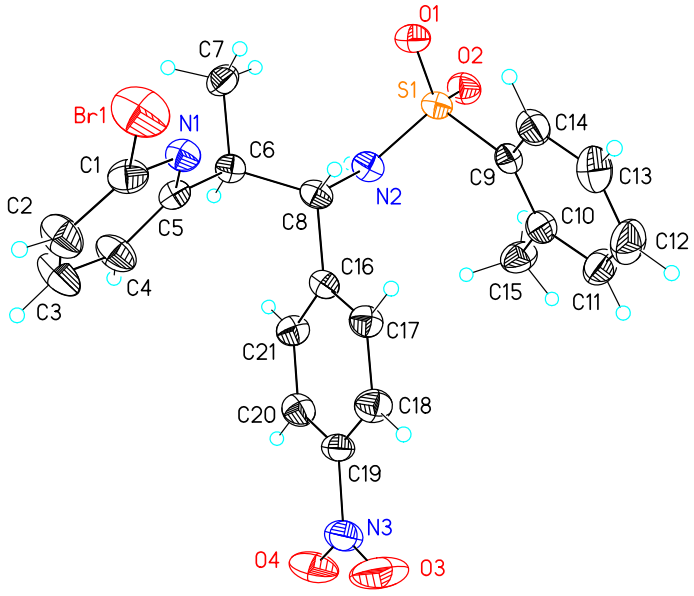
$CDCl_3$ in $CHCl_3$

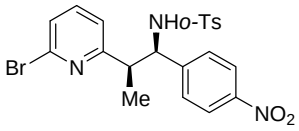



200
180
160
140
120
100
80
60
40
20
0
ppm

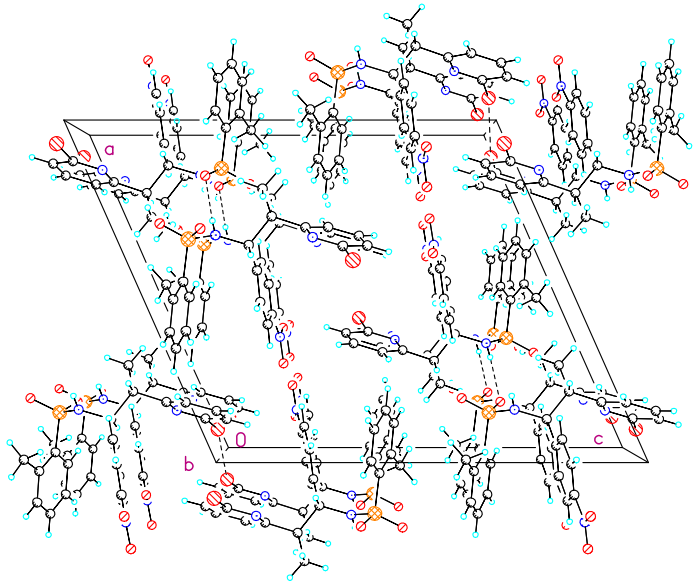
IV. X-Ray Crystallographic Data for Compound 3a

View of **3a** showing the atom labeling scheme. Displacement ellipsoids are scaled to the 50% probability level.





Unit cell packing diagram for **3a**. The view is approximately down the **b** axis.



X-ray Experimental

Table 1. Crystallographic Data for **3a**.

Table 2. Fractional coordinates and equivalent isotropic thermal parameters ($Å^2$) for the non-hydrogen atoms of **3a**.

Table 3. Bond Lengths (Å) and Angles (^{o}) for the non-hydrogen atoms of **3a**.

Table 4. Anisotropic thermal parameters for the non-hydrogen atoms of **3a**.

Table 5. Fractional coordinates and isotropic thermal parameters ($Å^2$) for the hydrogen atoms of **3a**.

Table 6. Torsion Angles (^{o}) for the non-hydrogen atoms of **3a**.

Table 7. Observed and calculated structure factor amplitudes for **3a**. Values for Fo, Fc and σ(Fo) have been multiplied by 10.

Figure 1. View of **3a** showing the atom labeling scheme. Displacement ellipsoids are scaled to the 50% probability level.

Figure 2. Unit cell packing diagram for **3a**. The view is approximately down the **b** axis.

Table 7. Observed and calculated structure factor amplitudes for **3a**. Values for Fo, Fc and σ(Fo) have been multiplied by 10.

X-ray Experimental for $C_{21}H_{20}N_3O_4SBr$: Crystals grew as colorless laths by slow evaporation from ether and hexanes. The data crystal was cut from a larger crystal and had approximate dimensions; 0.40x 0.07 x 0.06 mm. The data were collected on a Nonius Kappa CCD diffractometer using a graphite monochromator with MoKα radiation (λ = 0.71073Å). A total of 215 frames of data were collected using ω-scans with a scan range of 1.4° and a counting time of 259 seconds per frame. The data were collected at 153 K using an Oxford Cryostream low temperature device. Details of crystal data, data collection and structure refinement are listed in Table 1. Data reduction were performed using DENZO-SMN.[1] The structure was solved by direct methods using SIR97[2] and refined by full-matrix least-squares on F^2 with anisotropic displacement parameters for the non-H atoms using SHELXL-97.[3] The hydrogen atoms on carbon were calculated in ideal positions with isotropic displacement parameters set to 1.2xUeq of the attached atom (1.5xUeq for methyl hydrogen atoms). The hydrogen atom bound to N2 was observed in a ΔF map and refined with an isotropic displacement parameter. The function, $\Sigma w(|F_o|^2 - |F_c|^2)^2$, was minimized, where $w = 1/[(\sigma(F_o))^2 + (0.0359*P)^2 + (1.2475*P)]$ and $P = (|F_o|^2 + 2|F_c|^2)/3$. $R_w(F^2)$ refined to 0.108, with R(F) equal to 0.0502 and a goodness of fit, S, = 1.04. Definitions used for calculating R(F), $R_w(F^2)$ and the goodness of fit, S, are given below.[4] The data were checked for secondary extinction effects but no correction was necessary. Neutral atom scattering factors and values used to calculate the linear absorption coefficient are from the International Tables for X-ray Crystallography (1992).[5] All figures were generated using SHELXTL/PC.[6] Tables of positional and thermal parameters, bond lengths and angles, torsion angles, figures and lists of observed and calculated structure factors are located in tables 1 through 7.

References

1) DENZO-SMN. (1997). Z. Otwinowski and W. Minor, Methods in Enzymology, **276**: Macromolecular Crystallography, part A, 307 – 326, C. W. Carter, Jr. and R. M. Sweets, Editors, Academic Press.

2) SIR97. (1999). A program for crystal structure solution. Altomare A., Burla M.C., Camalli M., Cascarano G.L., Giacovazzo C. , Guagliardi A., Moliterni A.G.G., Polidori G.,Spagna R. J. Appl. Cryst. 32, 115-119.

3) Sheldrick, G. M. (1994). SHELXL97. Program for the Refinement of Crystal Structures. University of Gottingen, Germany.

4) $R_w(F^2) = \{\Sigma w(|F_o|^2 - |F_c|^2)^2/\Sigma w(|F_o|)^4\}^{1/2}$ where w is the weight given each reflection.
$R(F) = \Sigma(|F_o| - |F_c|)/\Sigma|F_o|\}$ for reflections with $F_o > 4(\sigma(F_o))$.
$S = [\Sigma w(|F_o|^2 - |F_c|^2)^2/(n - p)]^{1/2}$, where n is the number of reflections and p is the number of refined parameters.

5) International Tables for X-ray Crystallography (1992). Vol. C, Tables 4.2.6.8 and 6.1.1.4, A. J. C. Wilson, editor, Boston: Kluwer Academic Press.

6) Sheldrick, G. M. (1994). SHELXTL/PC (Version 5.03). Siemens Analytical X-ray Instruments, Inc., Madison, Wisconsin, USA.

Table 1. Crystal data and structure refinement for **3a**.

Identification code	brpyr	
Empirical formula	C21 H20 Br N3 O4 S	
Formula weight	490.37	
Temperature	153(2) K	
Wavelength	0.71070 Å	
Crystal system	Monoclinic	
Space group	P21/n	
Unit cell dimensions	a = 16.3587(8) Å	α= 90°.
	b = 7.6346(5) Å	β= 113.997(2)°.
	c = 18.8937(12) Å	γ = 90°.
Volume	2155.7(2) $Å^3$	
Z	4	
Density (calculated)	1.511 Mg/m^3	
Absorption coefficient	2.036 mm^{-1}	
F(000)	1000	
Crystal size	0.40 x 0.07 x 0.06 mm	
Theta range for data collection	2.13 to 27.47°.	
Index ranges	-21<=h<=14, -9<=k<=9, -21<=l<=24	
Reflections collected	15100	
Independent reflections	4907 [R(int) = 0.0662]	
Completeness to theta = 27.47°	99.4 %	
Absorption correction	Analytical	
Max. and min. transmission	0.908 and 0.500	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4907 / 0 / 276	
Goodness-of-fit on F^2	1.038	
Final R indices [I>2sigma(I)]	R1 = 0.0502, wR2 = 0.0916	
R indices (all data)	R1 = 0.0986, wR2 = 0.1078	
Largest diff. peak and hole	0.445 and -0.408 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **3a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Br1	4165(1)	1463(1)	4775(1)	55(1)
S1	3563(1)	4255(1)	8159(1)	29(1)
O1	3298(1)	2612(3)	7751(1)	36(1)
O2	3124(1)	4750(3)	8651(1)	36(1)
O3	7113(2)	10575(4)	7433(2)	69(1)
O4	6088(2)	12550(3)	7115(2)	52(1)
N1	3510(2)	4013(3)	5423(1)	28(1)
N2	3425(2)	5860(3)	7572(2)	27(1)
N3	6342(2)	11033(4)	7251(2)	40(1)
C1	3756(2)	3770(4)	4851(2)	32(1)
C2	3728(2)	4992(4)	4306(2)	42(1)
C3	3434(3)	6638(4)	4387(2)	49(1)
C4	3179(2)	6966(4)	4988(2)	39(1)
C5	3211(2)	5631(4)	5491(2)	26(1)
C6	2896(2)	5865(4)	6135(2)	25(1)
C7	2163(2)	4544(4)	6052(2)	33(1)
C8	3704(2)	5745(4)	6926(2)	26(1)
C9	4737(2)	4142(4)	8682(2)	28(1)
C10	5220(2)	5562(4)	9128(2)	32(1)
C11	6142(2)	5330(5)	9517(2)	38(1)
C12	6565(2)	3801(5)	9467(2)	46(1)
C13	6073(2)	2410(5)	9024(2)	42(1)
C14	5153(2)	2585(4)	8634(2)	34(1)
C15	4808(2)	7271(4)	9209(2)	39(1)
C16	4405(2)	7149(4)	7019(2)	24(1)
C17	5302(2)	6694(4)	7254(2)	29(1)
C18	5941(2)	7954(4)	7336(2)	34(1)
C19	5672(2)	9672(4)	7181(2)	29(1)
C20	4788(2)	10171(4)	6951(2)	33(1)
C21	4159(2)	8906(4)	6881(2)	30(1)

Table 3. Bond lengths [Å] and angles [°] for **3a**.

Br1-C1	1.911(3)	C8-C16	1.527(4)
S1-O2	1.436(2)	C8-H8	1.00
S1-O1	1.444(2)	C9-C14	1.390(4)
S1-N2	1.607(3)	C9-C10	1.404(4)
S1-C9	1.770(3)	C10-C11	1.393(4)
O3-N3	1.217(4)	C10-C15	1.505(4)
O4-N3	1.221(3)	C11-C12	1.380(5)
N1-C1	1.312(4)	C11-H11	0.95
N1-C5	1.354(4)	C12-C13	1.388(5)
N2-C8	1.469(4)	C12-H12	0.95
N2-H2N	0.77(3)	C13-C14	1.387(5)
N3-C19	1.477(4)	C13-H13	0.95
C1-C2	1.375(4)	C14-H14	0.95
C2-C3	1.376(5)	C15-H15A	0.98
C2-H2	0.95	C15-H15B	0.98
C3-C4	1.384(4)	C15-H15C	0.98
C3-H3	0.95	C16-C17	1.393(4)
C4-C5	1.380(4)	C16-C21	1.395(4)
C4-H4	0.95	C17-C18	1.382(4)
C5-C6	1.512(4)	C17-H17	0.95
C6-C7	1.525(4)	C18-C19	1.377(4)
C6-C8	1.543(4)	C18-H18	0.95
C6-H6	1.00	C19-C20	1.383(4)
C7-H7A	0.98	C20-C21	1.377(4)
C7-H7B	0.98	C20-H20	0.95
C7-H7C	0.98	C21-H21	0.95
O2-S1-O1	116.98(13)	C8-N2-S1	121.7(2)
O2-S1-N2	106.21(13)	C8-N2-H2N	117(2)
O1-S1-N2	111.50(13)	S1-N2-H2N	114(2)
O2-S1-C9	111.54(13)	O3-N3-O4	123.9(3)
O1-S1-C9	106.11(13)	O3-N3-C19	118.0(3)
N2-S1-C9	103.76(14)	O4-N3-C19	118.1(3)
C1-N1-C5	116.8(3)	N1-C1-C2	126.4(3)

N1-C1-Br1	115.2(2)	C11-C10-C15	119.4(3)
C2-C1-Br1	118.3(2)	C9-C10-C15	124.4(3)
C1-C2-C3	116.3(3)	C12-C11-C10	122.5(3)
C1-C2-H2	121.8	C12-C11-H11	118.8
C3-C2-H2	121.8	C10-C11-H11	118.8
C2-C3-C4	119.5(3)	C11-C12-C13	120.3(3)
C2-C3-H3	120.3	C11-C12-H12	119.9
C4-C3-H3	120.3	C13-C12-H12	119.9
C5-C4-C3	119.5(3)	C14-C13-C12	119.0(3)
C5-C4-H4	120.3	C14-C13-H13	120.5
C3-C4-H4	120.3	C12-C13-H13	120.5
N1-C5-C4	121.5(3)	C13-C14-C9	120.1(3)
N1-C5-C6	116.0(2)	C13-C14-H14	120.0
C4-C5-C6	122.5(3)	C9-C14-H14	120.0
C5-C6-C7	110.4(2)	C10-C15-H15A	109.5
C5-C6-C8	109.5(2)	C10-C15-H15B	109.5
C7-C6-C8	112.9(2)	H15A-C15-H15B	109.5
C5-C6-H6	108.0	C10-C15-H15C	109.5
C7-C6-H6	108.0	H15A-C15-H15C	109.5
C8-C6-H6	108.0	H15B-C15-H15C	109.5
C6-C7-H7A	109.5	C17-C16-C21	119.0(3)
C6-C7-H7B	109.5	C17-C16-C8	120.5(3)
H7A-C7-H7B	109.5	C21-C16-C8	120.5(3)
C6-C7-H7C	109.5	C18-C17-C16	120.9(3)
H7A-C7-H7C	109.5	C18-C17-H17	119.6
H7B-C7-H7C	109.5	C16-C17-H17	119.6
N2-C8-C16	109.6(2)	C19-C18-C17	118.5(3)
N2-C8-C6	111.6(2)	C19-C18-H18	120.7
C16-C8-C6	112.2(2)	C17-C18-H18	120.7
N2-C8-H8	107.8	C18-C19-C20	122.1(3)
C16-C8-H8	107.8	C18-C19-N3	119.4(3)
C6-C8-H8	107.8	C20-C19-N3	118.5(3)
C14-C9-C10	121.9(3)	C21-C20-C19	118.8(3)
C14-C9-S1	117.0(2)	C21-C20-H20	120.6
C10-C9-S1	121.1(2)	C19-C20-H20	120.6
C11-C10-C9	116.3(3)	C20-C21-C16	120.6(3)

C20-C21-H21	119.7	C16-C21-H21	119.7

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **3a**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br1	78(1)	32(1)	71(1)	-5(1)	48(1)	11(1)
S1	29(1)	28(1)	31(1)	3(1)	13(1)	-5(1)
O1	37(1)	28(1)	40(1)	1(1)	11(1)	-8(1)
O2	32(1)	42(1)	38(1)	5(1)	19(1)	-3(1)
O3	36(2)	58(2)	113(2)	8(2)	29(2)	-14(1)
O4	66(2)	28(1)	73(2)	-2(1)	41(2)	-13(1)
N1	32(1)	23(1)	31(1)	-2(1)	16(1)	1(1)
N2	26(2)	27(1)	34(2)	2(1)	16(1)	4(1)
N3	46(2)	38(2)	40(2)	-2(1)	22(2)	-12(2)
C1	35(2)	26(2)	39(2)	-6(2)	18(2)	-2(1)
C2	61(2)	39(2)	42(2)	-1(2)	37(2)	5(2)
C3	74(3)	37(2)	49(2)	14(2)	40(2)	6(2)
C4	54(2)	26(2)	46(2)	6(2)	31(2)	7(2)
C5	23(2)	26(2)	28(2)	-4(1)	9(1)	-3(1)
C6	24(2)	25(2)	28(2)	0(1)	12(1)	1(1)
C7	31(2)	37(2)	29(2)	-7(2)	11(1)	-8(2)
C8	31(2)	19(1)	31(2)	0(1)	17(2)	3(1)
C9	33(2)	29(2)	22(2)	3(1)	10(1)	-3(1)
C10	34(2)	35(2)	28(2)	1(2)	14(2)	-2(2)
C11	30(2)	44(2)	35(2)	-2(2)	8(2)	-3(2)
C12	30(2)	59(2)	42(2)	7(2)	8(2)	8(2)
C13	42(2)	48(2)	36(2)	5(2)	15(2)	11(2)
C14	44(2)	31(2)	30(2)	2(2)	16(2)	1(2)
C15	38(2)	30(2)	45(2)	-8(2)	13(2)	-5(2)
C16	30(2)	21(1)	25(2)	0(1)	15(1)	1(1)
C17	29(2)	24(2)	34(2)	2(1)	14(2)	3(1)
C18	27(2)	37(2)	41(2)	1(2)	18(2)	1(2)
C19	34(2)	27(2)	29(2)	-4(1)	17(2)	-9(1)
C20	42(2)	23(2)	34(2)	-2(1)	17(2)	1(2)
C21	28(2)	26(2)	36(2)	-2(1)	13(2)	1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **3a**.

	x	y	z	U(eq)
H2	3903	4714	3898	51
H3	3406	7541	4032	58
H4	2983	8101	5055	46
H6	2634	7067	6087	30
H7A	1669	4676	5541	49
H7B	1944	4753	6456	49
H7C	2406	3355	6104	49
H8	3991	4576	6955	31
H11	6491	6259	9828	46
H12	7195	3700	9737	55
H13	6362	1356	8989	51
H14	4806	1639	8334	41
H15A	5264	8006	9594	59
H15B	4324	7043	9377	59
H15C	4565	7877	8708	59
H17	5477	5503	7359	34
H18	6552	7641	7495	41
H20	4618	11365	6844	39
H21	3552	9234	6736	36
H2N	3012(19)	6420(30)	7510(16)	13(8)

Table 6. Torsion angles [°] for **3a**.

O2-S1-N2-C8	-173.5(2)	C14-C9-C10-C11	0.5(4)
O1-S1-N2-C8	-45.0(3)	S1-C9-C10-C11	179.9(2)
C9-S1-N2-C8	68.8(3)	C14-C9-C10-C15	-179.3(3)
C5-N1-C1-C2	-1.0(5)	S1-C9-C10-C15	0.0(4)
C5-N1-C1-Br1	-179.6(2)	C9-C10-C11-C12	0.4(5)
N1-C1-C2-C3	1.7(5)	C15-C10-C11-C12	-179.8(3)
Br1-C1-C2-C3	-179.6(3)	C10-C11-C12-C13	-0.7(5)
C1-C2-C3-C4	-0.7(5)	C11-C12-C13-C14	0.0(5)
C2-C3-C4-C5	-1.0(6)	C12-C13-C14-C9	0.8(5)
C1-N1-C5-C4	-0.9(4)	C10-C9-C14-C13	-1.1(4)
C1-N1-C5-C6	177.7(3)	S1-C9-C14-C13	179.5(2)
C3-C4-C5-N1	1.8(5)	N2-C8-C16-C17	106.0(3)
C3-C4-C5-C6	-176.6(3)	C6-C8-C16-C17	-129.5(3)
N1-C5-C6-C7	-56.3(3)	N2-C8-C16-C21	-73.2(3)
C4-C5-C6-C7	122.3(3)	C6-C8-C16-C21	51.3(3)
N1-C5-C6-C8	68.6(3)	C21-C16-C17-C18	-1.2(4)
C4-C5-C6-C8	-112.9(3)	C8-C16-C17-C18	179.6(3)
S1-N2-C8-C16	-119.2(2)	C16-C17-C18-C19	0.1(4)
S1-N2-C8-C6	115.9(2)	C17-C18-C19-C20	0.3(5)
C5-C6-C8-N2	-176.6(2)	C17-C18-C19-N3	-178.9(3)
C7-C6-C8-N2	-53.1(3)	O3-N3-C19-C18	1.2(4)
C5-C6-C8-C16	60.0(3)	O4-N3-C19-C18	-179.6(3)
C7-C6-C8-C16	-176.5(2)	O3-N3-C19-C20	-178.0(3)
O2-S1-C9-C14	125.9(2)	O4-N3-C19-C20	1.2(4)
O1-S1-C9-C14	-2.5(3)	C18-C19-C20-C21	0.5(4)
N2-S1-C9-C14	-120.1(2)	N3-C19-C20-C21	179.7(3)
O2-S1-C9-C10	-53.5(3)	C19-C20-C21-C16	-1.6(4)
O1-S1-C9-C10	178.1(2)	C17-C16-C21-C20	2.0(4)
N2-S1-C9-C10	60.5(3)	C8-C16-C21-C20	-178.8(3)

Table 7. Observed and calculated structure factors for **3a**
Page 1

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
2	0	0	644	633	12	5	5	0	86	77	6	-10	1	1	82	89	9	4	3	1	498	489	5	-12	6	1	72	42	71
4	0	0	2001	1999	86	6	5	0	148	146	6	-9	1	1	192	207	3	5	3	1	175	169	4	-11	6	1	78	114	77
6	0	0	406	377	6	7	5	0	290	296	5	-8	1	1	76	56	7	6	3	1	561	566	7	-10	6	1	139	140	22
8	0	0	45	45	13	8	5	0	616	614	7	-7	1	1	110	94	5	7	3	1	425	422	5	-9	6	1	144	147	13
10	0	0	125	121	7	9	5	0	84	56	23	-6	1	1	665	653	6	8	3	1	102	114	11	-8	6	1	262	270	9
12	0	0	162	160	7	10	5	0	53	70	52	-5	1	1	718	715	6	9	3	1	157	154	5	-7	6	1	32	47	32
14	0	0	256	250	11	11	5	0	232	244	17	-4	1	1	837	841	10	10	3	1	104	107	22	-6	6	1	57	70	10
16	0	0	217	227	18	12	5	0	128	119	19	-3	1	1	459	448	5	11	3	1	53	44	18	-5	6	1	461	449	5
18	0	0	227	183	23	13	5	0	149	150	15	-2	1	1	2256	2302	92	12	3	1	182	193	8	-4	6	1	287	296	6
1	1	0	544	593	182	14	5	0	0	53	1	-1	1	1	193	168	10	13	3	1	71	77	23	-3	6	1	327	322	4
2	1	0	219	203	5	15	5	0	56	28	55	1	1	1	295	290	17	14	3	1	132	119	17	-2	6	1	175	171	6
3	1	0	1394	1405	14	16	5	0	0	12	1	2	1	1	182	187	3	15	3	1	116	113	35	-1	6	1	841	832	13
4	1	0	870	869	8	0	6	0	346	299	10	3	1	1	1796	1775	20	16	3	1	64	70	64	0	6	1	25	15	25
5	1	0	655	639	6	1	6	0	234	239	4	4	1	1	581	565	6	17	3	1	0	53	1	1	6	1	224	202	17
6	1	0	145	141	3	2	6	0	321	308	4	5	1	1	314	336	3	18	3	1	97	47	96	2	6	1	137	120	5
7	1	0	1445	1396	14	3	6	0	86	71	9	6	1	1	212	219	3	-18	4	1	0	104	1	3	6	1	64	50	10
8	1	0	96	116	5	4	6	0	205	195	10	7	1	1	1006	969	9	-17	4	1	111	49	111	4	6	1	536	526	6
9	1	0	282	293	3	5	6	0	58	27	20	8	1	1	223	239	4	-16	4	1	0	9	1	5	6	1	52	42	17
10	1	0	330	332	4	6	6	0	535	544	6	9	1	1	272	277	3	-15	4	1	102	71	19	6	6	1	77	71	12
11	1	0	357	365	6	7	6	0	114	111	7	10	1	1	149	158	5	-14	4	1	169	143	24	7	6	1	206	196	7
12	1	0	38	44	29	8	6	0	315	334	5	11	1	1	11	17	11	-13	4	1	174	147	22	8	6	1	244	229	7
13	1	0	160	185	17	9	6	0	204	177	10	12	1	1	529	508	9	-12	4	1	116	147	14	9	6	1	199	190	7
14	1	0	191	175	13	10	6	0	195	183	31	13	1	1	139	127	14	-11	4	1	244	247	22	10	6	1	82	88	31
15	1	0	53	10	52	11	6	0	11	13	11	14	1	1	114	100	15	-10	4	1	653	646	23	11	6	1	260	241	22
16	1	0	103	100	19	12	6	0	134	122	15	15	1	1	137	144	17	-9	4	1	98	97	8	12	6	1	0	17	1
17	1	0	56	9	55	13	6	0	93	36	37	16	1	1	214	209	10	-8	4	1	229	242	4	13	6	1	193	184	17
19	1	0	85	23	85	14	6	0	70	93	56	17	1	1	0	11	1	-7	4	1	70	78	14	14	6	1	0	69	1
0	2	0	321	326	4	15	6	0	123	104	102	18	1	1	0	52	1	-6	4	1	92	62	6	15	6	1	89	130	88
1	2	0	216	204	3	1	7	0	707	693	9	-19	2	1	184	135	32	-5	4	1	429	418	4	-14	7	1	64	9	64
2	2	0	846	816	8	2	7	0	199	195	12	-18	2	1	149	117	36	-4	4	1	383	377	4	-13	7	1	0	55	1
3	2	0	625	616	6	3	7	0	77	88	12	-16	2	1	198	170	11	-3	4	1	394	367	3	-12	7	1	314	286	12
4	2	0	27	41	26	4	7	0	343	349	5	-15	2	1	138	141	11	-2	4	1	404	379	3	-11	7	1	82	19	40
5	2	0	537	549	6	5	7	0	191	188	5	-14	2	1	77	57	42	-1	4	1	796	788	8	-10	7	1	119	72	18
6	2	0	483	468	4	6	7	0	87	74	27	-13	2	1	144	156	10	0	4	1	0	14	1	-9	7	1	80	109	80
7	2	0	156	169	5	7	7	0	54	54	27	-12	2	1	156	150	5	1	4	1	912	885	8	-8	7	1	528	520	10
8	2	0	147	153	5	8	7	0	0	56	1	-11	2	1	238	245	4	2	4	1	44	38	12	-7	7	1	138	115	13
9	2	0	894	884	9	9	7	0	113	134	32	-10	2	1	300	298	4	3	4	1	104	95	5	-6	7	1	306	316	7
10	2	0	158	155	12	10	7	0	103	11	23	-9	2	1	29	41	28	4	4	1	316	332	4	-5	7	1	295	308	5
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13	2	0	273	268	9	13	7	0	171	165	22	-6	2	1	557	526	7	7	4	1	627	642	8	-2	7	1	289	291	5
14	2	0	212	217	23	0	8	0	106	84	29	-5	2	1	439	446	5	8	4	1	220	222	6	-1	7	1	297	295	8
15	2	0	0	18	1	1	8	0	130	135	11	-4	2	1	963	976	10	9	4	1	168	192	8	0	7	1	414	404	6
16	2	0	86	3	29	2	8	0	174	180	8	-3	2	1	43	42	8	10	4	1	108	116	11	1	7	1	86	96	10
17	2	0	137	63	24	3	8	0	380	373	9	-2	2	1	1050	1027	9	11	4	1	295	287	12	2	7	1	435	434	5
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1	3	0	601	597	5	6	8	0	228	217	23	1	2	1	374	365	4	15	4	1	0	66	1	5	7	1	135	136	9
2	3	0	608	597	6	7	8	0	140	107	15	2	2	1	1211	1183	15	16	4	1	94	28	38	6	7	1	463	449	16
3	3	0	165	155	5	8	8	0	0	58	1	3	2	1	679	677	7	17	4	1	0	59	1	7	7	1	89	43	15
4	3	0	1092	1034	10	9	8	0	54	64	54	4	2	1	176	179	5	-17	5	1	212	161	20	8	7	1	59	56	33
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9	3	0	117	122	9	3	9	0	0	24	1	9	2	1	249	255	4	-12	5	1	0	18	1	13	7	1	159	107	30
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0	4	0	409	415	5	-7	0	1	1676	1609	31	-18	3	1	79	38	56	-2	5	1	332	322	3	-2	8	1	367	370	7
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2	4	0	69	89	8	-3	0	1	293	283	4	-16	3	1	110	102	46	0	5	1	117	116	6	0	8	1	16	14	16
3	4	0	666	626	6	1	0	1	1494	1523	27	-15	3	1	117	147	27	1	5	1	817	810	8	1	8	1	93	43	26
4	4	0	594	581	6	3	0	1	1390	1325	17	-14	3	1	186	185	8	2	5	1	216	214	4	2	8	1	224	234	12
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6	4	0	393	404	5	7	0	1	62	54	13	-12	3	1	337	334	6	4	5	1	103	102	10	4	8	1	209	193	8
7	4	0	83	82	9	9	0	1	85	103	8	-11	3	1	568	569	12	5	5	1	112	113	6	5	8	1	37	55	36
8	4	0	48	42	24	11	0	1	23	39	22	-10	3	1	226	223	9	6	5	1	150	145	6	6	8	1	90	69	26
9	4	0	20	30	20	13	0	1	65	81	28	-9	3	1	321	335	9	7	5	1	53	67	14	7	8	1	0	79	1
10	4	0	119	133	9	15	0	1	206	187	15	-8	3	1	329	343	10	8	5	1	270	280	5	8	8	1	215	213	14
11	4	0	43	68	43	17	0	1	18	64	18	-7	3	1	80	79	7	9	5	1	222	223	9	9	8	1	30	24	29
12	4	0	172	164	12	19	0	1	32	114	32	-6	3	1	955	931	11	10	5	1	328	335	15	10	8	1	119	133	25
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14	4	0	252	250	19	-18	1	1	192	176	20	-4	3	1	104	101	5	12	5	1	176	152	20	-8	9	1	128	62	40
15	4	0	264	248	20	-17	1	1	31	46	30	-3	3	1	242	232	3	13	5	1	114	68	26	-7	9	1	140	76	48
16	4	0	142	143	29	-16	1	1	99	67	21	-2	3	1	537	519	5	14	5	1	0	12	1	-6	9	1	189	185	26
17	4	0	60	67	60	-15	1	1	204	204	7	-1	3	1	38	15	8	15	5	1	34	18	33	-5	9	1	169	148	18
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2	5	0	484	478	6	-13	1	1	91	93	15	1	3	1	219	199	4	-15	6	1	88	100	48	-3	9	1	250	245	18
3	5	0	154	160	4	-12	1	1	8	34	7	2	3	1	367	360	4	-14	6	1	103	116	26	-2	9	1	112	108	39
4	5	0	617	617	6	-11	1	1	152	150	4	3	3	1	59	80	9	-13	6	1	0	54	1	-1	9	1	255	244	17

Table 7. Observed and calculated structure factors for **3a**
Page 2

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
0	9	1	121	108	25	3	2	2	1051	1060	12	16	4	2	32	38	31	8	7	2	111	125	20	5	1	3	52	18	8
1	9	1	158	191	15	4	2	2	66	82	7	-17	5	2	151	56	26	9	7	2	66	25	32	6	1	3	1195	1150	12
2	9	1	54	41	54	5	2	2	226	219	5	-16	5	2	212	189	24	10	7	2	95	101	95	7	1	3	518	514	5
3	9	1	276	251	17	6	2	2	0	20	1	-15	5	2	111	75	50	11	7	2	373	352	13	8	1	3	43	32	14
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5	9	1	42	30	42	8	2	2	83	89	7	-13	5	2	39	88	39	-12	8	2	100	68	51	10	1	3	512	520	8
6	9	1	0	39	1	9	2	2	393	379	5	-12	5	2	82	84	31	-11	8	2	95	54	36	11	1	3	110	143	28
7	9	1	0	36	1	10	2	2	83	77	11	-11	5	2	172	167	26	-10	8	2	62	52	62	12	1	3	181	180	8
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-16	0	2	182	162	17	12	2	2	113	106	7	-9	5	2	32	35	32	-8	8	2	81	17	36	14	1	3	108	96	16
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-6	0	2	637	684	7	17	2	2	94	96	50	-4	5	2	321	316	4	-3	8	2	332	328	10	-19	2	3	0	46	1
-4	0	2	643	595	9	18	2	2	195	111	29	-3	5	2	193	195	3	-2	8	2	80	60	33	-18	2	3	90	64	67
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-15	2	2	352	340	8	-2	4	2	229	241	3	-10	7	2	18	10	18	-13	1	3	85	93	10	-1	3	3	629	616	6
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-8	2	2	95	97	5	5	4	2	293	299	4	-3	7	2	297	306	7	-6	1	3	650	642	6	6	3	3	429	443	5
-7	2	2	189	184	2	6	4	2	332	330	5	-2	7	2	167	169	6	-5	1	3	96	68	6	7	3	3	327	337	8
-6	2	2	66	66	4	7	4	2	123	124	7	-1	7	2	234	233	6	-4	1	3	569	595	5	8	3	3	70	75	22
-5	2	2	937	914	9	8	4	2	282	292	6	0	7	2	133	126	6	-3	1	3	1448	1444	21	9	3	3	514	528	9
-4	2	2	496	476	5	9	4	2	46	36	45	1	7	2	208	190	5	-2	1	3	553	556	7	10	3	3	41	65	35
-3	2	2	351	353	3	10	4	2	0	31	1	2	7	2	202	207	5	-1	1	3	887	881	10	11	3	3	85	68	45
-2	2	2	136	141	2	11	4	2	118	112	19	3	7	2	67	27	17	0	1	3	587	578	9	12	3	3	200	184	14
-1	2	2	907	900	10	12	4	2	161	201	24	4	7	2	70	59	28	1	1	3	999	988	11	13	3	3	164	159	15
0	2	2	272	277	4	13	4	2	217	177	21	5	7	2	122	106	9	2	1	3	900	887	12	14	3	3	0	29	1
1	2	2	814	803	8	14	4	2	0	19	1	6	7	2	40	55	39	3	1	3	1014	989	13	15	3	3	329	294	23
2	2	2	182	171	5	15	4	2	84	53	84	7	7	2	315	326	7	4	1	3	236	238	4	16	3	3	58	92	57

Table 7. Observed and calculated structure factors for **3a**
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h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
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-18	4	3	64	29	63	3	6	3	91	85	20	4	0	4	2295	2151	33	-15	3	4	91	85	50	3	5	4	167	165	6
-17	4	3	117	73	29	4	6	3	83	90	11	6	0	4	831	793	11	-14	3	4	86	84	40	4	5	4	100	87	20
-16	4	3	198	170	14	5	6	3	376	393	5	8	0	4	213	232	7	-13	3	4	298	300	14	5	5	4	172	186	14
-15	4	3	88	130	33	6	6	3	20	30	20	10	0	4	96	52	26	-12	3	4	306	308	9	6	5	4	107	83	38
-14	4	3	107	66	107	7	6	3	322	330	8	12	0	4	138	151	22	-11	3	4	66	68	7	7	5	4	117	122	20
-13	4	3	225	203	10	8	6	3	148	139	10	14	0	4	0	38	1	-10	3	4	322	320	7	8	5	4	115	111	39
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-9	4	3	204	218	5	12	6	3	99	92	99	-18	1	4	0	67	1	-6	3	4	164	156	3	12	5	4	78	49	78
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2	4	3	981	948	10	-6	7	3	137	128	12	-7	1	4	389	395	3	5	3	4	747	741	9	-8	6	4	0	35	1
3	4	3	134	135	5	-5	7	3	130	116	9	-6	1	4	762	771	8	6	3	4	94	100	12	-7	6	4	35	52	34
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6	4	3	138	144	6	-2	7	3	353	350	5	-3	1	4	614	633	9	9	3	4	314	309	5	-4	6	4	90	86	17
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13	4	3	0	58	1	5	7	3	137	134	8	4	1	4	405	417	5	16	3	4	0	35	1	3	6	4	84	100	35
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-6	5	3	37	21	17	-5	8	3	95	101	32	-19	2	4	0	38	1	-4	4	4	33	18	26	-9	7	4	381	387	10
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-4	5	3	293	284	4	-3	8	3	103	103	14	-17	2	4	222	203	12	-2	4	4	573	577	5	-7	7	4	385	381	11
-3	5	3	322	330	5	-2	8	3	332	348	7	-16	2	4	128	131	17	-1	4	4	136	145	3	-6	7	4	75	31	58
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5	5	3	24	14	23	7	8	3	106	99	46	-8	2	4	142	136	7	7	4	4	749	751	12	2	7	4	26	42	26
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9	5	3	388	395	10	-8	9	3	0	16	1	-4	2	4	162	176	3	11	4	4	178	188	15	6	7	4	39	32	39
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12	5	3	0	23	1	-5	9	3	225	215	21	-1	2	4	546	546	6	14	4	4	0	31	1	9	7	4	64	44	37
13	5	3	149	163	35	-4	9	3	90	45	56	0	2	4	622	595	7	15	4	4	110	53	73	10	7	4	0	28	1
14	5	3	77	79	54	-3	9	3	114	129	29	1	2	4	1354	1321	14	16	4	4	91	79	91	11	7	4	90	79	45
15	5	3	182	90	34	-2	9	3	156	141	22	2	2	4	401	408	5	-17	5	4	114	58	40	-12	8	4	0	57	1
-16	6	3	173	159	36	-1	9	3	66	88	66	3	2	4	516	497	9	-16	5	4	113	122	30	-11	8	4	268	271	19
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-10	6	3	223	232	25	5	9	3	99	16	76	9	2	4	347	347	6	-10	5	4	107	122	13	-5	8	4	210	211	11
-9	6	3	97	82	21	6	9	3	0	63	1	10	2	4	176	182	4	-9	5	4	166	166	9	-4	8	4	87	91	28
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-7	6	3	665	672	9	-16	0	4	51	21	50	12	2	4	189	180	10	-7	5	4	101	101	4	-2	8	4	197	200	7
-6	6	3	75	74	11	-14	0	4	191	182	8	13	2	4	248	265	15	-6	5	4	125	135	4	-1	8	4	62	103	62
-5	6	3	252	252	7	-12	0	4	543	549	8	14	2	4	87	56	31	-5	5	4	107	120	5	0	8	4	132	131	13
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Table 7. Observed and calculated structure factors for **3a**
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h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
7	8	4	159	185	33	-6	2	5	389	408	9	9	4	5	0	40	1	6	7	5	186	172	9	8	1	6	362	360	8
8	8	4	109	4	68	-5	2	5	603	586	6	10	4	5	138	109	19	7	7	5	0	30	1	9	1	6	189	176	12
9	8	4	101	90	101	-4	2	5	985	970	9	11	4	5	129	124	19	8	7	5	0	5	1	10	1	6	0	16	1
-8	9	4	72	129	71	-3	2	5	37	41	5	12	4	5	216	197	22	9	7	5	59	35	58	11	1	6	294	288	10
-7	9	4	74	46	38	-2	2	5	356	356	4	14	4	5	79	52	78	10	7	5	77	78	38	12	1	6	65	43	30
-6	9	4	0	59	1	-1	2	5	31	48	20	15	4	5	143	119	43	11	7	5	69	17	69	13	1	6	98	87	30
-5	9	4	95	30	32	0	2	5	65	67	7	-18	5	5	113	93	63	-12	8	5	169	138	20	14	1	6	113	55	32
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1	9	4	0	6	1	6	2	5	658	652	8	-12	5	5	47	66	47	-6	8	5	141	169	11	-17	2	6	214	223	10
2	9	4	294	322	14	7	2	5	188	190	5	-11	5	5	269	240	11	-5	8	5	251	254	12	-16	2	6	0	27	1
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-9	0	5	102	105	9	16	2	5	84	13	68	-2	5	5	94	79	7	4	8	5	116	120	18	-7	2	6	683	676	6
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-6	1	5	327	318	3	7	3	5	212	213	7	-5	6	5	90	69	10	-2	0	6	1502	1462	15	-16	3	6	126	111	13
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Table 7. Observed and calculated structure factors for **3a**
Page 5

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
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-14	6	6	0	43	1	-15	0	7	41	71	40	14	2	7	282	285	15	-3	5	7	257	249	4	4	8	7	107	94	20
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-12	6	6	154	122	22	-11	0	7	142	140	6	-20	3	7	102	36	40	-1	5	7	365	374	5	6	8	7	162	161	25
-11	6	6	280	253	9	-9	0	7	981	1000	13	-19	3	7	89	90	30	0	5	7	46	52	14	7	8	7	108	43	82
-10	6	6	80	48	49	-7	0	7	491	506	5	-18	3	7	80	27	39	1	5	7	430	426	9	-8	9	7	145	40	54
-9	6	6	93	72	25	-5	0	7	327	331	5	-17	3	7	0	25	1	2	5	7	95	78	20	-7	9	7	66	38	66
-8	6	6	407	411	17	-3	0	7	250	221	5	-16	3	7	63	53	63	3	5	7	174	171	11	-6	9	7	87	52	30
-7	6	6	28	54	28	-1	0	7	248	236	3	-15	3	7	95	109	17	4	5	7	151	169	11	-5	9	7	233	220	13
-6	6	6	61	67	15	1	0	7	352	335	4	-14	3	7	266	273	8	5	5	7	143	85	36	-4	9	7	67	49	38
-5	6	6	201	209	17	3	0	7	119	116	8	-13	3	7	192	197	7	6	5	7	175	185	11	-3	9	7	303	301	13
-4	6	6	453	451	6	5	0	7	477	468	7	-12	3	7	254	248	6	7	5	7	203	197	22	-2	9	7	194	203	16
-3	6	6	249	257	6	7	0	7	62	83	61	-11	3	7	307	319	6	8	5	7	105	102	23	-1	9	7	136	118	48
-2	6	6	171	171	7	9	0	7	388	374	16	-10	3	7	328	341	9	9	5	7	153	143	17	0	9	7	132	95	28
-1	6	6	169	174	5	11	0	7	122	60	16	-9	3	7	312	317	5	10	5	7	22	32	22	1	9	7	228	258	22
0	6	6	183	184	4	13	0	7	119	18	21	-8	3	7	571	564	11	11	5	7	91	65	41	2	9	7	176	171	18
1	6	6	196	200	4	15	0	7	124	5	45	-7	3	7	156	167	3	12	5	7	0	51	1	3	9	7	95	83	76
2	6	6	45	44	44	-20	1	7	194	201	30	-6	3	7	296	310	6	13	5	7	204	131	23	-20	0	8	151	172	42
3	6	6	230	214	6	-19	1	7	178	176	13	-5	3	7	309	316	5	-16	6	7	114	114	33	-18	0	8	74	86	29
4	6	6	205	203	7	-18	1	7	78	66	25	-4	3	7	744	734	9	-15	6	7	208	186	22	-16	0	8	132	136	10
5	6	6	77	56	41	-17	1	7	35	45	34	-3	3	7	159	152	5	-14	6	7	163	139	17	-14	0	8	41	57	41
6	6	6	169	180	10	-16	1	7	205	197	6	-2	3	7	848	849	9	-13	6	7	27	66	26	-12	0	8	176	178	6
7	6	6	125	136	50	-15	1	7	58	17	16	-1	3	7	92	99	6	-12	6	7	239	235	12	-10	0	8	267	261	12
8	6	6	107	100	19	-14	1	7	36	24	36	0	3	7	248	260	4	-11	6	7	112	99	34	-8	0	8	1403	1399	24
9	6	6	159	145	13	-13	1	7	68	76	14	1	3	7	31	24	29	-10	6	7	325	323	17	-6	0	8	291	297	5
10	6	6	241	230	10	-12	1	7	115	113	6	2	3	7	203	184	4	-9	6	7	0	39	1	-4	0	8	1636	1571	17

Table 7. Observed and calculated structure factors for 1
Page 6

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
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0	0	8	84	83	4	-14	3	8	41	58	40	7	5	8	181	169	13	-21	0	9	97	77	96	13	2	9	149	134	21
2	0	8	214	206	5	-13	3	8	355	349	6	8	5	8	125	107	19	-19	0	9	165	125	29	14	2	9	66	6	66
4	0	8	65	66	15	-12	3	8	210	221	6	9	5	8	56	42	56	-17	0	9	0	62	1	-20	3	9	0	41	1
6	0	8	284	268	9	-11	3	8	0	33	1	10	5	8	0	92	1	-15	0	9	719	690	11	-19	3	9	0	35	1
8	0	8	0	33	1	-10	3	8	292	296	10	11	5	8	0	76	1	-13	0	9	63	70	20	-18	3	9	77	99	28
10	0	8	432	389	17	-9	3	8	673	684	12	12	5	8	50	19	50	-11	0	9	269	283	5	-17	3	9	101	95	18
12	0	8	75	31	36	-8	3	8	42	48	15	-16	6	8	107	147	38	-9	0	9	113	124	6	-16	3	9	92	48	17
14	0	8	105	58	34	-7	3	8	237	250	5	-15	6	8	147	120	23	-7	0	9	935	897	21	-15	3	9	94	97	12
-21	1	8	54	53	53	-6	3	8	136	142	5	-14	6	8	274	266	15	-5	0	9	58	39	9	-14	3	9	406	408	9
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-17	1	8	125	149	12	-2	3	8	160	172	4	-10	6	8	407	396	20	3	0	9	675	698	9	-10	3	9	478	478	6
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1	1	8	278	280	3	-18	4	8	49	43	48	8	6	8	0	15	1	-9	1	9	77	74	6	8	3	9	239	243	10
2	1	8	541	532	4	-17	4	8	56	64	55	9	6	8	118	120	23	-8	1	9	546	559	6	9	3	9	124	125	18
3	1	8	804	800	6	-16	4	8	70	88	36	10	6	8	113	63	31	-7	1	9	84	97	6	10	3	9	207	193	12
4	1	8	299	294	4	-15	4	8	173	177	13	11	6	8	98	99	36	-6	1	9	612	578	5	11	3	9	136	142	23
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6	1	8	155	163	8	-13	4	8	0	39	1	-13	7	8	0	71	1	-4	1	9	88	99	5	13	3	9	80	97	52
7	1	8	254	270	7	-12	4	8	81	76	16	-12	7	8	183	172	16	-3	1	9	840	807	6	-19	4	9	204	164	16
8	1	8	0	40	1	-11	4	8	62	31	13	-11	7	8	165	132	20	-2	1	9	654	658	4	-18	4	9	105	67	22
9	1	8	82	89	82	-10	4	8	115	108	7	-10	7	8	68	25	67	-1	1	9	454	453	3	-17	4	9	80	46	79
10	1	8	30	48	29	-9	4	8	79	78	5	-9	7	8	202	215	9	0	1	9	102	111	8	-16	4	9	79	66	36
11	1	8	79	87	38	-8	4	8	449	451	6	-8	7	8	267	266	8	1	1	9	239	247	2	-15	4	9	92	75	29
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14	1	8	71	91	71	-5	4	8	404	416	5	-5	7	8	143	154	13	4	1	9	182	183	4	-12	4	9	208	210	14
15	1	8	75	86	75	-4	4	8	421	432	6	-4	7	8	151	144	14	5	1	9	329	316	6	-11	4	9	97	95	18
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-18	2	8	126	105	17	-1	4	8	407	406	5	-1	7	8	133	124	11	8	1	9	34	12	34	-8	4	9	221	229	8
-17	2	8	192	197	12	0	4	8	149	159	5	0	7	8	42	9	41	9	1	9	36	15	36	-7	4	9	502	508	6
-16	2	8	0	33	1	1	4	8	242	257	5	1	7	8	232	213	9	10	1	9	122	102	16	-6	4	9	93	104	6
-15	2	8	266	267	8	2	4	8	167	153	8	2	7	8	100	121	22	11	1	9	60	74	52	-5	4	9	0	17	1
-14	2	8	99	114	9	3	4	8	0	22	1	3	7	8	156	162	11	12	1	9	67	67	66	-4	4	9	253	274	6
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-11	2	8	517	520	6	6	4	8	193	183	21	6	7	8	0	15	1	-20	2	9	155	149	13	-1	4	9	493	503	7
-10	2	8	335	339	8	7	4	8	0	53	1	7	7	8	27	51	26	-19	2	9	0	25	1	0	4	9	486	492	7
-9	2	8	380	365	6	8	4	8	219	225	11	8	7	8	0	25	1	-18	2	9	86	69	30	1	4	9	188	193	10
-8	2	8	53	51	13	9	4	8	405	383	11	9	7	8	82	35	42	-17	2	9	152	142	10	2	4	9	239	239	10
-7	2	8	233	241	3	10	4	8	123	113	18	-12	8	8	83	108	57	-16	2	9	132	104	11	3	4	9	487	512	8
-6	2	8	56	67	6	11	4	8	152	175	25	-11	8	8	192	160	18	-15	2	9	46	49	46	4	4	9	296	311	9
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-4	2	8	194	202	2	13	4	8	65	106	64	-9	8	8	184	179	16	-13	2	9	101	85	6	6	4	9	279	308	17
-3	2	8	495	515	5	-18	5	8	48	106	47	-8	8	8	95	121	37	-12	2	9	342	345	5	7	4	9	260	278	11
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-1	2	8	309	324	3	-16	5	8	176	175	14	-6	8	8	60	36	54	-10	2	9	679	688	10	9	4	9	202	204	25
0	2	8	380	382	4	-15	5	8	60	76	60	-5	8	8	385	359	9	-9	2	9	132	128	3	10	4	9	113	135	39
1	2	8	656	673	5	-14	5	8	93	65	23	-4	8	8	94	71	62	-8	2	9	119	112	5	11	4	9	0	30	1
2	2	8	81	64	6	-13	5	8	89	54	25	-3	8	8	0	24	1	-7	2	9	227	215	5	12	4	9	0	71	1
3	2	8	208	209	5	-12	5	8	517	516	17	-2	8	8	101	55	27	-6	2	9	1007	1000	15	-18	5	9	121	79	23
4	2	8	443	453	6	-11	5	8	188	193	10	-1	8	8	328	305	16	-5	2	9	408	412	5	-17	5	9	51	82	51
5	2	8	356	361	8	-10	5	8	94	86	23	0	8	8	136	117	13	-4	2	9	197	207	3	-16	5	9	99	45	29
6	2	8	151	176	6	-9	5	8	265	265	12	1	8	8	101	70	26	-3	2	9	316	319	5	-15	5	9	0	14	1
7	2	8	381	380	6	-8	5	8	216	217	10	2	8	8	0	27	1	-2	2	9	547	548	5	-14	5	9	83	49	27
8	2	8	391	396	9	-7	5	8	177	185	17	3	8	8	155	154	13	-1	2	9	89	94	5	-13	5	9	57	33	56
9	2	8	0	31	1	-6	5	8	517	523	6	4	8	8	207	201	11	0	2	9	424	415	3	-12	5	9	125	120	16
10	2	8	24	26	24	-5	5	8	94	102	9	5	8	8	0	40	1	1	2	9	35	25	24	-11	5	9	285	277	14
11	2	8	145	140	14	-4	5	8	532	553	8	6	8	8	72	47	71	2	2	9	492	502	5	-10	5	9	105	109	13
12	2	8	184	187	16	-3	5	8	229	223	4	-7	9	8	0	14	1	3	2	9	30	14	29	-9	5	9	173	143	26
13	2	8	61	9	61	-2	5	8	198	203	6	-6	9	8	120	109	25	4	2	9	210	209	10	-8	5	9	114	71	14
14	2	8	110	82	30	-1	5	8	56	49	8	-5	9	8	153	134	41	5	2	9	167	170	5	-7	5	9	497	498	7
15	2	8	146	142	23	0	5	8	298	313	5	-4	9	8	96	44	96	6	2	9	85	79	6	-6	5	9	170	183	5
-20	3	8	81	52	81	1	5	8	0	7	1	-3	9	8	0	23	1	7	2	9	295	288	9	-5	5	9	283	296	5
-19	3	8	96	61	29	2	5	8	431	437	10	-2	9	8	107	117	35	8	2	9	296	295	9	-4	5	9	183	190	6
-18	3	8	248	259	16	3	5	8	172	186	8	-1	9	8	81	73	50	9	2	9	139	118	10	-3	5	9	53	75	52
-17	3	8	0	5	1	4	5	8	261	264	8	0	9	8	198	186	15	10	2	9	39	18	39	-2	5	9	66	57	17
-16	3	8	82	48	23	5	5	8	95	84	32	1	9	8	57	70	56	11	2	9	53	49	52	-1	5	9	425	428	5

Table 7. Observed and calculated structure factors for **3a**
Page 7

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
0	5	9	0	6	1	-20	0	10	154	170	19	13	2	10	107	97	33	2	5	10	162	163	12	-3	0	11	849	855	9
1	5	9	390	390	9	-18	0	10	56	15	55	-20	3	10	80	105	79	3	5	10	19	30	18	-1	0	11	134	121	5
2	5	9	79	97	26	-16	0	10	146	132	10	-19	3	10	85	58	41	4	5	10	239	245	14	1	0	11	117	118	7
3	5	9	213	218	12	-14	0	10	463	458	7	-18	3	10	87	71	45	5	5	10	114	117	42	3	0	11	320	322	8
4	5	9	112	85	17	-12	0	10	213	218	11	-17	3	10	52	50	51	6	5	10	239	235	15	5	0	11	41	75	41
5	5	9	122	73	14	-10	0	10	471	502	13	-16	3	10	0	65	1	7	5	10	41	60	41	7	0	11	0	16	1
6	5	9	123	115	29	-8	0	10	568	596	9	-15	3	10	198	205	10	8	5	10	103	82	36	9	0	11	169	109	23
7	5	9	152	149	24	-6	0	10	333	319	4	-14	3	10	295	296	11	9	5	10	104	103	36	11	0	11	231	226	20
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Table 7. Observed and calculated structure factors for **3a**
Page 9

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
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1	2	13	188	200	7	0	5	13	112	56	51	-9	1	14	358	375	6	-11	4	14	0	29	1	-2	8	14	0	52	1
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-13	5	13	261	234	25	8	0	14	0	18	1	4	3	14	148	156	14	-4	7	14	0	34	1	8	2	15	0	9	1
-12	5	13	193	181	19	10	0	14	0	104	1	5	3	14	82	81	81	-3	7	14	347	350	17	-19	3	15	55	37	55
-11	5	13	25	32	25	-20	1	14	140	89	16	6	3	14	80	83	31	-2	7	14	117	114	42	-18	3	15	74	40	48
-10	5	13	136	144	21	-19	1	14	69	23	45	7	3	14	161	157	21	-1	7	14	93	8	92	-17	3	15	137	125	18

Table 7. Observed and calculated structure factors for **3a**
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h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
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-14	3	15	212	207	10	-1	6	15	197	179	12	4	2	16	116	112	17	-6	6	16	18	27	17	7	2	17	88	37	39
-13	3	15	249	257	9	0	6	15	0	19	1	5	2	16	103	11	47	-5	6	16	135	101	29	-18	3	17	169	153	22
-12	3	15	295	283	6	1	6	15	166	133	18	6	2	16	0	33	1	-4	6	16	133	114	20	-17	3	17	0	50	1
-11	3	15	100	78	14	2	6	15	64	20	63	7	2	16	58	3	57	-3	6	16	24	71	24	-16	3	17	207	209	13
-10	3	15	449	435	10	3	6	15	39	38	38	8	2	16	0	51	1	-2	6	16	53	35	52	-15	3	17	106	105	23
-9	3	15	19	53	19	4	6	15	110	32	62	-19	3	16	0	53	1	-1	6	16	86	105	32	-14	3	17	84	63	37
-8	3	15	90	98	11	-12	7	15	180	139	29	-18	3	16	106	73	36	0	6	16	157	148	32	-13	3	17	19	27	18
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-6	3	15	120	112	8	-10	7	15	159	167	19	-16	3	16	160	152	15	2	6	16	155	112	28	-11	3	17	84	25	20
-5	3	15	233	244	5	-9	7	15	129	155	22	-15	3	16	181	134	30	3	6	16	0	6	1	-10	3	17	197	191	13
-4	3	15	231	232	6	-8	7	15	115	86	30	-14	3	16	0	15	1	-10	7	16	6	43	6	-9	3	17	52	25	51
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6	4	15	100	93	35	-8	1	16	184	175	9	-3	4	16	83	83	25	-6	1	17	162	161	7	4	4	17	0	39	1
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1	5	15	107	99	27	-16	2	16	178	169	9	-6	5	16	246	244	10	-13	2	17	78	76	19	3	5	17	42	82	41
2	5	15	132	155	21	-15	2	16	201	205	8	-5	5	16	67	43	31	-12	2	17	254	242	8	4	5	17	115	77	68
3	5	15	112	128	21	-14	2	16	103	110	14	-4	5	16	0	61	1	-11	2	17	188	188	12	-13	6	17	150	135	25
4	5	15	112	132	31	-13	2	16	244	234	6	-3	5	16	129	91	15	-10	2	17	72	69	19	-12	6	17	144	152	18
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6	5	15	129	66	29	-11	2	16	22	72	22	-1	5	16	53	67	52	-8	2	17	302	284	10	-10	6	17	28	5	27
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-4	6	15	67	83	66	1	2	16	66	68	27	-9	6	16	130	115	26	4	2	17	165	162	15	-8	7	17	188	183	22

Table 7. Observed and calculated structure factors for **3a**
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h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
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-6	7	17	206	197	14	2	3	18	103	75	26	2	1	19	12	58	12	-6	6	19	97	13	66	-6	4	20	170	162	17
-5	7	17	128	24	32	3	3	18	0	8	1	3	1	19	0	8	1	-5	6	19	34	111	33	-5	4	20	41	8	41
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-18	0	18	254	236	20	5	3	18	33	5	32	5	1	19	96	84	95	-18	0	20	444	434	26	-3	4	20	162	131	19
-16	0	18	267	252	22	-16	4	18	235	185	16	-18	2	19	86	43	52	-16	0	20	56	96	56	-2	4	20	67	74	66
-14	0	18	27	4	27	-15	4	18	207	235	15	-17	2	19	95	71	94	-14	0	20	113	83	20	-1	4	20	114	5	29
-12	0	18	328	306	21	-14	4	18	92	86	46	-16	2	19	218	203	18	-12	0	20	0	72	1	0	4	20	42	86	42
-10	0	18	136	140	14	-13	4	18	153	164	13	-15	2	19	9	12	9	-10	0	20	50	41	50	1	4	20	101	83	37
-8	0	18	194	175	12	-12	4	18	263	272	11	-14	2	19	179	187	13	-8	0	20	124	102	13	-12	5	20	117	57	31
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-2	0	18	157	211	18	-9	4	18	182	160	15	-11	2	19	32	62	31	-2	0	20	157	113	20	-9	5	20	101	56	32
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-7	1	18	75	61	15	-12	5	18	94	51	64	-16	3	19	0	73	1	-5	1	20	187	196	15	1	0	21	184	192	28
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-3	1	18	132	127	13	-8	5	18	292	269	15	-12	3	19	209	213	25	-1	1	20	57	76	56	-14	1	21	0	36	1
-2	1	18	171	174	8	-7	5	18	192	175	33	-11	3	19	17	7	17	0	1	20	92	60	45	-13	1	21	77	74	77
-1	1	18	220	222	7	-6	5	18	293	275	12	-10	3	19	228	206	24	1	1	20	156	147	22	-12	1	21	53	62	52
0	1	18	167	168	9	-5	5	18	155	144	15	-9	3	19	323	322	20	2	1	20	191	182	13	-11	1	21	170	181	10
1	1	18	247	232	9	-4	5	18	160	162	12	-8	3	19	90	97	24	3	1	20	0	51	1	-10	1	21	138	148	17
2	1	18	0	45	1	-3	5	18	94	80	28	-7	3	19	251	239	23	4	1	20	106	8	65	-9	1	21	200	180	12
3	1	18	78	52	45	-2	5	18	211	185	21	-6	3	19	217	182	14	-17	2	20	52	37	52	-8	1	21	37	41	37
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6	1	18	78	32	78	1	5	18	109	108	39	-3	3	19	160	126	11	-14	2	20	0	36	1	-5	1	21	34	57	34
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-14	2	18	138	128	19	-9	6	18	146	145	25	2	3	19	86	71	61	-9	2	20	402	387	23	0	1	21	74	71	39
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-4	2	18	95	98	16	-15	0	19	146	130	17	-9	4	19	0	33	1	1	2	20	138	79	16	-9	2	21	107	70	80
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0	3	18	215	235	41	0	1	19	358	338	9	-8	6	19	169	127	17	-8	4	20	0	71	1	-11	4	21	161	142	24

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
-10	4	21	105	90	34	-13	1	22	0	75	1	-4	2	22	79	102	78	-7	0	23	61	38	60	-4	2	23	94	11	51
-9	4	21	0	74	1	-12	1	22	71	61	34	-3	2	22	237	218	14	-5	0	23	185	176	24	-3	2	23	0	54	1
-8	4	21	83	62	83	-11	1	22	48	13	47	-2	2	22	0	16	1	-3	0	23	0	42	1	-11	3	23	85	164	84
-7	4	21	64	51	64	-10	1	22	108	94	18	-1	2	22	154	120	35	-14	1	23	70	49	69	-10	3	23	0	63	1
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-4	4	21	0	62	1	-7	1	22	98	83	19	-11	3	22	76	106	75	-11	1	23	75	23	74	-7	3	23	79	40	78
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-9	5	21	42	91	42	-4	1	22	74	12	50	-8	3	22	118	129	27	-8	1	23	177	170	17	-12	0	24	135	144	25
-8	5	21	210	183	37	-3	1	22	0	8	1	-7	3	22	109	122	26	-7	1	23	124	115	19	-10	0	24	0	35	1
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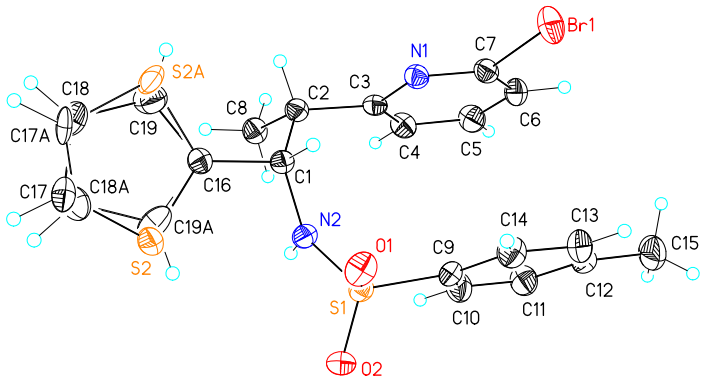
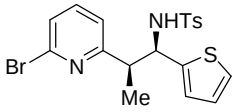
-14	0	22	38	75	37	-15	2	22	232	205	30	-3	3	22	0	1	1	-3	1	23	106	97	26	-10	1	24	164	123	31
-12	0	22	211	195	34	-14	2	22	122	111	26	-2	3	22	57	106	57	-2	1	23	0	52	1	-9	1	24	0	3	1
-10	0	22	148	144	15	-13	2	22	0	23	1	-11	4	22	181	114	27	-13	2	23	233	191	23	-8	1	24	63	19	62
-8	0	22	102	132	27	-12	2	22	0	25	1	-10	4	22	160	154	40	-12	2	23	40	43	40	-7	1	24	121	135	28
-6	0	22	333	295	26	-11	2	22	0	11	1	-9	4	22	172	161	37	-11	2	23	0	6	1	-6	1	24	144	128	16
-4	0	22	148	161	20	-10	2	22	127	56	23	-8	4	22	155	143	29	-10	2	23	157	124	24	-5	1	24	58	15	57
-2	0	22	0	36	1	-9	2	22	0	21	1	-7	4	22	0	2	1	-9	2	23	189	166	40	-9	2	24	0	58	1
0	0	22	210	184	23	-8	2	22	0	68	1	-6	4	22	0	49	1	-8	2	23	128	153	38	-8	2	24	94	51	93
-16	1	22	89	98	89	-7	2	22	54	56	53	-5	4	22	156	155	24	-7	2	23	110	136	26						
-15	1	22	13	19	12	-6	2	22	54	18	53	-11	0	23	47	33	47	-6	2	23	0	10	1						
-14	1	22	96	70	32	-5	2	22	0	16	1	-9	0	23	84	99	63	-5	2	23	0	22	1						

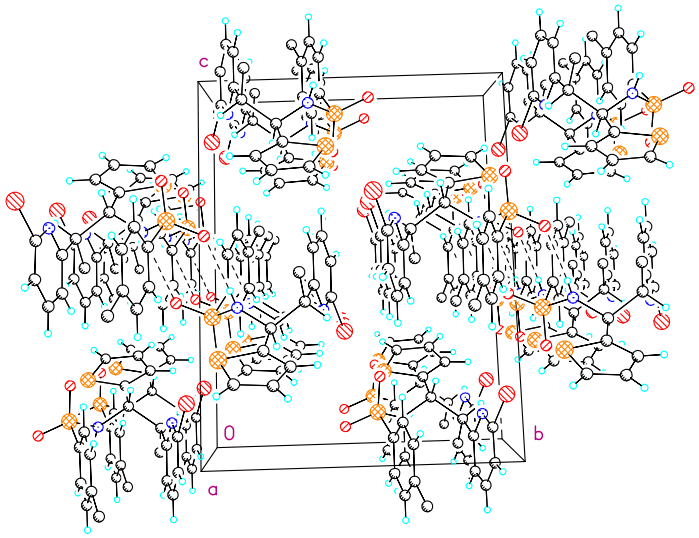
V. X-Ray Crystallographic Data for Compound 3f

View of **3f** showing the atom labeling scheme. Displacement ellipsoids are scaled to the 50% probability level. The disordered thiophene ring is shown.





Unit cell packing diagram for **3f**. The view is approximately down the **a** axis. Dashed lines are indicative of H-bonding interactions. The geometry of this interaction is: N2-H2···O2 (related by 1-x, -y, 1-z), N···O 2.983(2)Å, H···O 2.24(2)Å, N-H···O 166(2)°.



X-ray Experimental

Table 1. Crystallographic Data for **3f**.

Table 2. Fractional coordinates and equivalent isotropic thermal parameters ($Å^2$) for the non-hydrogen atoms of **3f**.

Table 3. Bond Lengths (Å) and Angles (°) for the non-hydrogen atoms of **3f**.

Table 4. Anisotropic thermal parameters for the non-hydrogen atoms of **3f**.

Table 5. Fractional coordinates and isotropic thermal parameters ($Å^2$) for the hydrogen atoms of **3f**.

Table 6. Torsion Angles (°) for the non-hydrogen atoms of **3f**.

Table 7. Observed and calculated structure factor amplitudes for **3f**. Values for Fo, Fc and σ(Fo) have been multiplied by 10.

Figure 1. View of **3f** showing the atom labeling scheme. Displacement ellipsoids are scaled to the 50% probability level. The disordered thiophene ring is shown.

Figure 2. Unit cell packing diagram for **3f**. The view is approximately down the **a** axis. Dashed lines are indicative of H-bonding interactions. The geometry of this interaction is: N2-H2···O2 (related by 1-x, -y, 1-z), N···O 2.983(2)Å, H···O 2.24(2)Å, N-H···O 166(2)°.

X-ray Experimental for $C_{19}H_{19}N_2O_2S_2Br$: Crystals grew as large, colorless prisms by slow evaporation from dichloromethane and hexanes. The data crystal was cut from a larger crystal and had approximate dimensions; 0.35 x 0.32 x 0.24 mm. The data were collected on a Nonius Kappa CCD diffractometer using a graphite monochromator with MoKα radiation (λ = 0.71073Å). A total of 209 frames of data were collected using ω-scans with a scan range of 2° and a counting time of 34 seconds per frame. The data were collected at 153 K using an Oxford Cryostream low temperature device. Details of crystal data, data collection and structure refinement are listed in Table 1. Data reduction were performed using DENZO-SMN.[1] The structure was solved by direct methods using SIR97[2] and refined by full-matrix least-squares on F^2 with anisotropic displacement parameters for the non-H atoms using SHELXL-97.[3] The

hydrogen atoms on carbon were calculated in ideal positions with isotropic displacement parameters set to 1.2xUeq of the attached atom (1.5xUeq for methyl hydrogen atoms). The hydrogen atom bound to N_2 was observed in a ΔF map and refined with an isotropic displacement parameter.

The thiophene ring was disordered by rotation about the C-C bond to the remainder of the molecule. The rings are rotated by about 180 degrees relative to each other. The disorder was modeled by assigning the variable x to the site occupancy factors of one orientation of the ring and (1-x) to the site occupancy factors for the alternate conformation. The geometry of the two rings was restrained to be equal throughout the refinement process. The variable x refined to a value very close to 0.5. The site occupancy factors were then set to 1/2 for the remainder of the refinement. The atoms were refined anisotropically with their displacement parameters restrained to be approximately isotropic.

The function, $\Sigma w(|F_o|^2 - |F_c|^2)^2$, was minimized, where $w = 1/[(\sigma(F_o))^2 + (0.0321*P)^2 + (1.1485*P)]$ and $P = (|F_o|^2 + 2|F_c|^2)/3$. $R_w(F^2)$ refined to 0.0700, with R(F) equal to 0.0291 and a goodness of fit, S, = 1.00. Definitions used for calculating R(F), $R_w(F^2)$ and the goodness of fit, S, are given below.[4] The data were corrected for secondary extinction effects. The correction takes the form: $F_{corr} = kF_c/[1 + (1.0(3)x10^{-6})* F_c^2 \lambda^3/(\sin 2\theta)]^{0.25}$ where k is the overall scale factor. Neutral atom scattering factors and values used to calculate the linear absorption coefficient are from the International Tables for X-ray Crystallography (1992).[5] All figures were generated using SHELXTL/PC.[6] Tables of positional and thermal parameters, bond lengths and angles, torsion angles, figures and lists of observed and calculated structure factors are located in tables1-7.

References

7) DENZO-SMN. (1997). Z. Otwinowski and W. Minor, Methods in Enzymology, **276**: Macromolecular Crystallography, part A, 307 – 326, C. W. Carter, Jr. and R. M. Sweets, Editors, Academic Press.

8) SIR97. (1999). A program for crystal structure solution. Altomare A., Burla M.C., Camalli M., Cascarano G.L., Giacovazzo C. , Guagliardi A., Moliterni A.G.G., Polidori G.,Spagna R. J. Appl. Cryst. 32, 115-119.

9) Sheldrick, G. M. (1994). SHELXL97. Program for the Refinement of Crystal Structures. University of Gottingen, Germany.

10) $R_w(F^2) = \{\Sigma w(|F_o|^2 - |F_c|^2)^2/\Sigma w(|F_o|)^4\}^{1/2}$ where w is the weight given each reflection.
$R(F) = \Sigma(|F_o| - |F_c|)/\Sigma|F_o|\}$ for reflections with $F_o > 4(\sigma(F_o))$.
$S = [\Sigma w(|F_o|^2 - |F_c|^2)^2/(n - p)]^{1/2}$, where n is the number of reflections and p is the number of refined parameters.

11) International Tables for X-ray Crystallography (1992). Vol. C, Tables 4.2.6.8 and 6.1.1.4, A. J. C. Wilson, editor, Boston: Kluwer Academic Press.

12) Sheldrick, G. M. (1994). SHELXTL/PC (Version 5.03). Siemens Analytical X-ray Instruments, Inc., Madison, Wisconsin, USA.

Table 1. Crystal data and structure refinement for **3f**.

Empirical formula	C19 H19 Br N2 O2 S2	
Formula weight	451.39	
Temperature	153(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 10.6171(3) Å	α= 90°.
	b = 12.0557(4) Å	β= 108.334(1)°.
	c = 15.7265(7) Å	γ = 90°.
Volume	1910.76(12) $Å^3$	
Z	4	
Density (calculated)	1.569 Mg/m^3	
Absorption coefficient	2.386 mm^{-1}	
F(000)	920	
Crystal size	0.35 x 0.32 x 0.24 mm	
Theta range for data collection	2.17 to 27.48°.	
Index ranges	-13<=h<=13, -15<=k<=15, -20<=l<=20	
Reflections collected	8165	
Independent reflections	4366 [R(int) = 0.0185]	
Completeness to theta = 27.48°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.56 and 0.47	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4366 / 108 / 280	
Goodness-of-fit on F^2	0.997	
Final R indices [I>2sigma(I)]	R1 = 0.0291, wR2 = 0.0653	
R indices (all data)	R1 = 0.0404, wR2 = 0.0700	
Extinction coefficient	$1.0(3)x10^{-6}$	
Largest diff. peak and hole	0.379 and -0.501 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 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)
Br1	71(1)	4557(1)	3344(1)	33(1)
N1	2695(1)	3922(1)	3934(1)	21(1)
N2	4474(2)	1371(1)	4065(1)	21(1)
O1	2495(1)	658(1)	2901(1)	29(1)
O2	3710(1)	-498(1)	4209(1)	26(1)
S1	3202(1)	565(1)	3838(1)	20(1)
S2	6076(2)	866(2)	2885(2)	27(1)
C17	7144(8)	1348(8)	2353(5)	28(2)
C18	7115(8)	2466(8)	2298(6)	29(2)
C19	6221(10)	2948(7)	2688(6)	34(3)
S2A	6147(3)	3207(2)	2585(2)	30(1)
C17A	7163(7)	2328(8)	2217(6)	27(2)
C18A	7025(9)	1254(8)	2456(6)	31(2)
C19A	6101(10)	1155(7)	2932(6)	36(3)
C1	4581(2)	2360(2)	3554(1)	20(1)
C2	4969(2)	3393(2)	4167(1)	21(1)
C3	3874(2)	3664(1)	4554(1)	20(1)
C4	4025(2)	3666(2)	5465(1)	26(1)
C5	2954(2)	3931(2)	5750(1)	29(1)
C6	1749(2)	4183(2)	5124(1)	27(1)
C7	1701(2)	4168(2)	4232(1)	22(1)
C8	6332(2)	3264(2)	4871(1)	25(1)
C9	2146(2)	1018(2)	4443(1)	22(1)
C10	2638(2)	1022(2)	5369(1)	30(1)
C11	1802(2)	1302(2)	5858(1)	33(1)
C12	484(2)	1582(2)	5433(1)	30(1)
C13	18(2)	1578(2)	4503(1)	34(1)
C14	836(2)	1300(2)	4001(1)	29(1)
C15	-409(2)	1910(2)	5971(2)	45(1)
C16	5560(2)	2157(2)	3048(1)	21(1)

Table 3. Bond lengths [Å] and angles [°] for **3f**.

Br1-C7	1.9090(18)	C2-C3	1.509(2)
N1-C7	1.316(2)	C2-C8	1.529(2)
N1-C3	1.359(2)	C2-H2	1.00
N2-C1	1.462(2)	C3-C4	1.389(2)
N2-S1	1.6100(16)	C4-C5	1.385(3)
N2-H2N	0.76(2)	C4-H4	0.95
O1-S1	1.4335(14)	C5-C6	1.381(3)
O2-S1	1.4411(13)	C5-H5	0.95
S1-C9	1.7693(18)	C6-C7	1.388(3)
S2-C16	1.696(3)	C6-H6	0.95
S2-C17	1.708(7)	C8-H8A	0.98
C17-C18	1.351(11)	C8-H8B	0.98
C17-H17A	0.95	C8-H8C	0.98
C18-C19	1.406(11)	C9-C10	1.385(3)
C18-H18A	0.95	C9-C14	1.387(3)
C19-C16	1.405(10)	C10-C11	1.386(3)
C19-H19A	0.95	C10-H10	0.95
S2A-C16	1.676(3)	C11-C12	1.390(3)
S2A-C17A	1.735(7)	C11-H11	0.95
C17A-C18A	1.368(11)	C12-C13	1.389(3)
C17A-H17B	0.95	C12-C15	1.509(3)
C18A-C19A	1.414(12)	C13-C14	1.386(3)
C18A-H18B	0.95	C13-H13	0.95
C19A-C16	1.374(9)	C14-H14	0.95
C19A-H19B	0.95	C15-H15A	0.98
C1-C16	1.514(2)	C15-H15B	0.98
C1-C2	1.550(2)	C15-H15C	0.98
C1-H1	1.00		

C7-N1-C3	117.11(15)	C3-C2-C8	113.85(15)
C1-N2-S1	125.11(13)	C3-C2-C1	109.72(14)
C1-N2-H2N	121.5(16)	C8-C2-C1	112.01(15)
S1-N2-H2N	113.4(16)	C3-C2-H2	107.0
O1-S1-O2	119.65(8)	C8-C2-H2	107.0
O1-S1-N2	108.18(8)	C1-C2-H2	107.0
O2-S1-N2	105.43(8)	N1-C3-C4	121.45(17)
O1-S1-C9	108.24(9)	N1-C3-C2	114.31(15)
O2-S1-C9	106.09(8)	C4-C3-C2	124.23(16)
N2-S1-C9	108.89(8)	C5-C4-C3	119.59(17)
C16-S2-C17	93.3(3)	C5-C4-H4	120.2
C18-C17-S2	111.4(5)	C3-C4-H4	120.2
C18-C17-H17A	124.3	C6-C5-C4	119.37(17)
S2-C17-H17A	124.3	C6-C5-H5	120.3
C17-C18-C19	112.9(6)	C4-C5-H5	120.3
C17-C18-H18A	123.6	C5-C6-C7	116.69(18)
C19-C18-H18A	123.5	C5-C6-H6	121.7
C16-C19-C18	112.7(7)	C7-C6-H6	121.7
C16-C19-H19A	123.6	N1-C7-C6	125.78(17)
C18-C19-H19A	123.6	N1-C7-Br1	116.03(13)
C16-S2A-C17A	92.2(3)	C6-C7-Br1	118.18(14)
C18A-C17A-S2A	110.8(5)	C2-C8-H8A	109.5
C18A-C17A-H17B	124.6	C2-C8-H8B	109.5
S2A-C17A-H17B	124.6	H8A-C8-H8B	109.5
C17A-C18A-C19A	112.2(7)	C2-C8-H8C	109.5
C17A-C18A-H18B	123.9	H8A-C8-H8C	109.5
C19A-C18A-H18B	123.9	H8B-C8-H8C	109.5
C16-C19A-C18A	112.6(7)	C10-C9-C14	120.89(17)
C16-C19A-H19B	123.7	C10-C9-S1	118.22(14)
C18A-C19A-H19B	123.7	C14-C9-S1	120.78(14)
N2-C1-C16	110.05(14)	C9-C10-C11	119.24(18)
N2-C1-C2	111.35(14)	C9-C10-H10	120.4
C16-C1-C2	111.35(14)	C11-C10-H10	120.4
N2-C1-H1	108.0	C10-C11-C12	121.06(19)
C16-C1-H1	108.0	C10-C11-H11	119.5
C2-C1-H1	108.0	C12-C11-H11	119.5

C13-C12-C11	118.52(19)	C12-C15-H15C	109.5
C13-C12-C15	120.85(19)	H15A-C15-H15C	109.5
C11-C12-C15	120.6(2)	H15B-C15-H15C	109.5
C14-C13-C12	121.37(19)	C19A-C16-C19	105.1(7)
C14-C13-H13	119.3	C19A-C16-C1	126.6(5)
C12-C13-H13	119.3	C19-C16-C1	128.0(4)
C13-C14-C9	118.92(18)	C19A-C16-S2A	112.2(5)
C13-C14-H14	120.5	C1-C16-S2A	121.18(16)
C9-C14-H14	120.5	C19-C16-S2	109.6(4)
C12-C15-H15A	109.5	C1-C16-S2	122.34(16)
C12-C15-H15B	109.5	S2A-C16-S2	116.44(17)
H15A-C15-H15B	109.5		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **3f**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br1	22(1)	46(1)	28(1)	-2(1)	5(1)	7(1)
N1	21(1)	19(1)	22(1)	-2(1)	7(1)	0(1)
N2	18(1)	21(1)	21(1)	3(1)	4(1)	-1(1)
O1	27(1)	36(1)	22(1)	-4(1)	5(1)	-7(1)
O2	30(1)	18(1)	31(1)	0(1)	10(1)	-1(1)
S1	20(1)	20(1)	20(1)	-2(1)	7(1)	-3(1)
S2	31(1)	25(1)	30(1)	1(1)	15(1)	5(1)
C17	23(2)	40(3)	24(3)	1(2)	12(2)	2(2)
C18	31(3)	38(3)	21(2)	-2(2)	10(2)	-6(2)
C19	43(4)	30(4)	32(3)	2(3)	14(2)	0(3)
S2A	39(1)	28(1)	34(1)	2(1)	26(1)	-6(1)
C17A	22(2)	43(3)	23(2)	-8(2)	18(2)	-2(2)
C18A	31(3)	36(3)	25(3)	-2(2)	8(2)	6(2)
C19A	41(4)	42(5)	29(3)	6(3)	14(2)	-11(3)
C1	20(1)	19(1)	20(1)	1(1)	7(1)	0(1)
C2	21(1)	19(1)	21(1)	0(1)	7(1)	0(1)
C3	22(1)	15(1)	23(1)	-1(1)	7(1)	0(1)
C4	27(1)	26(1)	23(1)	0(1)	7(1)	3(1)
C5	35(1)	32(1)	22(1)	1(1)	13(1)	4(1)
C6	27(1)	29(1)	29(1)	-1(1)	16(1)	3(1)
C7	20(1)	20(1)	26(1)	-1(1)	6(1)	0(1)
C8	22(1)	25(1)	27(1)	-3(1)	6(1)	-1(1)
C9	21(1)	22(1)	25(1)	2(1)	11(1)	-2(1)
C10	26(1)	37(1)	27(1)	6(1)	8(1)	6(1)
C11	36(1)	39(1)	27(1)	8(1)	16(1)	7(1)
C12	32(1)	25(1)	41(1)	7(1)	21(1)	2(1)
C13	21(1)	37(1)	43(1)	2(1)	10(1)	2(1)
C14	25(1)	33(1)	27(1)	0(1)	4(1)	-1(1)
C15	41(1)	50(2)	54(1)	8(1)	30(1)	9(1)
C16	21(1)	22(1)	20(1)	-1(1)	7(1)	1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 1.

	x	y	z	U(eq)
H17A	7689	887	2126	34
H18A	7642	2884	2025	35
H19A	6079	3725	2705	41
H17B	7737	2560	1894	32
H18B	7497	646	2319	37
H19B	5877	470	3147	44
H1	3692	2502	3105	23
H2	5033	4031	3776	25
H4	4858	3488	5889	31
H5	3047	3939	6371	35
H6	990	4359	5295	32
H8A	6543	3935	5240	37
H8B	7005	3152	4571	37
H8C	6323	2623	5251	37
H10	3539	835	5667	36
H11	2136	1303	6494	39
H13	-881	1771	4204	40
H14	506	1302	3365	35
H15A	-522	2717	5950	67
H15B	-10	1672	6594	67
H15C	-1276	1553	5718	67
H2N	5040(20)	1189(18)	4472(14)	22(6)

Table 6. Torsion angles [°] for 1.

C1-N2-S1-O1	25.20(17)
C1-N2-S1-O2	154.31(14)
C1-N2-S1-C9	-92.22(16)
C16-S2-C17-C18	-0.02(15)
S2-C17-C18-C19	0.0(2)
C17-C18-C19-C16	0.1(4)
C16-S2A-C17A-C18A	0.14(15)
S2A-C17A-C18A-C19A	0.07(19)
C17A-C18A-C19A-C16	-0.3(4)
S1-N2-C1-C16	-109.45(16)
S1-N2-C1-C2	126.58(14)
N2-C1-C2-C3	-64.89(18)
C16-C1-C2-C3	171.87(14)
N2-C1-C2-C8	62.57(19)
C16-C1-C2-C8	-60.66(19)
C7-N1-C3-C4	-0.4(3)
C7-N1-C3-C2	-179.89(16)
C8-C2-C3-N1	171.87(15)
C1-C2-C3-N1	-61.70(19)
C8-C2-C3-C4	-7.6(3)
C1-C2-C3-C4	118.82(19)
N1-C3-C4-C5	0.4(3)
C2-C3-C4-C5	179.79(18)
C3-C4-C5-C6	0.3(3)
C4-C5-C6-C7	-0.9(3)
C3-N1-C7-C6	-0.2(3)
C3-N1-C7-Br1	178.71(12)
C5-C6-C7-N1	0.9(3)
C5-C6-C7-Br1	-178.04(15)
O1-S1-C9-C10	-178.62(15)
O2-S1-C9-C10	51.81(17)
N2-S1-C9-C10	-61.24(18)
O1-S1-C9-C14	5.07(19)
O2-S1-C9-C14	-124.51(16)
N2-S1-C9-C14	122.45(17)
C14-C9-C10-C11	0.6(3)
S1-C9-C10-C11	-175.70(17)
C9-C10-C11-C12	-0.2(3)
C10-C11-C12-C13	-0.2(3)
C10-C11-C12-C15	-178.6(2)
C11-C12-C13-C14	0.3(3)
C15-C12-C13-C14	178.7(2)
C12-C13-C14-C9	0.1(3)
C10-C9-C14-C13	-0.6(3)
S1-C9-C14-C13	175.66(16)
C18A-C19A-C16-C19	-3.9(6)
C18A-C19A-C16-C1	-177.6(4)
C18A-C19A-C16-S2A	0.4(4)
C18A-C19A-C16-S2	140(5)
C18-C19-C16-C19A	3.4(6)
C18-C19-C16-C1	177.0(4)
C18-C19-C16-S2A	-147(3)
C18-C19-C16-S2	-0.1(4)
N2-C1-C16-C19A	11.4(4)
C2-C1-C16-C19A	135.4(4)
N2-C1-C16-C19	-160.9(4)
C2-C1-C16-C19	-36.9(4)
N2-C1-C16-S2A	-166.49(16)
C2-C1-C16-S2A	-42.5(2)
N2-C1-C16-S2	15.9(2)
C2-C1-C16-S2	139.88(17)
C17A-S2A-C16-C19A	-0.3(3)
C17A-S2A-C16-C19	31(3)
C17A-S2A-C16-C1	177.8(3)
C17A-S2A-C16-S2	-4.4(3)
C17-S2-C16-C19A	-37(5)
C17-S2-C16-C19	0.1(3)
C17-S2-C16-C1	-177.2(3)
C17-S2-C16-S2A	5.1(3)

Table 7. Observed and calculated structure factors for **3f**
Page 1

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
2	0	0	695	723	7	12	6	0	82	91	21	-4	1	1	554	563	4
7	4	1	628	627	4	-1	8	1	46	49	17						
3	0	0	2190	2231	26	1	7	0	419	401	3	-3	1	1	149	156	1
8	4	1	112	115	4	0	8	1	672	667	5						
4	0	0	996	974	11	2	7	0	119	115	2	-2	1	1	224	221	1
9	4	1	227	226	9	1	8	1	283	296	2						
5	0	0	1175	1165	12	3	7	0	49	52	12	-1	1	1	671	696	7
10	4	1	377	377	4	2	8	1	568	559	3						
6	0	0	751	748	8	4	7	0	404	396	2	0	1	1	0	64	1
11	4	1	396	389	7	3	8	1	349	350	2						
7	0	0	732	728	6	5	7	0	70	65	8	1	1	1	158	150	1
12	4	1	84	44	27	4	8	1	270	278	2						
8	0	0	629	610	6	6	7	0	58	56	6	2	1	1	813	832	4
13	4	1	101	93	14	5	8	1	378	381	3						
9	0	0	157	162	3	7	7	0	344	337	4	3	1	1	216	215	1
14	4	1	58	54	24	6	8	1	51	59	16						
10	0	0	586	582	6	8	7	0	108	115	5	4	1	1	202	213	1
15	4	1	203	202	6	7	8	1	330	328	5						
11	0	0	465	461	8	9	7	0	12	20	12	5	1	1	618	627	3
16	4	1	159	167	3	8	8	1	310	306	6						
12	0	0	262	252	10	10	7	0	414	402	12	6	1	1	573	572	3
17	4	1	273	277	4	9	8	1	0	16	1						
13	0	0	420	431	16	0	8	0	546	553	9	7	1	1	494	489	3
18	4	1	459	456	3	10	8	1	126	122	16						
1	1	0	487	496	5	1	8	0	323	318	2	8	1	1	828	818	6
19	4	1	194	203	4	11	8	1	0	19	1						
2	1	0	765	762	5	2	8	0	227	234	2	9	1	1	131	130	2
20	4	1	235	222	6	-10	9	1	23	27	23						
3	1	0	369	370	2	3	8	0	710	706	5	10	1	1	242	248	2
21	4	1	70	72	1	-9	9	1	12	22	12						
4	1	0	199	188	1	4	8	0	84	81	5	11	1	1	478	472	5
22	4	1	230	234	1	-8	9	1	249	246	10						
5	1	0	414	389	2	5	8	0	371	366	5	12	1	1	351	345	6
23	4	1	377	367	2	-7	9	1	62	67	16						
6	1	0	228	244	2	6	8	0	572	561	5	-12	2	1	153	146	6
24	4	1	146	150	1	-6	9	1	55	14	20						
7	1	0	376	372	3	7	8	0	74	62	9	-11	2	1	389	392	4
25	4	1	30	14	7	-5	9	1	159	160	5						
8	1	0	87	88	2	8	8	0	280	276	7	-10	2	1	31	36	30
26	4	1	332	325	2	-4	9	1	347	342	2						
9	1	0	51	54	4	9	8	0	255	260	10	-9	2	1	89	91	2
27	4	1	307	308	2	-3	9	1	352	348	3						
10	1	0	98	102	5	10	8	0	138	130	12	-8	2	1	894	881	6
28	4	1	146	135	3	-2	9	1	38	28	8						
11	1	0	97	102	5	11	8	0	0	34	1	-7	2	1	74	80	2
29	4	1	178	172	1	-1	9	1	575	583	5						
12	1	0	41	19	25	1	9	0	47	35	18	-6	2	1	627	623	4
30	4	1	282	275	2	0	9	1	52	39	6						
13	1	0	183	187	8	2	9	0	292	295	2	-5	2	1	427	438	2
31	4	1	225	219	2	1	9	1	218	221	2						
0	2	0	867	898	20	3	9	0	714	700	8	-4	2	1	93	90	1
32	4	1	85	98	1	2	9	1	714	708	5						
1	2	0	1166	1183	7	4	9	0	64	62	3	-3	2	1	447	438	3
33	4	1	36	30	9	3	9	1	193	199	5						
2	2	0	203	193	1	5	9	0	160	167	6	-2	2	1	556	569	3
34	4	1	129	141	5	4	9	1	131	137	4						
3	2	0	1030	1055	7	6	9	0	306	308	4	-1	2	1	773	776	6
35	4	1	268	268	4	5	9	1	392	385	5						
4	2	0	626	632	4	7	9	0	20	17	20	0	2	1	102	99	3
36	4	1	87	82	12	6	9	1	124	124	3						
5	2	0	617	609	4	8	9	0	91	92	13	1	2	1	958	985	6
37	4	1	90	85	17	7	9	1	88	95	10						
6	2	0	799	802	4	9	9	0	130	140	9	2	2	1	918	892	4
38	4	1	329	316	16	8	9	1	213	203	7						
7	2	0	504	503	3	10	9	0	116	69	14	3	2	1	42	38	2
39	4	1	361	367	6	9	9	1	154	145	17						
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42	4	1	426	424	3	-9	10	1	143	151	16						
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44	4	1	1027	1003	9	-7	10	1	68	51	22						
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47	4	1	1400	1397	17	-4	10	1	350	350	4						
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48	4	1	623	612	5	-3	10	1	194	188	5						
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49	4	1	678	673	5	-2	10	1	355	352	8						
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53	4	1	493	498	3	2	10	1	202	217	2						
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55	4	1	141	144	3	4	10	1	81	83	5						
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348   3
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223   2
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385  11
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96  19
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88  19
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216   5
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Table 7. Observed and calculated structure factors for **3f**
Page 2

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h  k  l 10Fo 10Fc 10s     h  k  l 10Fo 10Fc 10s     h  k  l 10Fo
10Fc 10s     h  k  l 10Fo 10Fc 10s     h  k  l 10Fo
10Fc 10s

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64   5
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391   2
  -7  1  2   70   64   3     2  4  2  404  402   4    -6  8
2   49   46   9     2 12  2  254  260   3     9  2  3  194
208   2
  -6  1  2  184  182   1     3  4  2   20   15   6    -5  8
2  110  111   6     3 12  2   70   83  11    10  2  3   63
72   7
  -5  1  2  221  219   1     4  4  2  224  215   1    -4  8
2  388  389   3     4 12  2   15   37  15    11  2  3  176
181   4
  -4  1  2   98   94   1     5  4  2  314  291   3    -3  8
2   51   45   5     5 12  2    0   26   1    12  2  3  132
127  15
  -3  1  2  229  233   1     6  4  2   43   33   5    -2  8
2   60   62   4     6 12  2  126  131  10   -13  3  3   87
87  11
  -2  1  2  128  134   1     7  4  2   17    4  16    -1  8
2  300  298   2     7 12  2   56   70  56   -12  3  3  201
207   6
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2  353  346   2    -7 13  2  212  213  10   -11  3  3  243
253   3
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2  262  262   4    -6 13  2   78   57  15   -10  3  3  309
318   3
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2  315  318   4    -5 13  2  129  125  18    -9  3  3  229
235   2
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2  304  295   2    -4 13  2   93   90   8    -8  3  3  389
384   3
   3  1  2  222  202   1    12  4  2   44   36  43     4  8
2  167  168   2    -3 13  2  337  357   5    -7  3  3  448
446   2
   4  1  2  518  508   3   -12  5  2  257  264  10     5  8
2  574  573   4    -2 13  2    0   14   1    -6  3  3   54
55   6
   5  1  2   56   40   1   -11  5  2   90   80  13     6  8
2  169  179   2    -1 13  2   48   18  48    -5  3  3 1254
1232   8
   6  1  2  153  169   4   -10  5  2  258  257   8     7  8
2  117  122  14     0 13  2  199  210   4    -4  3  3  179
198   1
   7  1  2  265  268   2    -9  5  2  346  348   3     8  8
2  136  151   8     1 13  2  108  115   5    -3  3  3  497
514   3
   8  1  2  121  118   1    -8  5  2  101  103   2     9  8
2  107  103  11     2 13  2   77   82  20    -2  3  3 1232
1246  10
   9  1  2  428  436   7    -7  5  2  707  698   5    10  8
2   61   67  18     3 13  2  155  163   7    -1  3  3  126
139   1
  10  1  2  239  240   3    -6  5  2  510  520   4   -11  9
2   84   71  39     4 13  2   98   86  13     0  3  3  804
810   4
  11  1  2   40   44  40    -5  5  2  185  192   2   -10  9
2  101   44  22     5 13  2  120  105  14     1  3  3  509
541   4
```

Table 7.Observed and calculated structure factors for **3f**
Page 3

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
2	3	3	614	620	3	-8	7	3	298	308	9	-3	11	3	224	218	6
-9	1	4	45	54	5	4	4	4	88	91	2						
3	3	3	510	513	2	-7	7	3	77	73	8	-2	11	3	581	573	5
-8	1	4	67	72	3	5	4	4	452	452	2						
4	3	3	318	345	1	-6	7	3	68	54	8	-1	11	3	232	227	3
-7	1	4	198	200	2	6	4	4	284	284	2						
5	3	3	259	272	1	-5	7	3	456	465	4	0	11	3	202	198	4
-6	1	4	303	285	2	7	4	4	95	93	6						
6	3	3	573	582	3	-4	7	3	70	56	4	1	11	3	681	677	7
-5	1	4	392	384	2	8	4	4	161	167	2						
7	3	3	255	266	3	-3	7	3	133	127	1	2	11	3	129	120	3
-4	1	4	59	42	2	9	4	4	164	163	3						
8	3	3	380	381	4	-2	7	3	538	535	8	3	11	3	362	372	3
-3	1	4	623	623	4	10	4	4	111	126	8						
9	3	3	269	272	10	-1	7	3	120	124	2	4	11	3	311	318	4
-2	1	4	541	537	3	11	4	4	103	115	8						
10	3	3	163	161	3	0	7	3	133	126	2	5	11	3	353	332	5
-1	1	4	965	980	5	-12	5	4	118	130	9						
11	3	3	295	288	9	1	7	3	396	393	2	6	11	3	136	139	18
0	1	4	580	576	3	-11	5	4	536	510	23						
12	3	3	0	25	1	2	7	3	70	65	6	7	11	3	262	260	12
1	1	4	753	753	3	-10	5	4	673	650	8						
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-11	4	3	48	40	12	4	7	3	238	248	2	-8	12	3	152	142	13
3	1	4	185	176	2	-8	5	4	782	767	7						
-10	4	3	74	68	8	5	7	3	77	78	11	-7	12	3	61	72	20
4	1	4	103	104	1	-7	5	4	831	818	7						
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5	1	4	389	391	3	-6	5	4	318	319	5						
-8	4	3	263	275	3	7	7	3	222	226	3	-5	12	3	181	179	8
6	1	4	144	129	1	-5	5	4	680	677	6						
-7	4	3	166	172	4	8	7	3	263	268	5	-4	12	3	42	42	16
7	1	4	97	106	2	-4	5	4	1071	1071	8						
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9	1	4	48	54	9	-2	5	4	806	799	5						
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10	1	4	78	66	6	-1	5	4	313	342	2						
-3	4	3	210	223	2	-10	8	3	80	69	17	0	12	3	23	35	23
11	1	4	24	40	23	0	5	4	1178	1165	9						
-2	4	3	44	29	5	-9	8	3	208	206	7	1	12	3	249	250	3
-13	2	4	72	43	37	1	5	4	280	299	2						
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-10	2	4	77	81	2	4	5	4	271	282	1						
2	4	3	45	62	3	-5	8	3	168	170	9	5	12	3	107	114	9
-9	2	4	22	18	12	5	5	4	611	615	3						
3	4	3	159	156	1	-4	8	3	62	70	12	6	12	3	19	56	19
-8	2	4	38	50	5	6	5	4	447	449	3						
4	4	3	369	357	2	-3	8	3	158	161	2	7	12	3	95	121	19
-7	2	4	144	142	1	7	5	4	46	38	8						
5	4	3	746	747	5	-2	8	3	244	244	5	-7	13	3	44	72	43
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6	4	3	140	142	2	-1	8	3	163	176	2	-6	13	3	97	78	15
-5	2	4	229	219	1	9	5	4	397	397	4						
7	4	3	94	85	2	0	8	3	167	182	1	-5	13	3	212	229	7
-4	2	4	55	42	2	10	5	4	38	53	37						
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-3	2	4	1200	1199	9	11	5	4	256	257	8						
9	4	3	38	48	10	2	8	3	287	293	2	-3	13	3	142	121	8
-2	2	4	281	279	1	-12	6	4	80	71	29						
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-1	2	4	289	294	1	-11	6	4	92	76	10						
11	4	3	460	454	8	4	8	3	156	159	2	-1	13	3	95	98	8
0	2	4	927	937	5	-10	6	4	61	71	23						
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-10	5	3	214	228	4	7	8	3	28	34	28	2	13	3	247	237	4
3	2	4	1034	1025	5	-7	6	4	70	70	16						
-9	5	3	265	268	3	8	8	3	120	118	13	3	13	3	98	83	9
4	2	4	107	124	4	-6	6	4	453	457	5						
-8	5	3	14	17	14	9	8	3	135	135	7	4	13	3	239	235	5
5	2	4	548	550	3	-5	6	4	174	177	2						
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6	2	4	504	510	4	-4	6	4	208	220	3						
-6	5	3	294	287	3	-11	9	3	303	314	13	6	13	3	155	162	15
7	2	4	358	359	2	-3	6	4	672	657	6						
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8	2	4	274	284	2	-2	6	4	56	34	2						
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9	2	4	382	380	3	-1	6	4	90	93	2						
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10	2	4	418	417	9	0	6	4	229	222	1						
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11	2	4	110	115	8	1	6	4	213	209	1						
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-13	3	4	332	294	11	2	6	4	46	51	4						
0	5	3	239	245	1	-4	9	3	96	102	2	0	14	3	147	158	6
-12	3	4	138	140	8	3	6	4	166	160	2						
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-11	3	4	280	279	5	4	6	4	60	66	2						
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-10	3	4	625	619	5	5	6	4	128	128	1						
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-9	3	4	151	155	1	6	6	4	67	70	5						
4	5	3	200	181	1	0	9	3	271	277	2	4	14	3	49	56	49
-8	3	4	727	714	5	7	6	4	21	8	21						
5	5	3	381	381	2	1	9	3	524	515	3	-3	15	3	177	172	7
-7	3	4	758	758	5	8	6	4	60	68	7						
6	5	3	33	9	5	2	9	3	612	602	5	-2	15	3	4	36	3
-6	3	4	144	151	2	9	6	4	125	130	5						
7	5	3	162	158	2	3	9	3	128	124	3	-1	15	3	154	123	8
-5	3	4	520	530	3	10	6	4	0	2	1						
8	5	3	121	127	8	4	9	3	504	493	4	0	15	3	195	199	10
-4	3	4	982	971	6	-12	7	4	54	57	54						
9	5	3	83	101	6	5	9	3	242	240	3	1	15	3	78	67	15
-3	3	4	1029	1018	7	-11	7	4	272	278	16						
10	5	3	95	104	8	6	9	3	161	173	11	2	15	3	68	36	22
-2	3	4	97	99	1	-10	7	4	329	322	6						
11	5	3	204	198	7	7	9	3	407	399	7	-13	0	4	41	46	40
-1	3	4	759	778	4	-9	7	4	312	308	6						
-12	6	3	251	237	10	8	9	3	192	196	6	-12	0	4	84	89	7
0	3	4	833	833	6	-8	7	4	282	273	4						

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 -11  6  3   56   62  22     9  9  3  184  188  16   -11  0
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 -10  6  3  227  216   7   -10 10  3  109   61  18   -10  0
4   48   58   9     2  3  4  372  379   2    -6  7  4  516
514  11
  -9  6  3   55   48  12    -9 10  3   48   43  34    -9  0
4  513  507   5     3  3  4  886  866   4    -5  7  4  248
242   3
  -8  6  3  166  172   3    -8 10  3   15   64  15    -8  0
4  549  547   5     4  3  4   97  100   3    -4  7  4  512
522   3
  -7  6  3   93  112   7    -7 10  3   84   86  14    -7  0
4  108  112   3     5  3  4  595  597   3    -3  7  4  552
546   6
  -6  6  3  471  467   4    -6 10  3   71  102  11    -6  0
4 1055 1035  11     6  3  4  314  308   2    -2  7  4  259
254   1
  -5  6  3   31   25   8    -5 10  3   63   57   8    -5  0
4  875  831   8     7  3  4  102  104   5    -1  7  4  731
718   5
  -4  6  3  213  204  10    -4 10  3  128  125   2    -4  0
4  357  367   3     8  3  4  465  462   3     0  7  4  514
515   3
  -3  6  3  601  583   4    -3 10  3  343  339   4    -3  0
4 1143 1143   9     9  3  4  197  195   3     1  7  4  639
614   4
  -2  6  3  284  274   2    -2 10  3  335  330   4    -2  0
4  349  335   2    10  3  4   77   74   6     2  7  4  568
571   4
  -1  6  3  306  302   3    -1 10  3  103   90   4    -1  0
4  871  878   7    11  3  4  123  119   9     3  7  4  333
334   2
   0  6  3   25   35   9     0 10  3   33   19  17     0  0
4  587  600   4   -12  4  4   42   34  34     4  7  4  331
329   2
   1  6  3  101   98   2     1 10  3    9    2   9     1  0
4  658  658   4   -11  4  4  191  197   5     5  7  4  660
653   4
   2  6  3  479  482   3     2 10  3   44   36   7     2  0
4 1363 1340   9   -10  4  4   63   61   8     6  7  4   75
66   4
   3  6  3  212  202   1     3 10  3    0   34   1     3  0
4  322  307   2    -9  4  4   47   39   6     7  7  4  119
121   4
   4  6  3   11   14  10     4 10  3   30   15  30     4  0
4 1191 1174  10    -8  4  4  183  185   2     8  7  4  250
251  11
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174   5
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4  615  622   5    -6  4  4   52   57   2    10  7  4   63
44  18
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4  475  477   4    -5  4  4  340  320   2   -10  8  4  140
146   9
   8  6  3  227  234   3     8 10  3   61   52  60     8  0
4  110  113   5    -4  4  4   70   73   2    -9  8  4  110
130  11
   9  6  3  221  223   5     9 10  3    7   35   7     9  0
4  737  728  10    -3  4  4  281  274   2    -8  8  4    0
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  10  6  3   42   33  33    -9 11  3    0  102   1    10  0
4  277  264   4    -2  4  4  285  279   1    -7  8  4  305
312   5
  11  6  3  251  246   7    -8 11  3  348  340   8    11  0
4  143  141  10    -1  4  4   55   45   5    -6  8  4  391
399   4
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301   2
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222   2
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4  192  200   2     2  4  4  234  230   1    -3  8  4  585
579   3
  -9  7  3  135  130  16    -4 11  3  152  159   3   -10  1
4  186  188   2     3  4  4  546  552   3    -2  8  4  156
160   2
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Table 7.Observed and calculated structure factors for **3f**
Page 4

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
-1	8	4	286	297	2	-6	13	4	89	70	16	-4	3	5	725	697	4
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-11	7	5	94	81	13	-5	11	5	137	131	5						
1	8	4	59	74	5	-4	13	4	305	299	6	-2	3	5	584	579	3
-10	7	5	80	63	12	-4	11	5	37	39	37						
2	8	4	138	153	2	-3	13	4	127	138	13	-1	3	5	61	47	2
-9	7	5	173	176	10	-3	11	5	334	335	4						
3	8	4	431	418	3	-2	13	4	109	115	5	0	3	5	198	206	1
-8	7	5	32	52	32	-2	11	5	179	180	9						
4	8	4	162	161	2	-1	13	4	164	166	7	1	3	5	76	99	2
-7	7	5	99	107	2	-1	11	5	133	144	3						
5	8	4	51	60	4	0	13	4	105	106	14	2	3	5	125	117	4
-6	7	5	649	642	6	0	11	5	483	484	4						
6	8	4	387	387	5	1	13	4	49	44	14	3	3	5	324	341	1
-5	7	5	109	111	2	1	11	5	137	140	3						
7	8	4	102	97	7	2	13	4	19	13	18	4	3	5	172	169	1
-4	7	5	135	131	2	2	11	5	83	78	14						
8	8	4	122	132	7	3	13	4	89	75	9	5	3	5	226	221	2
-3	7	5	388	378	10	3	11	5	196	196	3						
9	8	4	258	238	7	4	13	4	0	10	1	6	3	5	289	289	2
-2	7	5	111	119	1	4	11	5	67	77	9						
10	8	4	229	219	7	5	13	4	145	149	12	7	3	5	36	28	8
-1	7	5	132	128	2	5	11	5	50	21	49						
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0	7	5	34	17	7	6	11	5	71	78	13						
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1	7	5	134	139	2	7	11	5	128	125	10						
-9	9	4	183	173	10	-4	14	4	121	131	10	10	3	5	129	125	4
2	7	5	96	90	2	-8	12	5	224	213	10						
-8	9	4	22	34	22	-3	14	4	91	85	26	11	3	5	132	132	8
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6	7	5	247	251	2	-4	12	5	96	85	15						
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5   80   83   3     6  9  5  117  127  21    -6  0  6  595
608   5
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5   79   99   5     7  9  5  258  262   8    -5  0  6 1039
1000   9
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1468  13
   4 11  4  114   87  16    -1  2  5  773  760   4   -11  6
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502   4
   5 11  4  137  146   7     0  2  5  328  321   1   -10  6
5   79   91  14    -9 10  5  172  180   8    -1  0  6 1895
1912  16
   6 11  4   89   77  12     1  2  5  583  580   2    -9  6
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   7 11  4  176  176   6     2  2  5  304  313   2    -8  6
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146   2
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5  381  371  13    -7 11  5  148  144   7    -6  1  6  222
215   2
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Table 7. Observed and calculated structure factors for **3f**
Page 5

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-4	3	6	0	11	1	-11	7	6	444	437	9	-3	11	6	100	109	7
3	2	7	867	871	5	-5	6	7	431	429	6						
-3	3	6	219	209	1	-10	7	6	64	43	63	-2	11	6	57	45	20
4	2	7	331	335	3	-4	6	7	698	684	4						
-2	3	6	87	105	2	-9	7	6	45	46	27	-1	11	6	103	106	3
5	2	7	362	368	2	-3	6	7	525	529	3						
-1	3	6	412	404	2	-8	7	6	383	388	6	0	11	6	105	105	4
6	2	7	271	269	2	-2	6	7	262	281	3						
0	3	6	226	230	1	-7	7	6	175	173	3	1	11	6	25	11	24
7	2	7	151	150	2	-1	6	7	476	471	3						
1	3	6	305	288	1	-6	7	6	164	174	5	2	11	6	0	26	1
8	2	7	28	33	27	0	6	7	459	473	2						
2	3	6	30	27	11	-5	7	6	26	18	26	3	11	6	18	18	18
9	2	7	207	210	3	1	6	7	615	601	3						
3	3	6	427	422	2	-4	7	6	298	288	2	4	11	6	146	147	4
10	2	7	29	23	29	2	6	7	167	163	1						
4	3	6	44	36	2	-3	7	6	120	125	2	5	11	6	37	31	37
-13	3	7	131	112	8	3	6	7	615	605	3						

```
   5  3  6  346  353   2    -2  7  6   23    4  11     6 11
6   61   53  16   -12  3  7    0   31   1     4  6  7  375
378   2
   6  3  6  437  444   3    -1  7  6  248  251   2     7 11
6  131  118  17   -11  3  7   33   20  32     5  6  7  203
205   4
   7  3  6   75   74   3     0  7  6   56   41   5    -8 12
6  146  144  17   -10  3  7   19    3  18     6  6  7  455
450   4
   8  3  6  121  124   9     1  7  6  194  185   3    -7 12
6  317  311   8    -9  3  7   41   46   6     7  6  7  429
428   4
   9  3  6  272  274   7     2  7  6   58   55   4    -6 12
6   83   56  13    -8  3  7  324  337   2     8  6  7    0
28   1
  10  3  6   62   78  12     3  7  6  212  228   1    -5 12
6  269  268  10    -7  3  7   97  100   2     9  6  7  224
214   7
 -13  4  6  126   97  15     4  7  6  146  147   2    -4 12
6  372  371   7    -6  3  7  268  264   2   -12  7  7   86
104  22
 -12  4  6   80   73  17     5  7  6  180  182   3    -3 12
6   65   68   7    -5  3  7  330  342   2   -11  7  7   50
37  42
 -11  4  6  214  214   8     6  7  6  373  378   3    -2 12
6  350  345   4    -4  3  7   67   62   3   -10  7  7    0
20   1
 -10  4  6  380  379   5     7  7  6  120  115   9    -1 12
6  299  297   4    -3  3  7  762  744   4    -9  7  7   66
11  42
  -9  4  6  176  173   3     8  7  6   81   81  10     0 12
6  149  141   5    -2  3  7  227  226   2    -8  7  7  305
311   4
  -8  4  6  178  184   2     9  7  6  193  198  17     1 12
6  235  226   3    -1  3  7  123  103   1    -7  7  7  115
125   4
  -7  4  6  607  598   4   -11  8  6  414  388  11     2 12
6  289  290   4     0  3  7  287  286   1    -6  7  7   37
24  36
  -6  4  6  192  194   3   -10  8  6  317  324   7     3 12
6  218  210   3     1  3  7  146  165   1    -5  7  7  433
436   3
  -5  4  6   81   93   3    -9  8  6   74   73  16     4 12
6  219  222   5     2  3  7  183  193   3    -4  7  7   89
88   3
  -4  4  6  314  331   2    -8  8  6   96   89  16     5 12
6  167  166   6     3  3  7   86   78   6    -3  7  7  215
218   2
  -3  4  6   38   34   7    -7  8  6  604  606  10     6 12
6  293  287   8     4  3  7  448  447   2    -2  7  7  392
391   3
  -2  4  6  545  546   3    -6  8  6  246  260   3    -7 13
6   54    4  53     5  3  7   44   55   5    -1  7  7  221
223   2
  -1  4  6  106   81   3    -5  8  6  155  162   4    -6 13
6   74   85  19     6  3  7  100  109   3     0  7  7  216
222   2
   0  4  6 1057 1030   6    -4  8  6  712  716   6    -5 13
6   26   46  25     7  3  7  324  326   4     1  7  7  133
135   2
   1  4  6  379  374   2    -3  8  6  178  179   2    -4 13
6  181  189   7     8  3  7  330  343   3     2  7  7  156
156   2
   2  4  6  290  297   1    -2  8  6   67   55   3    -3 13
6  269  275   5     9  3  7    0   29   1     3  7  7   34
15   9
   3  4  6  154  158   1    -1  8  6  624  614   7    -2 13
6   66   67   9    10  3  7  299  305   7     4  7  7  218
229   2
   4  4  6  565  561   3     0  8  6  292  290   2    -1 13
6   59   35  13   -13  4  7  285  300  11     5  7  7   77
80   2
   5  4  6  246  251   2     1  8  6  223  231   2     0 13
6  166  156   4   -12  4  7  480  475  10     6  7  7  142
146   3
   6  4  6  182  183   2     2  8  6  412  408   2     1 13
6   80   79  11   -11  4  7   21   44  21     7  7  7  130
123   5
   7  4  6   84   92   3     3  8  6  121  118   2     2 13
6    0   14   1   -10  4  7  555  544   7     8  7  7  236
234   6
```

Table 7. Observed and calculated structure factors for **3f**
Page 6

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
9	7	7	85	94	22	4	12	7	0	29	1	5	2	8	258	267	2
0	6	8	19	28	19	-9	11	8	80	43	26						
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1	6	8	109	109	5	-8	11	8	67	53	66						
-10	8	7	72	81	16	-7	13	7	0	25	1	7	2	8	0	28	1
2	6	8	39	43	15	-7	11	8	187	206	14						
-9	8	7	276	266	6	-6	13	7	77	55	28	8	2	8	136	133	5
3	6	8	332	331	2	-6	11	8	110	108	16						
-8	8	7	218	211	15	-5	13	7	62	67	21	9	2	8	64	83	13
4	6	8	57	58	9	-5	11	8	116	96	12						
-7	8	7	302	304	7	-4	13	7	75	86	18	10	2	8	0	21	1
5	6	8	172	176	2	-4	11	8	67	71	6						
-6	8	7	233	226	3	-3	13	7	71	68	51	-13	3	8	224	223	7
6	6	8	175	178	3	-3	11	8	13	31	12						
-5	8	7	410	416	4	-2	13	7	133	137	6	-12	3	8	58	44	18
7	6	8	47	56	13	-2	11	8	68	75	5						
-4	8	7	229	223	3	-1	13	7	48	35	48	-11	3	8	177	184	4
8	6	8	193	188	7	-1	11	8	85	85	5						
-3	8	7	548	543	5	0	13	7	96	102	7	-10	3	8	285	285	3
9	6	8	0	42	1	0	11	8	94	95	4						
-2	8	7	246	244	2	1	13	7	98	103	7	-9	3	8	298	304	6
7	8	63	84	40	1	11	8	152	150	3							
-1	8	7	315	312	2	2	13	7	107	106	6	-8	3	8	333	334	4
7	8	204	226	11	2	11	8	67	72	8							
0	8	7	549	540	4	3	13	7	43	58	41	-7	3	8	197	200	2
7	8	263	267	6	3	11	8	67	72	9							
1	8	7	260	267	2	4	13	7	125	128	12	-6	3	8	664	649	3
7	8	54	75	22	4	11	8	132	122	9							
2	8	7	312	306	3	-4	14	7	63	35	23	-5	3	8	176	175	2
7	8	288	293	4	5	11	8	57	82	26							
3	8	7	121	131	2	-3	14	7	202	201	13	-4	3	8	628	633	4
7	8	503	485	5	6	11	8	68	62	45							
4	8	7	268	266	2	-2	14	7	70	58	13	-3	3	8	528	523	3
7	8	46	34	6	8	12	8	214	218	12							
5	8	7	90	88	5	-1	14	7	0	15	1	-2	3	8	401	393	2
7	8	428	423	4	7	12	8	218	223	12							
6	8	7	228	237	4	0	14	7	230	232	5	-1	3	8	729	746	4
7	8	406	406	3	6	12	8	71	74	17							
7	8	7	88	79	8	1	14	7	43	28	42	0	3	8	216	199	1
7	8	240	236	3	5	12	8	268	249	12							
8	8	7	80	88	13	2	14	7	0	20	1	1	3	8	516	496	3
7	8	422	428	3	4	12	8	41	22	30							
-11	9	7	149	147	19	-13	0	8	198	191	9	2	3	8	892	875	4
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-10	9	7	149	140	17	-12	0	8	148	152	7	3	3	8	338	344	2
0	7	8	490	481	4	2	12	8	320	316	4						
-9	9	7	125	128	9	-11	0	8	624	616	10	4	3	8	54	48	3
1	7	8	328	336	2	-1	12	8	0	17	1						
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2	7	8	446	444	3	0	12	8	104	100	5						
-7	9	7	0	15	1	-9	0	8	260	262	3	6	3	8	448	445	4
3	7	8	644	629	4	1	12	8	34	19	33						
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4	7	8	165	168	2	2	12	8	18	20	17						
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5	7	8	571	568	4	3	12	8	128	111	10						
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6	7	8	289	286	7	4	12	8	60	10	19						
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7	7	8	154	159	4	-6	13	8	76	75	25						
-2	9	7	305	311	4	-4	0	8	92	109	4	-13	4	8	39	47	38
8	7	8	393	386	7	-5	13	8	119	117	17						
-1	9	7	46	42	7	-3	0	8	454	454	4	-12	4	8	241	241	6
8	8	273	266	11	4	13	8	125	130	11							
0	9	7	211	226	2	-2	0	8	594	620	5	-11	4	8	71	73	20
8	8	90	78	15	3	13	8	61	71	22							
1	9	7	491	486	3	-1	0	8	101	73	3	-10	4	8	44	37	19
8	8	0	32	1	2	13	8	50	57	14							
2	9	7	33	22	10	0	0	8	482	453	4	-9	4	8	273	283	3
8	8	261	267	8	1	13	8	246	248	5							
3	9	7	203	212	2	1	0	8	1025	990	8	-8	4	8	90	83	2
8	12	16	12	0	13	8	38	54	27								
4	9	7	382	384	3	2	0	8	633	651	5	-7	4	8	313	322	7
8	8	146	150	2	1	13	8	66	65	11							
5	9	7	123	121	8	3	0	8	349	353	2	-6	4	8	133	131	1
8	8	204	209	3	2	13	8	160	165	5							
6	9	7	54	68	19	4	0	8	657	657	5	-5	4	8	450	441	2
8	8	343	342	3	3	13	8	33	34	32							
7	9	7	315	309	7	5	0	8	719	706	6	-4	4	8	127	133	1
8	8	29	29	9	4	14	8	108	108	17							
8	9	7	214	228	8	6	0	8	239	240	3	-3	4	8	268	267	3
8	8	236	232	3	3	14	8	106	90	14							
-10	10	7	133	116	15	7	0	8	144	138	4	-2	4	8	246	242	3
8	8	143	146	2	2	14	8	63	16	17							
-9	10	7	85	82	32	8	0	8	217	224	4	-1	4	8	226	231	1
8	8	144	138	2	1	14	8	146	155	7							
-8	10	7	241	238	6	9	0	8	55	17	20	0	4	8	120	112	2
8	8	402	387	3	0	14	8	0	11	1							
-7	10	7	128	126	9	10	0	8	0	8	1	1	4	8	107	119	2
8	8	193	194	2	1	14	8	85	113	13							
-6	10	7	68	77	10	-13	1	8	107	109	11	2	4	8	31	28	8
8	8	169	181	2	-13	1	9	239	231	6							
-5	10	7	64	65	35	-12	1	8	21	43	21	3	4	8	16	16	16
8	8	271	270	3	-12	1	9	489	474	7							
-4	10	7	138	140	4	-11	1	8	15	24	14	4	4	8	84	87	3
8	8	81	82	9	-11	1	9	77	74	6							
-3	10	7	118	112	4	-10	1	8	231	241	2	5	4	8	318	322	2
8	8	38	18	18	-10	1	9	486	499	4							
-2	10	7	200	202	4	-9	1	8	123	128	2	6	4	8	131	137	3
8	8	197	200	5	-9	1	9	720	697	5							
-1	10	7	185	170	2	-8	1	8	148	150	2	7	4	8	0	16	1
8	8	54	62	26	-8	1	9	238	243	2							
0	10	7	167	180	4	-7	1	8	428	423	3	8	4	8	40	47	25
8	8	115	111	17	-7	1	9	485	487	3							
1	10	7	78	64	4	-6	1	8	47	46	4	9	4	8	41	53	33
8	8	161	124	16	-6	1	9	535	536	3							
2	10	7	158	155	4	-5	1	8	235	231	2	-12	5	8	95	108	22
8	8	0	17	1	-5	1	9	850	841	5							
3	10	7	43	27	10	-4	1	8	259	268	2	-11	5	8	368	358	14
8	8	108	95	11	-4	1	9	717	710	4							
4	10	7	0	16	1	-3	1	8	285	278	5	-10	5	8	217	220	8
8	8	135	139	15	-3	1	9	867	874	5							
5	10	7	205	195	15	-2	1	8	249	250	2	-9	5	8	118	125	3
8	8	215	219	3	-2	1	9	653	655	3							
6	10	7	62	35	20	-1	1	8	173	200	1	-8	5	8	345	348	4
8	8	268	271	10	-1	1	9	463	475	2							
7	10	7	0	23	1	0	1	8	92	82	2	-7	5	8	493	490	3
8	64	56	6	0	1	9	1016	1008	5								
-9	11	7	91	99	22	1	1	8	596	585	3	-6	5	8	303	303	3
8	189	199	3	1	1	9	424	448	2								

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  -8 11  7  194  197  11     2  1  8   63   58   3    -5  5
8  149  157   1    -2  9  8   33   29  15     2  1  9  641
634   3
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8  663  671   4    -1  9  8   84   86   4     3  1  9  936
922   5
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8  668  660   4     0  9  8  423  414   3     4  1  9  204
206   2
  -5 11  7  124  129   6     5  1  8   90   98   2    -2  5
8  409  414   2     1  9  8  123  123   3     5  1  9  180
174   2
  -4 11  7   50   66  12     6  1  8  482  479   3    -1  5
8  869  862   5     2  9  8   47   29   7     6  1  9  546
535   4
  -3 11  7    9   22   8     7  1  8    0   23   1     0  5
8  583  584   3     3  9  8  211  210   4     7  1  9  495
488   4
  -2 11  7  215  218   3     8  1  8  194  202   3     1  5
8   62   61   4     4  9  8  129  139   7     8  1  9  217
224   5
  -1 11  7  100  109  11     9  1  8  159  160  10     2  5
8 1313 1301   7     5  9  8  304  304   4     9  1  9  274
267   5
   0 11  7   73   67  18    10  1  8   14   26  13     3  5
8  220  233   2     6  9  8  118  137   7   -13  2  9    0
15   1
   1 11  7  335  337   3   -13  2  8  151  162   7     4  5
8  398  397   2     7  9  8  188  179  12   -12  2  9  128
128   7
   2 11  7  128  130   3   -12  2  8  102   87   9     5  5
8  516  516   4   -10 10  8   72   70  31   -11  2  9   14
22  14
   3 11  7  115  116   8   -11  2  8  540  522   8     6  5
8  273  274   3    -9 10  8    0   38   1   -10  2  9  161
170   3
   4 11  7  236  239   6   -10  2  8  301  309   3     7  5
8  192  194   6    -8 10  8  446  451   9    -9  2  9   25
51  19
   5 11  7   89  105  10    -9  2  8   58   51   5     8  5
8  338  343   5    -7 10  8  138  126   9    -8  2  9  222
225   2
   6 11  7  100  118  26    -8  2  8  853  837   6     9  5
8  308  319   9    -6 10  8   40   30  18    -7  2  9   91
101   2
  -8 12  7    0   18   1    -7  2  8  248  243   2   -12  6
8  178  196  15    -5 10  8  432  417   7    -6  2  9  388
384   3
  -7 12  7   59   55  39    -6  2  8  233  232   2   -11  6
8  141  149   8    -4 10  8   80   66   6    -5  2  9  304
302   2
  -6 12  7    0   48   1    -5  2  8  807  798   5   -10  6
8   48   39  48    -3 10  8   11   24  11    -4  2  9  305
302   2
  -5 12  7   48   14  28    -4  2  8  387  386   2    -9  6
8  124  108   9    -2 10  8  587  570   5    -3  2  9   63
55   3
  -4 12  7   35   28  35    -3  2  8  407  410   2    -8  6
8  128  130   9    -1 10  8   54   57   7    -2  2  9  521
500   3
  -3 12  7  143  150   7    -2  2  8  516  527   3    -7  6
8   80   81   4     0 10  8   40   32  10    -1  2  9  429
437   2
  -2 12  7    0   15   1    -1  2  8   44   41   7    -6  6
8  109  114   3     1 10  8  344  344   3     0  2  9  152
147   4
  -1 12  7   50   46  16     0  2  8  317  324   2    -5  6
8  380  382   3     2 10  8   75   73   5     1  2  9   73
67   3
   0 12  7  280  287   4     1  2  8  426  427   2    -4  6
8  298  299   4     3 10  8  145  146   4     2  2  9  161
159   2
   1 12  7   11   18  10     2  2  8   92  110   2    -3  6
8  400  392   3     4 10  8  153  147   7     3  2  9  324
333   2
   2 12  7  113  108   5     3  2  8   87   92   2    -2  6
8  217  208   2     5 10  8  156  147   6     4  2  9  145
144   2
   3 12  7  250  255   4     4  2  8   30   24  12    -1  6
8  278  279   6     6 10  8   27    7  27     5  2  9   18
10  17
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Table 7. Observed and calculated structure factors for **3f**
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h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
6	2	9	329	335	3	3	6	9	255	260	3	-3	11	9	498	484	6
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-3	2	10	30	30	30	-3	6	10	274	280	2						
8	2	9	69	80	9	5	6	9	69	76	6	-1	11	9	301	303	4
-2	2	10	285	292	2	-2	6	10	93	86	4						
9	2	9	30	18	29	6	6	9	94	89	6	0	11	9	491	482	7
-1	2	10	492	496	3	-1	6	10	172	175	2						
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1	2	10	378	376	3	1	6	10	55	65	6						
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2	2	10	545	545	3	2	6	10	279	282	2						
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4	2	10	169	173	2	4	6	10	78	91	8						
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5	4	10	16	21	16	-7	9	10	133	125	8						
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8	4	10	90	90	10	-4	9	10	163	160	7						
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-11	5	10	556	540	11	-2	9	10	178	176	4						

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  -2  5  9  222  220   2     4  9  9  513  502   5    -8  1
10   59   55   8   -10  5 10  195  192   6    -1  9 10   61
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258   3
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10  349  352   2    -8  5 10  419  394   3     1  9 10   34
43  15
   1  5  9  408  397   2     7  9  9  205  211   8    -5  1
10  158  165   2    -7  5 10  488  487   3     2  9 10  232
227   3
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272   4
   3  5  9   72   63   3    -9 10  9  119   65  15    -3  1
10  159  163   2    -5  5 10  847  831   6     4  9 10  153
150   5
   4  5  9  369  375   2    -8 10  9  297  297  15    -2  1
10  145  158   2    -4  5 10  213  213   2     5  9 10   90
93  15
   5  5  9  115  132   4    -7 10  9   49   10  48    -1  1
10  250  250   2    -3  5 10  428  426   2     6  9 10   50
45  50
   6  5  9   23   31  23    -6 10  9   17   22  16     0  1
10   18   19  18    -2  5 10  497  505   3    -9 10 10  150
157  13
   7  5  9   40   10  18    -5 10  9  221  218   4     1  1
10  332  335   2    -1  5 10  582  587   4    -8 10 10  126
122  14
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10  266  276   2     0  5 10  197  198   2    -7 10 10  267
266  17
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10  274  286   2     1  5 10  740  730   4    -6 10 10   26
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13  24
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7   1
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Table 7. Observed and calculated structure factors for **3f**
Page 8

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
-4	11	10	76	75	8	3	3	11	132	137	5	-9	8	11	161	162	8
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5	0	12	335	329	6	-12	5	12	90	116	36						
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6	0	12	451	452	8	-11	5	12	62	78	19						
0	11	10	63	60	11	7	3	11	84	48	13	-5	8	11	65	76	8
7	0	12	211	209	7	-10	5	12	71	62	15						
1	11	10	93	113	7	8	3	11	105	107	14	-4	8	11	234	227	6
8	0	12	238	236	11	-9	5	12	167	164	5						
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3	11	10	164	172	7	-11	4	11	164	169	7	-2	8	11	153	150	4
-12	1	12	148	145	7	-7	5	12	111	108	2						
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-9	1	12	34	33	13	-4	5	12	138	137	3						
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7	1	12	35	50	35	-7	6	12	156	166	3						
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-2	2	12	804	796	5	6	6	12	89	89	14						
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1	1	11	172	182	2	3	5	11	36	37	12	0	10	11	142	143	5
0	2	12	263	267	2	-10	7	12	91	113	19						
2	1	11	58	58	5	4	5	11	101	106	16	1	10	11	81	82	11
1	2	12	685	670	4	-9	7	12	280	272	6						
3	1	11	281	288	2	5	5	11	59	78	12	2	10	11	158	148	7
2	2	12	357	368	3	-8	7	12	58	62	11						
4	1	11	131	138	3	6	5	11	0	33	1	3	10	11	23	53	23
3	2	12	235	236	6	-7	7	12	74	86	9						
5	1	11	156	146	5	7	5	11	77	80	10	4	10	11	101	98	12
4	2	12	422	414	3	-6	7	12	78	71	5						
6	1	11	270	274	3	-12	6	11	110	133	16	-8	11	11	131	143	16
5	2	12	433	430	4	-5	7	12	295	293	4						
7	1	11	188	188	4	-11	6	11	96	66	17	-7	11	11	0	54	1
6	2	12	102	102	6	-4	7	12	100	101	4						
8	1	11	135	138	15	-10	6	11	286	282	6	-6	11	11	188	192	14
7	2	12	385	379	9	-3	7	12	226	226	3						
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-12	3	12	84	88	15	-2	7	12	201	193	3						
-12	2	11	232	227	7	-8	6	11	172	181	8	-4	11	11	364	361	6
-11	3	12	109	101	12	-1	7	12	289	299	3						
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-9	3	12	119	114	6	1	7	12	120	119	3						
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-8	3	12	139	148	3	2	7	12	222	222	3						
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-7	3	12	72	78	4	3	7	12	20	17	20						
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-6	3	12	203	218	2	4	7	12	49	58	16						
-6	2	11	365	368	3	-2	6	11	309	308	5	2	11	11	250	244	7
-5	3	12	311	317	2	5	7	12	158	157	6						
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-4	3	12	287	288	3	6	7	12	51	74	32						
-4	2	11	353	361	3	0	6	11	821	809	5	-6	12	11	173	168	16
-3	3	12	507	506	3	-10	8	12	72	80	30						
-3	2	11	638	635	4	1	6	11	385	384	3	-5	12	11	95	96	20
-2	3	12	204	214	3	-9	8	12	0	40	1						

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413   7
  -1  2 11  108  110   3     3  6 11  912  883   8    -3 12
11  162  161   5     0  3 12  116  121   3    -7  8 12   46
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   0  2 11  664  653   4     4  6 11  272  278   3    -2 12
11  152  144   8     1  3 12   26   12  25    -6  8 12   82
94   6
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11    0   41   1     2  3 12  210  213   3    -5  8 12  536
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11  236  243   9     3  3 12   46   64  10    -4  8 12   84
94   7
   3  2 11   31   35  20     7  6 11  325  325  11     1 12
11   50   46  50     4  3 12  125  127   3    -3  8 12  183
185   5
   4  2 11  140  151   6   -11  7 11   74   17  26     2 12
11  152  144  14     5  3 12  180  185   3    -2  8 12  499
500   5
   5  2 11  358  354   3   -10  7 11  228  238  15    -4 13
11  126  130  16     6  3 12  117  129   7    -1  8 12   67
77   7
   6  2 11  240  237   3    -9  7 11   53   43  29    -3 13
11  168  176   9     7  3 12   81   75  11     0  8 12  147
155   3
   7  2 11  188  182   6    -8  7 11   61   60  12    -2 13
11    0   49   1   -12  4 12  130  101  13     1  8 12  222
219   3
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11    9   12   9   -11  4 12   47   19  46     2  8 12  202
201   3
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12   84   36  30   -10  4 12   54   75  15     3  8 12   97
89  15
 -12  3 11    0   29   1    -5  7 11   61   55  16   -12  0
12  321  319   8    -9  4 12   62   64   6     4  8 12   93
114  12
 -11  3 11  247  249   6    -4  7 11   96   95   4   -11  0
12  557  560  10    -8  4 12  443  436   4     5  8 12  282
283  14
 -10  3 11  301  304   4    -3  7 11  253  244   4   -10  0
12  187  198   4    -7  4 12   79   81   3    -9  9 12    0
30   1
  -9  3 11  125  125   6    -2  7 11    8   11   7    -9  0
12  270  287   4    -6  4 12  239  249   2    -8  9 12    0
69   1
  -8  3 11  146  149   4    -1  7 11   74   84   6    -8  0
12  389  382   4    -5  4 12  704  697   5    -7  9 12  108
102  16
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55  35
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206   6
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12  619  606   6    -2  4 12  168  167   4    -4  9 12    0
37   1
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65  12
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63   9
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Table 7. Observed and calculated structure factors for **3f**
Page 9

h k l 10Fo 10Fc 10s h k l 10Fo 10Fc 10s h k l 10Fo 10Fc 10s h k l 10Fo 10Fc 10s

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109   5
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98   7
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14   79   74  28     3  6 14    0   26   1     2  2 15   80
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14  218  223  10     4  6 14  121  122  15     3  2 15   32
39  32
  -8  3 13  141  156   5    -9  8 13  225  229  10   -11  2
14  235  236   8     5  6 14   63   81  62     4  2 15   32
37  31
  -7  3 13  212  219   3    -8  8 13  149  138  10   -10  2
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459   4
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Table 7.Observed and calculated structure factors for **3f**
Page 10

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3 3 15 194 185 5 -3 10 15 84 91 28 -5 5 16 229 216 5 -1 3 17 123 127 7 0 2 18 356 357 8
4 3 15 109 108 11 -2 10 15 0 9 1 -4 5 16 106 115 17 0 3 17 84 106 9 1 2 18 179 171 12
5 3 15 128 120 7 -1 10 15 55 40 54 -3 5 16 372 361 4 1 3 17 210 195 5 2 2 18 127 109 11
-10 4 15 85 67 11 -11 0 16 82 81 19 -2 5 16 349 345 4 2 3 17 66 51 16 -9 3 18 164 163 20
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-8 4 15 230 233 4 -9 0 16 133 134 8 0 5 16 297 288 4 -10 4 17 391 376 16 -7 3 18 101 106 9
-7 4 15 30 13 30 -8 0 16 142 166 10 1 5 16 297 302 4 -9 4 17 0 59 1 -6 3 18 91 104 7
-6 4 15 136 129 4 -7 0 16 37 57 36 2 5 16 71 60 12 -8 4 17 157 154 5 -5 3 18 135 138 6
-5 4 15 229 236 3 -6 0 16 88 68 10 3 5 16 325 332 7 -7 4 17 421 413 6 -4 3 18 236 233 4
-4 4 15 126 125 4 -5 0 16 281 277 5 -9 6 16 53 41 52 -6 4 17 164 161 5 -3 3 18 96 105 8
-3 4 15 185 190 3 -4 0 16 91 69 10 -8 6 16 137 123 27 -5 4 17 52 51 13 -2 3 18 146 136 7
-2 4 15 70 61 11 -3 0 16 201 199 7 -7 6 16 87 82 10 -4 4 17 350 347 4 -1 3 18 166 144 6
-1 4 15 38 48 19 -2 0 16 425 416 6 -6 6 16 145 148 5 -3 4 17 250 246 8 0 3 18 115 123 10
0 4 15 114 121 5 -1 0 16 30 28 30 -5 6 16 165 159 5 -2 4 17 107 103 13 1 3 18 155 140 9
1 4 15 0 22 1 0 0 16 283 289 5 -4 6 16 93 99 9 -1 4 17 343 329 4 -9 4 18 83 26 22
2 4 15 38 52 16 1 0 16 455 446 8 -3 6 16 63 73 10 0 4 17 207 203 4 -8 4 18 97 96 16
3 4 15 177 186 5 2 0 16 198 203 6 -2 6 16 97 109 6 1 4 17 138 134 7 -7 4 18 120 116 17
4 4 15 66 42 37 3 0 16 55 44 27 -1 6 16 127 129 6 2 4 17 295 296 6 -6 4 18 288 270 11
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-8 5 15 38 43 19 -8 1 16 51 59 19 -9 7 16 250 223 11 -5 5 17 0 20 1 -1 4 18 120 108 8
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-8 6 15 153 157 8 -9 2 16 85 78 7 -5 8 16 149 162 6 -1 6 17 400 393 12 -4 6 18 21 29 20
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4 6 15 49 41 49 3 2 16 154 154 6 -1 9 16 187 192 9 -5 8 17 158 155 10 -4 1 19 209 220 7
-9 7 15 48 79 48 4 2 16 191 189 9 -10 1 17 66 36 14 -4 8 17 181 178 8 -3 1 19 54 17 53
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-7 7 15 150 145 7 -10 3 16 70 84 13 -8 1 17 518 506 8 -2 8 17 94 110 16 -1 1 19 339 321 8
-6 7 15 0 25 1 -9 3 16 431 422 6 -7 1 17 121 119 6 -1 8 17 215 215 7 0 1 19 0 29 1
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-4 7 15 303 310 4 -7 3 16 163 168 6 -5 1 17 365 361 4 -8 0 18 143 133 8 -7 2 19 13 25 13
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  -2  7 15   18   35  18    -5  3 16  209  208  11    -3  1
17  116  107   9    -6  0 18  310  316   7    -5  2 19  110
114  10
  -1  7 15  140  153   9    -4  3 16  319  319   3    -2  1
17   93   95   8    -5  0 18  321  312   6    -4  2 19    0
44   1
   0  7 15  196  205   4    -3  3 16  224  230   4    -1  1
17  170  171   5    -4  0 18  223  226   6    -3  2 19  135
134   9
   1  7 15   56   54  11    -2  3 16  280  279   4     0  1
17  156  171   5    -3  0 18  617  593  11    -2  2 19   85
108  16
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17   15   33  14    -2  0 18  176  176   7    -1  2 19   88
100  14
   3  7 15    5   55   5     0  3 16  403  404   5     2  1
17  211  209   5    -1  0 18  340  349   8     0  2 19    0
15   1
  -9  8 15  166  132  14     1  3 16  178  174   5     3  1
17   39   12  38     0  0 18  330  311  11    -8  3 19   78
88  17
  -8  8 15    0   24   1     2  3 16    0   24   1   -10  2
17   46   56  21     1  0 18  323  335  12    -7  3 19    0
15   1
  -7  8 15   51   21  50     3  3 16  306  287   6    -9  2
17   65   28  13     2  0 18    0   65   1    -6  3 19    0
7   1
  -6  8 15    0   58   1     4  3 16  143  143  16    -8  2
17    0   30   1    -9  1 18   77   63  10    -5  3 19   76
71  28
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17  235  238   4    -8  1 18   27   10  26    -4  3 19   99
104  13
  -4  8 15   16    6  15    -9  4 16   23   14  23    -6  2
17  236  230   7    -7  1 18  162  163   5    -3  3 19  139
133   9
  -3  8 15   67   76  21    -8  4 16   26   15  25    -5  2
17  169  174   9    -6  1 18  132  142   6    -2  3 19  113
111  10
  -2  8 15    0   12   1    -7  4 16   60    5  14    -4  2
17  438  431   5    -5  1 18   54   53  14    -1  3 19  103
89  14
  -1  8 15  151  141  12    -6  4 16  112  116   7    -3  2
17  251  260   7    -4  1 18   74   43  10     0  3 19  186
167   9
   0  8 15  200  199   5    -5  4 16   48   11  19    -2  2
17  155  159   6    -3  1 18   94  101   8    -7  4 19  104
131  11
   1  8 15   97   55  12    -4  4 16   33   67  33    -1  2
17  358  345   5    -2  1 18   75   74  12    -6  4 19    0
31   1
   2  8 15   47   22  29    -3  4 16   95   86   6     0  2
17   76   68  10    -1  1 18   83   66   9    -5  4 19  322
320   8
  -7  9 15  292  289  11    -2  4 16   54   60  13     1  2
17   94   91   9     0  1 18   80   57  14    -4  4 19  206
193   6
  -6  9 15   93   71  14    -1  4 16  244  246   3     2  2
17  200  203   6     1  1 18   24   26  23    -3  4 19  121
126  11
  -5  9 15  125  130   9     0  4 16   47   34  17     3  2
17  139  124  11     2  1 18   31   28  30    -2  4 19  319
303   7
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17  207  201   7    -9  2 18  301  285   6    -1  4 19  141
143   7
  -3  9 15  152  156   6     2  4 16   78   53  13    -9  3
17  109  110   7    -8  2 18  121  128   9    -6  5 19   59
25  27
  -2  9 15    0   28   1     3  4 16   89  107  12    -8  3
17  180  182  10    -7  2 18  193  197   6    -5  5 19   47
22  37
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51  12
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17   90   92   9    -5  2 18  278  279   5    -3  5 19   50
67  24
   1  9 15  101  108  14    -9  5 16  374  371   8    -5  3
17  160  166   5    -4  2 18  231  233   5    -2  5 19   51
31  22
```

Table 7.Observed and calculated structure factors for **3f**
Page 11

h k l 10Fo 10Fc 10s h k l 10Fo 10Fc 10s h k l 10Fo 10Fc 10s h k l 10Fo 10Fc 10s h k l 10Fo 10Fc 10s h k l 10Fo 10Fc 10s

-6 0 20 301 299 12 -2 0 20 83 62 25 -3 1 20 187 188 16 -4 2 20 179 173 9
-5 0 20 0 21 1 -6 1 20 39 36 39 -2 1 20 105 97 18 -3 2 20 36 27 36
-4 0 20 263 252 11 -5 1 20 82 98 18 -6 2 20 20 47 19 -5 3 20 173 178 8
-3 0 20 0 19 1 -4 1 20 67 62 22 -5 2 20 169 163 9 -4 3 20 47 69 42