Supporting Information for

Stereocontrolled Reactions Mediated by a Remote Sulfoxide Group: Synthesis of Optically Pure *anti* β-Amino Alcohol.

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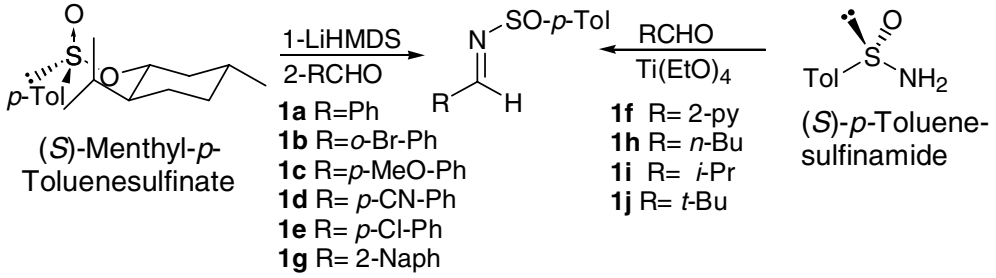
General Methods.

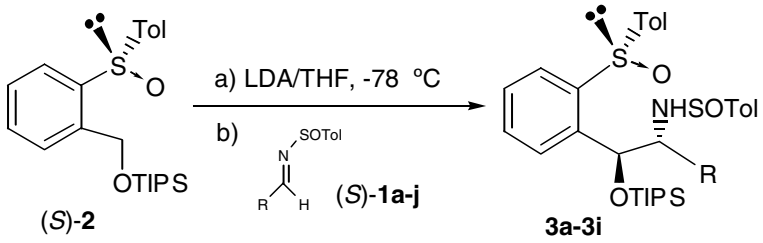
Melting points are uncorrected. ^{1}H NMR spectra were acquired at 300 MHz and ^{13}C NMR were acquired at 75 MHz (unless otherwise indicated). Chemical shifts (δ) are reported in ppm relative to $CDCl_3$ (7.26 and 77.0 ppm). Mass spectra (MS) were determined at an ionizing voltage of 70 eV. All reactions were carried out in anhydrous solvents and under argon atmosphere. THF and Et_2O were distilled from sodium-benzophenone under argon. CH_2Cl_2 was distilled from P_2O_5. Flash column chromatography was performed using silica gel Merk-60 (230-400 mesh) and *Varian* SCX column. *n*-BuLi (2.5M solution in hexanes) were purchased from Aldrich.

Sulfinylimines.

Enantiopure sulfinylimines were prepared according to Davis' procedures.[1]



General procedure for the reactions summarized in Table 1.



[1] (a) Davis, F. A.; Reddy, R. E.; Szewczyk, J. M.; Reddy, G. V.; Portonovo, P. S.; Zhang, H.; Fanelli, D.; Reddy; T. R.; Zhou, P.; Carroll, P. J. *J. Org. Chem.* **1997**, *62*, 2555; (b) Davis, F. A.; Zhang, Y.; Andemichael, Y.; Y. Fang ; Fanelli, D. L.; Zhang, H. *J. Org. Chem.* **1999**, *64*, 1403; (d) Sulfinylimines **1b** and **1d** was described in: Garcia Ruano, J. L.; Aleman, J.; Soriano, J. F. *Org. Lett.*, **2003**, *5*, 677.

A solution of *n*-BuLi (0.60 mmol, 2.5 M in hexane) was added over $^{i}Pr_2NH$ (0.89 mmol) in THF (3 mL) at 0 ºC. After 20 min stirring, the mixture was cooled at –78 ºC and then a solution of sulfoxide **2** (0.50 mmol) in THF (2 mL) was added. After 1 h stirring, the electrophile [sulfinilimine (**1a-j**), 0.52 mmol] dissolved in THF (4 mL) was added at –78 ºC. When the reaction was completed, the mixture was hydrolyzed (2 mL H_2O), extracted (3x10 mL Et_2O), washed (2x10 mL NaCl sat.), dried ($MgSO_4$) and the solvent evaporated. The residue was purified by flash-column chromatography.

[1*R*,2*S*,(S)*S*)]-*N*-{1-Phenyl-2-[(*S*)-2-(*p*-toluenesulfinyl)phenyl]-2-triisopropyl-silanyloxyethyl}-*p*-toluene sulfinamide (3a). Chromatography: *n*-hexane-AcOEt 3:1, yield: 81%; white solid; mp: 139-141 ºC (Et_2O); $[\alpha]_D^{20}$ = + 37.8 (*c* 2.7, $CHCl_3$); IR (NaCl): 3062, 2944, 2866, 1598, 1514, 1495 cm^{-1}; ^1H NMR: δ 7.90 (d, *J* = 7.6 Hz, 1H), 7.53–7.30 (m, 5H), 7.18-6.88 (m, 11H), 5.51 (d, *J* = 6.6 Hz, 1H), 5.47 (d, *J* = 9.4 Hz, 1H), 3.96 (dd, *J* = 9.4, 6.6 Hz, 1H), 2.30 (s, 3H), 2.28 (s, 3H), 0.71-0.50 (m, 21H); ^{13}C NMR: δ 142.9, 142.6, 142.4, 141.4, 141.3, 141.2, 141.1, 132.0, 130.8, 130.2, 129.6, 129.1 (2C), 128.3, 127.9, 126.7, 126.6, 126.4, 73.8, 64.6, 22.1, 21.9, 18.5, 18.4, 12.8; MS (FAB) *m/z* 632 (M+1, 5), 508 (100), 401 (11), 211 (15); Anal. Calcd for $C_{37}H_{47}NO_3S_2Si$: C. 68.79; H. 7.33; N. 2.17; S. 9.93; Found: C: 68,63, H, 7.29, N, 2.09, S, 10,05.

[1*R*,2*S*,(S)*S*)]-*N*-{1-(2-Bromophenyl)-2-[(*S*)-2-(*p*-toluenesulfinyl)phenyl]-2-triiso-propylsilanyloxyethyl}-*p*-toluene sulfinamide (3b). Chromatography: *n*-hexane-AcOEt 3:1; yield: 71%; white solid; mp: 72-74 ºC (Et_2O); $[\alpha]_D^{20}$ = +90.9 (*c* 1.0, $CHCl_3$); IR (NaCl): 3300, 2990, 2866, 1598, 1492, 1469, 1120 cm^{-1}; ^1H NMR: δ 7.92 (d, *J* = 7.7 Hz, 1H), 7.70-6.95 (m, 15H), 5.74 (m, 2H), 4.71 (dd, *J* = 8.5, 5.6 Hz, 1H),

2.34 (s, 3H), 2.29 (s, 3H), 0.90-0.60 (m, 21H); ^{13}C NMR: δ 141.7, 140.8, 140.5, 140.1, 137.4, 132.6, 131.7, 131.1, 130.1, 129.4, 128.7, 128.4, 127.7, 127.4, 125.9, 125.8 (2C),

124.7, 124.5, 122.7, 73.6, 55.2, 21.3, 20.8, 17.7, 17.5, 12.0; MS (FAB) *m/z* 726 (M+1, 28), 586 (11), 385 (100), 211(33); Anal. Calcd for $C_{37}H_{46}BrNO_3S_2Si$: C, 61.31; H, 6.40; N, 1.93; S, 8.85. Found: C, 61.39; H, 6.49; N, 1.94; S, 8.92.

[1*R*,2*S*,(S)*S*)]-*N*-{1-(4-Methoxyphenyl)-2-[(*S*)-2-(*p*-toluenesulfinyl)phenyl]-2-triiso-propylsilanyloxyethyl}-*p*-toluene sulfinamide (3c). Chromatography: *n*-hexane-AcOEt 3:2; yield: 78%; white solid; mp: 74-76 ºC (Et_2O); $[\alpha]_D^{20}$ = +75.2 (*c* 0.9, $CHCl_3$); IR (NaCl): 3210, 2943, 2866, 1612, 1513, 1463, 1248, 1093 cm^{-1}; ^1H NMR: δ 7.93 (d, *J* = 7.8 Hz, 1H), 7.52–7.45 (m, 3H), 7.38 (t, *J* = 7.7 Hz, 1H), 7.25 (d, *J* = 7.6 Hz, 1H), 7.14 (d, *J* = 8.3 Hz, 2H), 7.08 (d, *J* = 8.3 Hz, 2H), 7.03 (d, *J* = 8.7 Hz, 2H), 6.80 (d, *J* = 8.6 Hz, 2H), 6.63 (d, *J* = 8.6 Hz, 2H), 5.52 (d, *J* = 5.9 Hz, 1H), 5.24 (d, *J* = 9.5, 1H), 3.90 (dd, *J* = 9.5, 5.9 Hz, 1H), 3.70 (s, 3H), 2.31 (s, 6H), 0.80-0.51 (m, 21H); ^{13}C NMR: δ 158.7, 141.8 (2C), 140.7 (2C), 140.6, 132.2 (2C), 131.1, 130.0, 129.4, 128.8, 128.4 (2C), 126.1, 125.6 (2C), 113.0, 73.1, 63.5, 55.2, 21.4, 21.2, 17.7, 12.1; MS (FAB) *m/z* 676 (M+1, 55), 521 (100), 401 (88), 375 (69); Anal. Calcd for $C_{38}H_{49}NO_4S_2Si$: C, 67.51; H, 7.31; N, 2.07; S, 9.49. Found: C, 67.22; H, 7.02; N, 2.02; S, 9.44.

[1*R*,2*S*,(S)*S*)]-*N*-{1-(4-Cianophenyl-2-[(*S*)-2-(*p*-toluenesulfinyl)phenyl]-2-triiso-propylsilanyloxyethyl}-*p*-toluene sulfinamide (3d). Chromatography: *n*-hexane-AcOEt 3:1; yield: 74%; yellow oil; $[\alpha]_D^{20}$ = +65.8 (*c* 2.0, $CHCl_3$); IR (NaCl): 3443, 2965, 2866, 2228, 1645, 1608, 1492, 1462, 1095 cm^{-1}; ^1H NMR: δ 7.86 (d, *J* = 7.1 Hz, 1H), 7.58–7.34 (m, 7H), 7.23 (d, *J* = 8.2 Hz, 2H), 7.10 (d, *J* = 8.0 Hz, 2H), 7.01 (d, *J* = 8.0 Hz, 2H), 6.96 (d, *J* = 8.2 Hz, 2H), 6.47 (d, *J* = 8.7 Hz, 1H), 5.47 (d, *J* = 7.2 Hz, 1H), 4.13-4.05 (m, 1H), 2.34 (s, 3H), 2.28 (s, 3H), 0.54 (m, 18H), 0.20 (m, 3H); ^{13}C NMR: δ 147.1, 142.5, 141.6, 141.1, 140.7, 139.7, 132.0, 131.2, 130.0 (2C), 129.6, 129.2,

128.7, 128.5, 127.4, 125.6, 125.2, 118.9, 110.5, 72.6, 62.5, 21.3, 21.1, 17.6, 11.8; MS (FAB) *m/z* 671 (M+1, 42), 385 (100), 211 (32), 139 (19); HRMS [M+1]: Calcd. For $C_{38}H_{46}NO_3S_2Si$: 671.2719; found, 671.2707.

[1*R*,2*S*,(S)*S*)]-*N*-{1-(4-Chlorophenyl)-2-[(*S*)-2-(*p*-toluenesulfinyl)phenyl]-2-triiso-propylsilanyloxyethyl}-*p*-toluene sulfinamide (3e): Chromatography: *n*-hexane-AcOEt 3:2; yield: 76%; white solid; mp: 76-78 ºC (Et_2O); $[\alpha]_D^{20}$ = +75.0 (*c* 1.0, $CHCl_3$); IR (NaCl): 3206, 2943, 2866, 1596, 1492, 1463, 1092 cm^{-1}; ^1H NMR: δ 7.89 (dd, *J* = 7.6, 1.9 Hz, 1H), 7.50–7.35 (m, 5H), 7.20 (d, *J* = 7.9 Hz, 2H), 7.11-6.95 (m, 6H), 6.85 (d, *J* = 8.4 Hz, 2H), 5.81 (d, *J* = 9.1 Hz, 1H), 5.49 (d, *J* = 6.5 Hz, 1H), 3.95 (dd, *J* = 9.1, 6.5 Hz, 1H), 2.33 (s, 3H), 2.30 (s, 3H), 0.70-039 (m, 21); ^{13}C NMR: δ 142.1, 141.7, 141.3, 140.6, 140.2, 139.2, 132.7, 131.5, 130.0, 129.7, 129.5, 128.8 (2C), 128.4, 127.6, 126.4, 125.6, 125.5, 72.8, 62.7, 21.3, 21.1, 17.7, 17.6, 11.9; MS (FAB) *m/z* 680 (M+1, 45), 540 (23), 385 (100), 211 (31); Anal. Calcd for $C_{37}H_{46}ClNO_3S_2Si$: C, 65.31; H, 6.81; N, 2.06; S, 9.43. Found: C, 65.22; H, 6.49; N, 2.01; S, 9.30.

[1*R*,2*S*,(S)*S*)]-*N*-{1-(2-Pyridin)-2-[(*S*)-2-(*p*-toluenesulfinyl)phenyl]-2-triiso-propylsilanyloxyethyl}-*p*-toluene sulfinamide (3f). Cromatography solvent: n-Hexane-AcOEt 2:1; Yield: 77 %; yellow oil; $[\alpha]_D^{20}$= +37.5 (*c* 0.8, $CHCl_3$); IR (NaCl): 3300, 3288, 3055, 2892, 1592, 1572, 1493, 1093 cm^{-1}; ^1H NMR: δ 8.61 (d, *J* = 4.0 Hz, 1H), 8.19 (dd, *J* = 7.8, 2.0 Hz, 1H), 7.75 (m, 1H), 7.70-7.55 (m, 5H), 7.30 (d, *J* = 7.7 Hz, 1H), 7.20 (ddd, *J* = 7.5, 4.7, 1.0 Hz, 1H), 6.93 (d, *J* = 8.0 Hz, 2H), 6.76 (d, *J* = 8.1 Hz, 2H), 6.36 (d, *J* = 8.1 Hz, 2H), 5.70 (d, *J* = 8.5 Hz, 1H), 4.53 (dd, *J* = 10.1, 8.5 Hz, 1H), 3.87 (d, *J* = 10.1 Hz, 1H), 2.33 (s, 3H), 2.07 (s, 3H), 0.90-0.53 (m, 21H); ^{13}C NMR: δ 159.6, 149.4, 143.9, 141.8, 141.7, 141.4, 140.6, 140.5, 136.1, 131.2, 129.5,

129.0, 128.9, 128.0, 126.4, 124.8, 124.3, 123.5, 122.9, 72.2, 68.1, 21.2, 21.2, 17.7, 17.4, 12.2. MS (FAB) m/z 647 (M+1, 65), 509 (77), 401 (100), 211 (32), 107 (55); HMRS [M+1]: Calcd. for $C_{36}H_{46}N_2O_3S_2Si$: 647.2719; found 647.2781.

[1*R*,2*S*,(S)*S*)]-*N*-{1-(2-Naphthyl)-2-[(*S*)-2-(*p*-toluenesulfinyl)phenyl]-2-triiso-propylsilanyloxyethyl}-*p*-toluene sulfinamide (3g). Chromatography: *n*-hexane-AcOEt 3:1; yield: 68%; white solid; mp: 77-79 ºC (Et_2O); $[\alpha]_D^{20}$ = +147.7 (*c* 1.0, $CHCl_3$); IR (NaCl): 3029, 3054, 2942, 2890, 2865, 1596, 1491, 1093 cm^{-1}; ^1H NMR: δ 7.93 (d, *J* = 7.6 Hz, 1H), 7.70–6.95 (m, 16H), 6.66 (d, *J* = 8.0 Hz, 2H), 6.11 (d, *J* = 7.7 Hz, 1H), 5.78 (d, *J* = 5.8 Hz, 1H), 4.99 (m, 1H), 2.37 (s, 3H), 2.02 (s, 3H), 0.77-0.34 (m, 21H); ^{13}C NMR: δ 141.7, 140.8, 140.5, 140.1, 137.5, 132.7, 131.7, 131.1, 130.1, 130.0, 129.6, 129.5, 128.7, 128.5, 127.8, 127.4, 126.0, 125.9, 125.7, 125.6, 124.7, 124.6, 122.7, 73.6, 55.2, 21.4, 20.8, 17.7, 17.5, 12.0; Anal. Calcd for $C_{41}H_{49}NO_3S_2Si$: C. 70.75; H. 7.10; N. 2.01; S. 9.21; Found: C, 70.35; H, 7.04; N, 1.97; S, 9.28.

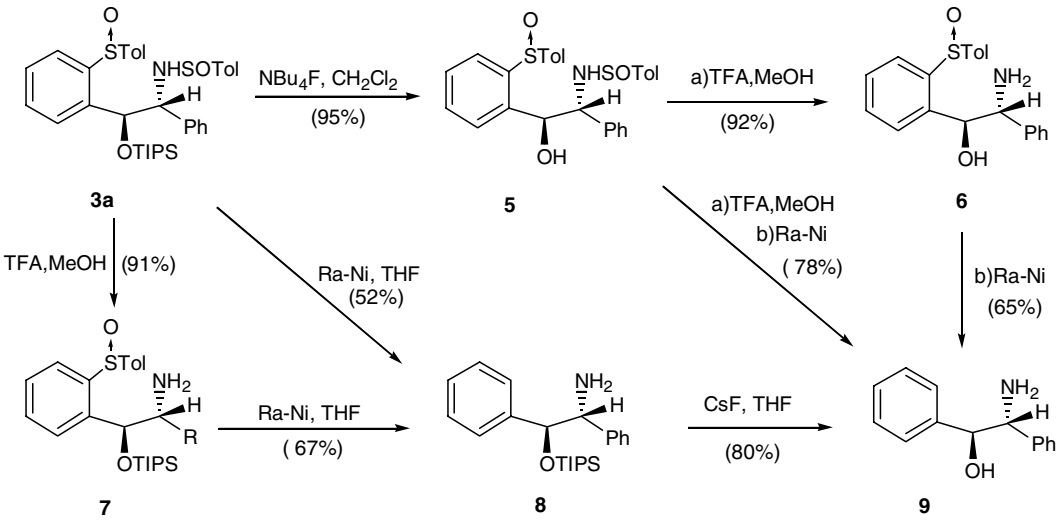
[1*R*,2*S*,(S)*S*)]-*N*-{1-Butyl-2-[(*S*)-2-(*p*-toluenesulfinyl)phenyl]-2-triiso-propylsilanyloxyethyl}-*p*-toluenesulfinamide (3h). Chromatography: *n*-hexane-AcOEt 5:2; yield: 74%; yellow oil; $[\alpha]_D^{20}$ = +33.8 (*c* 1.0, $CHCl_3$); IR (NaCl): 3583, 3221, 2944, 2866, 1595, 1492, 1463, 1090 cm^{-1}; ^1H NMR: δ 7.99 (d, *J* = 9.2 Hz, 1H), 7.68 (m, 1H), 7.57 (m, 2H), 7.24 (d, *J* = 8.0 Hz, 2H), 7.05 (d, *J* = 8.2 Hz, 2H), 6.82 (d, *J* = 8.0 Hz, 2H), 6.71 (d, *J* = 8.2 Hz, 2H), 5.21 (d, *J* = 6.8 Hz, 1H), 3.30 (m, 1H), 2.89 (d, *J* = 10.3 Hz, 1H), 2.35 (s, 3H), 2.21 (s, 3H), 1.50-1.10 (m, 6H), 1.00-0.80 (m, 24H); ^{13}C NMR: δ 142.4 (2C), 142.0, 141.9, 140.8, 140.6, 131.3, 129.7, 129.0, 128.6, 128.5, 126.4, 124.9, 72.6, 63.9, 32.5, 27.5, 22.4, 21.3, 21.2, 17.9, 17.7, 13.9, 12.3; MS (FAB) *m/z* 626 (M+1, 70), 488 (21), 385 (100), 211(46); HRMS [M+1]: Calcd. for $C_{35}H_{51}NO_3S_2Si$: 626.3157; found, 626.3165.

[1*R*,2*S*,(S)*S*)]-*N*-{1-Isopropyl-2-[(*S*)-2-(*p*-toluenesulfinyl)phenyl]-2-triiso-propylsilanyloxyethyl}-*p*-toluenesulfinamide (3i). Chromatography: *n*-hexane-AcOEt 2:1; yield: 72%; white solid; mp: 138-140 ºC (Et_2O); $[\alpha]_D^{20}$ = + 17.5 (*c* 1.8, $CHCl_3$); IR (NaCl): 3251, 3056, 2944, 2867, 1595, 1492, 1179 cm^{-1}; ^1H NMR: δ 7.95 (d, *J* = 9.2 Hz, 1H), 7.79 (m, 1H), 7.63 (m, 2H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.01 (d, *J* = 8.0 Hz, 2H), 6.83 (d, *J* = 8.0 Hz, 2H), 6.53 (d, *J* = 8.0 Hz, 2H), 5.15 (d, *J* = 8.2 Hz, 1H), 3.43 (d, *J* = 10.9 Hz, 1H), 3.32 (m, 1H), 2.35 (s, 3H), 2.22 (s, 3H), 1.07 (d, *J* = 7.0 Hz, 3H), 0.97-0.70 (m, 24H); ^{13}C NMR: δ 143.7, 142.7, 141.9, 141.7, 140.6, 140.2, 131.7, 129.7, 129.0, 128.7, 128.4, 126.1, 125.7, 125.1, 70.5, 70.4, 27.3, 21.3, 21.2, 21.1, 17.9, 17.7, 16.0, 12.3. Anal. Calcd for $C_{34}H_{49}NO_3S_2Si$: C. 66.73; H. 8.07; N. 2.29; S. 10.48;. Found: C: 66.47; H: 8.11; N: 2.22; S: 10.26.

[1*R*,2*S*,(S)*S*)]-*N*-{1-*tert*-Butyl-2-[(*S*)-2-(*p*-toluenesulfinyl)phenyl]-2-triiso-propylsilanyloxyethyl}-*p*-toluenesulfinamide (3j).[2] ^1H NMR: δ 7.95–7.20 (m, 6H), 7.09 (d, *J* = 8.0 Hz, 2H), 6.97 (d, *J* = 8.1 Hz, 2H), 6.91 (d, *J* = 8.1 Hz, 2H), 5.72 (d, *J* = 6 Hz, 1H), 3.53 (m, 2H), 2.37 (s, 3H), 2.29 (s, 3H), 1.10-0.70 (m, 30H);

Protocols for the Scheme 3

[2] The compound decomposes in chromatographic column.



[1*R*,2*S*,(S)*S*)]-*N*-{2-Hydroxyl-1-phenyl-2-[(*S*)-2-(*p*-toluenesulfinyl)phenyl]ethyl}-*p*-toluene sulfinamide (5): A solution of compound **3a** (1 mmol) in 2 mL of CH_2Cl_2 was treated with a 1M solution of NBu_4F (100 μL, 1.2 mmol). After the mixture was stirred for 3 h at rt, the solvent was evaporated. The residue was purified by flash chromatography (Hexane/AcOEt, 1:3), affording the corresponding alcohol. Yield: 95%; yellow oil; $[\alpha]_D^{20}$ = +18.9 (*c* 0.7, $CHCl_3$); IR (NaCl): 3316, 2922, 1595, 1493, 1454, 1085 cm^{-1}; ^1H NMR: δ 7.71 (d, *J* = 6.5 Hz, 1H), 7.40 (d, *J* = 8.2 Hz, 2H), 7.30–7.00 (m, 5H), 6.79 (d, *J* = 6.9 Hz, 2H), 6.03 (d, *J* = 8.2 Hz, 1H), 5.50 (bs, 1H), 4.40 (bs, 1H), 4.15 (dd, *J* = 8.2, 5.8 Hz, 1H), 2.31 (s, 3H), 2.26 (s, 3H); ^{13}C NMR: δ 141.8, 141.3, 141.1, 140.7, 140.4, 140.3, 138.7, 131.1, 129.8, 129.4, 128.9, 128.8, 128.4, 127.9, 127.2, 126.1, 125.7, 125.3, 72.6, 61.2, 21.2, 21.1; MS (FAB) m/z 490 (M+1, 100), 334 (31), 245 (46), 106 (85); HRMS [M+1]: Calcd. for $C_{28}H_{27}NO_3S_2$: 409.1432; found 409.1410.

(1*R*,2*S*)-2-Amine-2-phenyl-1-{(*S*)-2-(*p*-toluenesulfinyl)phenyl}-ethanol (6): To a stirred solution of **3a** (0.2 mmol) in methanol (3 mL) was added TFA (0.6 mmol, 50 μL). After the mixture was stirred for 3 h at 0 ºC, the solvent was evaporated, and the

residue was chromatography by SCX column, affording the corresponding amine. Yield: 92 %; colourless oil; $[\alpha]_D^{20}$ = +5.0 (*c* 0.6, $CHCl_3$); ^{1}H NMR ($MeOD_4$): δ 7.77 (d, *J* = 7.6 Hz, 1H), 7.50 (d, *J* = 8.0 Hz, 2H), 7.38-7.11 (m, 12H), 5.21 (m, 1H), 3.89 (m, 1H), 2.52 (bs, 1H), 2.31 (s, 3H); ^{13}C NMR: δ 142.9, 141.7, 141.3, 140.9, 140.7, 139.1, 131.0, 129.8, 129.6, 128.7, 128.5, 128.3, 128.1, 128.0, 127.8, 127.7, 125.9, 125.8, 66.6, 50.4, 21.3.

(1*R*,2*S*)-*N*-1-Phenyl-2-{(*S*)-2-(*p*-toluenesulfinyl)phenyl}-2-triisopropyl-silanyloxyethylamine (7): To a stirred solution of **3a** (0.2 mmol) in methanol (3 mL) was added TFA (0.6 mmol, 50 μL). After the mixture was stirred for 3 h at 0 ºC, the solvent was evaporated, and the residue was chromatography by SCX column, affording the corresponding amine. Yield: 91%; colourless oil; $[\alpha]_D^{20}$ = -1.2 (*c* 0.6, $CHCl_3$); IR (NaCl): 3583, 2865, 1596, 1056 cm^{-1}; ^{1}H NMR: δ 7.81 (d, *J* = 7.7 Hz, 1H), 7.55 (d, *J* = 8.1 Hz, 2H), 7.44-7.02 (m, 10H), 5.22 (d, *J* = 5.2 Hz, 1H), 3.62 (m, 1H), 2.37 (s, 3H), 1.96 (bs, 2H), 1.10-0.6 (m, 21H); ^{13}C NMR: δ 142.3, 142.0, 141.9, 141.7, 141.3, 130.9, 130.0, 128.9, 128.8, 128.3, 127.8, 126.3, 125.4, 73.9, 62.3, 21.4, 17.9, 17.7, 12.3. MS (FAB) m/z 508 (M+1, 100), 401 (38), 334 (18), 211 (26), 106 (30); HMRS [M+1] Calcd. For $C_{30}H_{41}NO_2SSi$: 508.2627; found, 508.2706.

(1*R*,2*S*)-1,2-Diphenyl-2-triisopropylsilanyloxyethylamine (8) (by directed double desulfinylation with Ra-Ni)**:**[3] To a stirred solution of **4a** (0.2 mmol) in THF (2 mL) was added a suspension of activated Raney-nickel (1.2 g). The reaction was stirred 2 hours, and then the crude was purified by SCX column to afford the amine. Yield: 51%; $[\alpha]_D^{20}$ = +19.0 (*c 0.3* ,MeOH); IR (NaCl): 3440, 1600, 1550 cm^{-1}; ^{1}H NMR ($MeOD_4$): δ 7.50–7.20 (m, 10H), 5.07 (d, *J* = 6.7 Hz, 1H), 4.50 (m, 1H), 1.00-0.70 (m, 21H); ^{13}C NMR: δ 130.7, 120.1, 120.0, 119.8, 119.8, 119.7, 119.3, 118.9, 69.0, 53.1, 8.3, 3.6;

Anal. Calcd for $C_{23}H_{35}NOSi$: C. 74.74; H. 9.54; N. 3.79; Found: C, 74.70; H, 9.61; N, 3.82.

(1*S*,2*R*)-2-Amino-1,2-diphenylethanol (9):[4] To a stirred solution of **4** (0.2 mmol) in methanol (3 mL) was added TFA (0.6 mmol, 50 μL). After the mixture was stirred for 3 h at 0 ºC, the solvent was evaporated, and the residue was chromatography by SCX column, affording the corresponding amine. To a solution of this amine in EtOH was added a suspension of activated Raney nickel (1.2 g). The reaction was stirred 2 hours, and the residue was purified by SCX column to afford the amine. Yield: 78%; $[\alpha]_D^{20}$ = + 6.6 (*c* 0.50, EtOH) {enantiomer was described; Lit [5] $[\alpha]_D^{20}$= -7.0 (*c* 0.98, EtOH)}; ^{1}H NMR ($MeOD_4$): δ 7.50–7.05 (m, 10H), 5.30 (d, *J* = 4.0 Hz, 1H), 4.50 (d, *J* = 4.0 Hz, 2H).

[3] Compound **8** can be obtained from **7** with the same procedure.
[4] Aminoalcohol **9** could be obtained by deprotection of **8** with CsF in THF and the same purification.
[5] The enantiomer was described in: Kanematsu, K.; Sasaki, T. *J. Med. Chem*., **1966**, 847.

X-Ray structure of **3i.** [6]

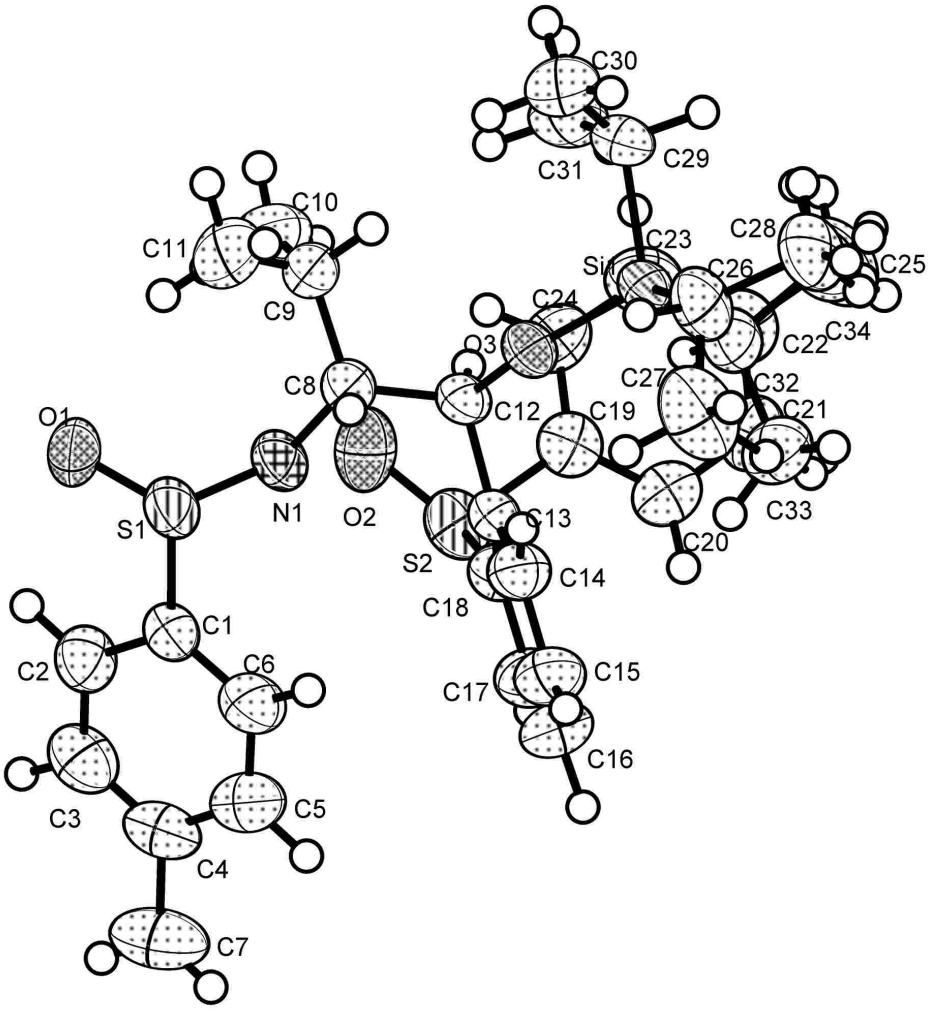


Figure 1.Ortep diagram for compound of **3i**

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

Identification code	otips_m
Empirical formula	C34 H49 N O3 S2 Si
Formula weight	611.95
Temperature	296(2) K
Wavelength	1.54178 Å

[6] The authors have deposited atomic coordinates for **3i** with the Cambridge Crystallographic data Centre (deposition number CCDC 208928). The coordinates can be obtained, on request, from the Director, Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge Cb2 1EZ, U.K.

Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 15.0361(8) Å	α= 90°.
	b = 15.2631(8) Å	β= 90°.
	c = 15.5706(10) Å	γ = 90°.
Volume	3573.4(4) $Å^3$	
Z	4	
Density (calculated)	1.137 Mg/m^3	
Absorption coefficient	1.912 mm^{-1}	
F(000)	1320	
Crystal size	0.33 x 0.29 x 0.27 mm^3	
Theta range for data collection	4.06 to 70.50°.	
Index ranges	-14<=h<=16, -13<=k<=18, -10<=l<=16	
Reflections collected	10768	
Independent reflections	5154 [R(int) = 0.0322]	
Completeness to theta = 70.50°	85.0 %	
Absorption correction	YES, SADABS v. 2.03	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5154 / 0 / 567	
Goodness-of-fit on F^2	1.036	
Final R indices [I>2sigma(I)]	R1 = 0.0335, wR2 = 0.0933	
R indices (all data)	R1 = 0.0351, wR2 = 0.0953	
Absolute structure parameter	-0.019(13)	
Extinction coefficient	0.00054(14)	
Largest diff. peak and hole	0.227 and -0.203 $e.Å^{-3}$	

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

	x	y	z	U(eq)
C(1)	2048(2)	-1626(1)	10952(2)	51(1)
C(2)	1272(2)	-1594(2)	11413(2)	61(1)
C(3)	474(2)	-1570(2)	10976(2)	70(1)
C(4)	434(2)	-1579(2)	10108(2)	69(1)
C(5)	1214(2)	-1604(3)	9650(3)	87(1)
C(6)	2019(2)	-1629(2)	10071(2)	79(1)
C(7)	-450(3)	-1529(4)	9638(5)	105(2)
C(8)	4514(2)	-795(2)	11025(2)	52(1)
C(9)	5049(2)	-614(2)	11849(2)	71(1)
C(10)	4630(3)	71(4)	12400(3)	103(2)
C(11)	5214(4)	-1462(5)	12341(4)	114(2)
C(12)	4708(1)	-123(1)	10306(2)	45(1)
C(13)	4102(2)	-265(1)	9535(2)	45(1)
C(14)	4296(2)	-959(2)	8988(2)	55(1)
C(15)	3794(2)	-1128(2)	8262(2)	72(1)
C(16)	3080(2)	-605(2)	8067(2)	78(1)
C(17)	2863(2)	66(2)	8602(2)	69(1)
C(18)	3360(2)	237(2)	9336(2)	53(1)
C(19)	3637(2)	1984(1)	9747(2)	55(1)
C(20)	3661(2)	2313(2)	8921(2)	61(1)
C(21)	4191(2)	3031(2)	8748(2)	67(1)
C(22)	4683(2)	3434(2)	9380(2)	70(1)
C(23)	4630(2)	3097(2)	10200(2)	74(1)
C(24)	4108(2)	2377(2)	10397(2)	67(1)
C(25)	5254(4)	4223(3)	9183(4)	106(2)
C(26)	7150(2)	-410(2)	9078(2)	69(1)
C(27)	6716(3)	-1046(3)	8480(3)	102(1)
C(28)	7934(2)	71(3)	8651(3)	79(1)
C(29)	7061(2)	860(2)	10589(2)	66(1)
C(30)	7546(3)	174(3)	11128(3)	90(1)
C(31)	6494(3)	1449(3)	11169(3)	88(1)
C(32)	5937(2)	1290(2)	9004(2)	59(1)
C(33)	5568(3)	1006(2)	8137(2)	76(1)

C(34)	6596(3)	2058(2)	8878(3)	86(1)
N(1)	3553(1)	-865(2)	11141(1)	52(1)
O(1)	2872(1)	-1719(1)	12423(1)	68(1)
O(2)	3014(2)	900(1)	10920(1)	75(1)
O(3)	5607(1)	-265(1)	10061(1)	50(1)
S(1)	3092(1)	-1756(1)	11498(1)	52(1)
S(2)	2891(1)	1105(1)	9989(1)	63(1)
Si(1)	6407(1)	375(1)	9680(1)	47(1)

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

C(1)-C(2)	1.372(4)
C(1)-C(6)	1.372(4)
C(1)-S(1)	1.795(3)
C(2)-C(3)	1.380(4)
C(2)-H(2)	1.01(4)
C(3)-C(4)	1.354(5)
C(3)-H(3)	0.95(4)
C(4)-C(5)	1.374(5)
C(4)-C(7)	1.520(5)
C(5)-C(6)	1.377(5)
C(5)-H(5)	1.01(4)
C(6)-H(6)	0.91(4)
C(7)-H(7A)	0.77(6)
C(7)-H(7B)	0.84(5)
C(7)-H(7C)	0.97(6)
C(8)-N(1)	1.460(3)
C(8)-C(9)	1.539(4)
C(8)-C(12)	1.546(3)
C(8)-H(8)	0.95(3)
C(9)-C(10)	1.491(6)
C(9)-C(11)	1.524(6)
C(9)-H(9)	0.96(3)
C(10)-H(10A)	0.97(3)
C(10)-H(10B)	0.95(4)
C(10)-H(10C)	0.85(6)
C(11)-H(11A)	0.91(5)
C(11)-H(11B)	0.97(6)
C(11)-H(11C)	0.75(5)
C(12)-O(3)	1.421(3)
C(12)-C(13)	1.522(3)
C(12)-H(12)	0.96(2)
C(13)-C(18)	1.389(3)
C(13)-C(14)	1.390(3)
C(14)-C(15)	1.383(4)
C(14)-H(14)	1.00(3)
C(15)-C(16)	1.373(5)

C(15)-H(15)	1.02(3)
C(16)-C(17)	1.360(5)
C(16)-H(16)	1.03(3)
C(17)-C(18)	1.389(4)
C(17)-H(17)	0.86(3)
C(18)-S(2)	1.813(3)
C(19)-C(24)	1.373(4)
C(19)-C(20)	1.381(4)
C(19)-S(2)	1.790(3)
C(20)-C(21)	1.381(4)
C(20)-H(20)	0.99(3)
C(21)-C(22)	1.376(5)
C(21)-H(21)	0.95(3)
C(22)-C(23)	1.380(5)
C(22)-C(25)	1.510(5)
C(23)-C(24)	1.384(4)
C(23)-H(23)	0.89(4)
C(24)-H(24)	0.96(3)
C(25)-H(25A)	0.91(5)
C(25)-H(25B)	1.07(8)
C(25)-H(25C)	0.93(7)
C(26)-C(27)	1.494(5)
C(26)-C(28)	1.539(4)
C(26)-Si(1)	1.888(3)
C(26)-H(26)	1.245(17)
C(27)-H(26)	1.488(19)
C(27)-H(27A)	1.24(7)
C(27)-H(27B)	1.12(5)
C(27)-H(27C)	1.05(4)
C(28)-H(28A)	0.96(4)
C(28)-H(28B)	0.95(4)
C(28)-H(28C)	0.89(4)
C(29)-C(30)	1.527(5)
C(29)-C(31)	1.533(5)
C(29)-Si(1)	1.877(3)
C(29)-H(29)	1.06(3)
C(30)-H(30A)	0.94(4)
C(30)-H(30B)	0.89(4)

C(30)-H(30C)	1.00(4)
C(31)-H(31A)	0.99(4)
C(31)-H(31B)	1.04(3)
C(31)-H(31C)	0.94(4)
C(32)-C(33)	1.522(4)
C(32)-C(34)	1.547(4)
C(32)-Si(1)	1.886(3)
C(32)-H(32)	0.97(3)
C(33)-H(33A)	1.00(4)
C(33)-H(33B)	1.02(4)
C(33)-H(33C)	1.00(3)
C(34)-H(34A)	1.00(5)
C(34)-H(34B)	0.90(4)
C(34)-H(34C)	1.09(4)
N(1)-S(1)	1.625(2)
N(1)-H(1)	0.71(3)
O(1)-S(1)	1.480(2)
O(2)-S(2)	1.495(2)
O(3)-Si(1)	1.6595(16)

C(2)-C(1)-C(6)	119.8(3)
C(2)-C(1)-S(1)	120.0(2)
C(6)-C(1)-S(1)	120.0(2)
C(1)-C(2)-C(3)	118.9(3)
C(1)-C(2)-H(2)	120(3)
C(3)-C(2)-H(2)	121(3)
C(4)-C(3)-C(2)	122.0(3)
C(4)-C(3)-H(3)	122(2)
C(2)-C(3)-H(3)	115(2)
C(3)-C(4)-C(5)	118.8(3)
C(3)-C(4)-C(7)	121.2(4)
C(5)-C(4)-C(7)	119.9(4)
C(4)-C(5)-C(6)	120.2(4)
C(4)-C(5)-H(5)	119(2)
C(6)-C(5)-H(5)	121(2)
C(1)-C(6)-C(5)	120.3(3)
C(1)-C(6)-H(6)	123(2)
C(5)-C(6)-H(6)	117(2)

C(4)-C(7)-H(7A)	107(5)
C(4)-C(7)-H(7B)	116(3)
H(7A)-C(7)-H(7B)	105(6)
C(4)-C(7)-H(7C)	112(3)
H(7A)-C(7)-H(7C)	114(6)
H(7B)-C(7)-H(7C)	103(4)
N(1)-C(8)-C(9)	115.3(2)
N(1)-C(8)-C(12)	109.0(2)
C(9)-C(8)-C(12)	112.7(2)
N(1)-C(8)-H(8)	106.9(16)
C(9)-C(8)-H(8)	106.6(15)
C(12)-C(8)-H(8)	105.8(15)
C(10)-C(9)-C(11)	112.0(4)
C(10)-C(9)-C(8)	112.6(3)
C(11)-C(9)-C(8)	110.6(3)
C(10)-C(9)-H(9)	110.6(18)
C(11)-C(9)-H(9)	104.5(18)
C(8)-C(9)-H(9)	106.1(19)
C(9)-C(10)-H(10A)	120(2)
C(9)-C(10)-H(10B)	107(2)
H(10A)-C(10)-H(10B)	108(3)
C(9)-C(10)-H(10C)	109(4)
H(10A)-C(10)-H(10C)	105(5)
H(10B)-C(10)-H(10C)	107(5)
C(9)-C(11)-H(11A)	110(3)
C(9)-C(11)-H(11B)	117(3)
H(11A)-C(11)-H(11B)	107(4)
C(9)-C(11)-H(11C)	98(4)
H(11A)-C(11)-H(11C)	92(5)
H(11B)-C(11)-H(11C)	131(6)
O(3)-C(12)-C(13)	109.61(18)
O(3)-C(12)-C(8)	105.82(18)
C(13)-C(12)-C(8)	111.33(18)
O(3)-C(12)-H(12)	112.5(15)
C(13)-C(12)-H(12)	108.6(15)
C(8)-C(12)-H(12)	108.9(14)
C(18)-C(13)-C(14)	116.8(2)
C(18)-C(13)-C(12)	125.4(2)

C(14)-C(13)-C(12)	117.8(2)
C(15)-C(14)-C(13)	121.9(3)
C(15)-C(14)-H(14)	121.1(16)
C(13)-C(14)-H(14)	116.5(16)
C(16)-C(15)-C(14)	120.0(3)
C(16)-C(15)-H(15)	125.2(17)
C(14)-C(15)-H(15)	114.9(17)
C(17)-C(16)-C(15)	119.3(3)
C(17)-C(16)-H(16)	125.1(16)
C(15)-C(16)-H(16)	115.5(16)
C(16)-C(17)-C(18)	121.1(3)
C(16)-C(17)-H(17)	121(2)
C(18)-C(17)-H(17)	118(2)
C(17)-C(18)-C(13)	120.8(2)
C(17)-C(18)-S(2)	112.9(2)
C(13)-C(18)-S(2)	126.18(19)
C(24)-C(19)-C(20)	121.0(3)
C(24)-C(19)-S(2)	119.7(2)
C(20)-C(19)-S(2)	119.0(2)
C(21)-C(20)-C(19)	119.0(3)
C(21)-C(20)-H(20)	116.0(18)
C(19)-C(20)-H(20)	124.3(18)
C(22)-C(21)-C(20)	121.7(3)
C(22)-C(21)-H(21)	111.7(18)
C(20)-C(21)-H(21)	126.6(18)
C(21)-C(22)-C(23)	117.7(3)
C(21)-C(22)-C(25)	121.1(4)
C(23)-C(22)-C(25)	121.2(4)
C(22)-C(23)-C(24)	122.2(3)
C(22)-C(23)-H(23)	121(3)
C(24)-C(23)-H(23)	116(3)
C(19)-C(24)-C(23)	118.4(3)
C(19)-C(24)-H(24)	115.7(16)
C(23)-C(24)-H(24)	125.8(15)
C(22)-C(25)-H(25A)	113(3)
C(22)-C(25)-H(25B)	118(4)
H(25A)-C(25)-H(25B)	115(5)
C(22)-C(25)-H(25C)	116(4)

H(25A)-C(25)-H(25C)	83(5)
H(25B)-C(25)-H(25C)	107(5)
C(27)-C(26)-C(28)	112.0(3)
C(27)-C(26)-Si(1)	117.5(2)
C(28)-C(26)-Si(1)	111.4(2)
C(27)-C(26)-H(26)	65.1(8)
C(28)-C(26)-H(26)	122.8(9)
Si(1)-C(26)-H(26)	119.7(9)
C(26)-C(27)-H(26)	49.3(7)
C(26)-C(27)-H(27A)	99(3)
H(26)-C(27)-H(27A)	148(4)
C(26)-C(27)-H(27B)	107(2)
H(26)-C(27)-H(27B)	83(3)
H(27A)-C(27)-H(27B)	109(4)
C(26)-C(27)-H(27C)	119(2)
H(26)-C(27)-H(27C)	85(2)
H(27A)-C(27)-H(27C)	118(4)
H(27B)-C(27)-H(27C)	103(3)
C(26)-C(28)-H(28A)	116(2)
C(26)-C(28)-H(28B)	108(2)
H(28A)-C(28)-H(28B)	100(3)
C(26)-C(28)-H(28C)	106(2)
H(28A)-C(28)-H(28C)	112(3)
H(28B)-C(28)-H(28C)	116(3)
C(30)-C(29)-C(31)	110.1(3)
C(30)-C(29)-Si(1)	113.2(3)
C(31)-C(29)-Si(1)	112.7(2)
C(30)-C(29)-H(29)	108.3(15)
C(31)-C(29)-H(29)	111.6(15)
Si(1)-C(29)-H(29)	100.6(15)
C(29)-C(30)-H(30A)	102(3)
C(29)-C(30)-H(30B)	105(2)
H(30A)-C(30)-H(30B)	119(4)
C(29)-C(30)-H(30C)	114(2)
H(30A)-C(30)-H(30C)	116(3)
H(30B)-C(30)-H(30C)	100(3)
C(29)-C(31)-H(31A)	117(2)
C(29)-C(31)-H(31B)	111.9(16)

H(31A)-C(31)-H(31B)	104(3)
C(29)-C(31)-H(31C)	108(2)
H(31A)-C(31)-H(31C)	103(3)
H(31B)-C(31)-H(31C)	114(3)
C(33)-C(32)-C(34)	109.7(3)
C(33)-C(32)-Si(1)	114.8(2)
C(34)-C(32)-Si(1)	113.1(2)
C(33)-C(32)-H(32)	101.7(17)
C(34)-C(32)-H(32)	111.3(16)
Si(1)-C(32)-H(32)	105.5(16)
C(32)-C(33)-H(33A)	106(2)
C(32)-C(33)-H(33B)	122(2)
H(33A)-C(33)-H(33B)	102(3)
C(32)-C(33)-H(33C)	110.4(18)
H(33A)-C(33)-H(33C)	109(3)
H(33B)-C(33)-H(33C)	107(3)
C(32)-C(34)-H(34A)	116(2)
C(32)-C(34)-H(34B)	118(3)
H(34A)-C(34)-H(34B)	111(3)
C(32)-C(34)-H(34C)	114(2)
H(34A)-C(34)-H(34C)	97(3)
H(34B)-C(34)-H(34C)	96(3)
C(8)-N(1)-S(1)	121.76(19)
C(8)-N(1)-H(1)	122(2)
S(1)-N(1)-H(1)	113(2)
C(12)-O(3)-Si(1)	134.10(14)
O(1)-S(1)-N(1)	113.35(12)
O(1)-S(1)-C(1)	105.17(11)
N(1)-S(1)-C(1)	96.83(11)
O(2)-S(2)-C(19)	106.45(13)
O(2)-S(2)-C(18)	110.03(11)
C(19)-S(2)-C(18)	100.74(11)
O(3)-Si(1)-C(29)	109.99(11)
O(3)-Si(1)-C(32)	111.36(10)
C(29)-Si(1)-C(32)	108.95(13)
O(3)-Si(1)-C(26)	103.49(11)
C(29)-Si(1)-C(26)	108.38(14)
C(32)-Si(1)-C(26)	114.51(14)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for otips_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}
C(1)	46(1)	54(1)	52(2)	0(1)	3(1)	-7(1)
C(2)	49(2)	71(1)	62(2)	4(1)	7(1)	4(1)
C(3)	45(2)	76(2)	89(3)	2(2)	4(1)	2(1)
C(4)	55(2)	61(1)	91(3)	-6(1)	-16(1)	-7(1)
C(5)	75(2)	118(3)	69(3)	-10(2)	-11(2)	-19(2)
C(6)	53(2)	117(2)	65(2)	-12(2)	6(1)	-20(2)
C(7)	73(3)	107(3)	134(5)	-10(3)	-42(3)	-3(2)
C(8)	36(1)	73(1)	46(2)	4(1)	2(1)	-5(1)
C(9)	47(2)	119(2)	48(2)	9(2)	-2(1)	-21(2)
C(10)	76(3)	171(5)	61(3)	-34(3)	1(2)	-27(3)
C(11)	85(4)	178(5)	78(3)	52(3)	-29(3)	-25(4)
C(12)	33(1)	59(1)	45(1)	-5(1)	2(1)	-5(1)
C(13)	37(1)	57(1)	42(1)	-1(1)	2(1)	-8(1)
C(14)	50(2)	64(1)	53(2)	-7(1)	0(1)	0(1)
C(15)	76(2)	80(2)	58(2)	-19(1)	-4(1)	-13(2)
C(16)	83(2)	96(2)	54(2)	-4(2)	-20(2)	-13(2)
C(17)	56(2)	80(2)	70(2)	8(1)	-18(1)	0(1)
C(18)	46(1)	58(1)	54(2)	1(1)	-3(1)	-2(1)
C(19)	51(1)	53(1)	61(2)	-6(1)	5(1)	10(1)
C(20)	62(2)	63(1)	58(2)	-4(1)	-4(1)	13(1)
C(21)	79(2)	61(1)	63(2)	6(1)	5(1)	14(1)
C(22)	76(2)	53(1)	82(2)	-7(1)	9(2)	7(1)
C(23)	82(2)	64(1)	77(2)	-20(2)	-2(2)	-2(1)
C(24)	75(2)	68(1)	57(2)	-8(1)	2(1)	9(1)
C(25)	108(4)	64(2)	146(5)	-6(2)	13(3)	-13(2)
C(26)	50(2)	78(2)	77(2)	-3(1)	21(1)	-1(1)
C(27)	96(3)	78(2)	132(4)	-22(2)	41(3)	1(2)
C(28)	53(2)	99(2)	85(3)	-5(2)	24(2)	-1(2)
C(29)	48(2)	90(2)	59(2)	-4(1)	-7(1)	-21(1)
C(30)	73(3)	126(3)	70(3)	10(2)	-22(2)	-14(2)
C(31)	86(3)	103(2)	74(3)	-30(2)	-6(2)	-24(2)
C(32)	53(2)	64(1)	60(2)	4(1)	4(1)	-1(1)
C(33)	72(2)	91(2)	64(2)	8(2)	-10(2)	4(2)

C(34)	76(3)	71(2)	112(3)	13(2)	-2(2)	-11(2)
N(1)	37(1)	62(1)	57(1)	4(1)	6(1)	-2(1)
O(1)	57(1)	97(1)	52(1)	19(1)	7(1)	-7(1)
O(2)	87(2)	70(1)	68(1)	1(1)	27(1)	10(1)
O(3)	34(1)	65(1)	52(1)	0(1)	5(1)	-4(1)
S(1)	41(1)	60(1)	56(1)	4(1)	6(1)	-3(1)
S(2)	46(1)	63(1)	79(1)	0(1)	9(1)	8(1)
Si(1)	33(1)	61(1)	47(1)	-3(1)	1(1)	-6(1)

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

	x	y	z	U(eq)
H(1)	3284(18)	-491(18)	11202(17)	47(8)
H(2)	1290(30)	-1570(30)	12060(30)	111(13)
H(3)	-50(30)	-1560(20)	11330(20)	100(12)
H(5)	1180(30)	-1610(20)	9000(30)	98(12)
H(6)	2510(20)	-1680(20)	9740(20)	80(9)
H(7A)	-780(40)	-1820(40)	9890(40)	160(30)
H(7B)	-690(30)	-1040(30)	9620(30)	106(15)
H(7C)	-390(30)	-1680(30)	9040(40)	132(19)
H(8)	4714(17)	-1347(17)	10810(16)	45(6)
H(9)	5630(20)	-430(19)	11660(20)	69(8)
H(10A)	4480(30)	640(20)	12160(30)	85(12)
H(10B)	4110(30)	-180(20)	12640(20)	87(10)
H(10C)	4980(40)	190(40)	12810(40)	160(20)
H(11A)	5540(30)	-1340(30)	12820(30)	112(14)
H(11B)	4690(40)	-1790(30)	12530(30)	131(16)
H(11C)	5620(40)	-1610(40)	12110(40)	120(20)
H(12)	4609(16)	458(16)	10526(16)	43(6)
H(14)	4860(20)	-1288(17)	9105(18)	59(7)
H(15)	4000(20)	-1655(18)	7912(19)	66(8)
H(16)	2750(20)	-755(18)	7500(20)	70(8)
H(17)	2400(20)	385(18)	8504(19)	64(8)
H(20)	3400(20)	2016(19)	8420(20)	69(8)
H(21)	4272(19)	3304(19)	8210(20)	64(8)
H(23)	4990(30)	3280(30)	10610(30)	99(12)
H(24)	4068(17)	2097(16)	10949(19)	49(7)
H(25A)	5830(30)	4080(30)	9070(30)	104(15)
H(25B)	4970(50)	4720(50)	8790(50)	220(30)
H(25C)	5510(40)	4510(40)	9650(40)	170(20)
H(26)	7192(12)	-1191(10)	9305(12)	18(4)
H(27A)	6470(50)	-530(50)	7910(40)	220(30)
H(27B)	7250(30)	-1480(30)	8210(30)	140(16)
H(27C)	6250(30)	-1490(20)	8720(20)	95(11)

H(28A)	8320(30)	-290(30)	8310(30)	102(12)
H(28B)	7700(30)	440(30)	8210(30)	99(13)
H(28C)	8220(20)	340(20)	9080(20)	79(11)
H(29)	7540(20)	1228(17)	10243(18)	60(7)
H(30A)	7960(30)	-50(30)	10730(30)	113(15)
H(30B)	7740(30)	460(20)	11590(30)	90(11)
H(30C)	7150(20)	-260(20)	11420(20)	77(9)
H(31A)	6810(30)	1790(30)	11620(30)	107(12)
H(31B)	6030(20)	1092(18)	11516(19)	63(8)
H(31C)	6240(20)	1890(20)	10820(20)	81(11)
H(32)	5404(19)	1481(17)	9298(18)	58(7)
H(33A)	5250(30)	1530(20)	7900(20)	91(10)
H(33B)	5090(30)	530(30)	8080(20)	100(12)
H(33C)	6060(20)	834(18)	7740(20)	70(8)
H(34A)	7200(30)	1900(30)	8660(30)	107(13)
H(34B)	6390(30)	2550(20)	8630(20)	92(11)
H(34C)	6810(30)	2370(30)	9470(30)	101(12)

Table 6. Torsion angles [°] for otips_m.

C(6)-C(1)-C(2)-C(3)	0.3(4)
S(1)-C(1)-C(2)-C(3)	-174.5(2)
C(1)-C(2)-C(3)-C(4)	0.2(4)
C(2)-C(3)-C(4)-C(5)	-0.7(5)
C(2)-C(3)-C(4)-C(7)	-178.4(3)
C(3)-C(4)-C(5)-C(6)	0.7(5)
C(7)-C(4)-C(5)-C(6)	178.4(4)
C(2)-C(1)-C(6)-C(5)	-0.3(5)
S(1)-C(1)-C(6)-C(5)	174.4(3)
C(4)-C(5)-C(6)-C(1)	-0.2(6)
N(1)-C(8)-C(9)-C(10)	-43.8(4)
C(12)-C(8)-C(9)-C(10)	82.1(4)
N(1)-C(8)-C(9)-C(11)	82.3(4)
C(12)-C(8)-C(9)-C(11)	-151.8(4)
N(1)-C(8)-C(12)-O(3)	-164.05(19)
C(9)-C(8)-C(12)-O(3)	66.7(3)
N(1)-C(8)-C(12)-C(13)	-45.0(3)
C(9)-C(8)-C(12)-C(13)	-174.3(2)
O(3)-C(12)-C(13)-C(18)	-140.7(2)
C(8)-C(12)-C(13)-C(18)	102.6(3)
O(3)-C(12)-C(13)-C(14)	40.2(3)
C(8)-C(12)-C(13)-C(14)	-76.5(3)
C(18)-C(13)-C(14)-C(15)	2.2(4)
C(12)-C(13)-C(14)-C(15)	-178.7(2)
C(13)-C(14)-C(15)-C(16)	-0.2(4)
C(14)-C(15)-C(16)-C(17)	-1.4(5)
C(15)-C(16)-C(17)-C(18)	0.9(5)
C(16)-C(17)-C(18)-C(13)	1.1(4)
C(16)-C(17)-C(18)-S(2)	-175.4(3)
C(14)-C(13)-C(18)-C(17)	-2.6(3)
C(12)-C(13)-C(18)-C(17)	178.3(2)
C(14)-C(13)-C(18)-S(2)	173.44(19)
C(12)-C(13)-C(18)-S(2)	-5.6(3)
C(24)-C(19)-C(20)-C(21)	2.1(4)
S(2)-C(19)-C(20)-C(21)	175.5(2)
C(19)-C(20)-C(21)-C(22)	-1.1(4)

C(20)-C(21)-C(22)-C(23)	-0.1(4)
C(20)-C(21)-C(22)-C(25)	-179.5(3)
C(21)-C(22)-C(23)-C(24)	0.3(5)
C(25)-C(22)-C(23)-C(24)	179.7(4)
C(20)-C(19)-C(24)-C(23)	-1.9(4)
S(2)-C(19)-C(24)-C(23)	-175.3(2)
C(22)-C(23)-C(24)-C(19)	0.7(5)
C(9)-C(8)-N(1)-S(1)	-79.8(3)
C(12)-C(8)-N(1)-S(1)	152.37(17)
C(13)-C(12)-O(3)-Si(1)	90.1(2)
C(8)-C(12)-O(3)-Si(1)	-149.74(18)
C(8)-N(1)-S(1)-O(1)	99.6(2)
C(8)-N(1)-S(1)-C(1)	-150.6(2)
C(2)-C(1)-S(1)-O(1)	-5.3(2)
C(6)-C(1)-S(1)-O(1)	179.9(2)
C(2)-C(1)-S(1)-N(1)	-121.8(2)
C(6)-C(1)-S(1)-N(1)	63.4(2)
C(24)-C(19)-S(2)-O(2)	-6.2(2)
C(20)-C(19)-S(2)-O(2)	-179.75(19)
C(24)-C(19)-S(2)-C(18)	-121.0(2)
C(20)-C(19)-S(2)-C(18)	65.5(2)
C(17)-C(18)-S(2)-O(2)	143.0(2)
C(13)-C(18)-S(2)-O(2)	-33.3(3)
C(17)-C(18)-S(2)-C(19)	-104.9(2)
C(13)-C(18)-S(2)-C(19)	78.8(2)
C(12)-O(3)-Si(1)-C(29)	89.8(2)
C(12)-O(3)-Si(1)-C(32)	-31.1(2)
C(12)-O(3)-Si(1)-C(26)	-154.6(2)
C(30)-C(29)-Si(1)-O(3)	63.3(3)
C(31)-C(29)-Si(1)-O(3)	-62.5(3)
C(30)-C(29)-Si(1)-C(32)	-174.4(3)
C(31)-C(29)-Si(1)-C(32)	59.8(3)
C(30)-C(29)-Si(1)-C(26)	-49.2(3)
C(31)-C(29)-Si(1)-C(26)	-175.0(3)
C(33)-C(32)-Si(1)-O(3)	-71.5(3)
C(34)-C(32)-Si(1)-O(3)	161.5(2)
C(33)-C(32)-Si(1)-C(29)	167.0(2)
C(34)-C(32)-Si(1)-C(29)	40.0(3)

C(33)-C(32)-Si(1)-C(26)	45.4(3)
C(34)-C(32)-Si(1)-C(26)	-81.5(3)
C(27)-C(26)-Si(1)-O(3)	47.4(3)
C(28)-C(26)-Si(1)-O(3)	178.6(3)
C(27)-C(26)-Si(1)-C(29)	164.2(3)
C(28)-C(26)-Si(1)-C(29)	-64.6(3)
C(27)-C(26)-Si(1)-C(32)	-74.0(3)
C(28)-C(26)-Si(1)-C(32)	57.2(3)

Symmetry transformations used to generate equivalent atoms: