Supporting Information for Highly Stereoselectivity Benzylation of *N*-Sulfinylketimines.

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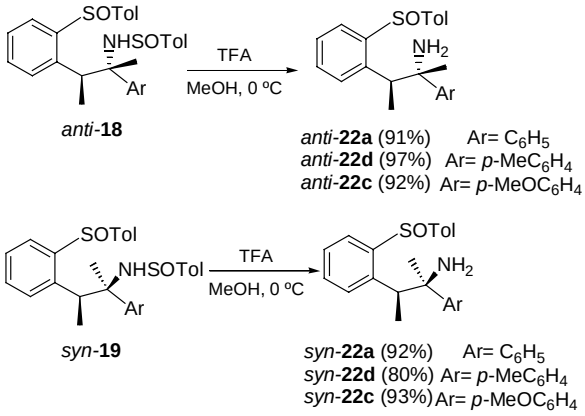
Experimental Section.

General Procedures. All flasks were flame-dried under a stream of argon and cooled before use. Solvents and solutions were transferred with syringes and cannulas using stardard inerts atmosphere techniques. ^{1}H-NMR spectra were acquired at either 200 or 300 MHz and ^{13}C-NMR were acquired at 75 MHz (unless otherwise indicated). Chemical shifts (δ are reported in ppm relative to $CDCl_3$ (7.26 and 77.0 ppm). Mass spectra (MS) were determined at FAB. All reactions were carried out in anhydrous solvents and under Argon atmosphere. THF and Et_2O were distilled from sodium-benzophenone under Argon. Dichlorometane was distilled from calcium hydride. *i*-Pr_2NH was distilled from KOH. Flash silica gel column chromatography was performed using silica gel Merk-60 (230-400 mesh). *n*-BuLi (2.5 M solution in hexane) was purchased from Aldrich.

***N*–α–Methyl-(4-bromobenzylidene)-*p*-toluenesulfinamide (3e).** This compound was obtained using Davis' methodology.[1] Chromatography: *n*-hexane-AcOEt 6:1; yield: 73%; yellow oil; $[\alpha]_D^{20}$ +87.4 (*c* 1, acetone); IR (NaCl): 1595, 1580, 1553, 1097, 1077 cm^{-1}; ^{1}H NMR (200 MHz, $CDCl_3$): δ 7.70–7.50 (m, 4H), 7.46 (d, *J* = 8.7 Hz, 2H), 7.28 (d, *J* = 8.3 Hz, 2H), 2.70 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (50 MHz, $CDCl_3$): δ 172.5, 142.8, 141.8, 136.6, 131.5, 129.7, 128.8, 126.6, 124.9, 21.3, 19.8; MS (FAB) *m/z* 68 (M+1, 45), 40 (23), 385 (100), 211 (31); Anal. Calcd for $C_{15}H_{14}$BrNOS: C, 53.58; H, 4.20; N, 4.17; S, 9.54. Found: C, 53.50; H, 4.26; N, 4.15; S, 9.38.

General procedure for N-S desulfinylation

[1] Davis, F. A.; Seung, Lee; Zhang, H.; Fanelli, D. L. *J. Org. Chem.* **2000**, *65*, 8704.



To a stirred solution of compound *syn* or *anti*-**4** (0.2 mmol) in methanol (3 mL) was added TFA (1.0 mmol, 50 μL). After the mixture was stirred for 3 h, the solvent was evaporated, and the residue was chromatography by SCX column, affording the corresponding amine.

(2*S*,3*S*)-2-Phenyl-3-[(*S*)-2-(*p*-toluenesulfinyl)phenyl]butyl-2-amine (*anti*-**22a**): SCX Chromatography; yield: 91%; colorless oil; $[\alpha]_D^{20}$ +27.0 (*c* 0.93, CH_3OH); IR (NaCl): 3358, 3285, 1682, 1472 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 7.62-7.54 (m, 4H), 7.51-7.42 (m, 5H), 7.35-7.33 (m, 2H), 7.26-7.23 (m, 2H), 4.07 (q, *J* = 7.1 Hz, 1H), 2.38 (s, 3H), 2.32 (bs, 2H), 1.58 (s, 3H), 0.92 (d, *J* = 7.1, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 144.9, 144.3, 141.1, 140.5, 131.5, 129.7, 129.5, 128.7, 128.2, 128.0, 127.4, 126.5, 126.1, 125.2, 58.3, 44.5, 24.2, 21.3, 16.8; MS (FAB^+) *m/z* 364 (M+1,100), 347 (36), 327 (71), 283 (65); HRMS calcd for $C_{23}H_{26}N_1O_1S_1$ 364.1735, found 364.1730.

(2*S*,3*S*)-2-(4-Methylphenyl)-3-[(*S*)-2-(*p*-toluenesulfinyl)phenyl]-butyl-2-amine (*anti*-**22d**): SCX Chromatography; yield: 97%; colorless oil; $[\alpha]_D^{20}$ -44.4 (*c* 1.0, $CHCl_3$); IR (NaCl): 3352, 3248, 3055, 3022, 2975, 2923, 2876, 1591, 1510, 1492, 1471, 1030, 1016 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 7.50-7.37 (m, 7H), 7.31-7.28 (m, 1H), 7.16 (dd, *J* = 8.3, 2.1 Hz, 4H), 4.05 (q, *J* = 7.1 Hz, 1H), 2.36 (s, 3H), 2.33 (s, 3H), 2.16 (bs, 2H), 1.52 (s, 3H), 0.94 (d, *J* = 7.1 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$):

δ 145.63, 145.0, 144.6, 141.1, 140.4, 135.9, 131.3, 129.5, 129.4, 128.6, 128.5, 127.3, 126.0, 125.4, 57.9, 44.6, 24.8, 21.2, 20.8, 16.9.

(2*S*,3*S*)-2-(4-Methoxyphenyl)-3-[(*S*)-2-(*p*-toluenesulfinyl)phenyl]butyl-2-amine (*anti*-**22c**): SCX Chromatography; yield: 92%; colorless oil; $[\alpha]_D^{20}$ -5.1 (*c*1.0, $CHCl_3$); IR (NaCl): 3367, 3276,2970, 2934, 1688, 1610, 1591, 1510, 1492 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 7.56 (d, *J* = 7.6 H, 1H), 7.47-7.30 (m, 7H), 7.19 (d, *J* = 7.6 Hz, 2H), 6.84 (dd, *J* = 7.5, 1.2 Hz, 2H), 3.98 (q, *J* = 6.8, 1H), 2.42 (bs, 2H), 2.34 (s, 3H), 1.52 (s, 3H), 0.82 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 158.2, 144.6, 144.3, 141.1, 140.5, 139.8, 131.6, 129.9, 129.5, 128.6, 127.4, 127.3, 125.2, 113.3, 58.2, 55.1, 44.8, 23.9, 21.2, 16.7. MS (FAB^+) *m/z* 394 (M+1, 76), 377 (100), 378 (28); HRMS (FAB^+) calcd for $C_{24}H_{27}N_1O_2S$ [M+1] 394.5416, found 394.1840.

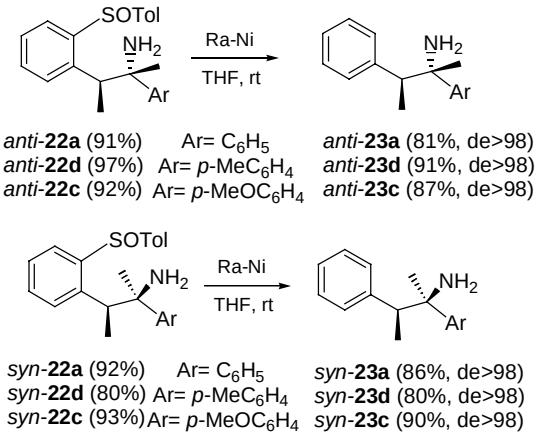
(2*R*,3*S*)-2-Phenyl-3-[(*S*)-2-(*p*-toluenesulfinyl)phenyl]butyl-2-amine (*syn*-**22a**): SCX Chromatography; yield: 92%; colorless oil; $[\alpha]_D^{20}$ +40.3 (*c* 1.1, CH_3OH); IR (NaCl): 3358, 3286, 1688, 1493 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 7.62-7.55 (m, 3H), 7.51-7.49 (m, 2H), 7.43 (d, *J* = 8.3 Hz, 2H), 7.37-7.22 (m, 6H), 4.07 (q, *J* = 7.1Hz, 1H), 2.75 (bs, 2H), 2.38 (s, 3H), 1.59 (s, 3H), 0.91 (d, *J* = 7.1 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 148.2, 144.7, 144.3, 141.0, 140.5, 131.5, 129.7, 129.5, 128.8, 128.0, 127.4, 126.5 (2C), 125.2, 58.4, 44.2, 24.0, 21.2, 16.7; MS (FAB^+) *m/z* 364 (M+1,100), 348 (10), 347 (41), 327 (18); HRMS calcd for $C_{23}H_{26}NOS$ 364.1735, found 364.1731.

(2*R*,3*S*)-2-(4-Methylphenyl)-3-[(*S*)-2-(*p*-toluenesulfinyl)phenyl]butyl-2-amine (*syn*-**22d**): SCX Chromatography; yield: 80%; colorless oil; $[\alpha]_D^{20}$ -120.1 (*c* 1.0, $HCCl_3$); ^1H NMR (200 MHz, $CDCl_3$): δ 7.52–7.28 (m, 8H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.11 (d, *J* = 8.0 Hz, 2H), 4.03 (q, *J* = 6.6 Hz, 1H), 2.35 (s, 3H), 2.33 (s, 3H), 1.53 (s, 3H), 0.90 (d, *J* = 6.6 Hz, 3H); ^{13}C NMR (50 MHz, $CDCl_3$): δ 144.8, 141.0, 140.5, 136.1, 131.5, 129.6, 129.5 (2C), 128.7 (2C), 127.5, 126.0 (2C), 125.3, 58.1, 44.5, 24.4,

21.3, 20.9, 16.8 ; MS (FAB$^+$) *m/z* 378 (M+1,100), 371 (37), 361 (56), 327 (18); HRMS calcd for $C_{24}H_{27}NOS$ [M+1] 378.5422, found 378.1883.

(2*R*,3*S*)-2-(4-Methoxyphenyl)-3-[(*S*)-2-(*p*-toluenesulfinyl)phenyl]butyl-2-amine (*syn*-**22c**): SCX Chromatography; yield: 92%; colorless oil; $[\alpha]_D^{20}$ +82.1 (*c* 1.0, acetone); IR (NaCl): 3187, 1513, 1492, 1086 cm^{-1}; ^{1}H NMR (200 MHz, $CDCl_3$): δ 7.60-7.18 (m, 10H), 6.83 (d, *J* = 8.9 Hz, 2H), 3.99 (q, *J* = 7.1 Hz, 1H), 3.79 (s, 3H), 2.35 (s, 3H), 1.92 (bs, 2H), 1.51 (s, 3H), 0.88 (d, *J* = 7.1 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 158.1, 152.1, 148.9, 131.4, 129.6, 129.5, 128.7 (2C), 127.3 (2C), 125.3 (2C), 113.2 (2C), 57.9, 55.2, 44.8, 21.2, 16.8 (2C).

Representative procedure for C-S desulfinylation



A solution of the corresponding compound **6** (0.18 mmol) in THF (2 mL) was added activated Raney nickel (1.2 g) in THF (3 mL). The reaction was followed by TLC and then it was stirred for 2 hours, filtered, and the residue was purified by SCX column, affording the pure free amine.

(2*S*,3*S*)-2-Phenyl-3-phenylbutyl-2-amine (***anti*-23a**): SCX Chromatography; yield: 81%; colorless oil; $[\alpha]_D^{20}$ -37.9 (*c* 2.0, $CHCl_3$); IR (NaCl): 3269, 3203, 1602, 1494, 1451, 1029 cm^{-1}; ^{1}H NMR (200 MHz, CD_3OD): δ 7.41−7.21 (m, 8H), 7.10-7.07 (m, 2H), 3.23 (d, *J* = 7.2 Hz, 1H), 1.55 (s, 3H), 1.30 (bs, 2H), 1.17 (d, *J* = 7.2Hz, 3H); ^{13}C NMR (75 MHz, CD_3OD): δ 146.7, 143.3, 130.9 (2C), 129.6,

129.4, 128.4, 127.6, 60.5, 52.5, 24.7, 16.7; MS (FAB^+) *m/z* 226 (M+1, 61), 209 (100), 195 (71); HRMS calcd for $C_{16}H_{17}N_1$ 226.1595, found 226.1607.

(2*S*,3*S*)-2-(4-Methylphenyl)-3-phenylbutyl-2-amine (***anti*-23d**): SCX Chromatography; yield: 91%; colorless oil; $[\alpha]_D^{20}$ -52.3 (*c* 1.0, $CHCl_3$); IR (NaCl): 3385, 3031, 2923, 2855, 1517, 1453, 815, 704 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 7.23-7.08 (m, 9H), 6.98 (bs, 2H), 3.39 (d, *J* = 8.8 Hz, 1H), 2.33 (s, 3H), 1.65 (s, 3H), 1.27 (d, *J* = 8.8 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 140.4, 137.3, 129.6, 128.8, 127.9, 127.1, 126.6, 29.7, 24.1, 20.9, 15.9, 14.1; MS (FAB^+) *m/z* 240 (M+1, 24), 224 (19), 223 (100), 209 (14); HRMS calcd for $C_{17}H_{22}N$ 240.1762, found 240.1742.

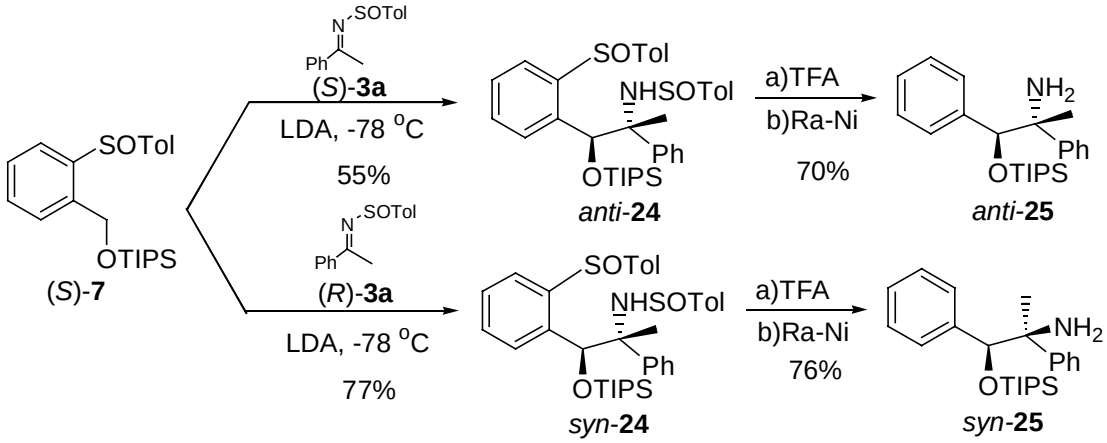
(2*S*,3*S*)-2-(4-Methoxyphenyl)-3-phenylbutyl-2-amine (***anti*-23c**): SCX Chromatography; yield: 95 %; colorless oil; $[\alpha]_D^{20}$ -47.9 (*c* 1.0, $CHCl_3$); IR (NaCl): 3361, 3059, 3028, 2969, 2935, 2836, 2876, 1610, 1512, 1453, 1299, 1249, 1181, 1034 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 7.29 (d, *J* = 8.79 Hz, 3H), 7.19 (d, *J* = 4.4 Hz, 2H), 7.02 (d, *J*= 7.4 Hz, 2H), 6.82 (d, *J* = 8.8 Hz, 2H), 3.80 (s, 3H), 3.17 (q, *J* = 7.2 Hz, 1H), 1.52 (s, 3H), 1.20 (d, *J* = 7.2 Hz, 3H), 0.52 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 158.2, 142.6, 129.5, 129.3, 127.5 (2C), 126.5, 113.0 (2C), 58.5, 55.2, 50.8, 26.1, 15.9; HRMS calcd for $C_{17}H_{19}NO$ 239.1435 found 239.1443.

(2*R*,3*S*)-2-Phenyl-3-phenylbutyl-2-amine (***syn*-23a**): SCX Chromatography; yield: 90%; colorless oil; $[\alpha]_D^{20}$ -20.4 (*c* 1.0, $CHCl_3$); IR (NaCl): 3270 (bs), 1602, 1451 cm^{-1}; ^1H NMR (200 MHz, CD_3OD): δ 7.40-7.21 (m, 8H), 7.09 (dd, *J* = 7.8, 2.3 Hz, 2H), 3.28 (q, *J* = 7.0 Hz, 1H), 1.59 (s, 3H), 1.25 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (50 MHz, CD_3OD): δ 145.9, 142.7, 130.5, 129.2, 129.0, 128.2, 128.0, 127.2, 60.3, 51.9, 23.9, 16.2; MS (FAB^+) *m/z* 209 (M+1, 24), 195 (55); HRMS calcd for $C_{16}H_{17}N_1$ 209.1330, found 209.1329.

(2*R*,3*S*)-2-(4-Methylphenyl)-3-phenylbutyl-2-amine (*syn*-23d): SCX Chromatography; yield: 80%; colorless oil; $[\alpha]_D^{20}$ -0.6 (*c* 0.5, $CHCl_3$); IR (NaCl): 3200 (bs), 1611, 1451 cm^{-1}; ^1H NMR (300 MHz, CD_3OD): δ 7.35-7.20 (m, 9H), 3.37 (q, *J* = 7.2 Hz, 1H), 2.38 (s, 3H), 1.93 (s, 3H), 1.13 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, CD_3OD): δ 140.8, 139.7, 138.5, 130.6, 130.5, 129.6, 128.9, 127.0, 62.7, 30.7, 21.0, 20.6, 16.3.

(2*R*,3*S*)-2-(4-Methoxylphenyl)-3-phenylbutyl-2-amine (*syn*-23c): SCX Chromatography; yield: 80%; colorless oil; $[\alpha]_D^{20}$ -6.2 (*c* 1.0, $CHCl_3$); IR (NaCl): 3200 (bs), 1611, 1517, 1258 cm^{-1}; ^1H NMR (300 MHz, CD_3OD): δ 7.35-7.20 (m, 7H), 6.83 (d, *J* = 8.7 Hz, 2H), 3.79 (s, 3H), 3.34 (q, *J* = 7.2 Hz, 1H), 1.61 (s, 3H), 1.22 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, CD_3OD): δ 158.7, 140.9, 129.5, 127.8, 127.7 (2C), 126.9, 113.2, 55.1, 49.7, 29.6, 24.5, 15.8.

Synthesis of the aminealcohols (Scheme 5).



Procedure for the synthesis of compounds anti- *and* syn-***24*** A solution of *n*-BuLi (0.7 mmol, 2.3 M in hexane) was added to $^iPr_2NH$ (1.0 mmol) in THF (3 mL) at 0 ºC. After stirring for 20 min, the mixture was cooled to –78 ºC. A solution of sulfoxide **7** (0.5 mmol) in THF (2 mL) was added. After stirring for 30 min., the corresponding (*R*) or (*S*) *N*-sulfinylketimine **3a** (0.5 mmol) was added at –78 ºC. When the reaction was completed (5 min), the mixture was hydrolysed (1 mL H_2O), extracted (3x10 mL

Et_2O), washed (2x10 mL NaCl sat.), dried ($MgSO_4$) and the solvent was removed under reduced pressure.

[2*S*,3*S*,(S)*S*]-*N*-{2-Phenyl-3-triisopropylsilyloxi-3-[(*S*)-2-(*p*-toluenesulfinyl)phenyl]propyl}-*p*-toluene sulfinamide (*anti*-24): Chromatography: *n*-hexane-AcOEt 1:1; yield: 55%; colorless oil; $[\alpha]_D^{20}$ –0.92 (*c* 1.0, $CHCl_3$); IR (NaCl): 3302, 1492, 1463, 1125, 1090 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 7.52 (d, *J* = 7.4 Hz, 1H), 7.65 (d, *J* =7.8 Hz, 2H), 7.54-7.50 (m, 4H), 7.31-7.28 (m, 5H), 7.13 (d, *J* = 7.2 Hz, 2H), 7.04 (d, *J* = 1.2 Hz, 1H), 6.68 (d, *J* =7.2 Hz, 2H), 6.15 (s, 1H), 5.43 (s, 1H), 2.45 (s, 3H), 2.39 (s, 3H), 2.04 (s, 3H), 0.91-0.88 (m, 18H), 0.88-0.76 (m, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 144.1, 143.6, 141.1, 140.9, 140.6, 140.4, 130.9, 130.5, 129.8, 129.5, 129.3, 129.2, 128.4, 128.2, 128.1, 127.5, 127.4, 125.6, 124.7, 76.0, 66.5, 23.1, 21.3, 17.8, 17.7, 12.2; Anal. Calcd for $C_{38}H_{49}NO_3S_2Si$: C, 69.15; H, 7.48; N, 2.12; S, 9.72. Found: C, 68.71; H, 7.36; N, 2.19; S, 9.43.

[2*R*,3*S*,(S)*S*]-*N*-{2-Phenyl-3-triisopropylsilyloxi-3-[(*S*)-2-(*p*-toluenesulfinyl)phenyl]propyl}-*p*-toluene sulfinamide (*syn*-24): Chromatography: *n*-hexane-AcOEt 1:1; yield: 77%; colorless oil; $[\alpha]_D^{20}$ –7.25 (*c* 0.4, EtOH); IR (NaCl): 3182, 1492, 1462, 1093 cm^{-1}; ^1H NMR (200 MHz, $CDCl_3$): δ 7.70-7.17 (m, 11H), 7.04 (d, *J* = 8.7 Hz, 2H), 6.84 (dd, *J* = 8.3, 1.7 Hz, 2H), 5.99 (d, *J* = 1.5 Hz, 1H), 5.09 (s, 1H), 2.33 (s, 6H), 2.06 (s, 3H), 0.90-0.65 (m, 21H); ^{13}C NMR (50 MHz, $CDCl_3$): δ 143.8, 143.3. 142.6, 141.5, 140.9, 140.6, 138.6, 130.9, 130.1, 129.3 (2C), 128.8, 127.8, 127.4, 125.3 (2C), 124.9 (2C), 76.4, 65.9, 23.9, 21.2, 17.8 (2C), 12.1; Anal. Calcd for $C_{38}H_{49}NO_3S_2Si$: C, 69.15; H, 7.48; N, 2.12; S, 9.72. Found: C, 68.71; H, 7.36; N, 2.19; S, 9.43.

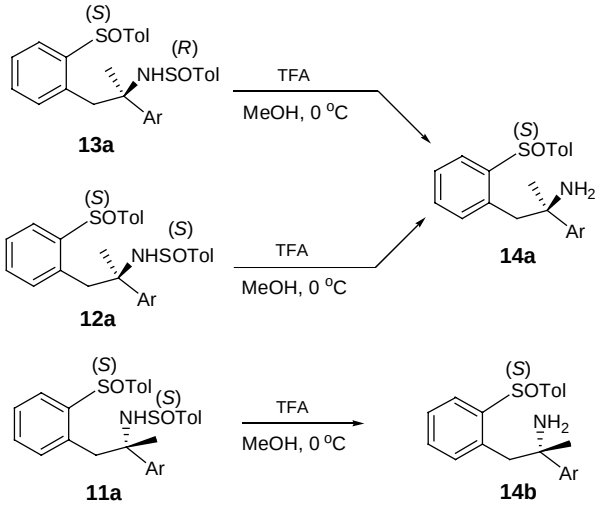
Synthesis of compounds anti *and* syn-***25*** To a stirred solution of *anti* or *syn*-**24** (0.2 mmol) in methanol (3 mL) was added TFA (1.0 mmol, 50 μL). After the mixture was stirred for 3 h, the solvent was evaporated, and the residue was chromatography by SCX column. To the corresponding free-amine in

THF (2 mL), was added a suspension of activated Raney nickel (1.2 g) in THF (3 mL). The reaction was stirred 2 hours, filtered, and the residue was purified by SCX column to afford the amine.

(2*S*,3*S*)-2,3-Diphenyltriisopropylsilyloxipropyl-2-amine (*anti*-25): SCX Chromatography; yield: 70%; colorless oil; $[\alpha]_D^{20}$ +256.0 (*c* 0.55, CH_3OH); IR (NaCl): 3021, 1602, 1462 , 1100, 1065 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 7.40 (d, *J* =7.2Hz, 2H), 7.27-7.19 (m, 6H), 7.09 (m, 2H), 4.98 (s, 1H), 3.10 (bs, 2H), 1.35 (s, 3H), 0.87-0.84 (m, 21H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 140.6, 128.1, 127.7, 127.6, 127.3, 126.6 (2C), 126.5, 82.8, 60.2, 25.8, 18.0, 17.9, 12.6; MS (FAB) *m/z* 384 (M+1, 100), 371 (26), 368 (31), 367 (93); HRMS calcd for $C_{24}H_{38}NOSi$ 384.2724, found 384.2724.

(2*S*,3*R*)-2,3-Diphenyl-3-triisopropylsilyloxipropyl-2-amine (*syn*-25): SCX Chromatography; yield: 77%; colorless oil; $[\alpha]_D^{20}$ -1.0 (*c* 0.55, CH_3OH); IR (NaCl): 1494, 1463, 1907, 1064 cm^{-1}; ^1H NMR (200 MHz, $CDCl_3$): δ 7.27-7.19 (m, 8H), 7.00-6.85 (m, 2H), 4.94 (s, 1H), 2.38 (bs, 2H), 1.58 (s, 3H), 1.10-0.80 (m, 21H); ^{13}C NMR (50 MHz, $CDCl_3$): δ 145.2, 140.7, 128.1, 127.5, 127.2, 126.9, 126.5, 126.4, 82.9, 59.6, 26.9, 18.0, 12.2; Anal. Calcd for $C_{24}H_{38}NOSi$: C, 75.14; H, 9.72; N, 3.65; Found: C, 75.06; H, 9.98; N, 3.47.

<u>Scheme and compounds for correlation of compounds 11a, 12a, 13a.</u>



(1*R*)-1-Methyl-1-phenyl-2-[(*S*)-2-*p*-tolylsulfinylphenyl]-ethylamine (14a). This amine was obtained using the general procedure for N-S desulfinilation from *N*-sulfinilamide **13a** or **12a.** SCX Chromatography; yield: 85%; colorless oil; $[\alpha]_D^{20}$ -190.5 (*c* 0.4, CH_3OH); ^1H NMR (300 MHz, $CDCl_3$): δ 7.73 (dd, *J* = 6.4, 1.3 Hz, 1H), 7.41-7.12 (m, 11H), 6.80 (dd, *J* = 6.6, 1.1 Hz, 1H), 3.16 (dd, *J* = 13.7 Hz, 2H), 2.28 (s, 3H), 1.86 (bs, 2H), 1.53 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 148.0, 145.5, 141.9, 141.2, 136.1, 131.6, 130.5, 129.9, 128.3, 128.1, 129.7, 125.7, 125.5, 125.4, 56.2, 46.2, 30.7, 21.3.

(1*S*)-1-Methyl-1-phenyl-2-[(*S*)-2-*p*-tolylsulfinylphenyl]-ethylamine (14b). This amine was obtained using the general procedure for N-S desulfinilation from *N*-sulfinilamide **11a.** SCX Chromatography; yield: 92%; colorless oil; $[\alpha]_D^{20}$ -210.0 (*c* 0.2, $(CH_3)_2CO$); IR (NaCl): 3057, 3022, 2970, 2926, 1596, 1470, 1082, 1058, 1031, 753 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 7.70 (d, 1H), 7.38-7.12 (m, 11H), 6.81 (d, *J* = 6.6 Hz, 1H), 3.18 (dd, *J* = 13.7 Hz, 2H), 2.27 (s, 3H), 1.84 (bs, 2H), 1.54 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 147.7, 145.4, 141.6, 141.3, 136.1, 131.8, 130.5, 129.9, 128.4, 128.1, 126.8, 125.8, 125.5(2C), 56.5, 46.1, 30.2, 21.4.

X-Ray structure of *anti*-**18b.** [2]

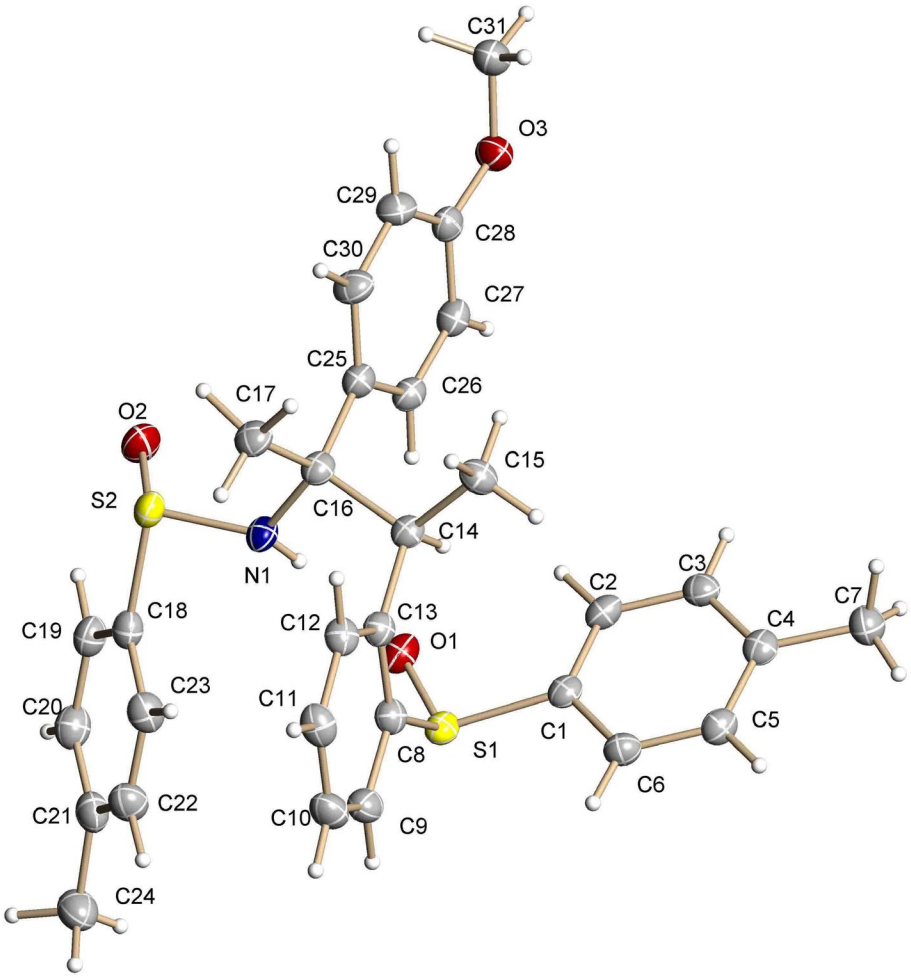


Figure 1. Ortep diagram for compound *anti*-**18b**

[2] The authors have deposited atomic coordinates for *anti*-**18b** and **17b** with the Cambridge Crystallographic data Centre (deposition number CCDC 254168 and 271792 respectively). The coordinates can be obtained, on request, from the Director, Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge Cb2 1EZ, U.K.

Table 1. Crystal data and structure refinement for *anti*-**18b**

Identification code	datos_m	
Empirical formula	C31 H33 N O3 S2	
Formula weight	531.70	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 7.33490(10) Å	α= 90°.
	b = 18.72360(10) Å	β= 90°.
	c = 20.2187(2) Å	γ = 90°.
Volume	2776.75(5) $Å^3$	
Z	4	
Density (calculated)	1.272 Mg/m^3	
Absorption coefficient	1.993 mm^{-1}	
F(000)	1128	
Crystal size	0.30 x 0.15 x 0.15 mm^3	
Theta range for data collection	3.22 to 70.44°.	
Index ranges	-8<=h<=8, -22<=k<=22, -17<=l<=23	
Reflections collected	11918	
Independent reflections	4807 [R(int) = 0.0259]	
Completeness to theta = 70.44°	94.9 %	
Absorption correction	YES, SADABS v. 2.03	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4807 / 0 / 466	
Goodness-of-fit on F^2	1.051	
Final R indices [I>2sigma(I)]	R1 = 0.0267, wR2 = 0.0697	
R indices (all data)	R1 = 0.0278, wR2 = 0.0707	
Absolute structure parameter	-0.002(10)	
Largest diff. peak and hole	0.194 and -0.186 $e.Å^{-3}$	

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

	x	y	z	U(eq)
S(1)	9175(1)	6191(1)	1586(1)	23(1)
S(2)	7238(1)	3798(1)	2478(1)	25(1)
N(1)	6999(2)	4471(1)	1958(1)	23(1)
O(1)	9746(2)	5428(1)	1479(1)	26(1)
O(2)	8192(2)	3169(1)	2197(1)	34(1)
O(3)	6879(2)	2903(1)	-876(1)	30(1)
C(1)	8638(2)	6541(1)	781(1)	22(1)
C(2)	8913(2)	6129(1)	224(1)	25(1)
C(3)	8647(2)	6427(1)	-396(1)	25(1)
C(4)	8131(2)	7140(1)	-466(1)	24(1)
C(5)	7863(2)	7544(1)	104(1)	25(1)
C(6)	8100(3)	7254(1)	726(1)	25(1)
C(7)	7932(3)	7469(1)	-1141(1)	30(1)
C(8)	6964(2)	6241(1)	1971(1)	23(1)
C(9)	6906(3)	6741(1)	2478(1)	28(1)
C(10)	5286(3)	6873(1)	2807(1)	32(1)
C(11)	3744(3)	6494(1)	2623(1)	30(1)
C(12)	3819(2)	5984(1)	2129(1)	25(1)
C(13)	5436(2)	5840(1)	1784(1)	22(1)
C(14)	5484(2)	5298(1)	1227(1)	21(1)
C(15)	4033(3)	5449(1)	702(1)	26(1)
C(16)	5475(2)	4499(1)	1477(1)	23(1)
C(17)	3710(3)	4302(1)	1836(1)	28(1)
C(18)	8939(3)	4250(1)	2973(1)	25(1)
C(19)	10544(3)	3892(1)	3110(1)	28(1)
C(20)	11873(3)	4222(1)	3486(1)	31(1)

C(21)	11624(3)	4913(1)	3734(1)	30(1)
C(22)	9969(3)	5255(1)	3600(1)	32(1)
C(23)	8633(3)	4930(1)	3225(1)	29(1)
C(24)	13106(3)	5283(1)	4116(1)	38(1)
C(25)	5832(2)	4025(1)	871(1)	23(1)
C(26)	7497(2)	4070(1)	533(1)	24(1)
C(27)	7800(3)	3694(1)	-44(1)	26(1)
C(28)	6455(2)	3249(1)	-301(1)	25(1)
C(29)	4814(3)	3184(1)	31(1)	29(1)
C(30)	4518(3)	3576(1)	608(1)	29(1)
C(31)	5508(3)	2460(1)	-1160(1)	33(1)

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

S(1)-O(1)	1.5034(12)
S(1)-C(1)	1.7990(18)
S(1)-C(8)	1.8011(18)
S(2)-O(2)	1.4830(13)
S(2)-N(1)	1.6511(14)
S(2)-C(18)	1.8091(19)
N(1)-C(16)	1.482(2)
N(1)-H(1)	0.85(2)
O(3)-C(28)	1.366(2)
O(3)-C(31)	1.425(2)
C(1)-C(2)	1.379(2)
C(1)-C(6)	1.396(2)
C(2)-C(3)	1.387(3)
C(2)-H(2)	0.979(18)
C(3)-C(4)	1.394(2)
C(3)-H(3)	0.91(2)
C(4)-C(5)	1.391(3)
C(4)-C(7)	1.504(2)
C(5)-C(6)	1.381(3)
C(5)-H(5)	0.95(2)
C(6)-H(6)	0.94(2)
C(7)-H(7A)	0.95(3)
C(7)-H(7B)	0.95(3)
C(7)-H(7C)	0.96(3)
C(8)-C(9)	1.390(2)
C(8)-C(13)	1.401(2)
C(9)-C(10)	1.383(3)
C(9)-H(9)	0.98(2)
C(10)-C(11)	1.387(3)
C(10)-H(10)	0.92(2)

C(11)-C(12)	1.384(3)
C(11)-H(11)	0.94(2)
C(12)-C(13)	1.402(3)
C(12)-H(12)	0.936(19)
C(13)-C(14)	1.517(2)
C(14)-C(15)	1.529(2)
C(14)-C(16)	1.579(2)
C(14)-H(14)	0.969(19)
C(15)-H(15A)	0.98(2)
C(15)-H(15B)	0.94(2)
C(15)-H(15C)	0.96(2)
C(16)-C(17)	1.529(2)
C(16)-C(25)	1.535(2)
C(17)-H(17A)	0.97(2)
C(17)-H(17B)	0.99(2)
C(17)-H(17C)	1.00(2)
C(18)-C(19)	1.383(3)
C(18)-C(23)	1.391(2)
C(19)-C(20)	1.382(3)
C(19)-H(19)	1.00(2)
C(20)-C(21)	1.399(3)
C(20)-H(20)	1.04(2)
C(21)-C(22)	1.399(3)
C(21)-C(24)	1.503(3)
C(22)-C(23)	1.380(3)
C(22)-H(22)	0.97(2)
C(23)-H(23)	0.90(3)
C(24)-H(24A)	1.02(3)
C(24)-H(24B)	1.01(3)
C(24)-H(24C)	0.78(4)
C(25)-C(30)	1.385(2)
C(25)-C(26)	1.402(3)

C(26)-C(27)	1.380(2)
C(26)-H(26)	0.96(2)
C(27)-C(28)	1.392(2)
C(27)-H(27)	0.96(2)
C(28)-C(29)	1.383(3)
C(29)-C(30)	1.396(3)
C(29)-H(29)	0.94(2)
C(30)-H(30)	0.98(2)
C(31)-H(31A)	1.00(2)
C(31)-H(31B)	0.95(3)
C(31)-H(31C)	0.98(2)

O(1)-S(1)-C(1)	106.12(8)
O(1)-S(1)-C(8)	111.20(7)
C(1)-S(1)-C(8)	100.11(8)
O(2)-S(2)-N(1)	114.26(8)
O(2)-S(2)-C(18)	104.92(8)
N(1)-S(2)-C(18)	93.93(7)
C(16)-N(1)-S(2)	121.67(11)
C(16)-N(1)-H(1)	111.4(15)
S(2)-N(1)-H(1)	117.6(15)
C(28)-O(3)-C(31)	117.28(15)
C(2)-C(1)-C(6)	120.83(16)
C(2)-C(1)-S(1)	120.13(12)
C(6)-C(1)-S(1)	118.78(14)
C(1)-C(2)-C(3)	119.45(15)
C(1)-C(2)-H(2)	118.9(11)
C(3)-C(2)-H(2)	121.7(11)
C(2)-C(3)-C(4)	120.99(17)
C(2)-C(3)-H(3)	120.4(13)
C(4)-C(3)-H(3)	118.4(13)
C(5)-C(4)-C(3)	118.33(16)

C(5)-C(4)-C(7)	121.03(15)
C(3)-C(4)-C(7)	120.62(16)
C(6)-C(5)-C(4)	121.52(15)
C(6)-C(5)-H(5)	119.7(13)
C(4)-C(5)-H(5)	118.8(13)
C(5)-C(6)-C(1)	118.87(17)
C(5)-C(6)-H(6)	123.4(13)
C(1)-C(6)-H(6)	117.7(13)
C(4)-C(7)-H(7A)	115.9(17)
C(4)-C(7)-H(7B)	110.7(16)
H(7A)-C(7)-H(7B)	114(2)
C(4)-C(7)-H(7C)	110.2(14)
H(7A)-C(7)-H(7C)	100(2)
H(7B)-C(7)-H(7C)	104(2)
C(9)-C(8)-C(13)	122.37(16)
C(9)-C(8)-S(1)	112.44(13)
C(13)-C(8)-S(1)	125.17(13)
C(10)-C(9)-C(8)	120.10(17)
C(10)-C(9)-H(9)	123.9(11)
C(8)-C(9)-H(9)	116.0(11)
C(9)-C(10)-C(11)	118.73(17)
C(9)-C(10)-H(10)	119.2(16)
C(11)-C(10)-H(10)	122.0(17)
C(12)-C(11)-C(10)	120.96(18)
C(12)-C(11)-H(11)	121.5(13)
C(10)-C(11)-H(11)	117.5(13)
C(11)-C(12)-C(13)	121.68(17)
C(11)-C(12)-H(12)	121.5(11)
C(13)-C(12)-H(12)	116.8(11)
C(8)-C(13)-C(12)	116.12(15)
C(8)-C(13)-C(14)	122.73(15)
C(12)-C(13)-C(14)	121.12(15)

C(13)-C(14)-C(15)	112.01(13)
C(13)-C(14)-C(16)	113.38(14)
C(15)-C(14)-C(16)	113.27(14)
C(13)-C(14)-H(14)	106.0(10)
C(15)-C(14)-H(14)	106.4(11)
C(16)-C(14)-H(14)	105.0(10)
C(14)-C(15)-H(15A)	110.3(12)
C(14)-C(15)-H(15B)	112.8(13)
H(15A)-C(15)-H(15B)	106.2(17)
C(14)-C(15)-H(15C)	110.9(13)
H(15A)-C(15)-H(15C)	108.0(16)
H(15B)-C(15)-H(15C)	108.4(18)
N(1)-C(16)-C(17)	108.61(14)
N(1)-C(16)-C(25)	112.00(14)
C(17)-C(16)-C(25)	112.53(14)
N(1)-C(16)-C(14)	103.92(13)
C(17)-C(16)-C(14)	112.56(14)
C(25)-C(16)-C(14)	106.93(13)
C(16)-C(17)-H(17A)	109.8(11)
C(16)-C(17)-H(17B)	112.7(13)
H(17A)-C(17)-H(17B)	109.2(17)
C(16)-C(17)-H(17C)	110.1(13)
H(17A)-C(17)-H(17C)	108.7(17)
H(17B)-C(17)-H(17C)	106.1(18)
C(19)-C(18)-C(23)	120.53(18)
C(19)-C(18)-S(2)	118.17(13)
C(23)-C(18)-S(2)	121.28(15)
C(20)-C(19)-C(18)	119.63(16)
C(20)-C(19)-H(19)	121.8(12)
C(18)-C(19)-H(19)	118.5(12)
C(19)-C(20)-C(21)	121.24(18)
C(19)-C(20)-H(20)	119.1(13)

C(21)-C(20)-H(20)	119.6(13)
C(22)-C(21)-C(20)	117.79(18)
C(22)-C(21)-C(24)	121.12(17)
C(20)-C(21)-C(24)	121.07(18)
C(23)-C(22)-C(21)	121.47(17)
C(23)-C(22)-H(22)	119.1(14)
C(21)-C(22)-H(22)	119.4(14)
C(22)-C(23)-C(18)	119.31(19)
C(22)-C(23)-H(23)	116.9(14)
C(18)-C(23)-H(23)	123.8(14)
C(21)-C(24)-H(24A)	112.0(17)
C(21)-C(24)-H(24B)	113.7(19)
H(24A)-C(24)-H(24B)	103(2)
C(21)-C(24)-H(24C)	114(2)
H(24A)-C(24)-H(24C)	111(3)
H(24B)-C(24)-H(24C)	103(3)
C(30)-C(25)-C(26)	117.09(16)
C(30)-C(25)-C(16)	122.59(16)
C(26)-C(25)-C(16)	120.18(15)
C(27)-C(26)-C(25)	121.43(17)
C(27)-C(26)-H(26)	118.0(13)
C(25)-C(26)-H(26)	120.6(13)
C(26)-C(27)-C(28)	120.45(17)
C(26)-C(27)-H(27)	119.7(12)
C(28)-C(27)-H(27)	119.8(12)
O(3)-C(28)-C(29)	124.69(16)
O(3)-C(28)-C(27)	116.11(16)
C(29)-C(28)-C(27)	119.20(17)
C(28)-C(29)-C(30)	119.67(17)
C(28)-C(29)-H(29)	121.0(14)
C(30)-C(29)-H(29)	119.3(14)
C(25)-C(30)-C(29)	122.14(18)

C(25)-C(30)-H(30)	122.9(12)
C(29)-C(30)-H(30)	115.0(12)
O(3)-C(31)-H(31A)	108.1(13)
O(3)-C(31)-H(31B)	108.8(14)
H(31A)-C(31)-H(31B)	110.2(18)
O(3)-C(31)-H(31C)	113.0(12)
H(31A)-C(31)-H(31C)	111.1(17)
H(31B)-C(31)-H(31C)	105.7(19)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for datos_m. 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}
S(1)	18(1)	24(1)	27(1)	2(1)	-2(1)	-2(1)
S(2)	28(1)	21(1)	25(1)	4(1)	3(1)	-1(1)
N(1)	19(1)	24(1)	27(1)	5(1)	1(1)	-3(1)
O(1)	19(1)	24(1)	37(1)	6(1)	2(1)	1(1)
O(2)	44(1)	21(1)	36(1)	1(1)	1(1)	3(1)
O(3)	34(1)	29(1)	25(1)	-4(1)	3(1)	-3(1)
C(1)	16(1)	22(1)	28(1)	2(1)	0(1)	-3(1)
C(2)	22(1)	19(1)	33(1)	1(1)	3(1)	-1(1)
C(3)	24(1)	25(1)	27(1)	-3(1)	2(1)	-3(1)
C(4)	16(1)	26(1)	29(1)	2(1)	1(1)	-2(1)
C(5)	22(1)	22(1)	31(1)	2(1)	0(1)	3(1)
C(6)	24(1)	23(1)	28(1)	-3(1)	1(1)	0(1)
C(7)	32(1)	31(1)	27(1)	2(1)	0(1)	2(1)
C(8)	21(1)	24(1)	23(1)	2(1)	-1(1)	3(1)
C(9)	29(1)	27(1)	26(1)	0(1)	-4(1)	-1(1)
C(10)	39(1)	30(1)	25(1)	-5(1)	-1(1)	4(1)

C(11)	28(1)	35(1)	26(1)	1(1)	3(1)	8(1)
C(12)	19(1)	28(1)	26(1)	3(1)	-1(1)	3(1)
C(13)	21(1)	23(1)	23(1)	3(1)	-1(1)	2(1)
C(14)	16(1)	22(1)	25(1)	1(1)	1(1)	0(1)
C(15)	24(1)	30(1)	25(1)	-3(1)	-3(1)	3(1)
C(16)	18(1)	24(1)	27(1)	2(1)	-1(1)	-2(1)
C(17)	24(1)	28(1)	31(1)	0(1)	4(1)	-4(1)
C(18)	26(1)	25(1)	23(1)	4(1)	4(1)	2(1)
C(19)	30(1)	25(1)	28(1)	5(1)	3(1)	3(1)
C(20)	28(1)	33(1)	33(1)	7(1)	1(1)	3(1)
C(21)	32(1)	35(1)	24(1)	5(1)	1(1)	-2(1)
C(22)	37(1)	29(1)	29(1)	-3(1)	0(1)	4(1)
C(23)	30(1)	30(1)	28(1)	0(1)	1(1)	7(1)
C(24)	37(1)	44(1)	32(1)	2(1)	-4(1)	-6(1)
C(25)	23(1)	21(1)	26(1)	2(1)	1(1)	0(1)
C(26)	23(1)	20(1)	28(1)	3(1)	-1(1)	-1(1)
C(27)	25(1)	24(1)	28(1)	4(1)	3(1)	0(1)
C(28)	31(1)	20(1)	25(1)	3(1)	-1(1)	2(1)
C(29)	28(1)	27(1)	33(1)	-3(1)	-2(1)	-4(1)
C(30)	26(1)	28(1)	34(1)	-3(1)	5(1)	-7(1)
C(31)	41(1)	29(1)	27(1)	-2(1)	-3(1)	-3(1)

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

	x	y	z	U(eq)
H(1)	7970(30)	4656(11)	1798(11)	32(6)
H(2)	9290(30)	5631(10)	279(9)	21(5)
H(3)	8730(30)	6153(11)	-765(11)	30(5)
H(5)	7490(30)	8027(11)	60(10)	31(5)

H(6)	7950(30)	7514(11)	1118(11)	32(5)
H(7A)	8860(40)	7350(14)	-1454(14)	64(8)
H(7B)	7690(40)	7965(15)	-1107(13)	58(7)
H(7C)	6870(30)	7277(12)	-1361(12)	45(7)
H(9)	8070(30)	6969(10)	2592(9)	23(5)
H(10)	5250(40)	7225(13)	3127(12)	48(7)
H(11)	2650(30)	6592(11)	2852(11)	35(6)
H(12)	2780(30)	5735(9)	1993(9)	14(4)
H(14)	6650(30)	5358(9)	1011(9)	15(4)
H(15A)	4170(30)	5934(10)	531(9)	26(5)
H(15B)	2840(30)	5417(10)	869(10)	24(5)
H(15C)	4150(30)	5124(11)	337(11)	33(5)
H(17A)	3640(30)	4555(10)	2251(10)	20(5)
H(17B)	2600(30)	4408(11)	1569(11)	34(6)
H(17C)	3680(30)	3776(12)	1927(11)	40(6)
H(19)	10720(30)	3406(10)	2920(10)	29(5)
H(20)	13100(30)	3960(12)	3566(11)	45(6)
H(22)	9760(30)	5735(12)	3764(11)	40(6)
H(23)	7600(30)	5184(12)	3150(11)	41(6)
H(24A)	13670(40)	4958(16)	4469(15)	72(9)
H(24B)	12660(50)	5707(17)	4382(15)	80(10)
H(24C)	13870(50)	5450(17)	3892(16)	78(11)
H(26)	8480(30)	4349(11)	708(11)	37(6)
H(27)	8960(30)	3727(10)	-260(10)	30(5)
H(29)	3880(30)	2887(11)	-132(11)	37(6)
H(30)	3310(30)	3515(10)	806(10)	30(5)
H(31A)	6030(30)	2230(11)	-1565(11)	36(5)
H(31B)	4490(40)	2750(12)	-1275(11)	45(6)
H(31C)	5040(30)	2103(11)	-852(11)	31(5)

Table 6. Torsion angles [°] for datos_m.

O(2)-S(2)-N(1)-C(16)	83.80(15)
C(18)-S(2)-N(1)-C(16)	-167.89(14)
O(1)-S(1)-C(1)-C(2)	-4.26(16)
C(8)-S(1)-C(1)-C(2)	-119.97(14)
O(1)-S(1)-C(1)-C(6)	-178.55(13)
C(8)-S(1)-C(1)-C(6)	65.73(15)
C(6)-C(1)-C(2)-C(3)	-0.2(3)
S(1)-C(1)-C(2)-C(3)	-174.34(13)
C(1)-C(2)-C(3)-C(4)	1.0(3)
C(2)-C(3)-C(4)-C(5)	-1.0(3)
C(2)-C(3)-C(4)-C(7)	177.07(17)
C(3)-C(4)-C(5)-C(6)	0.1(3)
C(7)-C(4)-C(5)-C(6)	-177.90(17)
C(4)-C(5)-C(6)-C(1)	0.7(3)
C(2)-C(1)-C(6)-C(5)	-0.7(3)
S(1)-C(1)-C(6)-C(5)	173.60(13)
O(1)-S(1)-C(8)-C(9)	135.67(12)
C(1)-S(1)-C(8)-C(9)	-112.51(13)
O(1)-S(1)-C(8)-C(13)	-45.71(17)
C(1)-S(1)-C(8)-C(13)	66.11(16)
C(13)-C(8)-C(9)-C(10)	-1.8(3)
S(1)-C(8)-C(9)-C(10)	176.86(14)
C(8)-C(9)-C(10)-C(11)	0.6(3)
C(9)-C(10)-C(11)-C(12)	1.0(3)
C(10)-C(11)-C(12)-C(13)	-1.4(3)
C(9)-C(8)-C(13)-C(12)	1.4(2)
S(1)-C(8)-C(13)-C(12)	-177.13(12)
C(9)-C(8)-C(13)-C(14)	179.47(15)
S(1)-C(8)-C(13)-C(14)	1.0(2)
C(11)-C(12)-C(13)-C(8)	0.2(2)
C(11)-C(12)-C(13)-C(14)	-177.91(15)

C(8)-C(13)-C(14)-C(15)	-124.60(17)
C(12)-C(13)-C(14)-C(15)	53.4(2)
C(8)-C(13)-C(14)-C(16)	105.69(18)
C(12)-C(13)-C(14)-C(16)	-76.28(19)
S(2)-N(1)-C(16)-C(17)	45.66(18)
S(2)-N(1)-C(16)-C(25)	-79.24(17)
S(2)-N(1)-C(16)-C(14)	165.69(12)
C(13)-C(14)-C(16)-N(1)	-52.59(18)
C(15)-C(14)-C(16)-N(1)	178.34(14)
C(13)-C(14)-C(16)-C(17)	64.73(19)
C(15)-C(14)-C(16)-C(17)	-64.35(19)
C(13)-C(14)-C(16)-C(25)	-171.20(14)
C(15)-C(14)-C(16)-C(25)	59.72(18)
O(2)-S(2)-C(18)-C(19)	-12.83(16)
N(1)-S(2)-C(18)-C(19)	-129.22(14)
O(2)-S(2)-C(18)-C(23)	168.92(15)
N(1)-S(2)-C(18)-C(23)	52.53(16)
C(23)-C(18)-C(19)-C(20)	-1.8(3)
S(2)-C(18)-C(19)-C(20)	179.90(14)
C(18)-C(19)-C(20)-C(21)	0.4(3)
C(19)-C(20)-C(21)-C(22)	1.1(3)
C(19)-C(20)-C(21)-C(24)	-177.18(19)
C(20)-C(21)-C(22)-C(23)	-1.2(3)
C(24)-C(21)-C(22)-C(23)	177.12(19)
C(21)-C(22)-C(23)-C(18)	-0.2(3)
C(19)-C(18)-C(23)-C(22)	1.8(3)
S(2)-C(18)-C(23)-C(22)	179.98(14)
N(1)-C(16)-C(25)-C(30)	135.12(17)
C(17)-C(16)-C(25)-C(30)	12.4(2)
C(14)-C(16)-C(25)-C(30)	-111.66(18)
N(1)-C(16)-C(25)-C(26)	-49.3(2)
C(17)-C(16)-C(25)-C(26)	-171.97(15)

C(14)-C(16)-C(25)-C(26)	63.94(19)
C(30)-C(25)-C(26)-C(27)	1.2(2)
C(16)-C(25)-C(26)-C(27)	-174.68(15)
C(25)-C(26)-C(27)-C(28)	-0.9(2)
C(31)-O(3)-C(28)-C(29)	1.7(2)
C(31)-O(3)-C(28)-C(27)	-178.24(15)
C(26)-C(27)-C(28)-O(3)	179.55(15)
C(26)-C(27)-C(28)-C(29)	-0.4(3)
O(3)-C(28)-C(29)-C(30)	-178.61(16)
C(27)-C(28)-C(29)-C(30)	1.3(3)
C(26)-C(25)-C(30)-C(29)	-0.2(3)
C(16)-C(25)-C(30)-C(29)	175.52(16)
C(28)-C(29)-C(30)-C(25)	-1.0(3)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for datos_m [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1)...O(1)	0.85(2)	2.05(2)	2.8652(19)	159(2)

Symmetry transformations used to generate equivalent atoms:

X-Ray structure of **17b.**

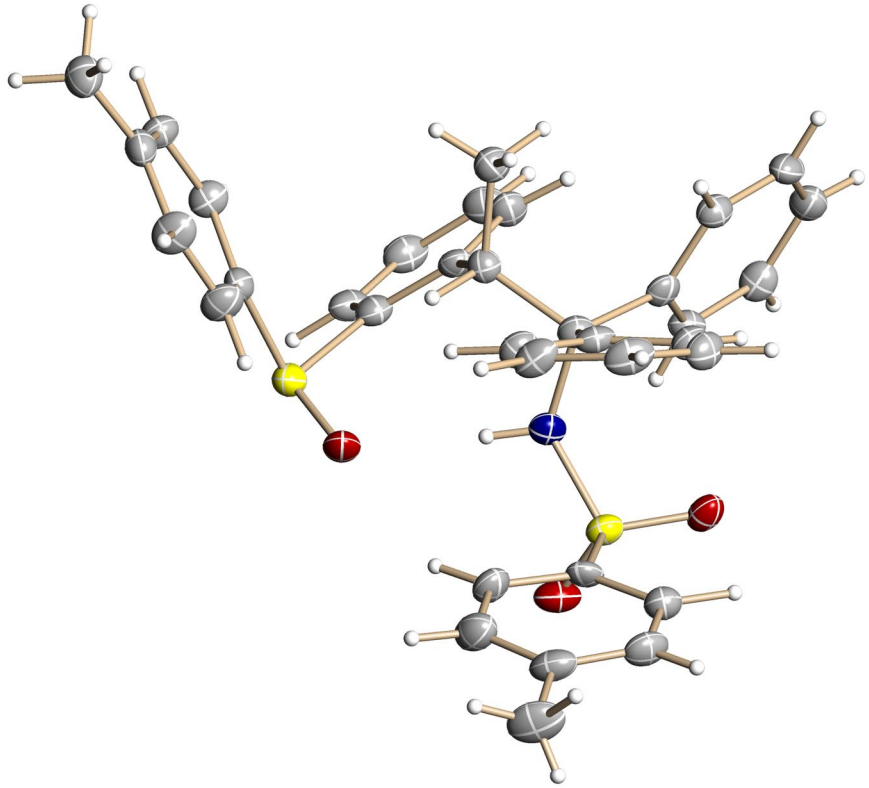


Figure 2. ORTEP diagram for compound **17b**

Table 7. Crystal data and structure refinement for **17b**

Project name: 2004 Alejandro Parra SULFO 100K parte 69498

Project path: F:\2004\Alejandro_Parra\69498\work\Sulfo_m.*

Identification code	sulfo_m	
Empirical formula	C35 H33 N O3 S2	
Formula weight	579.74	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 8.2042(3) Å	α= 90°.

	b = 15.1998(6) Å	β= 90°.
	c = 23.3340(9) Å	γ = 90°.
Volume	2909.80(19) Å^3	
Z	4	
Density (calculated)	1.323 Mg/m^3	
Absorption coefficient	1.951 mm^{-1}	
F(000)	1224	
Crystal size	0.10 x 0.06 x 0.02 mm^3	
Theta range for data collection	3.47 to 63.94°.	
Index ranges	-9<=h<=9, -15<=k<=17, -24<=l<=26	
Reflections collected	11104	
Independent reflections	4445 [R(int) = 0.0552]	
Completeness to theta = 63.94°	95.7 %	
Absorption correction	YES, SADABS v. 2.03	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4445 / 0 / 503	
Goodness-of-fit on F^2	1.011	
Final R indices [I>2sigma(I)]	R1 = 0.0408, wR2 = 0.0825	
R indices (all data)	R1 = 0.0590, wR2 = 0.0898	
Absolute structure parameter	0.03(2)	
Extinction coefficient	0.00011(9)	
Largest diff. peak and hole	0.203 and -0.279 e.Å^{-3}	

Table 8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **17b**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	5057(1)	3981(1)	2023(1)	24(1)
S(2)	7427(1)	5567(1)	381(1)	26(1)
N(1)	4720(4)	4698(2)	1522(1)	23(1)
O(1)	6728(3)	4107(2)	2173(1)	33(1)
O(2)	3832(3)	4064(2)	2449(1)	29(1)
O(3)	7087(3)	4668(2)	622(1)	30(1)
C(1)	4921(4)	2896(2)	1742(2)	25(1)
C(2)	5848(5)	2665(3)	1269(2)	29(1)
C(3)	5900(5)	1789(3)	1099(2)	36(1)
C(4)	5027(5)	1150(2)	1394(2)	33(1)
C(5)	4052(5)	1402(3)	1846(2)	31(1)
C(6)	3995(4)	2280(2)	2028(2)	27(1)
C(7)	5184(8)	189(3)	1233(3)	45(1)
C(8)	3101(4)	4929(2)	1270(2)	24(1)
C(9)	2207(4)	4075(2)	1081(2)	23(1)
C(10)	946(5)	3718(3)	1413(2)	26(1)
C(11)	177(5)	2949(2)	1239(2)	29(1)
C(12)	636(5)	2527(3)	751(2)	33(1)
C(13)	1925(5)	2843(3)	434(2)	31(1)
C(14)	2709(5)	3616(2)	597(2)	28(1)
C(15)	2090(4)	5488(2)	1687(2)	22(1)
C(16)	430(4)	5635(3)	1596(2)	25(1)
C(17)	-445(4)	6196(3)	1940(2)	27(1)
C(18)	318(5)	6651(3)	2378(2)	30(1)
C(19)	1948(5)	6517(3)	2475(2)	28(1)
C(20)	2830(4)	5936(2)	2137(2)	25(1)
C(21)	3549(4)	5505(3)	725(2)	22(1)

C(22)	2093(4)	5762(3)	361(2)	28(1)
C(23)	4577(4)	6311(2)	874(2)	22(1)
C(24)	3866(5)	7041(2)	1132(2)	27(1)
C(25)	4762(5)	7786(3)	1279(2)	32(1)
C(26)	6399(5)	7829(3)	1155(2)	32(1)
C(27)	7131(5)	7131(3)	881(2)	28(1)
C(28)	6240(4)	6385(2)	747(2)	25(1)
C(29)	6459(4)	5615(3)	-308(2)	23(1)
C(30)	6176(5)	6404(3)	-579(2)	26(1)
C(31)	5619(4)	6418(3)	-1132(2)	26(1)
C(32)	5318(4)	5640(3)	-1434(2)	26(1)
C(33)	5576(5)	4852(3)	-1151(2)	34(1)
C(34)	6170(5)	4828(3)	-591(2)	33(1)
C(35)	4790(5)	5666(3)	-2043(2)	33(1)

Table 9. Bond lengths [Å] and angles [°] for **17b**.

S(1)-O(2)	1.419(3)
S(1)-O(1)	1.428(3)
S(1)-N(1)	1.623(3)
S(1)-C(1)	1.778(4)
S(2)-O(3)	1.504(3)
S(2)-C(29)	1.795(4)
S(2)-C(28)	1.795(4)
N(1)-C(8)	1.495(4)
N(1)-H(1)	0.85(4)
C(1)-C(6)	1.378(5)
C(1)-C(2)	1.386(5)
C(2)-C(3)	1.390(6)
C(2)-H(2)	0.95(4)
C(3)-C(4)	1.390(6)
C(3)-H(3)	0.94(4)
C(4)-C(5)	1.378(6)
C(4)-C(7)	1.513(6)
C(5)-C(6)	1.401(5)
C(5)-H(5)	0.90(3)
C(6)-H(6)	1.05(3)
C(7)-H(7A)	0.99(6)
C(7)-H(7B)	0.80(5)
C(7)-H(7C)	0.93(6)
C(8)-C(15)	1.536(5)
C(8)-C(9)	1.554(5)
C(8)-C(21)	1.586(5)
C(9)-C(14)	1.389(5)
C(9)-C(10)	1.402(5)
C(10)-C(11)	1.388(5)
C(10)-H(10)	0.92(3)

C(11)-C(12)	1.361(6)
C(11)-H(11)	0.94(4)
C(12)-C(13)	1.377(6)
C(12)-H(12)	0.95(4)
C(13)-C(14)	1.394(5)
C(13)-H(13)	0.92(3)
C(14)-H(14)	0.99(4)
C(15)-C(20)	1.392(5)
C(15)-C(16)	1.396(5)
C(16)-C(17)	1.374(5)
C(16)-H(16)	0.92(4)
C(17)-C(18)	1.384(6)
C(17)-H(17)	0.89(4)
C(18)-C(19)	1.371(6)
C(18)-H(18)	0.92(3)
C(19)-C(20)	1.388(5)
C(19)-H(19)	1.03(4)
C(20)-H(20)	0.93(3)
C(21)-C(22)	1.517(5)
C(21)-C(23)	1.527(5)
C(21)-H(21)	1.00(3)
C(22)-H(22A)	0.97(4)
C(22)-H(22B)	0.91(3)
C(22)-H(22C)	0.99(4)
C(23)-C(24)	1.391(5)
C(23)-C(28)	1.400(5)
C(24)-C(25)	1.392(5)
C(24)-H(24)	0.97(3)
C(25)-C(26)	1.375(6)
C(25)-H(25)	0.89(3)
C(26)-C(27)	1.377(6)
C(26)-H(26)	0.91(4)

C(27)-C(28)	1.385(5)
C(27)-H(27)	0.96(3)
C(29)-C(30)	1.375(5)
C(29)-C(34)	1.386(5)
C(30)-C(31)	1.369(5)
C(30)-H(30)	0.89(4)
C(31)-C(32)	1.398(5)
C(31)-H(31)	0.94(3)
C(32)-C(33)	1.384(5)
C(32)-C(35)	1.486(5)
C(33)-C(34)	1.396(6)
C(33)-H(33)	0.98(4)
C(34)-H(34)	0.95(4)
C(35)-H(35A)	1.01(5)
C(35)-H(35B)	0.95(4)
C(35)-H(35C)	0.96(5)

O(2)-S(1)-O(1)	119.79(17)
O(2)-S(1)-N(1)	108.94(16)
O(1)-S(1)-N(1)	104.45(16)
O(2)-S(1)-C(1)	107.26(16)
O(1)-S(1)-C(1)	105.91(16)
N(1)-S(1)-C(1)	110.31(17)
O(3)-S(2)-C(29)	106.82(16)
O(3)-S(2)-C(28)	110.55(16)
C(29)-S(2)-C(28)	99.10(16)
C(8)-N(1)-S(1)	126.3(2)
C(8)-N(1)-H(1)	113(3)
S(1)-N(1)-H(1)	113(3)
C(6)-C(1)-C(2)	121.1(3)
C(6)-C(1)-S(1)	119.0(3)
C(2)-C(1)-S(1)	119.6(3)

C(1)-C(2)-C(3)	119.1(4)
C(1)-C(2)-H(2)	123(2)
C(3)-C(2)-H(2)	117(2)
C(2)-C(3)-C(4)	120.9(4)
C(2)-C(3)-H(3)	117(2)
C(4)-C(3)-H(3)	122(2)
C(5)-C(4)-C(3)	118.9(4)
C(5)-C(4)-C(7)	120.6(4)
C(3)-C(4)-C(7)	120.5(4)
C(4)-C(5)-C(6)	121.1(4)
C(4)-C(5)-H(5)	120(2)
C(6)-C(5)-H(5)	119(2)
C(1)-C(6)-C(5)	118.8(4)
C(1)-C(6)-H(6)	121.8(18)
C(5)-C(6)-H(6)	119.4(18)
C(4)-C(7)-H(7A)	111(4)
C(4)-C(7)-H(7B)	116(4)
H(7A)-C(7)-H(7B)	96(5)
C(4)-C(7)-H(7C)	108(3)
H(7A)-C(7)-H(7C)	100(5)
H(7B)-C(7)-H(7C)	123(5)
N(1)-C(8)-C(15)	111.1(3)
N(1)-C(8)-C(9)	109.6(3)
C(15)-C(8)-C(9)	112.7(3)
N(1)-C(8)-C(21)	103.8(3)
C(15)-C(8)-C(21)	109.1(3)
C(9)-C(8)-C(21)	110.1(3)
C(14)-C(9)-C(10)	118.2(3)
C(14)-C(9)-C(8)	120.6(3)
C(10)-C(9)-C(8)	121.0(3)
C(11)-C(10)-C(9)	120.0(4)
C(11)-C(10)-H(10)	122(2)

C(9)-C(10)-H(10)	118(2)
C(12)-C(11)-C(10)	121.1(4)
C(12)-C(11)-H(11)	128(3)
C(10)-C(11)-H(11)	111(3)
C(11)-C(12)-C(13)	119.8(4)
C(11)-C(12)-H(12)	120(3)
C(13)-C(12)-H(12)	121(3)
C(12)-C(13)-C(14)	120.1(4)
C(12)-C(13)-H(13)	126(2)
C(14)-C(13)-H(13)	114(2)
C(9)-C(14)-C(13)	120.6(4)
C(9)-C(14)-H(14)	121(2)
C(13)-C(14)-H(14)	119(2)
C(20)-C(15)-C(16)	117.5(3)
C(20)-C(15)-C(8)	120.9(3)
C(16)-C(15)-C(8)	121.3(3)
C(17)-C(16)-C(15)	121.4(4)
C(17)-C(16)-H(16)	119(2)
C(15)-C(16)-H(16)	119(2)
C(16)-C(17)-C(18)	120.4(3)
C(16)-C(17)-H(17)	118(3)
C(18)-C(17)-H(17)	121(2)
C(19)-C(18)-C(17)	119.2(4)
C(19)-C(18)-H(18)	118(2)
C(17)-C(18)-H(18)	123(2)
C(18)-C(19)-C(20)	120.6(4)
C(18)-C(19)-H(19)	118(2)
C(20)-C(19)-H(19)	121(2)
C(19)-C(20)-C(15)	120.9(3)
C(19)-C(20)-H(20)	117.2(19)
C(15)-C(20)-H(20)	122.0(18)
C(22)-C(21)-C(23)	110.8(3)

C(22)-C(21)-C(8)	114.1(3)
C(23)-C(21)-C(8)	112.9(3)
C(22)-C(21)-H(21)	104.8(19)
C(23)-C(21)-H(21)	110.3(18)
C(8)-C(21)-H(21)	103.3(19)
C(21)-C(22)-H(22A)	116(2)
C(21)-C(22)-H(22B)	114(2)
H(22A)-C(22)-H(22B)	102(3)
C(21)-C(22)-H(22C)	109(2)
H(22A)-C(22)-H(22C)	105(3)
H(22B)-C(22)-H(22C)	109(3)
C(24)-C(23)-C(28)	115.8(3)
C(24)-C(23)-C(21)	120.5(3)
C(28)-C(23)-C(21)	123.7(3)
C(23)-C(24)-C(25)	122.3(4)
C(23)-C(24)-H(24)	118(2)
C(25)-C(24)-H(24)	119(2)
C(26)-C(25)-C(24)	120.1(4)
C(26)-C(25)-H(25)	125(2)
C(24)-C(25)-H(25)	115(2)
C(25)-C(26)-C(27)	119.2(4)
C(25)-C(26)-H(26)	120(3)
C(27)-C(26)-H(26)	121(3)
C(26)-C(27)-C(28)	120.3(4)
C(26)-C(27)-H(27)	121.1(19)
C(28)-C(27)-H(27)	118.6(19)
C(27)-C(28)-C(23)	122.2(4)
C(27)-C(28)-S(2)	112.8(3)
C(23)-C(28)-S(2)	125.0(3)
C(30)-C(29)-C(34)	120.3(3)
C(30)-C(29)-S(2)	121.5(3)
C(34)-C(29)-S(2)	117.8(3)

C(31)-C(30)-C(29)	120.2(4)
C(31)-C(30)-H(30)	123(3)
C(29)-C(30)-H(30)	116(3)
C(30)-C(31)-C(32)	121.3(4)
C(30)-C(31)-H(31)	122(2)
C(32)-C(31)-H(31)	117(2)
C(33)-C(32)-C(31)	117.8(3)
C(33)-C(32)-C(35)	121.5(4)
C(31)-C(32)-C(35)	120.6(4)
C(32)-C(33)-C(34)	121.4(4)
C(32)-C(33)-H(33)	117(2)
C(34)-C(33)-H(33)	122(2)
C(29)-C(34)-C(33)	118.9(4)
C(29)-C(34)-H(34)	116(2)
C(33)-C(34)-H(34)	125(2)
C(32)-C(35)-H(35A)	117(3)
C(32)-C(35)-H(35B)	114(2)
H(35A)-C(35)-H(35B)	115(3)
C(32)-C(35)-H(35C)	113(3)
H(35A)-C(35)-H(35C)	99(4)
H(35B)-C(35)-H(35C)	95(3)

Symmetry transformations used to generate equivalent atoms:

Table 10. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **17b**. 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}
S(1)	29(1)	20(1)	24(1)	2(1)	-3(1)	2(1)
S(2)	24(1)	26(1)	27(1)	3(1)	0(1)	2(1)
N(1)	25(2)	16(2)	28(2)	0(1)	-2(2)	0(1)
O(1)	32(1)	27(2)	39(2)	4(1)	-11(1)	2(1)
O(2)	43(1)	21(2)	24(2)	3(1)	4(1)	4(1)
O(3)	33(1)	26(2)	33(2)	8(1)	4(1)	10(1)
C(1)	26(2)	17(2)	31(2)	5(2)	-1(2)	8(2)
C(2)	38(2)	21(2)	28(2)	8(2)	3(2)	2(2)
C(3)	48(3)	30(3)	30(3)	1(2)	2(2)	10(2)
C(4)	44(2)	24(2)	30(2)	1(2)	-10(2)	7(2)
C(5)	37(2)	20(2)	36(3)	9(2)	-5(2)	-3(2)
C(6)	29(2)	25(2)	28(2)	3(2)	-1(2)	2(2)
C(7)	67(4)	19(3)	50(4)	-3(2)	-11(3)	5(2)
C(8)	26(2)	20(2)	26(2)	1(2)	-3(2)	0(2)
C(9)	27(2)	17(2)	25(2)	4(2)	-8(2)	0(2)
C(10)	30(2)	23(2)	27(2)	4(2)	-1(2)	-2(2)
C(11)	28(2)	26(2)	33(2)	7(2)	-1(2)	-8(2)
C(12)	43(2)	18(2)	39(3)	2(2)	-12(2)	-6(2)
C(13)	50(2)	19(2)	24(2)	-3(2)	-4(2)	0(2)
C(14)	37(2)	18(2)	29(2)	3(2)	0(2)	-2(2)
C(15)	30(2)	13(2)	24(2)	5(2)	2(2)	0(2)
C(16)	26(2)	24(2)	25(2)	3(2)	-3(2)	-3(2)
C(17)	21(2)	31(2)	30(2)	8(2)	0(2)	3(2)
C(18)	36(2)	24(2)	29(3)	1(2)	3(2)	8(2)
C(19)	40(2)	19(2)	26(2)	-4(2)	1(2)	-3(2)
C(20)	23(2)	22(2)	29(2)	3(2)	-3(2)	1(2)
C(21)	24(2)	20(2)	23(2)	-2(2)	1(2)	0(2)

C(22)	29(2)	24(3)	30(3)	3(2)	1(2)	0(2)
C(23)	28(2)	16(2)	21(2)	4(2)	-1(2)	4(1)
C(24)	32(2)	19(2)	32(2)	5(2)	3(2)	0(2)
C(25)	40(2)	17(2)	39(2)	-2(2)	-2(2)	2(2)
C(26)	37(2)	24(2)	35(3)	5(2)	-7(2)	-7(2)
C(27)	26(2)	25(2)	33(2)	7(2)	-7(2)	-2(2)
C(28)	27(2)	26(2)	23(2)	4(2)	-5(2)	1(2)
C(29)	18(2)	27(2)	25(2)	2(2)	3(2)	2(2)
C(30)	32(2)	19(2)	28(2)	-3(2)	-2(2)	-3(2)
C(31)	30(2)	22(2)	26(2)	4(2)	-3(2)	-1(2)
C(32)	23(2)	32(2)	24(2)	-1(2)	4(2)	0(2)
C(33)	50(3)	18(2)	31(3)	-7(2)	-1(2)	-1(2)
C(34)	45(2)	20(2)	33(3)	3(2)	0(2)	3(2)
C(35)	34(2)	37(3)	28(2)	-3(2)	1(2)	0(2)

Table 11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **17b**

	x	y	z	U(eq)
H(1)	5500(50)	4730(30)	1280(19)	44(14)
H(2)	6500(50)	3070(30)	1061(17)	33(11)
H(3)	6540(40)	1660(20)	777(16)	20(10)
H(5)	3440(40)	1000(20)	2029(14)	14(9)
H(6)	3260(40)	2450(20)	2379(15)	16(9)
H(7A)	4100(80)	-90(40)	1190(30)	100(20)
H(7B)	5510(60)	-130(30)	1480(20)	65(19)
H(7C)	5540(70)	160(30)	860(20)	80(20)
H(10)	650(40)	4020(20)	1741(15)	13(9)
H(11)	-660(50)	2800(30)	1495(18)	39(12)
H(12)	50(50)	2020(30)	629(18)	42(11)
H(13)	2390(40)	2560(20)	122(15)	14(9)
H(14)	3640(40)	3830(20)	366(17)	34(11)
H(16)	-90(50)	5340(20)	1307(16)	30(11)
H(17)	-1500(50)	6270(20)	1869(16)	29(11)
H(18)	-230(40)	7030(20)	2622(15)	12(9)
H(19)	2510(50)	6870(20)	2792(15)	26(10)
H(20)	3930(40)	5860(20)	2225(12)	6(8)
H(21)	4190(40)	5090(20)	480(15)	13(8)
H(22A)	1380(50)	5290(30)	244(16)	31(11)
H(22B)	2360(40)	6010(20)	19(14)	11(8)
H(22C)	1390(40)	6170(20)	580(15)	19(9)
H(24)	2740(40)	7000(20)	1247(14)	15(9)
H(25)	4210(40)	8190(20)	1477(15)	12(9)
H(26)	6980(50)	8320(30)	1258(18)	42(13)
H(27)	8270(40)	7140(20)	787(13)	7(8)

H(30)	6390(40)	6890(30)	-378(17)	32(11)
H(31)	5430(40)	6950(20)	-1327(15)	11(9)
H(33)	5300(40)	4310(20)	-1360(15)	27(10)
H(34)	6400(40)	4310(30)	-381(17)	30(11)
H(35A)	3970(60)	5210(30)	-2170(19)	57(14)
H(35B)	5650(50)	5770(20)	-2307(17)	31(11)
H(35C)	4200(60)	6190(30)	-2140(20)	61(16)

Table 12. Torsion angles [°] for **17b**.

O(2)-S(1)-N(1)-C(8)	-42.0(3)
O(1)-S(1)-N(1)-C(8)	-171.1(3)
C(1)-S(1)-N(1)-C(8)	75.5(3)
O(2)-S(1)-C(1)-C(6)	-13.0(3)
O(1)-S(1)-C(1)-C(6)	116.0(3)
N(1)-S(1)-C(1)-C(6)	-131.5(3)
O(2)-S(1)-C(1)-C(2)	172.2(3)
O(1)-S(1)-C(1)-C(2)	-58.8(3)
N(1)-S(1)-C(1)-C(2)	53.7(3)
C(6)-C(1)-C(2)-C(3)	-3.1(6)
S(1)-C(1)-C(2)-C(3)	171.5(3)
C(1)-C(2)-C(3)-C(4)	0.6(6)
C(2)-C(3)-C(4)-C(5)	2.6(6)
C(2)-C(3)-C(4)-C(7)	-175.7(4)
C(3)-C(4)-C(5)-C(6)	-3.3(6)
C(7)-C(4)-C(5)-C(6)	174.9(4)
C(2)-C(1)-C(6)-C(5)	2.4(5)
S(1)-C(1)-C(6)-C(5)	-172.3(3)
C(4)-C(5)-C(6)-C(1)	0.9(6)
S(1)-N(1)-C(8)-C(15)	74.1(4)
S(1)-N(1)-C(8)-C(9)	-51.2(4)
S(1)-N(1)-C(8)-C(21)	-168.8(3)
N(1)-C(8)-C(9)-C(14)	-73.4(4)
C(15)-C(8)-C(9)-C(14)	162.3(3)
C(21)-C(8)-C(9)-C(14)	40.3(4)
N(1)-C(8)-C(9)-C(10)	102.5(4)
C(15)-C(8)-C(9)-C(10)	-21.9(5)
C(21)-C(8)-C(9)-C(10)	-143.9(3)
C(14)-C(9)-C(10)-C(11)	-3.3(5)
C(8)-C(9)-C(10)-C(11)	-179.3(3)

C(9)-C(10)-C(11)-C(12)	0.6(6)
C(10)-C(11)-C(12)-C(13)	2.6(6)
C(11)-C(12)-C(13)-C(14)	-3.0(6)
C(10)-C(9)-C(14)-C(13)	2.9(5)
C(8)-C(9)-C(14)-C(13)	178.9(3)
C(12)-C(13)-C(14)-C(9)	0.2(6)
N(1)-C(8)-C(15)-C(20)	19.2(5)
C(9)-C(8)-C(15)-C(20)	142.7(3)
C(21)-C(8)-C(15)-C(20)	-94.7(4)
N(1)-C(8)-C(15)-C(16)	-167.0(3)
C(9)-C(8)-C(15)-C(16)	-43.5(4)
C(21)-C(8)-C(15)-C(16)	79.1(4)
C(20)-C(15)-C(16)-C(17)	-0.3(5)
C(8)-C(15)-C(16)-C(17)	-174.3(3)
C(15)-C(16)-C(17)-C(18)	1.8(6)
C(16)-C(17)-C(18)-C(19)	-1.8(6)
C(17)-C(18)-C(19)-C(20)	0.3(6)
C(18)-C(19)-C(20)-C(15)	1.2(6)
C(16)-C(15)-C(20)-C(19)	-1.2(5)
C(8)-C(15)-C(20)-C(19)	172.8(3)
N(1)-C(8)-C(21)-C(22)	175.1(3)
C(15)-C(8)-C(21)-C(22)	-66.3(4)
C(9)-C(8)-C(21)-C(22)	57.8(4)
N(1)-C(8)-C(21)-C(23)	-57.2(4)
C(15)-C(8)-C(21)-C(23)	61.4(4)
C(9)-C(8)-C(21)-C(23)	-174.4(3)
C(22)-C(21)-C(23)-C(24)	54.1(5)
C(8)-C(21)-C(23)-C(24)	-75.3(4)
C(22)-C(21)-C(23)-C(28)	-123.7(4)
C(8)-C(21)-C(23)-C(28)	106.9(4)
C(28)-C(23)-C(24)-C(25)	-2.7(6)
C(21)-C(23)-C(24)-C(25)	179.3(3)

C(23)-C(24)-C(25)-C(26)	1.9(6)
C(24)-C(25)-C(26)-C(27)	0.5(6)
C(25)-C(26)-C(27)-C(28)	-2.0(6)
C(26)-C(27)-C(28)-C(23)	1.1(6)
C(26)-C(27)-C(28)-S(2)	179.1(3)
C(24)-C(23)-C(28)-C(27)	1.2(5)
C(21)-C(23)-C(28)-C(27)	179.1(3)
C(24)-C(23)-C(28)-S(2)	-176.5(3)
C(21)-C(23)-C(28)-S(2)	1.3(5)
O(3)-S(2)-C(28)-C(27)	136.1(3)
C(29)-S(2)-C(28)-C(27)	-112.0(3)
O(3)-S(2)-C(28)-C(23)	-45.9(4)
C(29)-S(2)-C(28)-C(23)	66.0(3)
O(3)-S(2)-C(29)-C(30)	163.2(3)
C(28)-S(2)-C(29)-C(30)	48.4(3)
O(3)-S(2)-C(29)-C(34)	-24.0(3)
C(28)-S(2)-C(29)-C(34)	-138.8(3)
C(34)-C(29)-C(30)-C(31)	-0.6(5)
S(2)-C(29)-C(30)-C(31)	172.0(3)
C(29)-C(30)-C(31)-C(32)	0.3(6)
C(30)-C(31)-C(32)-C(33)	1.0(5)
C(30)-C(31)-C(32)-C(35)	-177.1(4)
C(31)-C(32)-C(33)-C(34)	-2.1(5)
C(35)-C(32)-C(33)-C(34)	175.9(4)
C(30)-C(29)-C(34)-C(33)	-0.5(5)
S(2)-C(29)-C(34)-C(33)	-173.4(3)
C(32)-C(33)-C(34)-C(29)	1.9(6)

Symmetry transformations used to generate equivalent atoms:

Table 13. Hydrogen bonds for **17b** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1)...O(3)	0.85(4)	2.02(4)	2.861(4)	170(4)

Symmetry transformations used to generate equivalent atoms: