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Supporting Information

Control of Vicinal Stereocenters through Nickel-Catalyzed Alkyl–Alkyl Cross-Coupling

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Supporting Information

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I. General Information

Unless otherwise noted, anhydrous THF and CH_2Cl_2 were purified and dried using a solvent purification system that contained activated alumina. All reagents were purchased from Sigma-Aldrich, unless otherwise noted. ZnI_2 and $Ni(acac)_2$ were purchased from Strem Chemicals. (1*S*,2*S*)-*N*,*N*′-Dimethyl-1,2-di(naphthalene-1-yl)ethane-1,2-diamine and (1*R*,2*R*)-*N*,*N*′-dimethyl-1,2-di(naphthalene-1-yl)ethane-1,2-diamine were synthesized according to previously reported procedures.[1]

HPLC analysis was carried out on an Agilent 1100 Series system, using Daicel CHIRALCEL® columns or Daicel CHIRALPAK® columns (internal diameter 4.6 mm, column length 250 mm, particle size 5 μm). GC analysis was performed on a Hewlett Packard HP 6850 Series apparatus with a Varian GC capillary column (WCOT fused silica 25 m × 0.25 mm; stationary phase: CP CHIRASIL-DEX CB; film thickness 0.25 μm). Flash chromatography was performed on SiO_2 (visualization by thin layer chromatography, staining with I_2/SiO_2).

II. Synthesis of Electrophiles

The procedures and yields have not been optimized.

General Procedure: Preparation of cyclohexyl iodides from cyclohexyl alcohols.[2] A 250 mL round-bottom flask was charged with a stir bar, triphenyl phosphine (15.7 g, 60 mmol; 1.2 equiv), and imidazole (4.1 g, 60 mmol; 1.2 equiv). CH_2Cl_2 (100 mL) was then added, and the mixture was stirred for 10 min, at which point it was homogeneous. Next, I_2 (15.2 g, 60 mmol; 1.2 equiv) was added in several portions over 10 min to the stirred solution. Then, the alcohol (50 mmol; 1.0 equiv) was added to the reaction mixture, which was then stirred overnight at r.t. After the reaction was complete, hexane was added, the reaction mixture was stirred for 10 min, and then the resulting precipitate was removed by filtration and the filtrate was concentrated. The crude product was purified by flash chromatography or distillation. The diastereoisomer ratio was determined via analysis by ^{1}H NMR spectroscopy or by GC.

1-Iodo-4-methylcyclohexane [65500-78-9]. The title compound was prepared according to the General Procedure from 4-methylcyclohexan-1-ol. A colorless oil (5.32 g, 48%) was obtained. Cis:trans = 83:17.

^{1}H NMR (400 MHz, $CDCl_3$) δ 4.73 (t, 0.83H, J = 4.0 Hz), 4.04 (tt, 0.17H, J = 4.0, 12.1 Hz), 2.38-2.22 (m, 0.4H), 2.09-1.82 (m, 2H), 1.62-1.29 (m, 6.5H), 1.01-0.83 (m, 3H).

The ^{1}H NMR spectra data are in agreement with literature data.[2]

1-Iodo-4-ethylcyclohexane [1342026-09-8]. The title compound was prepared according to the General Procedure from 4-ethylcyclohexan-1-ol. A colorless oil (4.82 g, 50%) was obtained. Cis:trans = 87:13.

^{1}H NMR (400 MHz, $CDCl_3$) δ 4.74 (t, 0.87H, J = 4.0 Hz), 4.05 (tt, 0.13H, J = 4.0, 12.0 Hz), 2.38-2.29 (m, 0.27H), 2.09-1.82 (m, 2H), 1.62-1.30 (m, 5.8H), 1.30-1.04 (m, 3H), 1.00-0.75 (m, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 40.4, 38.4, 37.8, 37.0, 36.2, 35.1, 30.8, 29.6, 29.0, 11.4, 11.3;

IR (film) 2959, 2919, 2853, 2832, 1437, 1379, 1348, 1271, 1221, 1104, 982, 847, 664, 494 cm^{-1};

LRMS (GC-MS EI): calcd for $C_8H_{15}I$ [M] 238.0, found 238.1.

1-(*tert*-Butyl)-4-iodocyclohexane [85592-89-8]. The title compound was prepared according to the General Procedure from 4-(*tert*-butyl)cyclohexan-1-ol. A white solid (3.56 g, 60%) was obtained. Cis:trans = 90:10.

^{1}H NMR (400 MHz, $CDCl_3$) δ 4.88-4.75 (m, 0.9H), 4.02 (tt, 0.10H, *J* = 4.0, 12.0 Hz), 2.48-2.32 (m, 0.2H), 2.17-1.82 (m, 2H), 1.68-1.32 (m, 6H), 1.10-0.94 (m, 1.3H), 0.93-0.76 (m, 8.5H);

The ^{1}H NMR spectra data are in agreement with literature data.[2]

1-Iodo-4-(trifluoromethyl)cyclohexane. The title compound was prepared according to the General Procedure from 4-(trifluoromethyl)cyclohexan-1-ol. A colorless oil (0.72 g, 52%) was obtained. Cis:trans = 62:38.

^{1}H NMR (400 MHz, $CDCl_3$) δ 4.74 (t, 0.62H, *J* = 4.0 Hz), 3.97 (tt, 0.38H, *J* = 4.0, 16.0 Hz), 2.51-2.35 (m, 0.81H), 2.18-1.93 (m, 2H), 1.92-1.68 (m, 4H), 1.57-1.43 (m, 1H), 1.36 (td, 1H, *J* = 4.0, 16.0 Hz);

^{13}C NMR (100 MHz, $CDCl_3$) δ 127.5 (q, *J* = 280 Hz), 127.3 (q, *J* = 276 Hz), 41.3 (q, *J* = 27 Hz), 40.4 (q, *J* = 26 Hz), 38.4, 32.7, 27.3 (q, *J* = 2 Hz), 21.3 (q, *J* = 2 Hz);

^{19}F NMR (282 MHz, $CDCl_3$) δ 73.7 (d, *J* = 8.5 Hz), 73.8 (d, *J* = 8.5 Hz);

IR (film) 2952, 2872, 1453, 1443, 1392, 1333, 1282, 1257, 1216, 1202, 1168, 1150, 1108, 1069, 1054, 989, 904, 839, 810, 706, 636 cm^{-1};

LRMS (GC-MS EI): calcd for $C_7H_{10}F_3I$ [M] 278.0, found 278.1.

(4-Iodocyclohexyl)benzene [1342026-09-8 (cis)]. The title compound was prepared according to the General Procedure from 4-phenylcyclohexan-1-ol. A white solid (4.72 g, 65%) was obtained. Cis:trans = 91:9.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26-7.02 (m, 5H), 4.85 (t, 0.91H, *J* = 4.0 Hz), 4.12 (tt, 0.09H, *J* = 4.0, 12.0 Hz), 2.58-2.40 (m, 1H), 2.18-2.03 (m, 2H), 2.02-1.87 (m, 2H), 1.77-1.55 (m, 4H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 146.6, 146.1, 128.4, 126.8, 126.6, 126.2, 126.1, 43.8, 42.8, 40.7, 36.5, 36.0, 30.0, 29.0;

IR (film) 2930, 2855, 1491, 1449, 1436, 1220, 1199, 1150, 1066, 991, 909, 892, 828, 755, 698, 672, 526 cm^{-1};

LRMS (GC-MS EI): calcd for $C_{12}H_{15}I$ [M] 286.0, found 286.1.

4-Iodo-1-isopropyl-1-methoxycyclohexane. The title compound was prepared according to the General Procedure from 4-isopropyl-4-methoxycyclohexan-1-ol. A colorless oil (2.52 g) was obtained. Cis:trans > 95:5.

^{1}H NMR (400 MHz, $CDCl_3$) δ 4.84-4.78 (m, 1H), 3.03 (s, 3H), 1.91-1.66 (m, 7H), 1.52-1.39 (m, 2H), 0.86 (d, 6H, *J* = 4.0 Hz);

^{13}C NMR (100 MHz, $CDCl_3$) δ 76.8, 47.1, 38.4, 31.9, 31.5, 25.9, 16.8;

IR (film) 2957, 2938, 2890, 2823, 1463, 1433, 1369, 1245, 1230, 1073, 1012, 943, 888, 866, 693, 658 cm^{-1};

LRMS (GC-MS EI): calcd for $C_{10}H_{19}IO$ [M] 282.0, found 282.3.

1-Iodo-3,5-dimethylcyclohexane. The title compound was prepared according to the General Procedure from 4-isopropyl-4-methoxycyclohexan-1-ol. A colorless oil (4.42 g, 46%) was obtained. Cis:trans = 67:33.

^{1}H NMR (400 MHz, $CDCl_3$) δ 4.83 (t, 0.67H, *J* = 4.0 Hz), 4.09 (tt, 0.33H, *J* = 4.0, 12.0 Hz), 2.37-2.26 (m, 0.7H), 2.03-1.85 (m, 2.7H), 1.70-1.59 (m, 1H), 1.57-1.33 (m, 1.5H), 1.08-0.94 (m, 1.4H), 0.86 (d, 4H, *J* = 4.0 Hz), 0.82 (d, 2H, *J* = 8.0 Hz), 0.59 (ddd, 1H, *J* = 4.0, 12.0, 24 Hz);

^{13}C NMR (100 MHz, $CDCl_3$) δ 48.5, 44.1, 43.8, 42.4, 36.2, 34.9, 29.1, 28.6, 21.9, 21.8;

IR (film) 2949, 2925, 2903, 2867, 1454, 1246, 1167, 1115, 974, 846, 661, 496 cm^{-1};

LRMS (GC-MS EI): calcd for $C_8H_{15}I$ [M] 238.0, found 238.2.

4-Iodo-2,6-dimethyltetrahydro-2*H*-pyran. The title compound was prepared according to the General Procedure from 2,6-dimethyltetrahydro-2*H*-pyran-4-ol. A colorless oil (2.11 g, 60%) was obtained. Cis:trans = 82:18.

^{1}H NMR (400 MHz, $CDCl_3$) δ 4.76 (t, 0.82H, *J* = 4.0 Hz), 4.19 (tt, 0.18H, *J* = 4.0, 12.0 Hz), 3.97-3.83 (m, 1.7H), 3.38 (ddd, 0.4H, *J* = 4.0, 8.0, 12.0 Hz), 2.28-2.18 (m, 0.4H), 1.97-1.70 (m, 2.0H), 1.38 (ddd, 1.7H, *J* = 4.0, 12.0, 16.0 Hz), 1.16 (d, 5H, *J* = 4.0 Hz), 1.11 (d, 1H, *J* = 4.0 Hz);

^{13}C NMR (100 MHz, $CDCl_3$) δ 74.7, 69.4, 46.5, 41.9, 30.9, 22.5, 21.3, 21.2;

IR (film) 2970, 2932, 2885, 2862, 1443, 1370, 1316, 1192, 1070, 1021, 957, 832, 668 cm^{-1};

LRMS (GC-MS EI): calcd for $C_7H_{13}IO$ [M] 240.0, found 240.1.

(3*R*)-1-Iodo-3-methylcyclohexane. The title compound was prepared from (*R*)-3-methylcyclohexan-1-one through reduction and then iodination according to the General Procedure. A colorless oil (1.58 g, 47%) was obtained. Cis:trans = 90:10.

^{1}H NMR (400 MHz, $CDCl_3$) δ 4.80 (t, 0.9H, *J* = 4.0 Hz), 4.09 (tt, 0.1H, *J* = 4.0, 12.0 Hz), 2.42-2.28 (m, 0.2H), 2.09-1.83 (m, 2.8H), 1.82-1.32 (m, 4H), 1.31-1.11 (m, 1H), 1.08-0.78 (m, 4H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 44.7, 40.1, 36.4, 36.2, 36.1, 35.6, 34.2, 33.5, 29.9, 28.7, 28.5, 22.7, 22.1, 21.4;

IR (film) 2924, 2865, 2844, 1454, 1444, 1245, 1166, 841, 649, 498 cm^{-1};

LRMS (GC-MS EI): calcd for $C_7H_{13}I$ [M] 224.0, found 224.1;

$[\alpha]^{25}_{D}$ = +0.02° (c = 1.0, $CHCl_3$).

1-Bromo-4-((1*R*)-3-iodocyclohexyl)benzene. (*R*)-3-(4-Bromophenyl)cyclohexan-1-one (0.67 g, 88% yield, >99% ee) was prepared according to a literature procedure.[3] The title compound was prepared from the ketone via reduction and then iodination according to the General Procedure. A white solid (0.73 g, 36%) was obtained. Cis:trans = 83:17.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45-7.26 (m, 2H), 7.05-6.95 (m, 2H), 4.91 (m, 0.83H), 4.16 (tt, 0.17H, *J* = 4.0, 12.0 Hz), 3.04 (tt, 0.8H, *J* = 4.0, 12.0 Hz), 2.57-2.33 (m, 0.6H), 2.21-1.98 (m, 2H), 1.96-1.78 (m, 2H), 1.75-1.31 (m, 4H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 144.9, 144.1, 131.5, 131.4, 128.8, 128.4, 120.0, 119.8, 47.7, 46.1, 43.3, 39.9, 39.5, 35.8, 35.5, 33.3, 32.4, 28.5, 28.0, 22.8;

IR (film) 2931, 2856, 1489, 1444, 1234, 1148, 1075, 1009, 815, 525 cm^{-1};

LRMS (GC-MS EI): calcd for $C_{12}H_{14}BrI$ [M] 363.9, found 364.0;

$[\alpha]^{25}_D$ = -32° (c = 1.0, $CHCl_3$).

(2*S*,4*R*)-4-Iodo-2-phenyltetrahydro-2*H*-pyran [936699-93-3].[4] A mixture of 3-buten-1-ol (1.44 g, 20 mmol), benzaldehyde (1.06 g, 10 mmol), and I_2 (2.54 g, 10 mmol) in CH_2Cl_2 (40 mL) was stirred at r.t. for 24 h. Next, water was added to quench the reaction, and the reaction mixture was extracted with Et_2O. The organic layer was washed with saturated aqueous $Na_2S_2O_3$, dried over Na_2SO_4, and concentrated. Flash chromatography furnished a light-orange oil (1.47 g, 55%). Chiral separation: IC column, 10% *i*-PrOH, 1.0 mL/min. Cis:trans > 99:1. The absolute stereochemistry was determined through X-ray crystallographic analysis of the cross-coupling product (vide infra).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36-7.12 (m, 5H), 4.43-4.20 (m, 2H), 4.02-3.88 (m, 1H), 3.70-3.55 (m, 1H), 2.59-2.42 (m, 1H), 2.38-2.11 (m, 3H).

The ^{1}H NMR spectra data are in agreement with literature data.[4]

1-Chloro-4-((1*R*)-3-iodo-1-methylcyclohexyl)benzene. The title compound was prepared from (*R*)-3-(4-chlorophenyl)-3-methylcyclohexan-1-one (94% ee) through reduction and then iodination according to the General Procedure. A colorless oil (1.01 g, 45%) was obtained. Cis:trans = 50:50.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27-7.14 (m, 4H), 4.41 (tt, 0.5H, *J* = 4.0, 12.0 Hz), 4.01 (tt, 0.5H, *J* = 4.0, 12.0 Hz), 2.96 (dq, 0.5H, *J* = 4.0, 16.0 Hz), 2.56-2.21 (m, 2H), 2.19-1.97 (m, 1.4H), 1.96-1.35 (m, 1.6H), 1.69-1.31 (m, 2.5H), 1.31-1.16 (m, 1.5H), 1.10-1.01 (m, 1.5H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 149.0, 144.1, 131.7, 131.5, 128.9, 128.6, 128.3, 127.6, 127.3, 126.3, 51.5, 51.2, 42.9, 40.8, 40.4, 40.1, 36.1, 36.0, 35.0, 26.8, 26.4, 24.9, 24.5, 23.8.

LRMS (GC-MS EI): calcd for $C_{13}H_{16}ClI$ [M] 334.0, found 334.0;
$[\alpha]^{25}_{D} = -69°$ (c = 1.0, $CHCl_3$).

(1*R*,4*aS*,7*R*,8*aS*)-3-Iodo-7-isopropyl-1,8a-dimethyldecahydronaphthalene. The title compound was prepared from (+)-nootkatone. (+)-Nootkatone (1.24 g, 5.7 mmol) was dissolved in EtOAc (10 mL) in a 50 mL round-bottom flask charged with a stir bar, and then Pd/C (200 mg) was added. A H_2 balloon was attached to the flask, and the reaction mixture was stirred for 16 h. Next, the reaction mixture was filtered, the solvent was removed, and the product was purified by flash chromatography, which furnished a colorless oil (1.31 g, 95%). The title compound was prepared according to the General Procedure. A colorless oil (1.42 g, 95%) was obtained. Cis:trans = 85:15.

^{1}H NMR (400 MHz, $CDCl_3$) δ 4.93-4.82 (m, 0.85H), 4.16 (tt, 0.15H, *J* = 4.0, 12.0 Hz), 2.11-1.91 (m, 0.5H), 1.75-1.42 (m, 6.5H), 1.40-1.14 (m, 7H), 1.06-0.92 (m, 1H), 0.85-0.63 (m, 11H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 48.9, 46.1, 44.7, 42.9, 42.1, 41.7, 41.5, 41.0, 38.9, 38.8, 38.7, 38.6, 38.5, 37.5, 37.1, 36.0, 33.1, 33.0, 31.6, 29.6, 28.3, 27.9, 20.0, 19.9, 19.6, 19.5, 14.4, 14.1, 12.2, 11.5;

IR (film) 2926, 2864, 1448, 1425, 1383, 1367, 1285, 1261, 1237, 1178, 1119, 1098, 981, 950, 886, 720, 661 cm^{-1};

LRMS (GC-MS EI): calcd for $C_{15}H_{27}I$ [M] 334.1, found 333.4;
$[\alpha]^{25}_{D} = +26°$ (c = 1.0, $CHCl_3$).

(3*R*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-3-Iodo-10,13-dimethyl-17-((*R*)-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[a]-phenanthrene [36049-79-3]. The title compound was prepared as in a previous report.[5] A white solid (3.5 g, 65%) was obtained. Cis:trans >20:1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 5.35 (dt, 1H, *J* = 2.0, 6.0 Hz), 4.06 (tt, 1H, *J* = 4.0, 12.0 Hz), 3.01-2.87 (m, 1H), 2.70 (ddd, 1H, *J* = 4.0, 8.0, 12.0 Hz), 2.37-2.14 (m, 2H), 2.08-1.92 (m, 2H), 1.91-1.68 (m, 2H), 1.65-1.23 (m, 10H), 1.21-0.96 (m, 13H), 0.93 (m, 3H), 0.91-0.85 (dd, 6H, *J* = 4.0, 8.0 Hz), 0.69 (s, 3H).

The ^{1}H NMR spectra data are in agreement with literature data.[5]

III. Stereoselective Cross-Couplings

Preparation of the nucleophile. An oven-dried Schlenk flask was charged with a stir bar, and then it was evacuated and backfilled with N_2 (three cycles). Next, *N*-Boc-pyrrolidine (1.2 g, 7.0 mmol) and TMEDA (freshly distilled over CaH_2; 1.05 mL, 7.0 mmol, 1.0 equiv) were added, followed by anhydrous Et_2O (14.0 mL). The resulting mixture was stirred for 5 min, and then it was cooled to –78 °C. *s*-BuLi (Sigma-Aldrich; 1.42 M in cyclohexane; 5.4 mL, 7.7 mmol, 1.1 equiv) was added dropwise over 1–2 min, resulting in a light-yellow reaction mixture. This mixture was stirred vigorously at –78 °C for 3.5 h. Meanwhile, ZnI_2 (1.12 g, 3.5 mmol; 0.50 equiv; the quality of the ZnI_2 is important: it should be a free-flowing white solid) and a stir bar were added to an oven-dried 20 mL vial in a glovebox. The vial was capped with a PTFE pierceable cap, and the joint was wrapped with electric tape. The vial was removed from the glovebox, anhydrous THF (7 mL) was added, and the resulting mixture was stirred vigorously for 1 h, at which time the ZnI_2 was completely dissolved. Then, the solution of ZnI_2 was added via syringe over 2 min to the solution of the lithiated *N*-Boc-pyrrolidine at –78 °C (during the addition of ZnI_2, the reaction mixture should be kept below –70 °C). The resulting white mixture was stirred at –78 °C for 30 min. Then, the flask was removed from the cooling bath and stirred for 1 h, at which time the almost-colorless mixture was nearly homogeneous. The resulting organozinc reagent was used in the cross-coupling reactions.

General procedure. An oven-dried 20 mL vial was charged with a stir bar, $Ni(acac)_2$ (27 mg, 0.105 mmol, 15 mol%), and (*S*,*S*)-**1** (40.6 mg, 0.119 mmol, 17 mol%). Then, the vial was capped with a PTFE pierceable cap, the joint was wrapped with electric tape, and the vial was placed under an N_2 atmosphere by evacuating and backfilling the vial (three cycles). Anhydrous THF (3.5 mL) was added via syringe, and the mixture was stirred for 10 min until a green-blue solution was formed. The alkyl iodide (0.70 mmol) was added via syringe (if the alkyl iodide was a solid, it was added as a solution in THF (0.5 mL)). The mixture was stirred for 10 min, and then the nucleophile (0.24 M with respect to the *N*-Boc-pyrrolidinyl group; 3.5 mL, 0.84 mmol) was added dropwise to the reaction mixture, which was gently stirred. After the addition of the nucleophile was complete, the mixture turned from blue-green to orange-red. Then, a balloon filled with N_2 was attached to the reaction vial, and the reaction mixture was stirred vigorously at r.t. for 72 h. Next, the reaction was quenched by the addition of 5% methanol in hexane (v/v; 10.5 mL), and the mixture was stirred for 15 min. Then, it was passed through a plug of silica gel, and the vial, the cap, and the silica gel were rinsed with Et_2O. The filtrate was concentrated, and the residue was purified by flash chromatography on silica gel.

***tert*-Butyl (*S*)-2-((1*r*,4*S*)-4-methylcyclohexyl)pyrrolidine-1-carboxylate (Table 1, entry 1)**. 1-Iodo-4-methylcyclohexane and the organozinc reagent were coupled under the standard cross-coupling conditions (0.70 mmol of the electrophile). Solvent system for chromatography: 20:1 hexane/ethyl acetate. The title compound was isolated as a colorless oil.

Run 1 with (*S,S*)-**1**: 143 mg (78% yield, 92:8 dr, 93% ee);

Run 2 with (*R,R*)-**1**: 149 mg (79% yield, 92:8 dr, 92% ee).

The ee was determined via SFC analysis with an AD-H column (10% MeOH/hexane, flow rate 3.0 mL/min); retention time for compound produced with (*S,S*)-**1**: 5.9 min (major), 8.1 min (minor).

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.75-3.52 (m, 1H), 3.47-3.27 (m, 1H), 3.21-3.06 (m, 1H), 1.80-1.60 (m, 6H), 1.59-1.46 (m, 3H), 1.39 (s, 9H), 1.25-1.13 (m, 1H), 1.05-0.71 (m, 7H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 155.0, 78.8, 61.6, 46.6, 40.8, 35.2, 35.0, 32.8, 31.6, 31.3, 30.0, 28.5, 27.8, 27.1, 24.0, 22.6.

IR (film) 2947, 2920, 2868, 2850, 1692, 1453, 1364, 1251, 1165, 1106, 941, 920, 865 cm^{-1};

LRMS (LCMS ESI): calcd for $C_{12}H_{22}NO_2$ [M − (isobutylene) + H] 212.2, found 212.2;

$[\alpha]^{25}_{D}$ = +40° (c = 1.0, $CHCl_3$) from (*R,R*)-**1**.

***tert*-Butyl (*S*)-2-((1*r*,4*S*)-4-ethylcyclohexyl)pyrrolidine-1-carboxylate (Table 1, entry 2)**. 1-Iodo-4-ethylcyclohexane and the organozinc reagent were coupled under the standard cross-coupling conditions (0.70 mmol of the electrophile). Solvent system for chromatography: 20:1 hexane/ethyl acetate. The title compound was isolated as a colorless oil.

Run 1 with (*S,S*)-**1**: 141 mg (72% yield, >99:1 dr, 93% ee);

Run 2 with (*R,R*)-**1**: 152 mg (77% yield, >99:1 dr, 92% ee).

The ee was determined via SFC analysis with an AD-H column (10% MeOH/hexane, flow rate 3.0 mL/min); retention time for compound produced with (*S,S*)-**1**: 7.3 min (major), 10.8 min (minor).

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.73-3.53 (m, 1H), 3.46-3.31 (m, 1H), 3.19-3.08 (m, 1H), 1.77-1.65 (m, 7H), 1.62-1.50 (m, 3H), 1.44-1.34 (m, 10H), 1.03-0.87 (m, 3H), 0.84-0.71 (m, 5H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 155.0, 78.8, 61.7, 46.6, 41.2, 39.6, 32.8, 32.5, 29.9, 29.8, 28.5, 28.4, 28.0, 27.7, 27.0, 23.9, 11.5;

IR (film) 2963, 2921, 2852, 1691, 1478, 1449, 1389, 1364, 1253, 1220, 1166, 1104, 951, 918, 876, 771 cm^{-1};

LRMS (LCMS ESI): calcd for $C_{13}H_{24}NO_2$ [M – (isobutylene) + H] 226.2, found 226.2;

$[\alpha]^{25}_D$ = -48° (c = 1.0, $CHCl_3$) from (*S,S*)-**1**.

***tert*-Butyl (*S*)-2-((1*r*,4*S*)-4-(*tert*-butyl)cyclohexyl)pyrrolidine-1-carboxylate (Table 1, entry 3)**. 1-(*tert*-Butyl)-4-iodocyclohexane and the organozinc reagent were coupled under the standard cross-coupling conditions (0.70 mmol of the electrophile). Solvent system for chromatography: 19:1 hexane/ethyl acetate. The title compound was isolated as a colorless oil.

Run 1 with (*S,S*)-**1**: 182 mg (84% yield, >99:1 dr, 91% ee);

Run 2 with (*R,R*)-**1**: 175 mg (81% yield, >99:1 dr, 91% ee).

The ee was determined via SFC analysis with an AS-H column (20% *i*-PrOH/hexane, flow rate 3.5 mL/min); retention time for compound produced with (*S,S*)-**1**: 3.7 min (minor), 5.6 min (major).

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.73-3.51 (m, 1H), 3.49-3.24 (m, 1H), 3.21-3.05 (m, 1H), l.85-1.51 (m, 9H), 1.39 (s, 9H), 1.03-0.81 (m, 5H), 0.79 (s, 9H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 154.9, 78.6, 61.5, 48.1, 46.7, 46.2, 41.4, 40.6, 32.2, 30.3, 28.4, 28.1, 27.5, 24.2, 23.4;

IR (film) 2964, 2935, 2859, 1691, 1478, 1451, 1389, 1363, 1247, 1167, 1104, 920, 877, 862, 771, 732 cm^{-1};

LRMS (LCMS ESI): calcd for $C_{15}H_{28}NO_2$ [M – (isobutylene) + H] 254.2, found 254.2;

$[\alpha]^{25}_D$ = -49° (c = 1.0, $CHCl_3$) from (*S,S*)-**1**.

***tert*-Butyl (*S*)-2-((1*r*,4*S*)-4-(trifluoromethyl)cyclohexyl)pyrrolidine-1-carboxylate (Table 1, entry 4)**. 1-Iodo-4-(trifluoromethyl)cyclohexane and the organozinc reagent were coupled under the standard cross-coupling conditions (0.70 mmol of the electrophile). Solvent system for chromatography: 18:1 hexane/ethyl acetate. The title compound was isolated as a white solid.

Run 1 with (*S,S*)-**1**: 185 mg (82% yield, >99:1 dr, 92% ee);

Run 2 with (*R,R*)-**1**: 183 mg (81% yield, >99:1 dr, 92% ee).

The ee was determined via SFC analysis with an AD-H column: (10% MeOH/hexane, flow rate 3.0 mL/min); retention time for compound produced with (*S,S*)-**1**: 5.2 min (major), 6.4 min (minor).

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.72-3.55 (m, 1H), 3.49-3.30 (m, 1H), 3.14 (ddd, 1H, *J* = 4.0, 8.0, 12.0 Hz), 1.98-1.82 (m, 3H), 1.79-1.52 (m, 7H), 1.39 (s, 9H), 1.29-1.11 (m, 2H), 1.08-0.83 (m, 2H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 155.1, 127.8 (q, *J* = 277 Hz), 79.1, 61.3, 46.7, 41.9 (q, *J* = 26.5 Hz), 40.4, 38.0, 28.5, 28.3, 27.2, 26.5, 24.9, 24.7;

^{19}F NMR (282 MHz, $CDCl_3$) δ -73.8 (d, *J* = 5.6 Hz);

IR (film) 2940, 2871, 1687, 1457, 1389, 1365, 1336, 1263, 1246, 1224, 1162, 1144, 1121, 1088, 1024, 979, 947, 918, 899, 867, 775 cm^{-1};

LRMS (LCMS ESI): calcd for $C_{12}H_{19}F_3NO_2$ [M – (isobutylene) + H] 266.1, found 266.2;

$[\alpha]^{25}_{D}$ = -41° (c = 1.0, $CHCl_3$) from (*S,S*)-**1**.

***tert*-Butyl (*S*)-2-((1*r*,4*S*)-4-phenylcyclohexyl)pyrrolidine-1-carboxylate (Table 1, entry 5)**. (4-Iodocyclohexyl)benzene and the organozinc reagent were coupled under the standard cross-coupling conditions (0.70 mmol of the electrophile). Solvent system for chromatography: 19:1 hexane/ethyl acetate. The title compound was isolated as a white solid.

Run 1 with (*S,S*)-**1**: 188 mg (81% yield, >99:1 dr, 90% ee);

Run 2 with (*R,R*)-**1**: 189 mg (82% yield, >99:1 dr, 92% ee).

The ee was determined via SFC analysis with an AD-H column(25% *i*-PrOH/hexane, flow rate 3.5 mL/min); retention time for compound produced with (*S,S*)-**1**: 3.8 min (minor), 5.5 min (major).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25-7.17 (m, 2H), 7.16-7.06 (m, 3H), 3.78-3.57 (m, 1H), 3.52-3.30 (m, 1H), 3.23-3.08 (m, 1H), 2.38 (tt, 1H, *J* = 4.0, 12.0 Hz), 1.91-1.80 (m, 2H), 1.80-1.62 (m, 7H), 1.48-1.29 (m, 11H), 1.23-1.00 (m, 2H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 155.1, 147.5, 128.3, 126.8, 125.8, 78.9, 61.6, 46.8, 46.7, 44.5, 40.8, 40.5, 34.2, 33.9, 30.2, 28.6, 28.1, 27.1, 24.1;

IR (film) 2971, 2923, 2853, 1688, 1449, 1389, 1364, 1340, 1253, 1163, 1103, 918, 875, 863, 756, 698 cm^{-1};

LRMS (LCMS ESI): calcd for $C_{17}H_{24}NO_2$ [M – (isobutylene) + H] 274.2, found 274.2;

$[\alpha]^{25}_{D}$ = -48° (c = 1.0, $CHCl_3$) from (*S,S*)-**1**.

***tert*-Butyl (*S*)-2-((1*s*,4*R*)-4-isopropyl-4-methoxycyclohexyl)pyrrolidine-1-carboxylate (Table 1, entry 6)**. 4-Iodo-1-isopropyl-1-methoxycyclohexane and the organozinc reagent were coupled under the standard cross-coupling conditions (0.70 mmol of the electrophile). Solvent system for chromatography: 15:1 hexane/ethyl acetate. The title compound was isolated as a colorless oil.

Run 1 with (*S,S*)-**1**: 218 mg (93% yield, 85:15 dr, 92% ee);

Run 2 with (*R,R*)-**1**: 222 mg (95% yield, 85:15 dr, 91% ee).

The ee was determined via HPLC analysis with an OD-H column (10% *i*-PrOH/hexane, flow rate 1.0 mL/min); retention time for compound with (*S,S*)-**1:** 8.1 min (major), 10.2 min (minor).

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.77-3.52 (m, 1H), 3.50-3.28 (m, 1H), 3.19-3.09 (m, 1H), 3.03 (s, 3H), 1.89-1.64 (m, 6H), 1.64-1.51 (m, 2H), 1.39 (s, 9H), 1.35-1.12 (m, 6H), 0.78 (d, 6H, *J* = 8.0 Hz);

^{13}C NMR (100 MHz, $CDCl_3$) δ 155.0, 78.8, 61.5, 47.1, 41.0, 39.8, 31.5, 28.9, 28.7, 28.5, 27.5, 26.2, 24.7, 22.5, 21.5, 17.1, 16.9.

IR (film) 2932, 2878, 1690, 1455, 1388, 1363, 1251, 1165, 1103, 1076, 904, 876, 772 cm^{-1};

LRMS (LCMS ESI): calcd for $C_{14}H_{24}NO_2$ [M − (isobutylene) - MeOH + H] 238.2, found 238.2;

$[\alpha]^{25}_{D}$ = -47° (c = 1.0, $CHCl_3$) from (*S,S*)-**1**.

***tert*-Butyl (*S*)-2-((1*s*,4*R*)-4-isopropyl-4-methoxycyclohexyl)pyrrolidine-1-carboxylate (Table 1, entry 7)**. 1-Iodo-3,5-dimethylcyclohexane and the organozinc reagent were coupled under the standard cross-coupling conditions (0.70 mmol of the electrophile). Solvent system for chromatography: 18:1 hexane/ethyl acetate. The title compound was isolated as a colorless oil.

Run 1 with (*S,S*)-**1**: 169 mg (85% yield, >99:1 dr, 91% ee);

Run 2 with (*R,R*)-**1**: 161 mg (83% yield, >99:1 dr, 92% ee).

The ee was determined via SFC analysis with an AD-H column (10% MeOH/hexane, flow rate 3.0 mL/min); retention time for compound produced with (*S,S*)-**1**: 3.3 min (major), 4.4 min (minor).

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.80-3.50 (m, 1H), 3.49-3.25 (m, 1H), 3.24-3.04 (ddd, 1H, *J* = 5.1, 6.9, 9.9 Hz), 1.93-1.60 (m, 5H), 1.58-1.13 (m, 14H), 0.82 (d, 3H, *J* = 4.0 Hz), 0.80 (d, 3H, *J* = 4.0 Hz), 0.64-0.35 (m, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 155.0, 78.8, 61.5, 46.4, 44.2, 41.0, 40.4, 38.4, 36.2, 32.4, 32.2, 28.5, 27.4, 24.3, 23.5, 22.8, 22.7;

IR (film) 2948, 2912, 2887, 1690, 1456, 1389, 1363, 1253, 1168, 1104, 771 cm^{-1};

LRMS (LCMS ESI): calcd for $C_{13}H_{24}NO_2$ [M – (isobutylene) + H] 226.2, found 226.2;

$[\alpha]^{25}_D$ = -52° (c = 1.0, $CHCl_3$) from (*S*,*S*)-**1**.

***tert*-Butyl (*S*)-2-((2*R*,4*r*,6*S*)-2,6-dimethyltetrahydro-2*H*-pyran-4-yl)pyrrolidine-1-carboxylate (Table 1, entry 8)**. 4-Iodo-2,6-dimethyltetrahydro-2*H*-pyran and the organozinc reagent were coupled under the standard cross-coupling conditions (0.70 mmol of the electrophile). Solvent system for chromatography: 12:1 hexane/ethyl acetate. The title compound was isolated as a colorless oil.

Run 1 with (*S*,*S*)-**1**: 159 mg (80% yield, >99:1 dr, 91% ee);

Run 2 with (*R*,*R*)-**1**: 169 mg (84% yield, >99:1 dr, 91% ee).

The ee was determined via SFC analysis with an AD-H column (10% MeOH/hexane, flow rate 3.0 mL/min); retention time for compound produced with (*S*,*S*)-**1**: 3.3 min (minor), 3.9 min (major).

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.80-3.51 (m, 1H), 3.52-3.26 (m, 3H), 3.15 (dt, 1H, *J* = 8.0, 12.0 Hz), 2.19-1.60 (m, 5H), 1.51-1.30 (m, 11H), 1.13 (d, 3H, *J* = 8.0 Hz), 1.12 (d, 3H, *J* = 4.0 Hz), 0.98-0.73 (m, 2H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 155.0, 79.0, 73.2, 73.1, 61.0, 46.7, 46.3, 39.2, 38.3, 36.8, 35.0, 28.5, 27.2, 24.2, 22.2, 22.1;

IR (film) 2970, 2930, 1689, 1450, 1387, 1318, 1255, 1167, 1106, 1080, 1028, 918, 770, 516 cm^{-1};

LRMS (LCMS ESI): calcd for $C_{12}H_{22}NO_3$ [M – (isobutylene) + H] 228.2, found 228.2;

$[\alpha]^{25}_D$ = -53° (c = 1.0, $CHCl_3$) from (*S*,*S*)-**1**.

***tert*-Butyl (*S*)-2-((1*S*,3*R*)-3-methylcyclohexyl)pyrrolidine-1-carboxylate (Table 2, entry 1)**. (3*R*)-1-Iodo-3-methylcyclohexane and the organozinc reagent were coupled under the standard cross-coupling conditions (0.70 mmol of the electrophile). Solvent system for chromatography: 20:1 hexane/ethyl acetate. The title compound was isolated as a colorless oil.

Run 1 with (*S,S*)-**1**: 153 mg (81% yield, 97:3 dr);

Run 2 with (*R,R*)-**1**: 151 mg (80% yield, 93:7 dr).

The dr was determined via HPLC analysis with an AD-H column (10% *i*-PrOH/hexane, flow rate 1.0 mL/min); retention time for compound produced with (*S,S*)-**1**: 7.1 min (major), 8.7 min (minor).

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.76-3.50 (m, 1H), 3.49-3.24 (m, 1H), 3.23-3.08 (m, 1H), 1.83-1.62 (m, 6H), 1.61-1.44 (m, 3H), 1.39 (s, 9H), 1.31-1.08 (m, 2H), 0.93-0.64 (m, 5H), 0.52 (q, 1H, J = 12.0 Hz);

^{13}C NMR (100 MHz, $CDCl_3$) δ 155.0, 78.7, 61.6, 46.7, 41.3, 40.6, 36.6, 36.3, 32.5, 29.6, 28.5, 27.3, 26.2, 23.0;

IR (film) 2947, 2920, 1690, 1455, 1388, 1364, 1253, 1168, 1104, 919, 863, 771 cm^{-1};

LRMS (LCMS ESI): calcd for $C_{12}H_{22}NO_2$ [M − (isobutylene) + H] 212.2, found 212.2;

$[\alpha]^{25}_{D}$ = -62° (c = 1.0, $CHCl_3$) from (*S,S*)-**1**.

***tert*-Butyl (*S*)-2-((1*S*,3*R*)-3-(4-bromophenyl)cyclohexyl)pyrrolidine-1-carboxylate (Table 2, entry 2)**. 1-Bromo-4-((1*R*)-3-iodocyclohexyl)benzene and the organozinc reagent were coupled under the standard cross-coupling conditions (0.70 mmol of the electrophile). Solvent system for chromatography: 18:1 hexane/ethyl acetate. The title compound was isolated as a colorless oil.

Run 1 with (*S,S*)-**1**: 170 mg (60% yield, 94:6 dr);

Run 2 with (*R,R*)-**1**: 178 mg (62% yield, 92:8 dr).

The dr was determined via HPLC analysis with an AD-H column (3% *i*-PrOH/hexane, flow rate 1.0 mL/min); retention time for compound produced with (*S,S*)-**1**: 5.2 min (major), 6.4 min (minor).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35-7.26 (m, 2H), 7.04-6.93 (m, 2H), 3.79-3.54 (m, 1H), 3.52-3.23 (m, 1H), 3.20-3.02 (m, 1H), 2.48-2.29 (m, 1H), 2.00-1.52 (m, 9H), 1.48-1.14 (m, 11H), 1.11-0.91 (m, 2H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 155.0, 131.2, 128.5, 119.4, 78.8, 61.5, 46.9, 46.4, 43.5, 35.9, 35.3, 34.0, 29.3, 28.52, 28.46, 26.3;

IR (film) 2971, 2926, 2854, 1690, 1489, 1451, 1390, 1365, 1170, 1109, 1075, 1009, 820 cm^{-1};

LRMS (LCMS ESI): calcd for $C_{17}H_{23}BrNO_2$ [M − (isobutylene) + H] 352.1, found 352.1;

$[\alpha]^{25}_{D}$ = -53° (c = 1.0, $CHCl_3$) from (*S,S*)-**1**.

***tert*-Butyl (*S*)-2-((2*S*,4*R*)-2-phenyltetrahydro-2*H*-pyran-4-yl)pyrrolidine-1-carboxylate (Table 2, entry 3)**. (2*R*,4*S*)-4-Iodo-2-phenyltetrahydro-2*H*-pyran and the organozinc reagent were coupled under the standard cross-coupling conditions (0.70 mmol of the electrophile). Solvent system for chromatography: 20:1 hexane/ethyl acetate. The title compound was isolated as a colorless oil.

Run 1 with (*S*,*S*)-**1**: 209 mg (90% yield, 96:4 dr);

Run 2 with (*R*,*R*)-**1**: 196 mg (84% yield, 94:6 dr).

The dr was determined via HPLC analysis with an IC column (10% *i*-PrOH/hexane, flow rate 1.0 mL/min); retention time for compound produced with (*S*,*S*)-**1**: 10.0 min (minor), 12.0 min (major).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30-7.21 (m, 4H), 7.20-7.13 (m, 1H), 4.31-4.17 (m, 1H), 4.13 (ddd, 1H, *J* = 2.0, 4.0, 12.0 Hz), 3.79-3.56 (m, 1H), 3.57-3.30 (m, 2H), 3.22-3.12 (m, 1H), 2.48-1.83 (m, 1H), 1.82-1.63 (m, 5H), 1.54-1.18 (m, 12H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 155.0, 142.9, 128.2, 127.3, 125.7, 79.7, 79.1, 68.2, 61.1, 47.0, 39.5, 38.5, 37.8, 28.5, 24.4, 23.4;

IR (film) 2970, 2932, 1686, 1452, 1388, 1364, 1252, 1167, 1142, 1097, 1033, 918, 894, 862, 757, 732, 698 cm^{-1};

LRMS (LCMS ESI): calcd for $C_{16}H_{22}NO_3$ [M − (isobutylene) + H] 276.2, found 276.2;

$[\alpha]^{25}_{D}$ = -40° (c = 1.0, $CHCl_3$) from (*S*,*S*)-**1**.

***tert*-Butyl (*S*)-2-((1*S*,3*R*)-3-(4-chlorophenyl)-3-methylcyclohexyl)pyrrolidine-1-carboxylate (Table 2, entry 4)**. (2*R*)-2-(4-Chlorophenyl)-4-iodo-2-methyltetrahydro-2*H*-pyran and the organozinc reagent were coupled under the standard cross-coupling conditions (0.70 mmol of the electrophile). Solvent system for chromatography: 20:1 hexane/ethyl acetate. The title compound was isolated as a colorless oil.

Run 1 with (*S*,*S*)-**1**: 172 mg (65% yield, 86:14 dr);

Run 2 with (*R*,*R*)-**1**: 168 mg (63% yield, 86:14 dr).

The dr was determined via HPLC analysis with an AD-H column (3% *i*-PrOH/hexane, flow rate 1.0 mL/min); retention time for compound produced with (*S*,*S*)-**1**: 8.1 min (minor), 11.7 min (minor), 14.2 (minor), 17.1 min (major).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34-7.05 (m, 4H), 3.82-3.22 (m, 2H), 3.21-3.02 (m, 1H), 2.26-1.95 (m, 1H), 1.81-1.45 (m, 8H), 1.44-1.20 (m, 9H), 1.16 (s, 3H), 1.06-0.98 (m, 1H), 0.98-0.78 (m, 1H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 151.1, 131.1, 130.8, 128.44, 128.41, 128.1, 127.9, 127.7, 126.6, 126.5, 61.5, 61.4, 46.8, 46.4, 39.3, 38.9, 38.7, 38.4, 37.5, 37.4, 37.3, 37.2, 36.3, 35.6, 35.1, 29.5, 28.5, 28.4, 27.4, 24.6, 22.4, 22.3.

IR (film) 2970, 2928, 2864, 1687, 1495, 1454, 1390, 1364, 1165, 1097, 1011, 823, 771, 735 cm^{-1};

LRMS (LCMS ESI): calcd for $C_{18}H_{25}ClNO_2$ [M − (isobutylene) + H] 322.2, found 322.2;

$[\alpha]^{25}_{D}$ = -81° (c = 1.0, $CHCl_3$) from (*S*,*S*)-**1**.

***tert*-Butyl (*S*)-2-((2*S*,4*R*,4a*S*,6*R*,8a*S*)-6-isopropyl-4,4a-dimethyldecahydronaphthalen-2-yl)pyrrolidine-1-carboxylate (Table 2, entry 5)**. (1*R*,4*aS*,7*R*,8*aS*)-3-Iodo-7-isopropyl-1,8a-dimethyldecahydronaphthalene and the organozinc reagent were coupled under the standard cross-coupling conditions (0.70 mmol of the electrophile). Solvent system for chromatography: 20:1 hexane/ethyl acetate. The title compound was isolated as a white solid.

Run 1 with (*S*,*S*)-**1**: 215 mg (81% yield, 95:5 dr);

Run 2 with (*R*,*R*)-**1**: 212 mg (80% yield, 94:6 dr).

The dr was determined via HPLC analysis with an AD-H column (2% *i*-PrOH/hexane, flow rate 1.0 mL/min); retention time for compound produced with (*S*,*S*)-**1**: 6.7 min (minor), 8.5 min (minor), 10.6 min (minor), 9.6 min (major).

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.74-3.51 (m, 1H), 3.43-3.26 (m, 1H), 3.20-3.06 (m, 1H), 1.95-1.49 (m, 7H), 1.39 (s, 9H), 1.33-0.96 (m, 8H), 0.97-0.68 (m, 12H), 0.62-0.46 (m, 4H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 155.0, 78.8, 61.5, 46.5, 46.0, 43.2, 42.2, 41.2, 38.8, 36.5, 34.3, 33.1, 30.3, 29.9, 29.2, 28.5, 27.6, 24.3, 24.0, 20.0, 19.6, 15.3, 15.2, 11.4;

IR (film) 2962, 2914, 2875, 2852, 1690, 1461, 1389, 1364, 1347, 1255, 1162, 1103, 1078, 874, 761 cm^{-1};

LRMS (LCMS ESI): calcd for $C_{20}H_{36}NO_2$ [M − (isobutylene) + H] 322.3, found 322.3;

$[\alpha]^{25}_{D}$ = -34° (c = 1.0, $CHCl_3$) from (*S*,*S*)-**1**.

***tert*-Butyl (*S*)-2-((3*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-10,13-dimethyl-17-((*R*)-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl)pyrrolidine-1-carboxylate (Table 2, entry 6)**. (3*R*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-3-Iodo-10,13-dimethyl-17-((R)-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[a]-phenanthrene and the organozinc reagent were coupled under the standard cross-coupling conditions (0.70 mmol of the electrophile). Solvent system for chromatography: 20:1 hexane/ethyl acetate. The title compound was isolated as a white solid.

Run 1 with (*S,S*)-**1**: 228 mg (62% yield, 87:13 dr);

Run 2 with (*R,R*)-**1**: 189 mg (52% yield, 68:32 dr).

The dr was determined via HPLC analysis with an AD-H column (2% *i*-PrOH/hexane, flow rate 1.0 mL/min); retention time for compound produced with (*S,S*)-**1**: 8.2 min (minor), 8.7 min(minor), 10.1 min (minor), 10.5 min (major).

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.75-3.53 (m, 1H), 3.52-3.24 (m, 1H), 3.24-3.05 (m, 1H), 2.00-1.64 (m, 10H), 1.61-1.15 (m, 23H), 1.14-0.70 (m, 22H), 0.60 (s, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 155.2, 142.7, 119.8, 78.9, 61.5, 56.8, 56.1, 50.4, 46.6, 42.8, 42.3, 39.8, 39.5, 37.2, 36.2, 35.8, 34.8, 32.0, 31.9, 28.6, 28.3, 28.0, 25.8, 24.3, 23.8, 22.9, 22.6, 20.9, 19.5, 18.7, 11.9;

IR (film) 2938, 2867, 2159, 1999, 1698, 1458, 1381, 1339, 1320, 1255, 1170, 1155, 1123, 1099, 967, 936, 888, 804, 770 cm^{-1};

LRMS (LCMS ESI): calcd for $C_{31}H_{54}N$ [M − (isobutylene) - CO_2 + H] 440.4, found 440.5;

$[\alpha]^{25}_{D}$ = -66° (c = 1.0, $CHCl_3$) from (*S,S*)-**1**.

IV. Determination of Stereochemistry of Cross-Coupling Products

(*S*)-2-((1*r*,4*S*)-4-Phenylcyclohexyl)-1-tosylpyrrolidine (Table 1, entry 5). This compound was synthesized under the standard cross-coupling conditions from (4-iodocyclohexyl)benzene and the organozinc reagent, using (*S*,*S*)-**1**, followed by tosylation.

A suitable crystal of $C_{23}H_{29}NO_2S$ was selected for analysis. All measurements were made on a Bruker AXS KAPPA APEX II diffractometer coupled to an APEX II CCD detector with graphite monochromated Cu K_α radiation (λ = 1.54178 Å) for the structure of compound P15146. Using Olex2, the structure was solved by direct methods using SHELXS[6] and refined against F^2 on all data by full-matrix least squares with SHELXL-2014[7] using established refinement techniques.[8]

Table S-1. Crystal data and structure refinement for P15146.

Identification code	P15146	
Empirical formula	$C_{23}H_{29}NO_2S$	
Formula weight	383.53	
Temperature	100(2) K	
Crystal system	monoclinic	
Space group	$P2_1$	
	a = 6.5074(2) Å	α = 90°
	b = 40.4713(16) Å	β = 103.7108(12)°
	c = 7.7313(3) Å	γ = 90°
Volume	1978.12(13) $Å^3$	
Z	4	
Density(calculated)	1.288 Mg/m^3	
Absorption coefficient	1.585 mm^{-1}	
F(000)	824.0	
Crystal size	0.200 × 0.180 × 0.070 mm^3	
Radiation	CuKα (λ = 1.54178)	
Theta range for data collection	4.366° to 149.05°	
Index ranges	$-8 \leq h \leq 7$, $-48 \leq k \leq 42$, $-9 \leq l \leq 9$	
Reflections collected	39151	
Independent reflections	7040 [Rint = 0.0270]	
Data/restraints/parameters	7040/1/489	
Goodness-of-fit on F^2	1.095	
R indexes [I>=2sigma (I)]	R1 = 0.0275, wR2 = 0.0697	
R indexes [all data]	R1 = 0.0283, wR2 = 0.0700	
Largest diff. peak/hole	0.24/-0.41 e/$Å^{-3}$	
Flack parameter	0.050(3)	

Table S-2. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for P15146. Ueq is defined as 1/3 of of the trace of the orthogonalised U^{ij} tensor.

Atom	x	y	z	U(eq)
S(1)	7927.3(7)	2636.1(2)	2326.0(6)	14.86(12)
O(1)	6412(2)	2853.6(4)	1243.4(19)	18.1(3)
O(2)	9856(2)	2556.5(4)	1818(2)	21.9(4)
N(1)	8606(3)	2797.0(5)	4302(2)	16.2(4)
C(1)	6925(3)	2930.7(6)	5142(3)	17.7(5)
C(2)	7701(4)	2818.8(7)	7092(3)	27.2(6)
C(3)	10100(4)	2770.2(7)	7367(3)	29.2(6)
C(4)	10313(3)	2626.5(7)	5615(3)	23.7(5)
C(5)	6644(3)	3303.5(6)	4832(3)	15.3(4)
C(6)	8561(3)	3508.9(6)	5747(3)	16.4(4)
C(7)	8199(3)	3876.5(6)	5335(3)	15.6(4)
C(8)	6228(3)	4008.1(6)	5867(3)	14.5(4)
C(9)	4301(3)	3796.9(6)	4967(3)	16.9(5)
C(10)	4666(3)	3429.2(6)	5376(3)	17.8(5)
C(11)	5833(3)	4374.1(6)	5496(3)	14.9(4)
C(12)	7196(3)	4573.3(6)	4786(3)	16.8(5)
C(13)	6808(4)	4907.8(6)	4462(3)	20.0(5)
C(14)	5030(4)	5056.0(6)	4829(3)	21.3(5)
C(15)	3654(4)	4861.4(6)	5535(3)	20.4(5)
C(16)	4060(3)	4529.1(6)	5870(3)	18.4(5)
C(17)	6618(3)	2257.8(6)	2462(3)	15.7(4)
C(18)	4416(3)	2249.6(6)	2032(3)	17.9(5)
C(19)	3394(4)	1949.1(6)	2013(3)	20.5(5)
C(20)	4508(4)	1653.6(6)	2415(3)	19.4(5)
C(21)	6715(4)	1669.8(6)	2913(3)	21.8(5)
C(22)	7765(3)	1967.2(6)	2935(3)	19.9(5)
C(23)	3377(4)	1326.5(7)	2238(3)	25.8(5)
S(2)	1303.5(7)	5805.0(2)	3124.5(6)	13.69(11)
O(3)	272(2)	5555.1(4)	3923.0(18)	17.4(3)

O(4)	3398(2)	5911.2(4)	4007.5(19)	17.9(3)
N(2)	1428(3)	5674.0(5)	1177(2)	15.8(4)
C(24)	-273(3)	5456.4(6)	90(3)	16.3(4)
C(25)	-206(4)	5549.3(6)	-1834(3)	22.0(5)
C(26)	2006(4)	5692.5(6)	-1701(3)	25.3(5)
C(27)	2468(4)	5879.1(6)	52(3)	23.0(5)
C(28)	150(3)	5091.8(6)	577(3)	13.4(4)
C(29)	-1736(3)	4879.4(6)	-340(3)	16.3(5)
C(30)	-1382(3)	4514.4(6)	130(3)	15.4(4)
C(31)	636(3)	4382.4(6)	-324(3)	13.5(4)
C(32)	2528(3)	4593.7(6)	660(3)	15.4(4)
C(33)	2190(3)	4959.4(6)	174(3)	15.3(4)
C(34)	1039(3)	4016.9(6)	55(3)	14.1(4)
C(35)	-301(3)	3816.8(6)	764(3)	17.3(5)
C(36)	144(4)	3485.4(6)	1130(3)	20.6(5)
C(37)	1958(4)	3343.2(6)	800(3)	20.5(5)
C(38)	3303(3)	3536.9(6)	69(3)	19.6(5)
C(39)	2845(3)	3867.7(6)	-308(3)	16.8(5)
C(40)	-303(3)	6163.2(6)	2896(3)	15.3(4)
C(41)	-2260(3)	6144.3(6)	3317(3)	18.2(5)
C(42)	-3480(3)	6429.7(7)	3230(3)	20.9(5)
C(43)	-2828(3)	6730.0(6)	2672(3)	19.5(5)
C(44)	-856(3)	6743.7(6)	2255(3)	20.1(5)
C(45)	409(3)	6464.9(6)	2383(3)	17.8(5)
C(46)	-4237(4)	7029.2(7)	2556(3)	26.1(5)

Table S-3. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for P15146. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11}+\ldots+2hka^*b^*U^{12}]$.

Atom	U11	U22	U33	U23	U13	U12
S(1)	15.9(2)	13.8(3)	15.9(2)	0.4(2)	5.81(18)	0.89(19)
O(1)	21.5(7)	17.2(10)	15.5(7)	1.9(6)	4.0(6)	1.9(6)
O(2)	19.3(7)	20.8(11)	28.8(8)	0.8(7)	12.1(6)	0.5(6)
N(1)	15.6(8)	15.1(11)	17.4(9)	0.1(7)	3.1(7)	0.8(7)
C(1)	20.7(10)	18.3(14)	15.5(10)	-2.7(9)	7.3(8)	-3.7(9)
C(2)	47.5(15)	19.3(15)	16.3(11)	2.6(9)	10.4(10)	-3.3(11)
C(3)	41.3(14)	20.6(15)	20.7(12)	1.1(10)	-2.3(10)	3.8(11)
C(4)	23.4(10)	19.6(14)	23.7(11)	3(1)	-3.4(8)	-0.1(10)
C(5)	17.3(10)	17.2(13)	12.1(9)	-2.2(8)	4.9(8)	-2.0(8)
C(6)	15.1(9)	16.6(13)	17(1)	-2.2(8)	2.6(8)	-0.2(8)
C(7)	14.9(9)	17.4(13)	15(1)	-0.9(8)	4.2(8)	-1.6(8)
C(8)	15.5(9)	16.9(13)	11.5(9)	-2.2(8)	3.8(8)	-1.2(8)
C(9)	13.4(10)	19.4(14)	18.2(11)	-3.0(8)	4.5(8)	-0.6(8)
C(10)	16.5(10)	19.9(14)	18.2(11)	-3.4(9)	6.5(8)	-3.2(8)
C(11)	16.4(9)	18.5(13)	8.5(9)	-2.1(8)	0.1(7)	1.2(8)
C(12)	17.5(10)	19.0(14)	13.7(10)	-2.1(8)	3.4(8)	1.1(8)
C(13)	24.4(11)	21.3(14)	13(1)	0.3(9)	2.2(8)	-2.1(9)
C(14)	28.5(11)	18.2(15)	14.6(10)	0.2(9)	-0.3(8)	4.1(9)
C(15)	22.2(11)	24.3(15)	13.9(10)	-2.1(9)	2.5(8)	8.2(9)
C(16)	19.7(10)	23.3(14)	12.5(10)	-1.1(8)	4.3(8)	1.0(9)
C(17)	17.3(10)	17.5(13)	12.7(9)	-2.3(8)	4.3(8)	-0.4(8)
C(18)	18.6(10)	18.3(13)	17.5(10)	-0.5(9)	5.9(8)	1.7(9)
C(19)	17.7(10)	24.9(15)	19.2(11)	-2.8(9)	5.0(8)	-2.2(9)
C(20)	24.6(11)	19.4(14)	14.1(10)	-1.2(8)	4.7(8)	-3.7(9)
C(21)	25.4(11)	16.6(14)	22.1(11)	0.2(9)	2.7(9)	2.5(9)
C(22)	19.4(10)	19.0(14)	21.0(11)	-0.8(9)	3.9(8)	2.4(9)
C(23)	30.0(12)	20.6(15)	25.5(12)	-0.3(10)	4.2(10)	-6.6(10)
S(2)	16.1(2)	13.3(3)	11.8(2)	-1.23(19)	3.44(17)	-0.69(19)
O(3)	23.1(7)	15.5(9)	14.8(7)	-1.1(6)	6.8(6)	-1.9(6)
O(4)	18.1(7)	19.5(10)	14.8(7)	-1.6(6)	1.5(6)	-0.5(6)

N(2)	22.1(9)	13.6(11)	12.2(8)	-2.3(7)	5.4(7)	-3.5(7)
C(24)	18.2(10)	15.9(13)	14(1)	-3.3(8)	1.9(8)	0.0(8)
C(25)	34.1(12)	15.6(14)	14.2(10)	1.4(9)	1.4(9)	0.9(9)
C(26)	43.8(14)	18.8(15)	16.1(11)	-1.0(9)	12.9(10)	-7(1)
C(27)	33.8(12)	19.6(15)	18.4(11)	-2.4(9)	11.7(9)	-9(1)
C(28)	14.6(9)	13.8(12)	12.0(9)	-2.5(8)	3.4(7)	-1.4(8)
C(29)	12.6(9)	18.1(14)	17.7(10)	-3.0(8)	2.5(8)	0.3(8)
C(30)	14.0(9)	15.6(13)	16.4(10)	-2.8(8)	3.2(8)	-1.0(8)
C(31)	15.3(9)	14.9(12)	10.6(9)	-0.6(8)	3.7(7)	-1.3(8)
C(32)	14.7(10)	14.3(13)	17(1)	-1.6(8)	3.1(8)	-0.1(8)
C(33)	14.8(9)	17.4(13)	14.4(9)	-1.4(8)	4.8(8)	-1.4(8)
C(34)	16.6(9)	15.9(13)	8.8(9)	-2.5(8)	0.8(7)	-0.7(8)
C(35)	18.8(10)	18.8(14)	14.1(10)	-2.0(8)	3.5(8)	-3.0(8)
C(36)	27.0(11)	18.6(14)	15.6(10)	1.3(9)	3.7(8)	-5.8(9)
C(37)	29.9(11)	14.5(14)	14.5(10)	-0.8(9)	-0.3(8)	-0.6(9)
C(38)	23.2(11)	18.8(14)	15.6(10)	-2.4(9)	2.5(8)	4.6(9)
C(39)	19.5(10)	19.0(14)	12.3(10)	-0.3(8)	4.3(8)	0.1(9)
C(40)	18.1(10)	14.6(13)	12.2(10)	-3.6(8)	1.5(8)	0.1(8)
C(41)	19(1)	17.8(14)	18.3(11)	-0.6(9)	5.3(8)	-2.3(8)
C(42)	15.4(10)	23.6(15)	23.7(12)	-1.7(9)	4.5(9)	-1.4(9)
C(43)	19.8(10)	18.3(14)	17.8(11)	-2.9(9)	-0.5(8)	1.8(9)
C(44)	22.7(11)	15.6(14)	20.8(11)	-0.8(9)	2.4(9)	-3.8(9)
C(45)	17.3(10)	17.0(13)	19.3(11)	-1.7(8)	4.5(8)	-2.7(8)
C(46)	23.8(11)	22.3(16)	31.1(13)	0.1(10)	4.3(10)	3.4(10)

Table S-4. Bond Lengths for P15146.

Atom	Atom	Length / Å	Atom	Atom	Length / Å
S(1)	O(1)	1.4337(16)	S(2)	O(3)	1.4324(16)
S(1)	O(2)	1.4379(15)	S(2)	O(4)	1.4377(15)
S(1)	N(1)	1.6229(18)	S(2)	N(2)	1.6164(17)
S(1)	C(17)	1.768(2)	S(2)	C(40)	1.771(2)
N(1)	C(4)	1.485(3)	N(2)	C(27)	1.477(3)
N(1)	C(1)	1.499(3)	N(2)	C(24)	1.505(3)
C(1)	C(5)	1.532(3)	C(24)	C(28)	1.532(3)
C(1)	C(2)	1.541(3)	C(24)	C(25)	1.545(3)
C(2)	C(3)	1.538(4)	C(25)	C(26)	1.532(3)
C(3)	C(4)	1.510(3)	C(26)	C(27)	1.518(3)
C(5)	C(6)	1.526(3)	C(28)	C(29)	1.528(3)
C(5)	C(10)	1.533(3)	C(28)	C(33)	1.531(3)
C(6)	C(7)	1.528(3)	C(29)	C(30)	1.526(3)
C(7)	C(8)	1.532(3)	C(30)	C(31)	1.534(3)
C(8)	C(11)	1.519(3)	C(31)	C(34)	1.519(3)
C(8)	C(9)	1.541(3)	C(31)	C(32)	1.543(3)
C(9)	C(10)	1.528(3)	C(32)	C(33)	1.530(3)
C(11)	C(16)	1.403(3)	C(34)	C(35)	1.394(3)
C(11)	C(12)	1.403(3)	C(34)	C(39)	1.407(3)
C(12)	C(13)	1.389(4)	C(35)	C(36)	1.387(4)
C(13)	C(14)	1.391(3)	C(36)	C(37)	1.390(3)
C(14)	C(15)	1.397(3)	C(37)	C(38)	1.391(3)
C(15)	C(16)	1.383(4)	C(38)	C(39)	1.388(3)
C(17)	C(18)	1.393(3)	C(40)	C(41)	1.390(3)
C(17)	C(22)	1.394(3)	C(40)	C(45)	1.397(3)
C(18)	C(19)	1.384(3)	C(41)	C(42)	1.394(3)
C(19)	C(20)	1.395(3)	C(42)	C(43)	1.389(4)
C(20)	C(21)	1.397(3)	C(43)	C(44)	1.397(3)
C(20)	C(23)	1.505(3)	C(43)	C(46)	1.508(3)
C(21)	C(22)	1.382(3)	C(44)	C(45)	1.387(3)

Table S-5. Bond Angles for P15146.

Atom	Atom	Atom	Angle / °	Atom	Atom	Atom	Angle / °
O(1)	S(1)	O(2)	120.13(9)	O(3)	S(2)	O(4)	119.67(9)
O(1)	S(1)	N(1)	107.42(10)	O(3)	S(2)	N(2)	107.58(9)
O(2)	S(1)	N(1)	106.66(9)	O(4)	S(2)	N(2)	106.82(9)
O(1)	S(1)	C(17)	106.99(10)	O(3)	S(2)	C(40)	107.16(10)
O(2)	S(1)	C(17)	106.65(10)	O(4)	S(2)	C(40)	105.85(10)
N(1)	S(1)	C(17)	108.61(10)	N(2)	S(2)	C(40)	109.52(10)
C(4)	N(1)	C(1)	112.10(17)	C(27)	N(2)	C(24)	112.28(16)
C(4)	N(1)	S(1)	116.70(16)	C(27)	N(2)	S(2)	119.69(15)
C(1)	N(1)	S(1)	119.26(14)	C(24)	N(2)	S(2)	121.28(14)
N(1)	C(1)	C(5)	111.11(18)	N(2)	C(24)	C(28)	111.17(17)
N(1)	C(1)	C(2)	102.37(18)	N(2)	C(24)	C(25)	102.13(17)
C(5)	C(1)	C(2)	116.24(19)	C(28)	C(24)	C(25)	115.26(18)
C(3)	C(2)	C(1)	105.01(19)	C(26)	C(25)	C(24)	105.53(17)
C(4)	C(3)	C(2)	103.39(18)	C(27)	C(26)	C(25)	103.44(18)
N(1)	C(4)	C(3)	102.8(2)	N(2)	C(27)	C(26)	102.98(18)
C(6)	C(5)	C(1)	114.18(18)	C(29)	C(28)	C(33)	110.37(17)
C(6)	C(5)	C(10)	109.80(18)	C(29)	C(28)	C(24)	110.49(17)
C(1)	C(5)	C(10)	111.16(18)	C(33)	C(28)	C(24)	113.65(17)
C(5)	C(6)	C(7)	111.42(17)	C(30)	C(29)	C(28)	112.01(17)
C(6)	C(7)	C(8)	112.31(18)	C(29)	C(30)	C(31)	111.80(18)
C(11)	C(8)	C(7)	113.77(18)	C(34)	C(31)	C(30)	114.40(18)
C(11)	C(8)	C(9)	111.85(17)	C(34)	C(31)	C(32)	111.33(17)
C(7)	C(8)	C(9)	109.23(17)	C(30)	C(31)	C(32)	108.68(17)
C(10)	C(9)	C(8)	112.11(18)	C(33)	C(32)	C(31)	111.32(17)
C(9)	C(10)	C(5)	111.46(18)	C(32)	C(33)	C(28)	111.69(17)
C(16)	C(11)	C(12)	116.8(2)	C(35)	C(34)	C(39)	117.3(2)
C(16)	C(11)	C(8)	120.5(2)	C(35)	C(34)	C(31)	123.11(19)
C(12)	C(11)	C(8)	122.68(19)	C(39)	C(34)	C(31)	119.57(19)
C(13)	C(12)	C(11)	121.7(2)	C(36)	C(35)	C(34)	121.5(2)
C(12)	C(13)	C(14)	120.5(2)	C(35)	C(36)	C(37)	120.5(2)
C(13)	C(14)	C(15)	118.5(2)	C(36)	C(37)	C(38)	119.0(2)

C(16) C(15) C(14)	120.7(2)	C(39) C(38) C(37)	120.3(2)
C(15) C(16) C(11)	121.7(2)	C(38) C(39) C(34)	121.3(2)
C(18) C(17) C(22)	119.9(2)	C(41) C(40) C(45)	119.9(2)
C(18) C(17) S(1)	119.31(18)	C(41) C(40) S(2)	118.94(18)
C(22) C(17) S(1)	120.71(16)	C(45) C(40) S(2)	121.08(16)
C(19) C(18) C(17)	119.2(2)	C(40) C(41) C(42)	119.1(2)
C(18) C(19) C(20)	121.9(2)	C(43) C(42) C(41)	121.8(2)
C(19) C(20) C(21)	117.8(2)	C(42) C(43) C(44)	118.1(2)
C(19) C(20) C(23)	121.1(2)	C(42) C(43) C(46)	119.7(2)
C(21) C(20) C(23)	121.0(2)	C(44) C(43) C(46)	122.2(2)
C(22) C(21) C(20)	121.1(2)	C(45) C(44) C(43)	120.9(2)
C(21) C(22) C(17)	119.9(2)	C(44) C(45) C(40)	120.0(2)

Table S-6. Torsion Angles for P15146.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O(1)	S(1)	N(1)	C(4)	-174.92(16)	O(3)	S(2)	N(2)	C(27)	-178.54(17)
O(2)	S(1)	N(1)	C(4)	-44.91(19)	O(4)	S(2)	N(2)	C(27)	-48.89(19)
C(17)	S(1)	N(1)	C(4)	69.69(18)	C(40)	S(2)	N(2)	C(27)	65.31(19)
O(1)	S(1)	N(1)	C(1)	45.22(19)	O(3)	S(2)	N(2)	C(24)	32.47(19)
O(2)	S(1)	N(1)	C(1)	175.23(16)	O(4)	S(2)	N(2)	C(24)	162.12(16)
C(17)	S(1)	N(1)	C(1)	-70.17(19)	C(40)	S(2)	N(2)	C(24)	-83.68(19)
C(4)	N(1)	C(1)	C(5)	123.1(2)	C(27)	N(2)	C(24)	C(28)	122.9(2)
S(1)	N(1)	C(1)	C(5)	-95.4(2)	S(2)	N(2)	C(24)	C(28)	-86.1(2)
C(4)	N(1)	C(1)	C(2)	-1.7(2)	C(27)	N(2)	C(24)	C(25)	-0.6(2)
S(1)	N(1)	C(1)	C(2)	139.89(17)	S(2)	N(2)	C(24)	C(25)	150.49(16)
N(1)	C(1)	C(2)	C(3)	23.8(2)	N(2)	C(24)	C(25)	C(26)	22.6(2)
C(5)	C(1)	C(2)	C(3)	-97.5(2)	C(28)	C(24)	C(25)	C(26)	-98.1(2)
C(1)	C(2)	C(3)	C(4)	-37.4(3)	C(24)	C(25)	C(26)	C(27)	-36.2(2)
C(1)	N(1)	C(4)	C(3)	-21.3(3)	C(24)	N(2)	C(27)	C(26)	-21.6(3)
S(1)	N(1)	C(4)	C(3)	-163.93(17)	S(2)	N(2)	C(27)	C(26)	-173.17(16)
C(2)	C(3)	C(4)	N(1)	35.2(2)	C(25)	C(26)	C(27)	N(2)	34.7(2)
N(1)	C(1)	C(5)	C(6)	-65.7(2)	N(2)	C(24)	C(28)	C(29)	172.06(16)
C(2)	C(1)	C(5)	C(6)	50.8(3)	C(25)	C(24)	C(28)	C(29)	-72.4(2)
N(1)	C(1)	C(5)	C(10)	169.39(16)	N(2)	C(24)	C(28)	C(33)	-63.2(2)
C(2)	C(1)	C(5)	C(10)	-74.1(2)	C(25)	C(24)	C(28)	C(33)	52.3(2)
C(1)	C(5)	C(6)	C(7)	178.20(17)	C(33)	C(28)	C(29)	C(30)	54.1(2)
C(10)	C(5)	C(6)	C(7)	-56.2(2)	C(24)	C(28)	C(29)	C(30)	-179.35(17)
C(5)	C(6)	C(7)	C(8)	57.0(2)	C(28)	C(29)	C(30)	C(31)	-56.6(2)
C(6)	C(7)	C(8)	C(11)	179.33(16)	C(29)	C(30)	C(31)	C(34)	-178.00(16)
C(6)	C(7)	C(8)	C(9)	-54.9(2)	C(29)	C(30)	C(31)	C(32)	56.9(2)
C(11)	C(8)	C(9)	C(10)	-178.47(17)	C(34)	C(31)	C(32)	C(33)	175.92(16)
C(7)	C(8)	C(9)	C(10)	54.7(2)	C(30)	C(31)	C(32)	C(33)	-57.2(2)
C(8)	C(9)	C(10)	C(5)	-56.5(2)	C(31)	C(32)	C(33)	C(28)	57.2(2)
C(6)	C(5)	C(10)	C(9)	56.1(2)	C(29)	C(28)	C(33)	C(32)	-54.5(2)
C(1)	C(5)	C(10)	C(9)	-176.58(17)	C(24)	C(28)	C(33)	C(32)	-179.27(16)
C(7)	C(8)	C(11)	C(16)	178.44(17)	C(30)	C(31)	C(34)	C(35)	-0.3(3)

C(9)	C(8)	C(11)	C(16)	54.1(2)	C(32)	C(31)	C(34)	C(35)	123.4(2)
C(7)	C(8)	C(11)	C(12)	-2.0(3)	C(30)	C(31)	C(34)	C(39)	-179.97(17)
C(9)	C(8)	C(11)	C(12)	-126.4(2)	C(32)	C(31)	C(34)	C(39)	-56.3(2)
C(16)	C(11)	C(12)	C(13)	-0.3(3)	C(39)	C(34)	C(35)	C(36)	1.2(3)
C(8)	C(11)	C(12)	C(13)	-179.81(19)	C(31)	C(34)	C(35)	C(36)	-178.52(19)
C(11)	C(12)	C(13)	C(14)	-0.3(3)	C(34)	C(35)	C(36)	C(37)	0.2(3)
C(12)	C(13)	C(14)	C(15)	0.2(3)	C(35)	C(36)	C(37)	C(38)	-1.1(3)
C(13)	C(14)	C(15)	C(16)	0.4(3)	C(36)	C(37)	C(38)	C(39)	0.6(3)
C(14)	C(15)	C(16)	C(11)	-0.9(3)	C(37)	C(38)	C(39)	C(34)	0.8(3)
C(12)	C(11)	C(16)	C(15)	0.8(3)	C(35)	C(34)	C(39)	C(38)	-1.7(3)
C(8)	C(11)	C(16)	C(15)	-179.60(19)	C(31)	C(34)	C(39)	C(38)	178.03(18)
O(1)	S(1)	C(17)	C(18)	-17.80(19)	O(3)	S(2)	C(40)	C(41)	-5.87(19)
O(2)	S(1)	C(17)	C(18)	-147.52(16)	O(4)	S(2)	C(40)	C(41)	-134.64(16)
N(1)	S(1)	C(17)	C(18)	97.87(18)	N(2)	S(2)	C(40)	C(41)	110.54(17)
O(1)	S(1)	C(17)	C(22)	160.01(17)	O(3)	S(2)	C(40)	C(45)	171.15(16)
O(2)	S(1)	C(17)	C(22)	30.3(2)	O(4)	S(2)	C(40)	C(45)	42.38(19)
N(1)	S(1)	C(17)	C(22)	-84.32(19)	N(2)	S(2)	C(40)	C(45)	-72.44(19)
C(22)	C(17)	C(18)	C(19)	-2.5(3)	C(45)	C(40)	C(41)	C(42)	-0.4(3)
S(1)	C(17)	C(18)	C(19)	175.31(16)	S(2)	C(40)	C(41)	C(42)	176.61(17)
C(17)	C(18)	C(19)	C(20)	0.1(3)	C(40)	C(41)	C(42)	C(43)	2.4(3)
C(18)	C(19)	C(20)	C(21)	2.5(3)	C(41)	C(42)	C(43)	C(44)	-2.4(3)
C(18)	C(19)	C(20)	C(23)	-174.8(2)	C(41)	C(42)	C(43)	C(46)	178.4(2)
C(19)	C(20)	C(21)	C(22)	-2.7(3)	C(42)	C(43)	C(44)	C(45)	0.5(3)
C(23)	C(20)	C(21)	C(22)	174.6(2)	C(46)	C(43)	C(44)	C(45)	179.7(2)
C(20)	C(21)	C(22)	C(17)	0.3(3)	C(43)	C(44)	C(45)	C(40)	1.4(3)
C(18)	C(17)	C(22)	C(21)	2.3(3)	C(41)	C(40)	C(45)	C(44)	-1.4(3)
S(1)	C(17)	C(22)	C(21)	-175.45(17)	S(2)	C(40)	C(45)	C(44)	-178.43(16)

Table S-7. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for P15146.

Atom	x	y	z	U(eq)
H(1)	5557	2818	4605	21
H(2A)	7393	2989	7914	33
H(2B)	7009	2610	7300	33
H(3A)	10860	2983	7612	35
H(3B)	10656	2616	8362	35
H(4A)	11720	2675	5395	28
H(4B)	10092	2384	5580	28
H(5)	6416	3342	3522	18
H(6A)	9817	3434	5343	20
H(6B)	8846	3475	7051	20
H(7A)	8044	3913	4044	19
H(7B)	9452	4002	5980	19
H(8)	6456	3976	7182	17
H(9A)	3050	3871	5381	20
H(9B)	3997	3831	3662	20
H(10A)	3418	3302	4730	21
H(10B)	4828	3392	6667	21
H(12)	8416	4477	4521	20
H(13)	7764	5036	3985	24
H(14)	4757	5285	4606	26
H(15)	2428	4958	5788	24
H(16)	3112	4402	6367	22
H(18)	3624	2448	1755	21
H(19)	1892	1944	1719	25
H(21)	7507	1473	3242	26
H(22)	9266	1974	3271	24
H(23A)	2022	1352	2568	39
H(23B)	4249	1164	3026	39
H(23C)	3123	1250	1003	39
H(24)	-1674	5522	306	20

H(25A)	-439	5352	-2611	26
H(25B)	-1308	5715	-2327	26
H(26A)	3055	5515	-1684	30
H(26B)	2013	5843	-2709	30
H(27A)	4009	5895	569	28
H(27B)	1857	6104	-103	28
H(28)	298	5071	1890	16
H(29A)	-3017	4957	18	20
H(29B)	-1981	4906	-1646	20
H(30A)	-2612	4385	-530	18
H(30B)	-1279	4484	1419	18
H(31)	484	4416	-1630	16
H(32A)	2715	4567	1961	19
H(32B)	3834	4515	344	19
H(33A)	2126	4988	-1110	18
H(33B)	3407	5089	854	18
H(35)	-1546	3910	1002	21
H(36)	-799	3355	1610	25
H(37)	2273	3117	1069	25
H(38)	4541	3442	-173	23
H(39)	3769	3996	-822	20
H(41)	-2761	5940	3659	22
H(42)	-4794	6419	3562	25
H(44)	-374	6947	1879	24
H(45)	1761	6479	2122	21
H(46A)	-5583	6987	1699	39
H(46B)	-3541	7220	2164	39
H(46C)	-4502	7075	3729	39

(*R*)-2-((1*s*,3*R*,5*S*)-3,5-Dimethylcyclohexyl)-1-tosylpyrrolidine (Table 1, entry 7). This compound was synthesized under the standard cross-coupling conditions from 1-iodo-3,5-dimethylcyclohexane and the organozinc reagent, using (*R*,*R*)-**1**, followed by tosylation.

A suitable crystal of $C_{19}H_{29}NO_2S$ was selected for analysis. All measurements were made on a Bruker AXS KAPPA APEX II diffractometer coupled to an APEX II CCD detector with graphite monochromated Mo K_α radiation (λ = 0.71073 Å) for the structure of compound A15018. Using Olex2, the structure was solved by direct methods using SHELXS[6] and refined against F^2 on all data by full-matrix least squares with SHELXL-2014[7] using established refinement techniques.[8]

Table S-1. Crystal data and structure refinement for A15018.

Identification code	A15018	
Empirical formula	$C_{19}H_{29}NO_2S$	
Formula weight	335.49	
Temperature	289 K	
Crystal system	orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 7.9804(6) Å	α = 90°
	b = 11.1586(9) Å	β = 90°
	c = 21.4932(17) Å	γ = 90°
Volume	1914.0(3) $Å^3$	
Z	4	
Density(calculated)	1.164 Mg/m^3	
Absorption coefficient	0.178 mm^{-1}	
F(000)	728.0	
Crystal size	0.400 × 0.330 × 0.190 mm^3	
Radiation	MoKα (λ = 0.71073)	
Theta range for data collection	4.112 to 61.006°	
Index ranges	$-11 \leq h \leq 11$, $-15 \leq k \leq 15$, $-30 \leq l \leq 30$	
Reflections collected	89468	
Independent reflections	5852 [Rint = 0.0355]	
Data/restraints/parameters	5852/0/211	
Goodness-of-fit on F^2	1.118	
R indexes [I>=2sigma(I)]	R1 = 0.0473, wR2 = 0.1190	
R indexes [all data]	R1 = 0.0611, wR2 = 0.1290	
Largest diff. peak/hole	0.32 and -0.19 e/$Å^{-3}$	
Flack parameter	0.013(12)	

Table S-2. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for A15018. Ueq is defined as 1/3 of of the trace of the orthogonalised U^{ij} tensor.

Atom	x	y	z	U(eq)
S(1)	5450.4(8)	1073.0(5)	2887.0(3)	53.94(16)
O(1)	4546(2)	2148.0(14)	3022.1(9)	62.3(4)
O(2)	4739(3)	-60.4(16)	3055.1(10)	77.9(6)
N(1)	7262(3)	1164.2(18)	3235.9(9)	58.8(5)
C(1)	8343(5)	80(3)	3242.9(16)	89(1)
C(2)	9996(5)	543(4)	3453.6(17)	99.2(13)
C(3)	10101(4)	1771(4)	3138.7(15)	87.7(10)
C(4)	8297(3)	2268(2)	3137.4(10)	57.2(5)
C(5)	7908(3)	3235(2)	3625.2(10)	50.6(5)
C(6)	8460(3)	2922(2)	4284.9(10)	56.7(5)
C(7)	8016(3)	3902(3)	4750.6(10)	59.3(5)
C(8)	8746(4)	5093(3)	4535.4(11)	66.1(6)
C(9)	8197(4)	5441(2)	3876.5(11)	61.1(6)
C(10)	8641(3)	4436(2)	3425.1(10)	59.8(6)
C(11)	8608(5)	3580(3)	5407.3(12)	85(1)
C(12)	8956(5)	6638(3)	3673.4(16)	88(1)
C(13)	5834(3)	1056.9(17)	2076.4(10)	48.8(4)
C(14)	6181(3)	-25.3(19)	1780.6(11)	53.3(5)
C(15)	6456(4)	-25(2)	1147.3(12)	63.0(6)
C(16)	6389(4)	1030(3)	799.4(12)	68.8(6)
C(17)	6054(4)	2092(3)	1109.2(14)	71.0(7)
C(18)	5779(4)	2116(2)	1742.4(12)	58.8(6)
C(19)	6619(6)	1001(4)	100.7(14)	103.7(12)

Table S-3. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for A15018. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11}+\ldots+2hka^*b^*U^{12}]$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	69.1(3)	35.2(2)	57.6(3)	-3.2(2)	7.1(2)	-3.6(2)
O(1)	65.4(10)	44.4(8)	77.2(11)	-11.9(7)	8.4(9)	-2.4(8)
O(2)	106.7(16)	43.1(8)	84.0(12)	0.7(8)	23.5(11)	-15.6(10)
N(1)	77.6(13)	49.3(10)	49.4(9)	0.6(8)	-1.1(9)	8.3(10)
C(1)	118(3)	71.7(18)	76.9(18)	-5.9(15)	-19.4(19)	37.6(19)
C(2)	107(3)	117(3)	73.3(19)	-14.5(19)	-12.1(18)	50(2)
C(3)	71.2(18)	133(3)	59.1(15)	-22.9(18)	11.3(13)	16(2)
C(4)	63.2(13)	67.8(14)	40.6(9)	-6.0(9)	-0.5(9)	-2.9(12)
C(5)	52.7(11)	59.1(12)	40.0(9)	-2.3(8)	-1.4(8)	-5(1)
C(6)	60.6(12)	67.7(14)	41.7(10)	0.0(9)	-1.0(9)	0.6(11)
C(7)	62.9(13)	75.2(14)	39.7(9)	-3.8(11)	1.2(9)	-2.0(13)
C(8)	74.6(15)	75.6(16)	48.2(11)	-10.6(11)	-2.8(11)	-14.9(14)
C(9)	67.8(14)	61.9(14)	53.6(12)	-1.6(10)	-2.6(11)	-13.2(12)
C(10)	65.9(13)	71.2(14)	42.3(10)	0.2(10)	-0.3(10)	-14.3(12)
C(11)	109(2)	106(2)	40.2(11)	-1.5(13)	-3.2(14)	4(2)
C(12)	120(3)	69.3(18)	75.0(18)	0.8(14)	0.8(18)	-26.1(19)
C(13)	57.8(10)	34.0(8)	54.5(10)	-3.7(9)	-5.8(9)	-2.0(8)
C(14)	63.2(13)	35.9(9)	60.8(12)	-5.3(9)	-7.7(10)	-0.9(9)
C(15)	66.0(14)	61.2(14)	62.0(13)	-18.6(11)	-9.7(11)	8.3(12)
C(16)	72.8(15)	80.2(17)	53.5(12)	0.2(13)	-8.6(11)	8.1(16)
C(17)	87.7(19)	59.1(14)	66.2(15)	14.3(12)	-9.7(14)	5.6(14)
C(18)	73.6(15)	39.1(9)	63.7(13)	-0.6(9)	-6.6(12)	2.8(10)
C(19)	120(3)	136(3)	55.0(14)	4.6(19)	-11.2(17)	19(3)

Table S-4. Bond Lengths for A15018.

Atom	Atom	Length / Å
S(1)	O(1)	1.4298(17)
S(1)	O(2)	1.4326(18)
S(1)	N(1)	1.632(2)
S(1)	C(13)	1.769(2)
N(1)	C(1)	1.486(4)
N(1)	C(4)	1.498(3)
C(1)	C(2)	1.488(6)
C(2)	C(3)	1.530(6)
C(3)	C(4)	1.543(4)
C(4)	C(5)	1.536(3)
C(5)	C(10)	1.524(3)
C(5)	C(6)	1.525(3)
C(6)	C(7)	1.524(3)
C(7)	C(8)	1.523(4)
C(7)	C(11)	1.531(3)
C(8)	C(9)	1.532(3)
C(9)	C(10)	1.525(4)
C(9)	C(12)	1.530(4)
C(13)	C(18)	1.383(3)
C(13)	C(14)	1.393(3)
C(14)	C(15)	1.379(4)
C(15)	C(16)	1.396(4)
C(16)	C(17)	1.385(4)
C(16)	C(19)	1.513(4)
C(17)	C(18)	1.379(4)

Table S-5. Bond Angles for A15018.

Atom	Atom	Atom	Angle / °	Atom	Atom	Atom	Angle / °
O(1)	S(1)	O(2)	119.29(12)	C(8)	C(7)	C(6)	109.72(19)
O(1)	S(1)	N(1)	107.56(11)	C(8)	C(7)	C(11)	111.5(2)
O(2)	S(1)	N(1)	106.88(14)	C(6)	C(7)	C(11)	111.4(2)
O(1)	S(1)	C(13)	107.21(11)	C(7)	C(8)	C(9)	113.1(2)
O(2)	S(1)	C(13)	107.93(11)	C(10)	C(9)	C(12)	111.6(2)
N(1)	S(1)	C(13)	107.45(10)	C(10)	C(9)	C(8)	109.6(2)
C(1)	N(1)	C(4)	110.6(2)	C(12)	C(9)	C(8)	111.9(2)
C(1)	N(1)	S(1)	117.9(2)	C(5)	C(10)	C(9)	112.21(19)
C(4)	N(1)	S(1)	118.35(16)	C(18)	C(13)	C(14)	120.7(2)
N(1)	C(1)	C(2)	103.6(3)	C(18)	C(13)	S(1)	119.80(16)
C(1)	C(2)	C(3)	103.0(3)	C(14)	C(13)	S(1)	119.52(16)
C(2)	C(3)	C(4)	105.8(3)	C(15)	C(14)	C(13)	118.8(2)
N(1)	C(4)	C(5)	111.70(19)	C(14)	C(15)	C(16)	121.5(2)
N(1)	C(4)	C(3)	102.6(2)	C(17)	C(16)	C(15)	118.1(2)
C(5)	C(4)	C(3)	116.1(2)	C(17)	C(16)	C(19)	121.3(3)
C(10)	C(5)	C(6)	110.66(19)	C(15)	C(16)	C(19)	120.6(3)
C(10)	C(5)	C(4)	110.33(18)	C(18)	C(17)	C(16)	121.4(2)
C(6)	C(5)	C(4)	114.5(2)	C(17)	C(18)	C(13)	119.4(2)
C(7)	C(6)	C(5)	112.3(2)				

Table S-6. Torsion Angles for A15018.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O(1)	S(1)	N(1)	C(1)	171.3(2)	C(6)	C(7)	C(8)	C(9)	55.5(3)
O(2)	S(1)	N(1)	C(1)	42.1(2)	C(11)	C(7)	C(8)	C(9)	179.4(3)
C(13)	S(1)	N(1)	C(1)	-73.5(2)	C(7)	C(8)	C(9)	C(10)	-55.5(3)
O(1)	S(1)	N(1)	C(4)	-51.17(19)	C(7)	C(8)	C(9)	C(12)	-179.8(3)
O(2)	S(1)	N(1)	C(4)	179.61(17)	C(6)	C(5)	C(10)	C(9)	-55.6(3)
C(13)	S(1)	N(1)	C(4)	63.97(18)	C(4)	C(5)	C(10)	C(9)	176.6(2)
C(4)	N(1)	C(1)	C(2)	26.6(3)	C(12)	C(9)	C(10)	C(5)	179.4(3)
S(1)	N(1)	C(1)	C(2)	167.1(2)	C(8)	C(9)	C(10)	C(5)	54.9(3)
N(1)	C(1)	C(2)	C(3)	-37.2(3)	O(1)	S(1)	C(13)	C(18)	20.9(2)
C(1)	C(2)	C(3)	C(4)	35.4(3)	O(2)	S(1)	C(13)	C(18)	150.6(2)
C(1)	N(1)	C(4)	C(5)	-129.4(2)	N(1)	S(1)	C(13)	C(18)	-94.5(2)
S(1)	N(1)	C(4)	C(5)	90.2(2)	O(1)	S(1)	C(13)	C(14)	-158.81(19)
C(1)	N(1)	C(4)	C(3)	-4.4(2)	O(2)	S(1)	C(13)	C(14)	-29.1(2)
S(1)	N(1)	C(4)	C(3)	-144.75(19)	N(1)	S(1)	C(13)	C(14)	85.8(2)
C(2)	C(3)	C(4)	N(1)	-19.0(3)	C(18)	C(13)	C(14)	C(15)	-0.6(4)
C(2)	C(3)	C(4)	C(5)	103.1(3)	S(1)	C(13)	C(14)	C(15)	179.15(19)
N(1)	C(4)	C(5)	C(10)	-166.16(19)	C(13)	C(14)	C(15)	C(16)	-0.1(4)
C(3)	C(4)	C(5)	C(10)	76.7(3)	C(14)	C(15)	C(16)	C(17)	0.7(4)
N(1)	C(4)	C(5)	C(6)	68.2(3)	C(14)	C(15)	C(16)	C(19)	-177.3(3)
C(3)	C(4)	C(5)	C(6)	-49.0(3)	C(15)	C(16)	C(17)	C(18)	-0.6(5)
C(10)	C(5)	C(6)	C(7)	55.6(3)	C(19)	C(16)	C(17)	C(18)	177.4(3)
C(4)	C(5)	C(6)	C(7)	-179.0(2)	C(16)	C(17)	C(18)	C(13)	-0.1(4)
C(5)	C(6)	C(7)	C(8)	-55.0(3)	C(14)	C(13)	C(18)	C(17)	0.7(4)
C(5)	C(6)	C(7)	C(11)	-179.0(2)	S(1)	C(13)	C(18)	C(17)	-179.0(2)

Table S-7. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×103) for A15018.

Atom	x	y	z	U(eq)
H(1A)	8424	-272	2831	107
H(1B)	7912	-516	3530	107
H(2A)	10901	24	3318	119
H(2B)	10034	619	3903	119
H(3A)	10519	1692	2717	105
H(3B)	10842	2299	3368	105
H(4)	8052	2592	2723	69
H(5)	6688	3331	3635	61
H(6A)	7927	2179	4411	68
H(6B)	9663	2796	4289	68
H(7)	6793	3981	4760	71
H(8A)	9959	5044	4548	79
H(8B)	8402	5717	4822	79
H(9)	6976	5530	3878	73
H(10A)	8222	4638	3015	72
H(10B)	9851	4367	3398	72
H(11A)	8100	2840	5534	127
H(11B)	8290	4205	5691	127
H(11C)	9805	3494	5409	127
H(12A)	10154	6569	3659	132
H(12B)	8649	7250	3966	132
H(12C)	8541	6846	3268	132
H(14)	6228	-736	2006	64
H(15)	6690	-745	947	76
H(17)	6015	2805	885	85
H(18)	5557	2837	1943	71
H(19A)	6936	208	-26	156
H(19B)	7480	1557	-17	156
H(19C)	5587	1219	-99	156

(*S*)-2-((1*S*,3*R*)-3-Methylcyclohexyl)-1-tosylpyrrolidine (Table 2, entry 1). This compound was synthesized under the standard cross-coupling conditions from (3*R*)-1-iodo-3-methylcyclohexane and the organozinc reagent, using (*S*,*S*)-**1**, followed by tosylation.

A suitable crystal of $C_{18}H_{27}NO_2S$ was selected for analysis. All measurements were made on a Bruker AXS KAPPA APEX II diffractometer coupled to an APEX II CCD detector with graphite monochromated Mo K_α radiation ($\lambda = 0.71073$ Å) for the structure of compound A15076. Using Olex2, the structure was solved by direct methods using SHELXS[6] and refined against F^2 on all data by full-matrix least squares with SHELXL-2014[7] using established refinement techniques.[8]

Table S-1. Crystal data and structure refinement for A15076.

Identification code	A15076	
Empirical formula	$C_{18}H_{27}NO_2S$	
Formula weight	321.46	
Temperature	100 K	
Crystal system	monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 7.8386(3) Å	α = 90°
	b = 11.2976(5) Å	β = 101.153(2) °
	c = 9.8622(4) Å	γ= 90°
Volume	856.88(6) $Å^3$	
Z	2	
Density(calculated)	1.246 Mg/m^3	
Absorption coefficient	0.196 mm^{-1}	
F(000)	348.0	
Crystal size	0.350 × 0.250 × 0.100 mm^3	
Radiation	MoKα (λ = 0.71073)	
Theta range for data collection	4.21° to 72.74°	
Index ranges	$-13 \leq h \leq 13$, $-18 \leq k \leq 18$, $-16 \leq l \leq 16$	
Reflections collected	31024	
Independent reflections	8293 [Rint = 0.0288]	
Data/restraints/parameters	8293/1/201	
Goodness-of-fit on F^2	1.049	
R indexes [I>=2sigma (I)]	R1 = 0.0314, wR2 = 0.0791	
R indexes [all data]	R1 = 0.0355, wR2 = 0.0811	
Largest diff. peak/hole	0.42/-0.21 e/$Å^{-3}$	
Flack parameter	0.030(14)	

Table S-2. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for A15076. Ueq is defined as 1/3 of of the trace of the orthogonalised U^{ij} tensor.

Atom	x	y	z	U(eq)
S(1)	10611.7(3)	7487.6(2)	4903.5(2)	13.50(6)
O(1)	11594.7(12)	6405.3(9)	4987.9(10)	19.90(17)
O(2)	11008.7(12)	8355.0(9)	5983.4(9)	19.48(17)
N(1)	8578.2(12)	7121.0(9)	4803.8(10)	14.00(16)
C(1)	7324.8(15)	8074.8(10)	5012.8(11)	14.85(18)
C(2)	5751.6(17)	7881.1(14)	3826.6(13)	22.1(2)
C(3)	6474.2(18)	7183.8(13)	2737.8(13)	22.6(2)
C(4)	7783.3(17)	6362.0(11)	3622.8(13)	19.1(2)
C(5)	6933.7(15)	8015(1)	6470.0(11)	15.01(18)
C(6)	6112.4(15)	6848.6(11)	6800.9(11)	15.84(19)
C(7)	5803.5(16)	6815.3(13)	8293.0(12)	19.4(2)
C(8)	4720.4(18)	7882.2(14)	8563.1(13)	23.9(2)
C(9)	5477(2)	9051.4(14)	8198.9(15)	26.4(3)
C(10)	5782.5(19)	9054.8(12)	6712.4(14)	21.9(2)
C(11)	4921(2)	5666.2(16)	8570.2(16)	29.6(3)
C(12)	10769.5(14)	8164.1(10)	3320.9(12)	13.99(18)
C(13)	10290.4(16)	9345.5(11)	3085.4(12)	16.72(19)
C(14)	10280.8(18)	9831.6(11)	1784.3(13)	19.1(2)
C(15)	10748.1(16)	9162.9(11)	722.4(12)	18.1(2)
C(16)	11246.5(17)	7986.5(12)	993.7(12)	18.7(2)
C(17)	11260.5(14)	7486.3(13)	2280.3(11)	16.59(17)
C(18)	10754(2)	9704.7(14)	-672.6(14)	24.8(3)

Table S-3. Anisotropic Displacement Parameters ($Å^2 \times 103$) for A15076. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11}+\ldots+2hka^*b^*U^{12}]$.

Atom	U11	U22	U33	U23	U13	U12
S(1)	11.45(10)	15.48(10)	13.57(9)	0.97(9)	2.43(7)	-1.01(9)
O(1)	16.2(4)	20.0(4)	24.1(4)	5.8(3)	5.3(3)	4.8(3)
O(2)	18.6(4)	23.7(4)	15.1(3)	-3.6(3)	0.8(3)	-5.2(3)
N(1)	12.4(4)	15.1(4)	15.1(4)	-0.7(3)	4.1(3)	-1.7(3)
C(1)	14.1(4)	15.2(5)	15.9(4)	2.4(3)	4.8(3)	1.2(3)
C(2)	16.3(5)	32.1(6)	17.1(5)	6.3(4)	1.6(4)	2.6(5)
C(3)	21.1(5)	29.3(6)	16.0(4)	0.5(4)	0.6(4)	-4.2(5)
C(4)	18.6(5)	18.3(5)	20.0(5)	-3.8(4)	3.0(4)	-5.4(4)
C(5)	13.4(4)	16.0(5)	16.0(4)	-1.1(3)	3.8(3)	0.7(4)
C(6)	15.8(5)	17.6(5)	14.7(4)	1.8(4)	4.3(3)	0.9(4)
C(7)	17.6(5)	26.7(6)	14.2(4)	3.1(4)	3.9(4)	2.9(4)
C(8)	21.0(5)	36.5(7)	15.8(5)	0.9(5)	7.2(4)	7.7(5)
C(9)	28.7(6)	28.1(7)	23.7(6)	-7.2(5)	8.4(5)	7.0(5)
C(10)	25.1(6)	17.7(5)	24.6(5)	-1.5(4)	8.8(4)	4.6(4)
C(11)	30.9(7)	35.0(7)	24.8(6)	10.6(5)	10.3(5)	-1.1(6)
C(12)	12.9(4)	13.9(4)	15.9(4)	0.1(3)	4.7(3)	-2.1(3)
C(13)	18.9(5)	14.1(4)	18.6(5)	-0.9(4)	7.3(4)	-1.6(4)
C(14)	22.5(6)	15.0(5)	21.1(5)	2.5(4)	7.6(4)	-0.8(4)
C(15)	18.0(5)	20.0(5)	17.0(4)	1.7(4)	4.8(4)	-4.0(4)
C(16)	20.9(5)	19.6(5)	17.4(5)	-1.5(4)	8.3(4)	-1.5(4)
C(17)	17.4(4)	15.2(4)	18.6(4)	-0.2(4)	6.9(3)	-0.4(5)
C(18)	29.7(7)	27.4(6)	18.0(5)	5.1(4)	5.9(4)	-3.4(5)

Table S-4. Bond Lengths for A15076.

Atom	Atom	Length / Å
S(1)	O(2)	1.4364(9)
S(1)	O(1)	1.4391(10)
S(1)	N(1)	1.6314(10)
S(1)	C(12)	1.7636(11)
N(1)	C(4)	1.4830(15)
N(1)	C(1)	1.4991(15)
C(1)	C(5)	1.5278(16)
C(1)	C(2)	1.5424(17)
C(2)	C(3)	1.526(2)
C(3)	C(4)	1.5265(19)
C(5)	C(10)	1.5280(17)
C(5)	C(6)	1.5293(16)
C(6)	C(7)	1.5373(16)
C(7)	C(11)	1.521(2)
C(7)	C(8)	1.5271(19)
C(8)	C(9)	1.519(2)
C(9)	C(10)	1.5305(19)
C(12)	C(17)	1.3930(15)
C(12)	C(13)	1.3938(16)
C(13)	C(14)	1.3945(17)
C(14)	C(15)	1.3964(18)
C(15)	C(16)	1.3965(18)
C(15)	C(18)	1.5066(17)
C(16)	C(17)	1.3872(16)

Table S-5. Bond Angles for A15076.

Atom	Atom	Atom	Angle / °	Atom	Atom	Atom	Angle / °
O(2)	S(1)	O(1)	120.00(6)	C(5)	C(6)	C(7)	112.09(10)
O(2)	S(1)	N(1)	106.67(5)	C(11)	C(7)	C(8)	110.78(11)
O(1)	S(1)	N(1)	107.08(6)	C(11)	C(7)	C(6)	110.76(11)
O(2)	S(1)	C(12)	108.56(6)	C(8)	C(7)	C(6)	110.09(10)
O(1)	S(1)	C(12)	106.92(5)	C(9)	C(8)	C(7)	112.91(11)
N(1)	S(1)	C(12)	106.96(5)	C(8)	C(9)	C(10)	111.66(11)
C(4)	N(1)	C(1)	109.67(9)	C(5)	C(10)	C(9)	110.76(11)
C(4)	N(1)	S(1)	116.83(8)	C(17)	C(12)	C(13)	120.51(11)
C(1)	N(1)	S(1)	117.90(8)	C(17)	C(12)	S(1)	119.37(9)
N(1)	C(1)	C(5)	110.71(9)	C(13)	C(12)	S(1)	119.98(9)
N(1)	C(1)	C(2)	104.06(9)	C(12)	C(13)	C(14)	118.93(11)
C(5)	C(1)	C(2)	115.51(10)	C(13)	C(14)	C(15)	121.44(12)
C(3)	C(2)	C(1)	104.82(10)	C(14)	C(15)	C(16)	118.38(11)
C(2)	C(3)	C(4)	102.21(10)	C(14)	C(15)	C(18)	120.84(12)
N(1)	C(4)	C(3)	103.37(10)	C(16)	C(15)	C(18)	120.76(12)
C(1)	C(5)	C(10)	110.19(10)	C(17)	C(16)	C(15)	121.02(12)
C(1)	C(5)	C(6)	114.09(9)	C(16)	C(17)	C(12)	119.70(12)
C(10)	C(5)	C(6)	110.08(10)				

Table S-6. Torsion Angles for A15076.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O(2)	S(1)	N(1)	C(4)	171.37(9)	C(5)	C(6)	C(7)	C(8)	54.86(13)
O(1)	S(1)	N(1)	C(4)	-58.99(10)	C(11)	C(7)	C(8)	C(9)	-175.71(12)
C(12)	S(1)	N(1)	C(4)	55.34(10)	C(6)	C(7)	C(8)	C(9)	-52.86(14)
O(2)	S(1)	N(1)	C(1)	37.37(9)	C(7)	C(8)	C(9)	C(10)	53.93(15)
O(1)	S(1)	N(1)	C(1)	167.01(8)	C(1)	C(5)	C(10)	C(9)	-176.33(11)
C(12)	S(1)	N(1)	C(1)	-78.66(9)	C(6)	C(5)	C(10)	C(9)	56.98(14)
C(4)	N(1)	C(1)	C(5)	121.78(10)	C(8)	C(9)	C(10)	C(5)	-55.45(15)
S(1)	N(1)	C(1)	C(5)	-101.20(10)	O(2)	S(1)	C(12)	C(17)	149.80(9)
C(4)	N(1)	C(1)	C(2)	-2.92(12)	O(1)	S(1)	C(12)	C(17)	19.00(11)
S(1)	N(1)	C(1)	C(2)	134.10(9)	N(1)	S(1)	C(12)	C(17)	-95.44(10)
N(1)	C(1)	C(2)	C(3)	-21.57(12)	O(2)	S(1)	C(12)	C(13)	-34.57(11)
C(5)	C(1)	C(2)	C(3)	-143.14(11)	O(1)	S(1)	C(12)	C(13)	-165.38(9)
C(1)	C(2)	C(3)	C(4)	37.28(13)	N(1)	S(1)	C(12)	C(13)	80.19(10)
C(1)	N(1)	C(4)	C(3)	26.15(12)	C(17)	C(12)	C(13)	C(14)	1.14(18)
S(1)	N(1)	C(4)	C(3)	-111.39(10)	S(1)	C(12)	C(13)	C(14)	-174.44(9)
C(2)	C(3)	C(4)	N(1)	-38.60(12)	C(12)	C(13)	C(14)	C(15)	-0.35(19)
N(1)	C(1)	C(5)	C(10)	175.06(10)	C(13)	C(14)	C(15)	C(16)	-0.57(19)
C(2)	C(1)	C(5)	C(10)	-67.02(14)	C(13)	C(14)	C(15)	C(18)	-179.19(12)
N(1)	C(1)	C(5)	C(6)	-60.52(12)	C(14)	C(15)	C(16)	C(17)	0.71(19)
C(2)	C(1)	C(5)	C(6)	57.39(14)	C(18)	C(15)	C(16)	C(17)	179.34(12)
C(1)	C(5)	C(6)	C(7)	177.99(10)	C(15)	C(16)	C(17)	C(12)	0.05(18)
C(10)	C(5)	C(6)	C(7)	-57.53(12)	C(13)	C(12)	C(17)	C(16)	-1.00(17)
C(5)	C(6)	C(7)	C(11)	177.72(11)	S(1)	C(12)	C(17)	C(16)	174.60(9)

Table S-7. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for A15076.

Atom	x	y	z	U(eq)
H(1)	7856	8862	4885	18
H(2A)	4828	7427	4152	26
H(2B)	5265	8648	3448	26
H(3A)	7050	7712	2163	27
H(3B)	5548	6730	2131	27
H(4A)	7196	5668	3940	23
H(4B)	8669	6082	3105	23
H(5)	8064	8100	7135	18
H(6A)	6885	6185	6661	19
H(6B)	4989	6739	6154	19
H(7)	6957	6859	8936	23
H(8A)	3528	7797	8014	29
H(8B)	4638	7893	9552	29
H(9A)	6594	9197	8842	32
H(9B)	4671	9701	8315	32
H(10A)	4652	9001	6063	26
H(10B)	6346	9807	6531	26
H(11A)	3826	5580	7902	44
H(11B)	4681	5680	9509	44
H(11C)	5686	4997	8478	44
H(13)	9976	9812	3800	20
H(14)	9949	10635	1617	23
H(16)	11581	7522	286	22
H(17)	11603	6685	2451	20
H(18A)	11560	10376	-567	37
H(18B)	9580	9979	-1079	37
H(18C)	11125	9111	-1280	37

(*S*)-2-((1*S*,3*R*)-3-(4-Bromophenyl)cyclohexyl)-1-tosylpyrrolidine (Table 2, entry 2). This compound was synthesized under the standard cross-coupling conditions from 1-bromo-4-((1*R*)-3-iodocyclohexyl)benzene and the organozinc reagent, using (*S*,*S*)-**1**, followed by tosylation.

A suitable crystal of $C_{23}H_{28}BrNO_2S$ was selected for analysis. All measurements were made on a Bruker AXS KAPPA APEX II diffractometer coupled to an APEX II CCD detector with graphite monochromated Mo K_α radiation (λ = 0.71073 Å) for the structure of compound a15119ja. Using Olex2, the structure was solved by direct methods using SHELXS[6] and refined against F^2 on all data by full-matrix least squares with SHELXL-2014[7] using established refinement techniques.[8]

Table S-1. Crystal data and structure refinement for a15119ja.

Identification code	a15119ja	
Empirical formula	$C_{23}H_{28}BrNO_2S$	
Formula weight	462.45	
Temperature/K	99.99 K	
Crystal system	orthorhombic	
Space group	$P2_12_12_1$	
	a = 7.5923(4) Å	$\alpha = 90°$
	b = 12.8176(8) Å	$\beta = 90°$
	c = 22.1203(11) Å	$\gamma = 90°$
Volume	2152.6(2) $Å^3$	
Z	4	
Density(calculated)	1.4268 Mg/m^3	
Absorption coefficient	2.025 mm^{-1}	
F(000)	959.7	
Radiation	Mo Kα (λ = 0.71073)	
Theta range for data collection	4.86° to 78.84°	
Index ranges	$-13 \leq h \leq 12$, $-21 \leq k \leq 21$, $-36 \leq l \leq 39$	
Reflections collected	138629	
Independent reflections	11526 [Rint = 0.0442]	
Data/restraints/parameters	11526/0/263	
Goodness-of-fit on F^2	1.005	
R indexes [I>=2sigma (I)]	R1 = 0.0308, wR2 = 0.0683	
R indexes [all data]	R1 = 0.0529, wR2 = 0.0728	
Largest diff. peak/hole	0.66/-0.71 e/$Å^{-3}$	
Flack parameter	0.022(4)	

Table S-2. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for a15119ja. Ueq is defined as 1/3 of of the trace of the orthogonalised U^{ij} tensor.

Atom	x	y	z	U(eq)
Br(01)	434.3(2)	371.56(10)	4738.25(6)	31.22(4)
S(002)	5167.5(3)	7371.91(19)	6286.81(11)	11.55(4)
O(003)	5513.9(11)	6912.6(6)	6870.7(3)	16.75(14)
O(004)	6198.9(11)	7067.1(6)	5771.8(4)	16.97(15)
C(005)	1148.7(15)	4012.4(8)	6586.0(5)	14.78(18)
N(006)	3125.5(12)	7126.6(7)	6125.5(4)	13.09(15)
C(007)	1143.7(14)	5124.7(8)	6328.3(5)	14.29(17)
C(008)	5027.7(14)	10318.7(9)	6946.2(5)	16.33(19)
C(009)	590.9(16)	1493.7(9)	5301.3(5)	20.9(2)
C(00A)	4818.7(15)	9241.1(8)	6887.3(5)	14.72(18)
C(00B)	6196.0(15)	9320.0(9)	5899.9(5)	16.91(19)
C(00C)	-113.6(16)	2461.8(9)	5155.7(5)	21.7(2)
C(00D)	6427.1(15)	10390.6(9)	5968.3(5)	18.4(2)
C(00E)	-255.4(17)	3928.8(8)	7088.2(5)	19.4(2)
C(00F)	1596.4(15)	2152.9(9)	6255.7(5)	18.6(2)
C(00G)	931.1(15)	3151.0(8)	6120.8(5)	15.29(18)
C(00H)	1771.8(14)	7042.3(8)	6612.5(5)	13.07(17)
C(00I)	78.5(17)	4726.5(9)	7591.6(5)	19.4(2)
C(00J)	68.5(16)	3285.1(9)	5566.2(5)	19.8(2)
C(00K)	194.5(16)	5837.5(8)	7340.3(5)	17.23(19)
C(00L)	2382.9(16)	7620.7(10)	5573.3(5)	20.4(2)
C(00M)	5407.3(14)	8743.9(7)	6362.0(4)	12.61(16)
C(00N)	5853.1(15)	10902.1(8)	6494.5(5)	16.10(19)
C(00O)	1573.9(13)	5908.9(8)	6831.6(5)	12.95(17)
C(00P)	1437.7(16)	1327.3(9)	5848.5(6)	21.0(2)
C(00Q)	6165.9(18)	12062.7(9)	6572.1(6)	22.9(2)
C(00R)	119.2(15)	7522.5(9)	6321.4(5)	19.9(2)
C(00S)	758(2)	8233.8(14)	5841.9(8)	22.5(4)
C(1)	490(5)	7466(3)	5627.4(14)	14.6(7)

Table S-3. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for a15119ja. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11}+\ldots+2hka^*b^*U^{12}]$.

Atom	U11	U22	U33	U12	U13	U23
Br(01)	33.87(8)	26.84(6)	32.95(7)	-5.54(5)	0.09(6)	-16.09(5)
S(002)	12.0(1)	11.22(9)	11.43(9)	-1.49(8)	-0.12(8)	0.35(7)
O(003)	16.7(3)	18.3(3)	15.3(3)	-1.2(3)	-2.7(3)	4.4(3)
O(004)	16.7(3)	16.8(3)	17.4(3)	0.1(3)	3.9(3)	-3.2(3)
C(005)	16.7(5)	12.3(4)	15.4(4)	-3.4(4)	1.0(3)	0.2(3)
N(006)	13.9(4)	13.9(4)	11.5(3)	-2.8(3)	-1.3(3)	1.9(3)
C(007)	16.0(4)	12.1(4)	14.8(4)	-3.2(3)	2.1(4)	-1.2(3)
C(008)	15.9(5)	17.2(4)	16.0(4)	-1.7(4)	-0.8(3)	-5.0(3)
C(009)	22.0(5)	18.0(5)	22.7(5)	-5.9(4)	1.8(5)	-7.9(4)
C(00A)	15.2(4)	16.6(4)	12.3(4)	-3.8(4)	1.0(3)	-2.0(3)
C(00B)	19.5(5)	16.5(5)	14.7(4)	-3.3(4)	3.3(4)	-0.4(4)
C(00C)	24.1(5)	21.1(5)	19.9(5)	-2.4(4)	-2.7(4)	-3.7(4)
C(00D)	21.1(5)	15.7(4)	18.4(5)	-5.0(4)	2.4(4)	1.6(4)
C(00E)	23.7(5)	15.5(4)	18.8(4)	-7.3(4)	5.4(4)	0.3(4)
C(00F)	21.0(5)	14.9(5)	20.0(5)	-2.1(4)	-1.0(4)	-0.2(4)
C(00G)	15.6(4)	13.1(4)	17.2(4)	-3.4(3)	1.8(4)	-1.4(3)
C(00H)	12.3(4)	12.1(4)	14.8(4)	-0.6(3)	0.1(3)	-1.4(3)
C(00I)	25.1(5)	17.8(5)	15.2(4)	-4.0(4)	6.2(4)	-0.2(4)
C(00J)	23.3(6)	16.3(4)	19.8(5)	-0.6(4)	-1.6(4)	-1.6(4)
C(00K)	18.8(5)	15.2(4)	17.6(4)	-1.9(4)	6.0(4)	-1.1(3)
C(00L)	23.9(5)	22.7(5)	14.6(4)	-4.0(4)	-7.8(4)	2.7(4)
C(00M)	13.2(4)	12.7(4)	12.0(4)	-2.6(3)	-0.5(3)	-0.6(3)
C(00N)	15.5(5)	13.6(4)	19.2(5)	-2.4(3)	-4.4(4)	-1.1(4)
C(00O)	12.6(4)	12.1(4)	14.1(4)	-1.4(3)	0.6(3)	-0.6(3)
C(00P)	23.2(5)	14.4(5)	25.4(5)	-1.4(4)	-0.6(4)	-3.0(4)
C(00Q)	26.2(6)	14.2(5)	28.4(6)	-4.8(4)	-4.2(5)	-2.7(4)
C(00R)	17.3(5)	18.5(5)	24.0(5)	5.9(4)	-4.1(4)	-2.0(4)
C(00S)	23.5(8)	18.3(8)	25.8(8)	3.1(6)	-9.7(7)	3.6(6)
C(1)	14.2(14)	16.5(14)	13.2(13)	2.5(12)	-6.0(11)	-0.1(10)

Table S-4. Bond Lengths for a15119ja.

Atom	Atom	Length/Å
Br(01)	C(009)	1.9064(11)
S(002)	O(003)	1.4436(8)
S(002)	O(004)	1.4366(8)
S(002)	N(006)	1.6217(9)
S(002)	C(00M)	1.7757(10)
C(005)	C(007)	1.5355(15)
C(005)	C(00E)	1.5432(15)
C(005)	C(00G)	1.5183(14)
N(006)	C(00H)	1.4928(14)
N(006)	C(00L)	1.4870(14)
C(007)	C(00O)	1.5351(14)
C(008)	C(00A)	1.3964(15)
C(008)	C(00N)	1.3964(16)
C(009)	C(00C)	1.3890(17)
C(009)	C(00P)	1.3871(17)
C(00A)	C(00M)	1.3985(14)
C(00B)	C(00D)	1.3917(16)
C(00B)	C(00M)	1.3961(14)
C(00C)	C(00J)	1.3992(15)
C(00D)	C(00N)	1.4054(16)
C(00E)	C(00I)	1.5329(15)
C(00F)	C(00G)	1.4074(16)
C(00F)	C(00P)	1.3948(16)
C(00G)	C(00J)	1.4012(16)
C(00H)	C(00O)	1.5388(14)
C(00H)	C(00R)	1.5388(15)
C(00I)	C(00K)	1.5313(16)
C(00K)	C(00O)	1.5398(15)
C(00L)	C(00S)	1.579(2)
C(00L)	C(1)	1.455(4)
C(00N)	C(00Q)	1.5162(16)
C(00R)	C(00S)	1.480(2)
C(00R)	C(1)	1.562(3)

Table S-5. Bond Angles for a15119ja.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O(004)	S(002)	O(003)	119.95(5)	C(00P)	C(00F)	C(00G)	121.45(11)
N(006)	S(002)	O(003)	106.98(5)	C(00F)	C(00G)	C(005)	118.57(10)
N(006)	S(002)	O(004)	107.09(5)	C(00J)	C(00G)	C(005)	123.71(10)
C(00M)	S(002)	O(003)	107.54(5)	C(00J)	C(00G)	C(00F)	117.70(10)
C(00M)	S(002)	O(004)	106.73(5)	C(00O)	C(00H)	N(006)	111.28(8)
C(00M)	S(002)	N(006)	108.10(5)	C(00R)	C(00H)	N(006)	103.32(8)
C(00E)	C(005)	C(007)	109.26(9)	C(00R)	C(00H)	C(00O)	115.46(9)
C(00G)	C(005)	C(007)	115.04(8)	C(00K)	C(00I)	C(00E)	111.47(9)
C(00G)	C(005)	C(00E)	111.23(9)	C(00G)	C(00J)	C(00C)	121.46(11)
C(00H)	N(006)	S(002)	120.89(7)	C(00O)	C(00K)	C(00I)	111.08(9)
C(00L)	N(006)	S(002)	117.43(7)	C(00A)	C(00M)	S(002)	119.76(8)
C(00L)	N(006)	C(00H)	111.26(9)	C(00B)	C(00M)	S(002)	119.95(8)
C(00O)	C(007)	C(005)	109.77(8)	C(00B)	C(00M)	C(00A)	120.29(9)
C(00N)	C(008)	C(00A)	120.93(10)	C(00D)	C(00N)	C(008)	118.82(10)
C(00C)	C(009)	Br(01)	119.89(9)	C(00Q)	C(00N)	C(008)	120.98(10)
C(00P)	C(009)	Br(01)	118.88(9)	C(00Q)	C(00N)	C(00D)	120.19(11)
C(00P)	C(009)	C(00C)	121.22(10)	C(00H)	C(00O)	C(007)	114.23(8)
C(00M)	C(00A)	C(008)	119.47(10)	C(00K)	C(00O)	C(007)	110.26(8)
C(00M)	C(00B)	C(00D)	119.74(10)	C(00K)	C(00O)	C(00H)	110.65(8)
C(00J)	C(00C)	C(009)	119.02(11)	C(00F)	C(00P)	C(009)	119.13(11)
C(00N)	C(00D)	C(00B)	120.73(10)	C(00R)	C(00S)	C(00L)	102.65(12)
C(00I)	C(00E)	C(005)	111.24(9)	C(00R)	C(1)	C(00L)	104.6(2)

Table S-6. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for a15119ja.

Atom	x	y	z	U(eq)
H(005)	2320.5(15)	3904.9(8)	6782.8(5)	17.7(2)
H(00a)	2029.2(14)	5181.1(8)	6001.5(5)	17.1(2)
H(00b)	-28.1(14)	5283.8(8)	6154.9(5)	17.1(2)
H(008)	4602.3(14)	10659.7(9)	7298.4(5)	19.6(2)
H(00c)	4280.9(15)	8848.9(8)	7201.5(5)	17.7(2)
H(00d)	6573.4(15)	8982.6(9)	5540.1(5)	20.3(2)
H(00e)	-710.2(16)	2563.3(9)	4782.8(5)	26.0(3)
H(00f)	6979.0(15)	10780.0(9)	5655.7(5)	22.1(2)
H(00g)	-1436.9(17)	4049.0(8)	6912.0(5)	23.2(2)
H(00h)	-236.0(17)	3216.5(8)	7261.1(5)	23.2(2)
H(00i)	2166.0(15)	2038.9(9)	6632.4(5)	22.3(2)
H(00j)	2140.5(14)	7487.6(8)	6961.5(5)	15.7(2)
H(00k)	-888.4(17)	4688.8(9)	7891.1(5)	23.2(2)
H(00l)	1192.1(17)	4552.0(9)	7801.3(5)	23.2(2)
H(00m)	-403.3(16)	3949.8(9)	5466.8(5)	23.7(3)
H(00n)	-971.0(16)	6049.4(8)	7181.6(5)	20.7(2)
H(00o)	517.0(16)	6323.9(8)	7669.9(5)	20.7(2)
H(00p)	3240.4(16)	8099.7(10)	5381.9(5)	24.5(3)
H(00q)	2005.0(16)	7090.9(10)	5274.5(5)	24.5(3)
H(00r)	2675.0(16)	8373(1)	5558.9(5)	24.5(3)
H(00s)	2843.0(16)	7280(1)	5203.9(5)	24.5(3)
H(00t)	2731.1(13)	5697.2(8)	7009.3(5)	15.5(2)
H(00u)	1903.6(16)	659.7(9)	5944.7(6)	25.2(3)
H(00v)	5503(11)	12446.5(10)	6264(3)	34.4(3)
H(00w)	5772(13)	12279.6(18)	6974.9(19)	34.4(3)
H(00x)	7425(3)	12212.2(14)	6528(5)	34.4(3)
H(00y)	-636.3(15)	6970.2(9)	6146.3(5)	23.9(2)
H	-572.7(15)	7912.8(9)	6625.9(5)	23.9(2)
H(a)	-946.5(15)	7117.1(9)	6427.8(5)	23.9(2)
H(b)	-43.8(15)	8254.0(9)	6453.8(5)	23.9(2)

H(00z)	1124(2)	8914.4(14)	6012.1(8)	27.0(5)
H(c)	-158(2)	8351.1(14)	5530.5(8)	27.0(5)
H(1a)	-161(5)	8020(3)	5409.3(14)	17.5(9)
H(1b)	140(5)	6779(3)	5462.1(14)	17.5(9)

Table S-7. Atomic Occupancy for a15119ja.

Atom	Occupancy	Atom	Occupancy	Atom	Occupancy
H(00p)	0.685(4)	H(00q)	0.685(4)	H(00r)	0.315(4)
H(00s)	0.315(4)	H(00y)	0.685(4)	H	0.685(4)
H(a)	0.315(4)	H(b)	0.315(4)	C(00S)	0.685(4)
H(00z)	0.685(4)	H(c)	0.685(4)	C(1)	0.315(4)
H(1a)	0.315(4)	H(1b)	0.315(4)		

(4-Bromophenyl)((*R*)-2-((2*S*,4*R*)-2-phenyltetrahydro-2*H*-pyran-4-yl)pyrrolidin-1-yl)methanone (Table 2, entry 3). This compound was synthesized under the standard cross-coupling conditions from (2*S*,4*R*)-4-iodo-2-phenyltetrahydro-2*H*-pyran and the organozinc reagent, using (*R*,*R*)-**1**, followed by benzoylation with 4-bromobenzoyl chloride.

A suitable crystal of $C_{22}H_{24}BrNO_2$ was selected for analysis. All measurements were made on a Bruker AXS KAPPA APEX II diffractometer coupled to an APEX II CCD detector with graphite monochromated Mo K_α radiation (λ = 0.71073 Å) for the structure of compound A17004. The structure was solved by direct methods using SHELXS[6] and refined against F^2 on all data by full-matrix least squares with SHELXL-2014[7] using established refinement techniques.[8]

Table S-1. Crystal data and structure refinement for a17004.

Identification code	A17004
Empirical formula	$C_{22}H_{24}BrNO_2$
Formula weight	414.34
Temperature/K	100.0
Crystal system	triclinic
Space group	P1
Unit cell dimensions	
	a = 5.401(2) Å α = 75.5°
	b = 8.114(3) Å β = 82.1°
	c = 11.573(4) Å γ = 89.3°
Volume	486.3(3) $Å^3$
Z	1
Density(calculated)	1.4146 Mg/m^3
Absorption coefficient	2.128 mm^{-1}
F(000)	213.8
Crystal size	0.33 × 0.11 × 0.1 mm^3
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection	3.66° to 67.84°
Index ranges	$-8 \leq h \leq 8$, $-12 \leq k \leq 12$, $-18 \leq l \leq 18$
Reflections collected	39606
Independent reflections	7831 [R_{int} = 0.0377]
Data/restraints/parameters	7831/3/235
Goodness-of-fit on F^2	1.017
Final R indexes [I>=2sigma (I)]	R_1 = 0.0274, wR_2 = 0.0584
Final R indexes [all data]	R_1 = 0.0303, wR_2 = 0.0592
Largest diff. peak/hole /	1.09/-0.39/ e $Å^{-3}$
Flack parameter	0.026(4)

Table S-2. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for a17004. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Br(0A)	11303.73(16)	2591.00(13)	-8388.2(1)	20.88(4)
O(0AA)	7508.0(19)	-3540.6(12)	1360.9(9)	21.8(2)
N(2)	7396(2)	1527.9(14)	-2336.4(10)	15.2(2)
C(3)	3410(2)	-3621.5(17)	3198.5(13)	17.5(2)
C(4)	2504(3)	-3534.8(18)	5277.1(13)	20.4(3)
C(1AA)	6708(3)	3025.5(17)	-855.8(13)	18.1(2)
C(6)	10956(2)	1025.4(17)	-5891.8(12)	16.2(2)
C(7)	6119(2)	-616.2(16)	1030.1(12)	14.8(2)
C(10)	6313(2)	1263.8(16)	-1066.8(11)	14.6(2)
C(12)	7538(2)	1357.2(16)	-4397.7(11)	14.0(2)
C(13)	6270(2)	911.7(17)	-3118.3(12)	15.4(2)
C(14)	5604(2)	-2657.4(16)	3070.5(11)	14.3(2)
O(16)	4357.2(18)	15.8(14)	-2820.5(10)	23.9(2)
C(17)	9748(2)	2083.2(16)	-6765.1(12)	14.6(2)
C(18)	7621(2)	-147.2(16)	-231.9(11)	14.4(2)
C(19)	9086(3)	-3132.1(19)	232.2(13)	24.3(3)
C(20)	7233(2)	-2108.3(16)	1871.5(12)	15.3(2)
C(21)	4679(3)	-2580.9(18)	5159.2(13)	20.0(3)
C(22)	1880(3)	-4061.2(18)	4299.3(13)	19.5(3)
C(25)	7993(3)	-1751.7(18)	-693.2(13)	21.2(3)
C(26)	9846(2)	684.6(17)	-4697.6(12)	16.3(2)
C(28)	6221(2)	-2151.7(17)	4060.2(12)	16.8(2)
C(29)	7468(2)	2794.1(17)	-6491.3(12)	16.0(2)
C(30)	6358(2)	2406.3(17)	-5296.3(12)	16.2(2)
C(31)	9309(3)	2898.3(19)	-2712.0(13)	23.0(3)
C(1)	9248(3)	3621.3(18)	-1608.0(13)	20.9(3)

Table S-3. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for a17004. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Br(0A)	22.58(6)	26.00(7)	12.44(5)	3.63(4)	1.79(4)	-4.16(4)
O(0AA)	34.1(6)	14.4(4)	14.4(5)	2.9(4)	3.4(4)	-2.7(4)
N(2)	16.5(5)	17.7(5)	10.3(5)	-5.1(4)	0.0(4)	-2.0(4)
C(3)	18.2(6)	17.4(6)	17.0(6)	0.3(5)	-3.5(5)	-3.9(5)
C(4)	23.8(7)	17.2(6)	16.5(6)	-2.4(5)	5.6(5)	-1.6(5)
C(1AA)	23.2(6)	16.4(6)	13.6(6)	-0.3(5)	1.2(5)	-3.6(5)
C(6)	13.4(5)	19.3(6)	15.9(6)	1.1(4)	-2.9(5)	-4.0(5)
C(7)	16.8(6)	13.8(5)	12.3(5)	0.8(4)	0.2(4)	-1.9(4)
C(10)	16.0(6)	16.4(6)	10.2(5)	-2.0(4)	0.3(4)	-1.9(4)
C(12)	13.9(5)	16.6(6)	11.5(5)	-1.7(4)	-1.7(4)	-3.5(4)
C(13)	14.7(6)	18.9(6)	12.2(5)	-0.4(4)	-2.3(4)	-3.0(4)
C(14)	16.2(6)	12.8(5)	12.2(5)	1.3(4)	-0.9(4)	-0.7(4)
O(16)	18.7(5)	34.4(6)	18.6(5)	-11.4(4)	0.0(4)	-7.2(4)
C(17)	15.6(6)	16.3(6)	12.0(5)	-1.9(4)	-0.7(4)	-4.4(4)
C(18)	15.7(6)	15.0(6)	11.4(5)	0.1(4)	0.3(4)	-2.4(4)
C(19)	36.8(9)	19.2(6)	14.4(6)	9.3(6)	3.0(6)	-3.5(5)
C(20)	18.0(6)	14.9(6)	12.0(5)	0.8(4)	-0.1(4)	-2.7(4)
C(21)	27.5(7)	17.8(6)	13.9(6)	-1.5(5)	-0.1(5)	-3.7(5)
C(22)	17.7(6)	16.4(6)	21.7(7)	-2.8(5)	0.6(5)	-1.5(5)
C(25)	32.2(8)	19.0(6)	12.4(6)	4.2(5)	-0.8(5)	-5.2(5)
C(26)	16.3(6)	19.3(6)	13.5(6)	0.9(5)	-4.8(5)	-3.0(5)
C(28)	18.6(6)	16.7(6)	14.4(6)	-2.5(5)	-1.2(5)	-3.0(5)
C(29)	16.9(6)	16.4(6)	14.2(6)	2.0(5)	-3.3(5)	-2.4(5)
C(30)	14.2(6)	18.7(6)	15.9(6)	0.9(4)	-1.9(5)	-4.8(5)
C(31)	25.9(7)	27.5(7)	15.7(6)	-13.7(6)	5.3(5)	-9.4(5)
C(1)	26.3(7)	21.6(7)	14.4(6)	-9.1(5)	2.2(5)	-6.2(5)

Table S-4. Bond Lengths for a17004.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Br(0A)	C(17)	1.8962(14)	C(7)	C(20)	1.5263(19)
O(0AA)	C(19)	1.4246(18)	C(10)	C(18)	1.5356(18)
O(0AA)	C(20)	1.4271(17)	C(12)	C(13)	1.5014(19)
N(2)	C(10)	1.4691(17)	C(12)	C(26)	1.3903(18)
N(2)	C(13)	1.3496(18)	C(12)	C(30)	1.3923(19)
N(2)	C(31)	1.4684(18)	C(13)	O(16)	1.2286(17)
C(3)	C(14)	1.3975(19)	C(14)	C(20)	1.5053(18)
C(3)	C(22)	1.388(2)	C(14)	C(28)	1.3904(19)
C(4)	C(21)	1.387(2)	C(17)	C(29)	1.3848(18)
C(4)	C(22)	1.387(2)	C(18)	C(25)	1.5270(19)
C(1AA)	C(10)	1.5308(19)	C(19)	C(25)	1.519(2)
C(1AA)	C(1)	1.534(2)	C(21)	C(28)	1.3891(19)
C(6)	C(17)	1.3847(19)	C(29)	C(30)	1.3900(19)
C(6)	C(26)	1.390(2)	C(31)	C(1)	1.530(2)
C(7)	C(18)	1.5305(18)			

Table S-5. Bond Angles for a17004.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C(20)	O(0AA)	C(19)	111.27(10)	C(28)	C(14)	C(20)	120.03(11)
C(13)	N(2)	C(10)	121.86(11)	C(6)	C(17)	Br(0A)	118.52(10)
C(31)	N(2)	C(10)	112.30(10)	C(29)	C(17)	Br(0A)	119.15(10)
C(31)	N(2)	C(13)	123.48(11)	C(29)	C(17)	C(6)	122.32(12)
C(22)	C(3)	C(14)	120.18(13)	C(10)	C(18)	C(7)	110.06(10)
C(22)	C(4)	C(21)	119.93(13)	C(25)	C(18)	C(7)	109.00(10)
C(1)	C(1AA)	C(10)	103.13(11)	C(25)	C(18)	C(10)	113.01(11)
C(26)	C(6)	C(17)	118.59(12)	C(25)	C(19)	O(0AA)	111.77(11)
C(20)	C(7)	C(18)	112.19(10)	C(7)	C(20)	O(0AA)	110.93(11)
C(1AA)	C(10)	N(2)	101.60(10)	C(14)	C(20)	O(0AA)	107.88(10)
C(18)	C(10)	N(2)	112.16(10)	C(14)	C(20)	C(7)	111.45(10)
C(18)	C(10)	C(1AA)	112.90(11)	C(28)	C(21)	C(4)	119.81(13)
C(26)	C(12)	C(13)	120.46(11)	C(4)	C(22)	C(3)	120.29(12)
C(30)	C(12)	C(13)	119.77(11)	C(19)	C(25)	C(18)	109.67(12)
C(30)	C(12)	C(26)	119.74(12)	C(12)	C(26)	C(6)	120.37(12)
C(12)	C(13)	N(2)	115.64(11)	C(21)	C(28)	C(14)	120.80(12)
O(16)	C(13)	N(2)	123.32(12)	C(30)	C(29)	C(17)	118.28(12)
O(16)	C(13)	C(12)	121.02(12)	C(29)	C(30)	C(12)	120.67(12)
C(20)	C(14)	C(3)	120.94(12)	C(1)	C(31)	N(2)	103.96(11)
C(28)	C(14)	C(3)	118.99(12)	C(31)	C(1)	C(1AA)	104.71(11)

Table S-6. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for a17004.

Atom	*x*	*y*	*z*	U(eq)
H(3)	2965(2)	-3976.9(17)	2530.2(13)	21.0(3)
H(4)	1442(3)	-3827.6(18)	6026.6(13)	24.5(3)
H(1Aa)	5369(3)	3804.1(17)	-1139.1(13)	21.7(3)
H(1Ab)	6755(3)	2951.4(17)	7.9(13)	21.7(3)
H(6)	12510(2)	542.7(17)	-6104.2(12)	19.4(3)
H(7a)	6073(2)	384.9(16)	1376.3(12)	17.7(3)
H(7b)	4379(2)	-916.1(16)	969.3(12)	17.7(3)
H(10)	4485(2)	987.0(16)	-968.3(11)	17.6(3)
H(18)	9303(2)	300.0(16)	-169.4(11)	17.3(3)
H(19a)	10745(3)	-2742.5(19)	347.0(13)	29.2(4)
H(19b)	9324(3)	-4167.7(19)	-72.7(13)	29.2(4)
H(20)	8916(2)	-1752.2(16)	2004.7(12)	18.3(3)
H(21)	5113(3)	-2221.9(18)	5828.0(13)	24.0(3)
H(22)	398(3)	-4725.5(18)	4383.6(13)	23.4(3)
H(25a)	6369(3)	-2153.4(18)	-841.3(13)	25.5(3)
H(25b)	9137(3)	-1493.1(18)	-1463.6(13)	25.5(3)
H(26)	10670(2)	-11.8(17)	-4083.0(12)	19.5(3)
H(28)	7716(2)	-1504.7(17)	3983.9(12)	20.2(3)
H(29)	6683(2)	3527.8(17)	-7104.2(12)	19.1(3)
H(30)	4778(2)	2861.6(17)	-5090.8(12)	19.4(3)
H(31a)	10976(3)	2446.5(19)	-2920.6(13)	27.6(4)
H(31b)	8897(3)	3780.2(19)	-3416.1(13)	27.6(4)
H(1a)	9386(3)	4879.9(18)	-1849.9(13)	25.1(3)
H(1b)	10632(3)	3174.5(18)	-1148.0(13)	25.1(3)

(*S*)-2-((1*S*,3*R*)-3-(4-Chlorophenyl)-3-methylcyclohexyl)-1-tosylpyrrolidine (Table 2, entry 4). This compound was synthesized under the standard cross-coupling conditions from 1-chloro-4-((1*R*)-3-iodo-1-methylcyclohexyl)benzene and the organozinc reagent, using (*S*,*S*)-**1**, followed by tosylation.

A suitable crystal of $C_{24}H_{30}NO_2S$ was selected for analysis. All measurements were made on a Bruker AXS KAPPA APEX II diffractometer coupled to an APEX II CCD detector with graphite monochromated Mo K_α radiation (λ = 0.71073 Å) for the structure of compound A17003. The structure was solved by direct methods using SHELXS[6] and refined against F^2 on all data by full-matrix least squares with SHELXL-2014[7] using established refinement techniques.[8]

Table S-1. Crystal data and structure refinement for A17003.

Identification code		A17003
Empirical formula		$C_{24}H_{30}ClNO_2S$
Formula weight		432.02
Temperature/K		293.15
Crystal system		orthorhombic
Space group		$P2_12_12_1$
Unit cell dimensions	$\alpha = 90°$	a = 7.6789(7) Å
	$\beta = 90°$	b = 13.3309(14) Å
	$\gamma = 90°$	c = 21.874(3) Å
Volume		2239.2(4) $Å^3$
Z		8
Density(Calculated)		1.281 Mg/m^3
Absorption coefficient		0.284 mm^{-1}
F(000)		920.0
Crystal size/mm^3		0.21 × 0.14 × 0.08 mm^3
Radiation		MoKα (λ = 0.71073)
Theta range for data collection		3.72° to 54.22°
Index ranges		$-9 \le h \le 9$, $-16 \le k \le 17$, $-28 \le l \le 27$
Reflections collected		35799
Independent reflections		4941 [R_{int} = 0.0330]
Data/restraints/parameters		4941/0/264
Goodness-of-fit on F^2		1.058
Final R indexes [I>=2sigma (I)]		R_1 = 0.0396, wR_2 = 0.1005
Final R indexes [all data]		R_1 = 0.0422, wR_2 = 0.1021
Largest diff. peak/hole		0.79/-0.45/ e $Å^{-3}$
Flack parameter		0.04(7)

Table S-2. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for A17003. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Cl(1)	10324.1(13)	11229.8(6)	4750.6(4)	61.1(3)
S(1)	-171.9(6)	6786.1(3)	6186.0(2)	17.97(11)
O(1)	-1081(2)	6969.1(12)	5627.2(7)	26.9(4)
O(2)	-644(2)	7327.4(11)	6729.1(7)	23.6(3)
N(1)	1880(2)	7009.3(13)	6056.8(8)	18.7(4)
C(1)	-174(4)	2308.0(15)	6686.7(11)	31.2(5)
C(2)	-271(3)	3420.9(14)	6569.5(9)	20.2(4)
C(3)	-598(3)	3789.0(17)	5987.7(10)	25.0(5)
C(4)	-628(3)	4818.4(17)	5868.2(10)	23.6(5)
C(5)	-342(3)	5486.7(14)	6344.8(9)	16.9(4)
C(6)	-73(3)	5134.6(15)	6935.4(9)	18.5(4)
C(7)	-36(3)	4105.6(15)	7041.8(9)	20.9(4)
C(8)	2648(3)	6537.7(17)	5501(1)	22.3(4)
C(9)	4592(3)	6528.5(16)	5643.2(10)	23.3(4)
C(10)	4651(3)	6362.5(16)	6330.9(10)	23.8(4)
C(11)	3116(3)	6966.8(16)	6587.4(10)	19.6(4)
C(12)	3541(3)	8023.4(17)	6829.7(10)	23.9(4)
C(13)	4523(3)	7949.3(18)	7440.1(10)	30.0(5)
C(14)	4914(3)	8996.1(19)	7703.0(11)	34.2(5)
C(15)	5934(3)	9622.7(19)	7247.6(11)	31.0(5)
C(16)	5069(3)	9720.7(16)	6612.3(10)	25.5(4)
C(17)	4580(3)	8649.9(15)	6377.3(10)	22.4(4)
C(18)	3427(3)	10369.2(19)	6653.9(14)	34.9(6)
C(19)	6377(3)	10154.0(15)	6156.3(11)	23.7(4)
C(20)	6045(3)	10970.8(17)	5779.6(12)	30.1(5)
C(21)	7262(4)	11300.5(19)	5349.5(13)	37.7(6)
C(22)	8821(4)	10822(2)	5299.4(13)	38.0(6)
C(23)	9228(3)	10014.3(19)	5667.8(12)	33.3(6)
C(24)	8004(3)	9683.8(17)	6087.4(11)	26.6(5)

Table S-3. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for A17003. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cl(1)	72.9(6)	42.8(4)	67.6(5)	-5.3(4)	32.1(5)	-21.9(4)
S(1)	13.7(2)	15.4(2)	24.8(2)	4.62(18)	-1.48(19)	0.15(17)
O(1)	22.2(8)	25.8(8)	32.6(8)	8.8(7)	-8.3(7)	0.4(6)
O(2)	19.5(7)	17.7(7)	33.5(8)	0.3(6)	1.2(6)	3.1(6)
N(1)	16.5(8)	16.9(8)	22.8(9)	2.8(7)	-0.2(7)	-2.4(6)
C(1)	40.1(13)	16.1(9)	37.3(12)	1.9(9)	-0.1(11)	-1.8(10)
C(2)	18.6(9)	16.5(9)	25.6(10)	0.3(7)	1.6(8)	-2.8(8)
C(3)	30.7(12)	21.1(10)	23.4(10)	-3.9(8)	-1.7(9)	-7.9(9)
C(4)	26.5(11)	23.9(10)	20.4(10)	1.2(8)	-5.0(8)	-6.1(9)
C(5)	13.4(9)	15.6(8)	21.8(9)	3.1(7)	-1.1(7)	-2.3(7)
C(6)	16.3(9)	19.7(9)	19.4(9)	0.2(7)	1.1(8)	-3.9(8)
C(7)	19.6(10)	22.6(9)	20.6(9)	5.3(7)	-0.8(8)	-3.6(8)
C(8)	22.5(10)	23.5(10)	20.8(10)	1.1(8)	3.0(8)	-5.6(8)
C(9)	20.1(10)	21.9(10)	27.8(10)	-0.7(8)	3.6(9)	-2.7(8)
C(10)	18.8(10)	21.6(10)	30.9(11)	-1.2(8)	-1.8(9)	0.3(8)
C(11)	15.6(9)	19.7(10)	23.5(10)	2.6(8)	-1.5(8)	-3.5(8)
C(12)	19.5(10)	23.0(11)	29.2(11)	-5.8(9)	0.2(8)	-1.3(8)
C(13)	30.6(12)	32.5(12)	26.8(11)	-2.2(9)	-1.4(9)	-4.6(10)
C(14)	31.7(13)	39.6(13)	31.2(12)	-11.7(10)	-3.6(11)	-6.5(12)
C(15)	26.1(12)	31.2(13)	35.6(13)	-8.7(10)	-5.9(10)	-4.9(10)
C(16)	19(1)	24.1(10)	33.5(11)	-7.2(9)	-1.4(9)	-2.6(9)
C(17)	19.1(10)	19.4(9)	28.7(10)	-2.9(8)	-3.2(8)	0.1(8)
C(18)	24.6(12)	25.9(12)	54.2(16)	-9.9(11)	0.0(11)	1(1)
C(19)	22.2(10)	15.5(9)	33.5(12)	-8.1(9)	-6.6(9)	-4.4(8)
C(20)	28.6(12)	19.1(11)	42.5(14)	-5.1(10)	-7.2(10)	-1.5(9)
C(21)	52.5(17)	18.4(11)	42.3(15)	0.4(10)	-6.0(13)	-9.8(11)
C(22)	44.2(15)	25.7(12)	44.0(15)	-10.3(11)	8.1(12)	-16.7(11)
C(23)	24.1(11)	30.4(13)	45.5(14)	-17.1(11)	1.9(11)	-5.2(10)
C(24)	24.8(11)	19.2(10)	35.9(13)	-7.0(9)	-5.6(10)	-1.0(8)

Table S-4. Bond Lengths for A17003.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cl(1)	C(22)	1.752(3)	C(10)	C(11)	1.534(3)
S(1)	O(1)	1.4286(16)	C(11)	C(12)	1.540(3)
S(1)	O(2)	1.4363(16)	C(12)	C(13)	1.537(3)
S(1)	N(1)	1.6280(18)	C(12)	C(17)	1.521(3)
S(1)	C(5)	1.7715(19)	C(13)	C(14)	1.539(3)
N(1)	C(8)	1.491(3)	C(14)	C(15)	1.518(4)
N(1)	C(11)	1.501(3)	C(15)	C(16)	1.546(3)
C(1)	C(2)	1.507(3)	C(16)	C(17)	1.563(3)
C(2)	C(3)	1.387(3)	C(16)	C(18)	1.531(3)
C(2)	C(7)	1.390(3)	C(16)	C(19)	1.529(3)
C(3)	C(4)	1.397(3)	C(19)	C(20)	1.389(3)
C(4)	C(5)	1.389(3)	C(19)	C(24)	1.406(3)
C(5)	C(6)	1.390(3)	C(20)	C(21)	1.397(4)
C(6)	C(7)	1.392(3)	C(21)	C(22)	1.360(4)
C(8)	C(9)	1.525(3)	C(22)	C(23)	1.381(4)
C(9)	C(10)	1.521(3)	C(23)	C(24)	1.386(3)

Table S-5. Bond Angles for A17003.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O(1)	S(1)	O(2)	119.90(9)	C(10)	C(11)	C(12)	116.34(17)
O(1)	S(1)	N(1)	107.05(10)	C(13)	C(12)	C(11)	110.13(19)
O(1)	S(1)	C(5)	107.38(10)	C(17)	C(12)	C(11)	112.92(17)
O(2)	S(1)	N(1)	107.20(9)	C(17)	C(12)	C(13)	110.07(18)
O(2)	S(1)	C(5)	108.09(9)	C(12)	C(13)	C(14)	111.2(2)
N(1)	S(1)	C(5)	106.51(9)	C(15)	C(14)	C(13)	110.8(2)
C(8)	N(1)	S(1)	116.60(14)	C(14)	C(15)	C(16)	114.5(2)
C(8)	N(1)	C(11)	111.37(16)	C(15)	C(16)	C(17)	108.76(18)
C(11)	N(1)	S(1)	118.11(14)	C(18)	C(16)	C(15)	110.4(2)
C(3)	C(2)	C(1)	120.89(19)	C(18)	C(16)	C(17)	109.73(19)
C(3)	C(2)	C(7)	118.23(18)	C(19)	C(16)	C(15)	109.62(18)
C(7)	C(2)	C(1)	120.88(19)	C(19)	C(16)	C(17)	106.75(17)
C(2)	C(3)	C(4)	121.5(2)	C(19)	C(16)	C(18)	111.5(2)
C(5)	C(4)	C(3)	119.1(2)	C(12)	C(17)	C(16)	114.42(18)
C(4)	C(5)	S(1)	119.45(15)	C(20)	C(19)	C(16)	124.2(2)
C(4)	C(5)	C(6)	120.30(18)	C(20)	C(19)	C(24)	116.7(2)
C(6)	C(5)	S(1)	120.10(15)	C(24)	C(19)	C(16)	119.0(2)
C(5)	C(6)	C(7)	119.43(18)	C(19)	C(20)	C(21)	121.5(2)
C(2)	C(7)	C(6)	121.35(18)	C(22)	C(21)	C(20)	119.7(2)
N(1)	C(8)	C(9)	102.98(17)	C(21)	C(22)	Cl(1)	119.3(2)
C(10)	C(9)	C(8)	103.41(17)	C(21)	C(22)	C(23)	121.2(3)
C(9)	C(10)	C(11)	105.22(17)	C(23)	C(22)	Cl(1)	119.5(2)
N(1)	C(11)	C(10)	102.89(16)	C(22)	C(23)	C(24)	118.7(2)
N(1)	C(11)	C(12)	111.45(17)	C(23)	C(24)	C(19)	122.2(2)

Table S-6. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for A17003.

Atom	*x*	*y*	*z*	U(eq)
H(1A)	187	2192	7101	47
H(1B)	653	2010	6412	47
H(1C)	-1299	2013	6622	47
H(3)	-802	3340	5670	30
H(4)	-838	5053	5475	28
H(6)	82	5583	7257	22
H(7)	149	3871	7437	25
H(8A)	2403	6932	5139	27
H(8B)	2208	5863	5442	27
H(9A)	5177	5989	5427	28
H(9B)	5131	7161	5533	28
H(10A)	5744	6601	6499	29
H(10B)	4525	5656	6427	29
H(11)	2573	6579	6917	23
H(12)	2437	8370	6906	29
H(13A)	5608	7590	7378	36
H(13B)	3827	7573	7731	36
H(14A)	3829	9332	7801	41
H(14B)	5580	8928	8078	41
H(15A)	7079	9326	7196	37
H(15B)	6095	10289	7416	37
H(17A)	3909	8717	6004	27
H(17B)	5643	8293	6277	27
H(18A)	2662	10099	6959	52
H(18B)	2846	10373	6265	52
H(18C)	3745	11042	6763	52
H(20)	4987	11306	5814	36
H(21)	7008	11844	5099	45
H(23)	10304	9698	5635	40
H(24)	8267	9133	6331	32

(*S*)-2-((2*S*,4*R*,4a*S*,6*R*,8a*S*)-6-Isopropyl-4,4a-dimethyldecahydronaphthalen-2-yl)-1-tosyl-pyrrolidine (Table 2, entry 5). This compound was synthesized under the standard cross-coupling conditions from (1*R*,4a*S*,7*R*,8a*S*)-3-iodo-7-isopropyl-1,8a-dimethyldecahydro naphthalene and the organozinc reagent, using (*S*,*S*)-**1**, followed by tosylation.

A suitable crystal of $C_{26}H_{41}NO_2S$ was selected for analysis. All measurements were made on a Bruker AXS KAPPA APEX II diffractometer coupled to an APEX II CCD detector with graphite monochromated Mo K_α radiation (λ = 0.71073 Å) for the structure of compound A15082. The structure was solved by direct methods using SHELXS[6] and refined against F^2 on all data by full-matrix least squares with SHELXL-2014[7] using established refinement techniques.[8]

Table S-1. Crystal data and structure refinement for A15082.

Identification code	A15082
Empirical formula	$C_{26}H_{41}NO_2S$
Formula weight	431.66
Temperature	100 K
Crystal system	orthorhombic
Space group	$P2_12_12_1$
Unit cell dimensions	a = 6.4513(3) Å α = 90°
	b = 12.5214(6) Å β = 90°
	c = 29.5670(13) Å γ = 90°
Volume	2388.40(19) $Å^3$
Z	4
Density(calculated)	1.200 Mg/m^3
Absorption coefficient	0.158 mm^{-1}
F(000)	944.0
Crystal size	0.600 × 0.500 × 0.500 mm^3
Radiation	MoKα (λ = 0.71073)
Theta range for data collection	2.754° to 72.686°
Index ranges	$-10 \leq h \leq 10$, $-10 \leq k \leq 20$, $-49 \leq l \leq 31$
Reflections collected	50566
Independent reflections	11566 [Rint = 0.0332]
Data/restraints/parameters	11566/0/276
Goodness-of-fit on F^2	1.076
R indexes [I>=2sigma (I)]	R1 = 0.0322, wR2 = 0.0829
R indexes [all data]	R1 = 0.0356, wR2 = 0.0846
Largest diff. peak/hole	0.42/-0.31 e/$Å^{-3}$
Flack parameter	0.027(13)

Table S-2. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for A15082. Ueq is defined as 1/3 of of the trace of the orthogonalised U^{ij} tensor.

Atom	x	y	z	U(eq)
S(1)	1638.8(4)	7068.3(2)	8918.0(2)	10.33(5)
O(1)	-469.9(13)	6989.2(7)	8768.8(3)	14.20(14)
O(2)	2715.7(15)	6128.4(7)	9068.0(3)	16.50(16)
N(1)	2948.0(14)	7569.0(8)	8497.2(3)	11.10(15)
C(1)	2074.9(17)	8543.1(8)	8272.4(3)	11.05(16)
C(2)	3955.2(19)	9300.2(9)	8224.8(4)	15.40(19)
C(3)	5531.2(19)	8893.2(11)	8570.5(4)	17.7(2)
C(4)	5219.7(17)	7687(1)	8549.4(4)	16.3(2)
C(5)	964.7(17)	8246.8(8)	7831.1(3)	10.42(16)
C(6)	2366.7(17)	7729.9(8)	7475.3(3)	11.33(17)
C(7)	1121.7(16)	7436.5(8)	7053.2(3)	10.36(16)
C(8)	94.4(17)	8430.3(8)	6832.4(3)	9.98(16)
C(9)	-1347.5(17)	8940.0(8)	7194.6(3)	10.79(16)
C(10)	-159.9(18)	9213.5(8)	7630.2(3)	11.76(17)
C(11)	2395.1(18)	6787.3(9)	6713.9(4)	13.39(18)
C(12)	1075.9(19)	6432.1(9)	6311.5(4)	14.74(19)
C(13)	32.6(17)	7388.1(9)	6079.7(4)	12.54(16)
C(14)	-1210.9(17)	8036.3(9)	6427.6(3)	12.63(17)
C(15)	-2529(2)	9927.3(10)	7030.6(4)	16.4(2)
C(16)	1702.6(19)	9251.3(8)	6666.9(4)	13.93(17)
C(17)	-1251.5(18)	7052.3(10)	5661.1(4)	15.35(18)
C(18)	-3181(3)	6400.2(14)	5772.6(5)	28.0(3)
C(19)	-1815(2)	8016.2(11)	5367.7(4)	22.3(2)
C(20)	1685.0(17)	7996.1(8)	9369.3(3)	11.17(15)
C(21)	-25.6(18)	8646.6(9)	9451.2(4)	13.40(17)
C(22)	10.9(19)	9356.4(9)	9812.9(4)	15.29(19)
C(23)	1760(2)	9442.6(8)	10090.0(4)	14.49(18)
C(24)	3467(2)	8795.3(9)	9998.8(4)	15.49(19)
C(25)	3438.7(19)	8061.2(9)	9643.9(3)	14.32(17)

C(26)	1789(2)	10198.8(10)	10484.3(4)	20.6(2)

Table S-3. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for A15082. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11}+\ldots+2hka^*b^*U^{12}]$.

Atom	U11	U22	U33	U23	U13	U12
S(1)	11.79(9)	10.86(9)	8.35(9)	1.03(7)	-1.11(8)	-0.27(8)
O(1)	11.5(3)	17.9(4)	13.2(3)	-0.1(3)	-1.6(3)	-3.7(3)
O(2)	23.0(4)	11.7(3)	14.8(3)	2.3(3)	-2.8(3)	3.9(3)
N(1)	10.0(3)	14.2(3)	9.1(3)	1.5(3)	-0.1(3)	0.9(3)
C(1)	12.2(4)	12.4(4)	8.6(3)	1.1(3)	-0.1(3)	0.3(3)
C(2)	17.0(5)	17.6(4)	11.6(4)	0.8(3)	-0.4(4)	-6.1(4)
C(3)	13.6(4)	25.5(5)	14.0(5)	0.9(4)	-1.0(4)	-6.1(4)
C(4)	9.4(4)	23.7(5)	16.0(4)	1.4(4)	0.7(3)	2.0(4)
C(5)	11.6(4)	11.9(4)	7.7(3)	0.9(3)	0.3(3)	0.5(3)
C(6)	11.7(4)	12.9(4)	9.4(4)	0.3(3)	-0.2(3)	2.1(3)
C(7)	11.7(4)	10.7(4)	8.6(3)	0.6(3)	0.6(3)	1.0(3)
C(8)	11.3(4)	10.3(4)	8.4(3)	0.8(3)	0.1(3)	0.6(3)
C(9)	11.8(4)	12.0(4)	8.5(3)	0.4(3)	-0.1(3)	2.3(3)
C(10)	14.2(4)	12.6(4)	8.5(4)	0.0(3)	0.1(3)	2.7(3)
C(11)	14.5(4)	14.2(4)	11.5(4)	-1.6(3)	-0.1(3)	3.8(3)
C(12)	18.3(5)	13.7(4)	12.2(4)	-2.3(3)	-0.5(4)	2.4(4)
C(13)	13.4(4)	14.7(4)	9.5(4)	-1.4(3)	0.0(4)	-0.2(3)
C(14)	12.9(4)	15.6(4)	9.5(4)	-1.3(3)	-1.1(3)	1.3(3)
C(15)	19.3(5)	16.9(5)	13.2(4)	0.6(3)	-0.7(4)	7.9(4)
C(16)	16.7(4)	13.1(4)	12.0(4)	1.7(3)	1.9(4)	-2.1(4)
C(17)	16.2(4)	20.1(4)	9.8(4)	-2.9(4)	-0.3(3)	-1.3(4)
C(18)	25.9(6)	42.6(8)	15.4(5)	-4.3(5)	-0.3(5)	-16.2(6)
C(19)	25.8(6)	26.4(6)	14.7(5)	-0.6(4)	-6.4(4)	2.1(5)
C(20)	13.0(4)	12.5(4)	8.0(3)	0.9(3)	-1.0(3)	0.0(4)
C(21)	12.9(4)	15.5(4)	11.9(4)	0.0(3)	-0.9(3)	0.4(4)
C(22)	16.1(5)	15.4(4)	14.4(4)	-1.9(3)	1.3(4)	0.2(4)
C(23)	19.8(5)	13.5(4)	10.1(4)	0.4(3)	0.5(4)	-3.0(4)
C(24)	19.3(5)	16.7(4)	10.4(4)	0.7(3)	-4.1(4)	-0.9(4)
C(25)	15.9(4)	16.0(4)	11.1(4)	0.7(3)	-3.2(4)	1.4(4)
C(26)	26.5(6)	20.6(5)	14.8(5)	-5.5(4)	1.6(4)	-5.2(5)

Table S-4. Bond Lengths for A15082.

Atom	Atom	Length / Å
S(1)	O(1)	1.4335(9)
S(1)	O(2)	1.4367(9)
S(1)	N(1)	1.6293(9)
S(1)	C(20)	1.7695(10)
N(1)	C(4)	1.4811(15)
N(1)	C(1)	1.4988(14)
C(1)	C(5)	1.5341(14)
C(1)	C(2)	1.5459(16)
C(2)	C(3)	1.5292(17)
C(3)	C(4)	1.5250(18)
C(5)	C(6)	1.5310(14)
C(5)	C(10)	1.5312(15)
C(6)	C(7)	1.5289(14)
C(7)	C(11)	1.5303(15)
C(7)	C(8)	1.5537(14)
C(8)	C(16)	1.5404(15)
C(8)	C(14)	1.5443(15)
C(8)	C(9)	1.5555(14)
C(9)	C(15)	1.5310(15)
C(9)	C(10)	1.5372(15)
C(11)	C(12)	1.5291(16)
C(12)	C(13)	1.5347(16)
C(13)	C(14)	1.5363(15)
C(13)	C(17)	1.5477(15)
C(17)	C(18)	1.5246(19)
C(17)	C(19)	1.5302(18)
C(20)	C(21)	1.3929(15)
C(20)	C(25)	1.3950(15)
C(21)	C(22)	1.3907(16)
C(22)	C(23)	1.3985(17)
C(23)	C(24)	1.3938(18)
C(23)	C(26)	1.5021(16)
C(24)	C(25)	1.3949(15)

Table S-5. Bond Angles for A15082.

Atom	Atom	Atom	Angle / °	Atom	Atom	Atom	Angle / °
O(1)	S(1)	O(2)	119.82(6)	C(14)	C(8)	C(9)	109.79(8)
O(1)	S(1)	N(1)	106.47(5)	C(7)	C(8)	C(9)	107.13(8)
O(2)	S(1)	N(1)	107.47(5)	C(15)	C(9)	C(10)	109.48(9)
O(1)	S(1)	C(20)	107.06(5)	C(15)	C(9)	C(8)	114.26(8)
O(2)	S(1)	C(20)	107.27(5)	C(10)	C(9)	C(8)	111.73(8)
N(1)	S(1)	C(20)	108.33(5)	C(5)	C(10)	C(9)	112.65(8)
C(4)	N(1)	C(1)	109.69(9)	C(12)	C(11)	C(7)	111.46(9)
C(4)	N(1)	S(1)	118.14(8)	C(11)	C(12)	C(13)	111.38(9)
C(1)	N(1)	S(1)	117.19(7)	C(12)	C(13)	C(14)	110.01(9)
N(1)	C(1)	C(5)	110.83(8)	C(12)	C(13)	C(17)	112.33(9)
N(1)	C(1)	C(2)	104.15(9)	C(14)	C(13)	C(17)	113.55(9)
C(5)	C(1)	C(2)	115.92(9)	C(13)	C(14)	C(8)	113.76(9)
C(3)	C(2)	C(1)	104.86(9)	C(18)	C(17)	C(19)	110.56(11)
C(4)	C(3)	C(2)	102.42(9)	C(18)	C(17)	C(13)	114.17(9)
N(1)	C(4)	C(3)	103.50(9)	C(19)	C(17)	C(13)	111.49(10)
C(6)	C(5)	C(10)	110.33(8)	C(21)	C(20)	C(25)	120.47(10)
C(6)	C(5)	C(1)	114.27(9)	C(21)	C(20)	S(1)	120.12(8)
C(10)	C(5)	C(1)	111.10(8)	C(25)	C(20)	S(1)	119.41(8)
C(7)	C(6)	C(5)	110.62(8)	C(22)	C(21)	C(20)	119.60(11)
C(6)	C(7)	C(11)	112.38(9)	C(21)	C(22)	C(23)	120.90(11)
C(6)	C(7)	C(8)	111.99(8)	C(24)	C(23)	C(22)	118.64(10)
C(11)	C(7)	C(8)	112.27(8)	C(24)	C(23)	C(26)	120.46(11)
C(16)	C(8)	C(14)	109.53(8)	C(22)	C(23)	C(26)	120.89(12)
C(16)	C(8)	C(7)	112.38(9)	C(23)	C(24)	C(25)	121.22(11)
C(14)	C(8)	C(7)	107.60(8)	C(24)	C(25)	C(20)	119.14(11)
C(16)	C(8)	C(9)	110.35(8)				

Table S-6. Torsion Angles for A15082.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O(1)	S(1)	N(1)	C(4)	-176.83(9)	C(7)	C(8)	C(9)	C(10)	56.10(11)
O(2)	S(1)	N(1)	C(4)	-47.28(10)	C(6)	C(5)	C(10)	C(9)	53.95(12)
C(20)	S(1)	N(1)	C(4)	68.33(9)	C(1)	C(5)	C(10)	C(9)	-178.26(9)
O(1)	S(1)	N(1)	C(1)	48.40(9)	C(15)	C(9)	C(10)	C(5)	176.71(9)
O(2)	S(1)	N(1)	C(1)	177.94(8)	C(8)	C(9)	C(10)	C(5)	-55.70(11)
C(20)	S(1)	N(1)	C(1)	-66.45(8)	C(6)	C(7)	C(11)	C(12)	175.75(9)
C(4)	N(1)	C(1)	C(5)	121.14(10)	C(8)	C(7)	C(11)	C(12)	-56.92(12)
S(1)	N(1)	C(1)	C(5)	-100.53(9)	C(7)	C(11)	C(12)	C(13)	55.53(12)
C(4)	N(1)	C(1)	C(2)	-4.20(11)	C(11)	C(12)	C(13)	C(14)	-54.44(12)
S(1)	N(1)	C(1)	C(2)	134.13(8)	C(11)	C(12)	C(13)	C(17)	178.03(9)
N(1)	C(1)	C(2)	C(3)	-20.11(11)	C(12)	C(13)	C(14)	C(8)	56.57(12)
C(5)	C(1)	C(2)	C(3)	-142.14(10)	C(17)	C(13)	C(14)	C(8)	-176.58(9)
C(1)	C(2)	C(3)	C(4)	36.15(11)	C(16)	C(8)	C(14)	C(13)	66.32(11)
C(1)	N(1)	C(4)	C(3)	26.82(11)	C(7)	C(8)	C(14)	C(13)	-56.11(11)
S(1)	N(1)	C(4)	C(3)	-111.06(9)	C(9)	C(8)	C(14)	C(13)	-172.37(9)
C(2)	C(3)	C(4)	N(1)	-38.36(11)	C(12)	C(13)	C(17)	C(18)	68.32(14)
N(1)	C(1)	C(5)	C(6)	-61.43(11)	C(14)	C(13)	C(17)	C(18)	-57.31(14)
C(2)	C(1)	C(5)	C(6)	56.99(12)	C(12)	C(13)	C(17)	C(19)	-165.50(10)
N(1)	C(1)	C(5)	C(10)	172.95(9)	C(14)	C(13)	C(17)	C(19)	68.87(13)
C(2)	C(1)	C(5)	C(10)	-68.64(12)	O(1)	S(1)	C(20)	C(21)	-13.18(10)
C(10)	C(5)	C(6)	C(7)	-55.43(11)	O(2)	S(1)	C(20)	C(21)	-142.98(9)
C(1)	C(5)	C(6)	C(7)	178.54(8)	N(1)	S(1)	C(20)	C(21)	101.28(9)
C(5)	C(6)	C(7)	C(11)	-172.52(9)	O(1)	S(1)	C(20)	C(25)	166.18(9)
C(5)	C(6)	C(7)	C(8)	60.01(11)	O(2)	S(1)	C(20)	C(25)	36.38(10)
C(6)	C(7)	C(8)	C(16)	62.38(11)	N(1)	S(1)	C(20)	C(25)	-79.36(9)
C(11)	C(7)	C(8)	C(16)	-65.15(11)	C(25)	C(20)	C(21)	C(22)	-0.76(16)
C(6)	C(7)	C(8)	C(14)	-176.97(8)	S(1)	C(20)	C(21)	C(22)	178.60(9)
C(11)	C(7)	C(8)	C(14)	55.50(11)	C(20)	C(21)	C(22)	C(23)	1.38(17)
C(6)	C(7)	C(8)	C(9)	-58.97(11)	C(21)	C(22)	C(23)	C(24)	-0.50(17)
C(11)	C(7)	C(8)	C(9)	173.50(9)	C(21)	C(22)	C(23)	C(26)	-179.19(11)
C(16)	C(8)	C(9)	C(15)	58.46(12)	C(22)	C(23)	C(24)	C(25)	-1.03(17)

C(14)	C(8)	C(9)	C(15)	-62.36(12)	C(26)	C(23)	C(24)	C(25)	177.68(11)
C(7)	C(8)	C(9)	C(15)	-178.91(9)	C(23)	C(24)	C(25)	C(20)	1.64(17)
C(16)	C(8)	C(9)	C(10)	-66.52(11)	C(21)	C(20)	C(25)	C(24)	-0.73(16)
C(14)	C(8)	C(9)	C(10)	172.66(8)	S(1)	C(20)	C(25)	C(24)	179.91(9)

Table S-7. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for A15082.

Atom	x	y	z	U(eq)
H(1)	1047	8880	8482	13
H(2A)	4533	9268	7915	18
H(2B)	3553	10046	8292	18
H(3A)	6962	9093	8484	21
H(3B)	5231	9174	8877	21
H(4A)	5964	7375	8288	20
H(4B)	5709	7339	8831	20
H(5)	-122	7709	7910	12
H(6A)	3489	8232	7392	14
H(6B)	3012	7079	7603	14
H(7)	-34	6963	7156	12
H(9)	-2407	8390	7276	13
H(10A)	866	9780	7564	14
H(10B)	-1146	9498	7857	14
H(11A)	3568	7226	6604	16
H(11B)	2974	6150	6867	16
H(12A)	-1	5927	6417	18
H(12B)	1964	6054	6090	18
H(13)	1169	7863	5968	15
H(14A)	-2360	7589	6543	15
H(14B)	-1831	8662	6274	15
H(15A)	-1553	10516	6983	25
H(15B)	-3556	10135	7258	25
H(15C)	-3233	9762	6745	25
H(16A)	2394	9576	6928	21
H(16B)	1003	9808	6491	21
H(16C)	2733	8892	6477	21
H(17)	-337	6584	5473	18
H(18A)	-2797	5797	5966	42
H(18B)	-3800	6132	5492	42

H(18C)	-4185	6853	5931	42
H(19A)	-2720	8497	5539	33
H(19B)	-2537	7772	5095	33
H(19C)	-548	8397	5281	33
H(21)	-1210	8606	9261	16
H(22)	-1168	9789	9873	18
H(24)	4672	8855	10182	19
H(25)	4599	7612	9590	17
H(26A)	3123	10143	10641	31
H(26B)	667	10015	10694	31
H(26C)	1596	10931	10375	31

(*R*)-2-((2*S*,4*R*,4a*S*,6*R*,8a*S*)-6-Isopropyl-4,4a-dimethyldecahydronaphthalen-2-yl)-1-tosyl-pyrrolidine (Table 2, entry 5). This compound was synthesized under the standard cross-coupling conditions from (1*R*,4a*S*,7*R*,8a*S*)-3-iodo-7-isopropyl-1,8a-dimethyldecahydro naphthalene and the organozinc reagent, using (*R*,*R*)-**1**, followed by tosylation.

A suitable crystal of $C_{26}H_{41}NO_2S$ was selected for analysis. All measurements were made on a Bruker AXS KAPPA APEX II diffractometer coupled to an APEX II CCD detector with graphite monochromated Mo K_α radiation ($\lambda = 0.71073$ Å) for the structure of compound A17007. The structure was solved by direct methods using SHELXS[6] and refined against F^2 on all data by full-matrix least squares with SHELXL-2014[7] using established refinement techniques.[8]

Table S-1. Crystal data and structure refinement for A17007.

Identification code	A17007
Empirical formula	$C_{26}H_{41}NO_2S$
Formula weight	431.66
Temperature/K	100.0
Crystal system	monoclinic
Space group	$P2_1$
Unit cell dimensions	a = 6.2849(19) Å, α = 90°
	b = 35.611(10) Å, β = 90.2°
	c = 10.788(4) Å, γ = 90°
Volume	2414.5(13) $Å^3$
Z	4
Density(calculated)	1.187 Mg / m^3
Absorption coefficient	0.156 mm^{-1}
F(000)	944.0
Crystal size	0.39 × 0.31 × 0.14 mm^3
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.288 to 65.678
Index ranges	$-9 \leq h \leq 9$, $-53 \leq k \leq 53$, $-16 \leq l \leq 16$
Reflections collected	154882
Independent reflections	17549 [R_{int} = 0.0332]
Data/restraints/parameters	17549/1/556
Goodness-of-fit on F^2	1.146
Final R indexes [I>=2sigma (I)]	R_1 = 0.0451, wR_2 = 0.1153
Final R indexes [all data]	R_1 = 0.0483, wR_2 = 0.1166
Largest diff. peak/hole	0.48/-0.34 / e $Å^{-3}$
Flack parameter	0.053(7)

Table S-2. Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for a17007. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
S1	8993.6(8)	4453.1(2)	12071.1(5)	16.71(10)
O1	9888(3)	4365.8(5)	13267.0(15)	23.0(3)
O2	10314(3)	4599.1(5)	11101.9(16)	22.2(3)
N1	7961(3)	4063.4(5)	11535.8(17)	16.3(3)
C1	1460(4)	5479.1(8)	12841(3)	33.1(6)
C2	4132(4)	5009.4(7)	13621(2)	24.4(4)
C3	5851(4)	4775.5(7)	13448(2)	21.3(4)
C4	6884(3)	4770.0(6)	12303(2)	17.9(4)
C5	6196(4)	5000.7(7)	11347(2)	20.3(4)
C6	4452(4)	5232.2(7)	11526(2)	23.8(4)
C7	3399(4)	5238.5(7)	12659(2)	23.2(4)
C8	6424(4)	3866.3(7)	12335(2)	20.3(4)
C9	4301(4)	3922.7(7)	11680(2)	22.9(4)
C10	4935(3)	3882.5(7)	10316(2)	22.3(4)
C11	7139(3)	4068.8(6)	10228.9(19)	17.1(4)
C12	8711(3)	3883.8(6)	9336.2(18)	15.1(3)
C13	9409(4)	3492.6(6)	9749.8(19)	17.4(4)
C14	10792(3)	3289.6(6)	8783.9(19)	16.4(4)
C15	9651(3)	3269.7(6)	7505.8(18)	14.8(3)
C16	9230(3)	3679.7(6)	7106.4(18)	14.6(3)
C17	7789(3)	3883.9(6)	8018.1(19)	16.4(3)
C18	8432(4)	3713.5(6)	5768(2)	20.0(4)
C19	9948(4)	3525.5(7)	4862(2)	21.2(4)
C20	10275(3)	3113.9(6)	5203.5(19)	16.9(4)
C21	11127(4)	3088.6(6)	6539.1(19)	16.6(4)
C22	7596(4)	3037.7(7)	7593(2)	21.0(4)
C23	11526(4)	2912.0(7)	9302(2)	26.0(5)
C24	11646(4)	2889.5(7)	4281(2)	19.7(4)
C25	10542(5)	2855(1)	3022(2)	33.0(6)
C26	13888(4)	3046.7(8)	4113(2)	27.1(5)
S1B	6058.0(9)	5545.3(2)	7449.5(5)	21.51(11)
O1B	5415(3)	5588.0(7)	8716.7(17)	33.0(4)
O2B	4532(3)	5448.5(5)	6509.7(17)	24.3(3)
N1B	7100(3)	5944.8(6)	7018.3(18)	21.9(4)
C1B	13431(5)	4467.6(10)	7047(4)	47.2(9)
C2B	11151(4)	4906.1(9)	8284(3)	35.7(7)
C3B	9456(5)	5151.9(9)	8395(2)	30.3(6)
C4B	8103(4)	5208.0(7)	7395(2)	22.1(4)
C5B	8431(4)	5013.7(7)	6286(2)	22.1(4)

C6B	10148(4)	4769.5(7)	6193(3)	26.5(5)
C7B	11521(4)	4717.4(8)	7184(3)	31.8(6)
C8B	8676(5)	6121.2(9)	7864(3)	32.4(6)
C9B	10722(4)	6094.5(9)	7177(3)	25.2(8)
C10B	10071(4)	6162.8(7)	5838(2)	24.3(4)
C11B	7913(4)	5961.8(6)	5717(2)	18.9(4)
C12B	6311(4)	6141.0(6)	4823(2)	18.5(4)
C13B	5580(4)	6533.5(7)	5214(2)	21.3(4)
C14B	4199(4)	6729.5(6)	4236(2)	19.8(4)
C15B	5334(4)	6744.7(6)	2963(2)	18.6(4)
C16B	5751(4)	6330.7(6)	2582(2)	18.2(4)
C17B	7203(4)	6133.0(7)	3501(2)	20.4(4)
C18B	6520(4)	6290.3(7)	1242(2)	24.8(5)
C19B	5000(4)	6478.1(8)	333(2)	26.4(5)
C20B	4702(4)	6892.4(7)	657(2)	20.7(4)
C21B	3856(4)	6922.3(7)	1980(2)	21.0(4)
C22B	7392(4)	6974.1(7)	3048(2)	26.0(5)
C23B	3461(5)	7110.2(8)	4731(3)	30.1(5)
C24B	3347(4)	7116.8(7)	-272(2)	23.8(4)
C25B	4425(5)	7141.9(10)	-1535(3)	36.4(6)
C26B	1079(4)	6969.3(9)	-423(3)	30.6(5)
C0AA	10320(30)	6337(6)	7121(17)	23(5)

Table S-3. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for a17007. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S1	13.04(19)	22.2(2)	14.9(2)	-3.46(18)	-1.11(15)	-0.94(18)
O1	19.7(7)	32.0(9)	17.2(7)	-2.5(6)	-5.2(6)	0.3(6)
O2	16.3(7)	29.2(8)	21.2(7)	-4.9(6)	3.3(6)	-4.2(6)
N1	14.3(7)	20.3(8)	14.3(7)	-1.9(6)	-2.5(6)	1.0(6)
C1	23.9(11)	25.9(13)	49.5(16)	-12.9(11)	3.2(11)	2.9(10)
C2	24.2(11)	27.2(11)	21.7(10)	-7.1(8)	5.6(8)	-2.9(9)
C3	21.3(10)	26.2(11)	16.4(9)	-2.4(8)	0.5(7)	-1.0(8)
C4	14.6(9)	19.5(9)	19.6(9)	-3.0(7)	1.3(7)	-0.1(7)
C5	20.9(10)	21.3(10)	18.7(9)	-2.0(7)	2.6(7)	-2.0(8)
C6	25.7(11)	19.1(10)	26.6(11)	-1.9(8)	-0.6(9)	0.4(8)
C7	17.9(9)	20.1(10)	31.6(12)	-9.1(8)	2.0(8)	-0.8(8)
C8	17.3(9)	21.8(10)	21.7(10)	2.8(8)	-2.9(7)	-1.4(8)
C9	14.1(9)	29.6(12)	25(1)	1.0(9)	0.2(7)	0.0(8)
C10	12.6(8)	30.9(12)	23.4(10)	-4.4(9)	-3.1(7)	-0.6(8)
C11	14.6(8)	19.9(9)	16.6(9)	-2.7(7)	-4.8(7)	1.2(7)
C12	15.1(8)	15.6(8)	14.5(8)	-2.7(6)	-3.5(6)	1.3(7)
C13	19.2(9)	19.1(9)	13.8(8)	0.2(7)	-3.4(7)	2.0(7)
C14	18.3(9)	16.8(9)	14.2(8)	-0.7(7)	-4.8(7)	3.3(7)
C15	18.1(9)	12.6(8)	13.7(8)	-0.3(6)	-4.3(7)	0.1(7)
C16	17.4(9)	13.6(8)	12.6(8)	-0.5(6)	-3.5(6)	0.2(7)
C17	17.7(9)	15.2(8)	16.3(8)	-1.7(7)	-3.9(7)	2.0(7)
C18	25.3(10)	18.4(9)	16.1(9)	0.1(7)	-5.5(8)	6.5(8)
C19	29.0(11)	21.5(10)	12.9(8)	1.4(7)	-1.7(8)	6.1(8)
C20	18.4(9)	18.9(9)	13.4(8)	-2.0(7)	-2.8(7)	1.3(7)
C21	19.5(9)	16.3(9)	13.9(8)	-1.1(6)	-2.3(7)	3.9(7)
C22	22.8(10)	19.1(10)	21.0(9)	-1.5(7)	-0.6(8)	-5.7(8)
C23	35.4(13)	24.0(11)	18.5(10)	2.7(8)	-5.0(9)	11.5(10)
C24	21.8(10)	22.8(10)	14.6(8)	-3.3(7)	-2.3(7)	1.7(8)
C25	31.0(13)	48.4(17)	19.5(11)	-12.6(11)	-3.0(9)	5.4(12)
C26	21.9(11)	34.2(13)	25.2(11)	-1.8(10)	2.3(9)	0.5(9)
S1B	21.7(2)	25.9(3)	16.9(2)	0.66(19)	4.14(18)	-6.3(2)
O1B	36.4(10)	42.8(11)	20.1(8)	-2.2(8)	13.4(7)	-7.6(9)
O2B	19.7(8)	28.1(9)	25.0(8)	2.0(6)	0.0(6)	-5.3(6)
N1B	24.4(9)	22.4(9)	18.8(8)	-2.6(7)	6.5(7)	-6.6(7)
C1B	25.0(12)	36.0(15)	81(3)	28.8(17)	3.3(14)	0.2(12)
C2B	24.4(12)	47.3(17)	35.4(14)	25.7(13)	-10(1)	-12.1(11)
C3B	32.0(13)	41.3(15)	17.6(10)	9.8(10)	-4.2(9)	-12.1(11)
C4B	21.2(10)	24.4(11)	20.6(10)	5.8(8)	-2.1(8)	-6.5(8)
C5B	24.7(11)	19(1)	22.6(10)	4.4(8)	-2.3(8)	-3.9(8)

C6B	26.7(11)	18.9(10)	33.9(12)	5.4(9)	1.8(9)	-2.4(9)
C7B	23.4(11)	27.5(13)	44.4(15)	20.3(11)	-1.4(10)	-5.8(9)
C8B	34.3(14)	36.8(14)	26.3(12)	-11.8(10)	7.7(10)	-14.6(11)
C9B	16.6(12)	31.0(17)	28.0(14)	-6.2(11)	2.0(9)	-1.6(10)
C10B	16.7(9)	26.9(11)	29.3(11)	3.3(9)	4.9(8)	-1.4(8)
C11B	20.1(9)	17.8(9)	18.9(9)	0.7(7)	5.8(7)	-1.2(7)
C12B	17.3(9)	15.5(9)	22.7(9)	-0.7(7)	6.1(7)	0.1(7)
C13B	24.2(10)	18.9(10)	21(1)	-1.1(7)	7.1(8)	3.7(8)
C14B	22.5(10)	16.2(9)	20.8(10)	-1.6(7)	6.8(8)	3.1(8)
C15B	20.7(10)	14.3(9)	20.7(9)	-0.8(7)	5.2(7)	-0.3(7)
C16B	19.9(9)	13.7(9)	20.9(9)	-1.0(7)	7.3(7)	2.2(7)
C17B	21.3(10)	20.0(9)	20.1(9)	-0.7(7)	5.1(7)	4.6(8)
C18B	30.2(12)	23.4(11)	20.9(10)	-1.2(8)	6.6(9)	7.6(9)
C19B	31.7(12)	27.0(12)	20.5(10)	-1.8(8)	3.0(9)	9.2(10)
C20B	18.5(9)	21.9(10)	21.7(10)	2.4(8)	3.9(8)	1.8(8)
C21B	22.4(10)	18.4(9)	22.2(10)	-1.2(7)	4.2(8)	3.2(8)
C22B	27.7(12)	21.8(11)	28.6(12)	1.7(9)	2.4(9)	-8.3(9)
C23B	40.6(14)	23.2(11)	26.5(12)	-4.0(9)	6.7(10)	10.2(10)
C24B	22.8(10)	26.0(11)	22.6(10)	2.9(8)	1.9(8)	2.1(9)
C25B	34.2(14)	51.2(18)	23.7(12)	9.8(12)	3.5(10)	5.6(13)
C26B	23.7(12)	36.6(14)	31.4(13)	1.4(11)	-1.2(10)	1.6(10)

Table S-4. Bond Lengths for A17007.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S1	O1	1.4392(18)	S1B	O2B	1.4347(19)
S1	O2	1.4350(18)	S1B	N1B	1.635(2)
S1	N1	1.636(2)	S1B	C4B	1.760(3)
S1	C4	1.760(2)	N1B	C8B	1.483(3)
N1	C8	1.476(3)	N1B	C11B	1.497(3)
N1	C11	1.500(3)	C1B	C7B	1.502(4)
C1	C7	1.503(4)	C2B	C3B	1.385(5)
C2	C3	1.377(3)	C2B	C7B	1.384(5)
C2	C7	1.397(4)	C3B	C4B	1.386(3)
C3	C4	1.398(3)	C4B	C5B	1.398(4)
C4	C5	1.387(3)	C5B	C6B	1.390(4)
C5	C6	1.385(3)	C6B	C7B	1.384(4)
C6	C7	1.394(3)	C8B	C9B	1.490(4)
C8	C9	1.520(3)	C8B	C0AA	1.52(2)
C9	C10	1.533(3)	C9B	C10B	1.519(4)
C10	C11	1.539(3)	C10B	C11B	1.538(3)
C11	C12	1.532(3)	C10B	C0AA	1.524(19)
C12	C13	1.526(3)	C11B	C12B	1.531(3)
C12	C17	1.533(3)	C12B	C13B	1.531(3)
C13	C14	1.540(3)	C12B	C17B	1.535(3)
C14	C15	1.553(3)	C13B	C14B	1.531(3)
C14	C23	1.527(3)	C14B	C15B	1.551(3)
C15	C16	1.545(3)	C14B	C23B	1.530(3)
C15	C21	1.540(3)	C15B	C16B	1.553(3)
C15	C22	1.536(3)	C15B	C21B	1.542(3)
C16	C17	1.524(3)	C15B	C22B	1.532(3)
C16	C18	1.532(3)	C16B	C17B	1.518(3)
C18	C19	1.523(3)	C16B	C18B	1.533(3)
C19	C20	1.525(3)	C18B	C19B	1.521(4)
C20	C21	1.538(3)	C19B	C20B	1.528(3)
C20	C24	1.542(3)	C20B	C21B	1.530(3)
C24	C25	1.528(3)	C20B	C24B	1.537(3)
C24	C26	1.528(4)	C24B	C25B	1.527(4)
S1B	O1B	1.4354(19)	C24B	C26B	1.527(4)

Table S-5. Bond Angles for A17007.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	S1	N1	106.62(11)	O2B	S1B	O1B	120.56(12)
O1	S1	C4	107.61(11)	O2B	S1B	N1B	105.99(11)
O2	S1	O1	120.43(11)	O2B	S1B	C4B	107.35(11)
O2	S1	N1	106.24(10)	N1B	S1B	C4B	106.91(11)
O2	S1	C4	108.05(11)	C8B	N1B	S1B	117.45(18)
N1	S1	C4	107.23(10)	C8B	N1B	C11B	109.27(19)
C8	N1	S1	117.19(15)	C11B	N1B	S1B	116.15(15)
C8	N1	C11	109.36(17)	C7B	C2B	C3B	120.9(2)
C11	N1	S1	117.10(15)	C2B	C3B	C4B	119.5(3)
C3	C2	C7	120.6(2)	C3B	C4B	S1B	121.2(2)
C2	C3	C4	119.7(2)	C3B	C4B	C5B	120.2(3)
C3	C4	S1	119.21(18)	C5B	C4B	S1B	118.47(18)
C5	C4	S1	120.44(17)	C6B	C5B	C4B	119.3(2)
C5	C4	C3	120.3(2)	C7B	C6B	C5B	120.6(3)
C6	C5	C4	119.6(2)	C2B	C7B	C1B	120.6(3)
C5	C6	C7	120.7(2)	C6B	C7B	C1B	120.0(3)
C2	C7	C1	120.1(2)	C6B	C7B	C2B	119.4(3)
C6	C7	C1	120.8(3)	N1B	C8B	C9B	104.0(2)
C6	C7	C2	119.1(2)	N1B	C8B	C0AA	110.1(7)
N1	C8	C9	103.94(18)	C8B	C9B	C10B	103.5(2)
C8	C9	C10	101.71(18)	C9B	C10B	C11B	103.9(2)
C9	C10	C11	104.81(18)	C0AA	C10B	C11B	110.6(8)
N1	C11	C10	104.12(18)	N1B	C11B	C10B	104.07(19)
N1	C11	C12	111.40(17)	N1B	C11B	C12B	112.43(18)
C12	C11	C10	115.85(18)	C12B	C11B	C10B	115.92(19)
C11	C12	C17	109.93(17)	C11B	C12B	C13B	113.84(19)
C13	C12	C11	113.21(18)	C11B	C12B	C17B	109.62(18)
C13	C12	C17	112.23(17)	C13B	C12B	C17B	112.58(19)
C12	C13	C14	113.14(17)	C12B	C13B	C14B	113.35(19)
C13	C14	C15	111.25(17)	C13B	C14B	C15B	111.37(19)
C23	C14	C13	109.66(18)	C23B	C14B	C13B	109.6(2)
C23	C14	C15	114.97(18)	C23B	C14B	C15B	114.8(2)
C16	C15	C14	106.40(16)	C14B	C15B	C16B	106.27(17)
C21	C15	C14	110.08(17)	C21B	C15B	C14B	110.17(19)
C21	C15	C16	108.06(17)	C21B	C15B	C16B	108.00(18)
C22	C15	C14	110.81(18)	C22B	C15B	C14B	110.9(2)
C22	C15	C16	112.45(18)	C22B	C15B	C16B	112.26(19)
C22	C15	C21	108.98(17)	C22B	C15B	C21B	109.16(19)
C17	C16	C15	111.87(17)	C17B	C16B	C15B	111.65(19)
C17	C16	C18	112.23(17)	C17B	C16B	C18B	112.41(18)

C18	C16	C15	113.10(17)	C18B	C16B	C15B	113.13(18)
C16	C17	C12	112.05(17)	C16B	C17B	C12B	112.16(18)
C19	C18	C16	111.54(18)	C19B	C18B	C16B	111.5(2)
C18	C19	C20	110.60(19)	C18B	C19B	C20B	110.8(2)
C19	C20	C21	109.17(17)	C19B	C20B	C21B	108.90(19)
C19	C20	C24	114.66(18)	C19B	C20B	C24B	114.9(2)
C21	C20	C24	112.40(17)	C21B	C20B	C24B	112.22(19)
C20	C21	C15	113.69(17)	C20B	C21B	C15B	113.70(19)
C25	C24	C20	111.26(19)	C25B	C24B	C20B	111.4(2)
C26	C24	C20	113.91(19)	C26B	C24B	C20B	113.9(2)
C26	C24	C25	109.8(2)	C26B	C24B	C25B	110.0(2)
O1B	S1B	N1B	107.07(12)	C8B	C0AA	C10B	101.9(11)
O1B	S1B	C4B	108.24(13)				

Table S-6. Torsion Angles for A17007.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
S1	N1	C8	C9	109.47(18)	S1B	N1B	C11B	C12B	97.7(2)
S1	N1	C11	C10	-132.99(16)	S1B	C4B	C5B	C6B	174.64(18)
S1	N1	C11	C12	101.45(19)	O1B	S1B	N1B	C8B	47.2(2)
S1	C4	C5	C6	176.19(18)	O1B	S1B	N1B	C11B	179.26(18)
O1	S1	N1	C8	53.83(18)	O1B	S1B	C4B	C3B	-28.5(2)
O1	S1	N1	C11	-173.21(15)	O1B	S1B	C4B	C5B	155.79(19)
O1	S1	C4	C3	-24.8(2)	O2B	S1B	N1B	C8B	177.12(19)
O1	S1	C4	C5	157.86(19)	O2B	S1B	N1B	C11B	-50.9(2)
O2	S1	N1	C8	-176.56(16)	O2B	S1B	C4B	C3B	-160.0(2)
O2	S1	N1	C11	-43.60(18)	O2B	S1B	C4B	C5B	24.2(2)
O2	S1	C4	C3	-156.26(18)	N1B	S1B	C4B	C3B	86.6(2)
O2	S1	C4	C5	26.4(2)	N1B	S1B	C4B	C5B	-89.2(2)
N1	S1	C4	C3	89.6(2)	N1B	C8B	C9B	C10B	37.4(3)
N1	S1	C4	C5	-87.8(2)	N1B	C8B	C0AA	C10B	-19.4(13)
N1	C8	C9	C10	39.0(2)	N1B	C11B	C12B	C13B	55.4(2)
N1	C11	C12	C13	51.9(2)	N1B	C11B	C12B	C17B	-177.46(18)
N1	C11	C12	C17	178.33(17)	C2B	C3B	C4B	S1B	-174.8(2)
C2	C3	C4	S1	-176.89(19)	C2B	C3B	C4B	C5B	0.9(4)
C2	C3	C4	C5	0.5(4)	C3B	C2B	C7B	C1B	176.6(3)
C3	C2	C7	C1	177.1(2)	C3B	C2B	C7B	C6B	-1.4(4)
C3	C2	C7	C6	-1.1(4)	C3B	C4B	C5B	C6B	-1.2(4)
C3	C4	C5	C6	-1.1(3)	C4B	S1B	N1B	C8B	-68.6(2)
C4	S1	N1	C8	-61.21(18)	C4B	S1B	N1B	C11B	63.4(2)
C4	S1	N1	C11	71.76(17)	C4B	C5B	C6B	C7B	0.1(4)
C4	C5	C6	C7	0.7(4)	C5B	C6B	C7B	C1B	-176.9(2)
C5	C6	C7	C1	-177.8(2)	C5B	C6B	C7B	C2B	1.1(4)
C5	C6	C7	C2	0.4(4)	C7B	C2B	C3B	C4B	0.4(4)
C7	C2	C3	C4	0.6(4)	C8B	N1B	C11B	C10B	-0.4(3)
C8	N1	C11	C10	3.4(2)	C8B	N1B	C11B	C12B	-126.6(2)
C8	N1	C11	C12	-122.18(19)	C8B	C9B	C10B	C11B	-37.7(3)
C8	C9	C10	C11	-37.1(2)	C9B	C10B	C11B	N1B	23.3(2)
C9	C10	C11	N1	21.2(2)	C9B	C10B	C11B	C12B	147.3(2)
C9	C10	C11	C12	143.9(2)	C10B	C11B	C12B	C13B	-64.1(3)
C10	C11	C12	C13	-66.8(2)	C10B	C11B	C12B	C17B	63.0(3)
C10	C11	C12	C17	59.6(2)	C11B	N1B	C8B	C9B	-23.1(3)
C11	N1	C8	C9	-26.9(2)	C11B	N1B	C8B	C0AA	12.9(9)
C11	C12	C13	C14	173.67(17)	C11B	C10B	C0AA	C8B	19.3(13)
C11	C12	C17	C16	-176.25(17)	C11B	C12B	C13B	C14B	172.79(18)
C12	C13	C14	C15	-55.0(2)	C11B	C12B	C17B	C16B	-176.14(19)
C12	C13	C14	C23	176.66(19)	C12B	C13B	C14B	C15B	-54.5(3)

C13	C12	C17	C16	-49.3(2)	C12B	C13B	C14B	C23B	177.3(2)
C13	C14	C15	C16	59.5(2)	C13B	C12B	C17B	C16B	-48.3(3)
C13	C14	C15	C21	176.33(17)	C13B	C14B	C15B	C16B	59.9(2)
C13	C14	C15	C22	-63.0(2)	C13B	C14B	C15B	C21B	176.67(19)
C14	C15	C16	C17	-61.3(2)	C13B	C14B	C15B	C22B	-62.4(3)
C14	C15	C16	C18	170.74(18)	C14B	C15B	C16B	C17B	-61.9(2)
C14	C15	C21	C20	-170.77(18)	C14B	C15B	C16B	C18B	170.1(2)
C15	C16	C17	C12	57.5(2)	C14B	C15B	C21B	C20B	-170.85(19)
C15	C16	C18	C19	-55.2(3)	C15B	C16B	C17B	C12B	57.3(2)
C16	C15	C21	C20	-55.0(2)	C15B	C16B	C18B	C19B	-54.5(3)
C16	C18	C19	C20	56.9(3)	C16B	C15B	C21B	C20B	-55.2(2)
C17	C12	C13	C14	48.5(2)	C16B	C18B	C19B	C20B	56.9(3)
C17	C16	C18	C19	177.04(19)	C17B	C12B	C13B	C14B	47.2(3)
C18	C16	C17	C12	-174.16(18)	C17B	C16B	C18B	C19B	177.9(2)
C18	C19	C20	C21	-57.5(2)	C18B	C16B	C17B	C12B	-174.3(2)
C18	C19	C20	C24	175.33(18)	C18B	C19B	C20B	C21B	-58.2(3)
C19	C20	C21	C15	58.5(2)	C18B	C19B	C20B	C24B	174.9(2)
C19	C20	C24	C25	-65.7(3)	C19B	C20B	C21B	C15B	59.2(3)
C19	C20	C24	C26	59.1(3)	C19B	C20B	C24B	C25B	-65.0(3)
C21	C15	C16	C17	-179.54(16)	C19B	C20B	C24B	C26B	60.2(3)
C21	C15	C16	C18	52.6(2)	C21B	C15B	C16B	C17B	179.89(18)
C21	C20	C24	C25	168.9(2)	C21B	C15B	C16B	C18B	51.9(3)
C21	C20	C24	C26	-66.4(3)	C21B	C20B	C24B	C25B	169.8(2)
C22	C15	C16	C17	60.1(2)	C21B	C20B	C24B	C26B	-65.0(3)
C22	C15	C16	C18	-67.8(2)	C22B	C15B	C16B	C17B	59.5(2)
C22	C15	C21	C20	67.5(2)	C22B	C15B	C16B	C18B	-68.5(3)
C23	C14	C15	C16	-175.12(19)	C22B	C15B	C21B	C20B	67.1(3)
C23	C14	C15	C21	-58.3(3)	C23B	C14B	C15B	C16B	-174.8(2)
C23	C14	C15	C22	62.4(3)	C23B	C14B	C15B	C21B	-58.0(3)
C24	C20	C21	C15	-173.09(18)	C23B	C14B	C15B	C22B	62.9(3)
S1B	N1B	C8B	C9B	112.0(2)	C24B	C20B	C21B	C15B	-172.4(2)
S1B	N1B	C8B	C0AA	148.0(9)	C0AA	C10B	C11B	N1B	-12.2(9)
S1B	N1B	C11B	C10B	-136.12(18)	C0AA	C10B	C11B	C12B	111.8(9)

Table S-7. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for a17007.

Atom	*x*	*y*	*z*	U(eq)
H1A	178	5328	12702	50
H1B	1484	5688	12250	50
H1C	1453	5578	13688	50
H2	3439	5015	14402	29
H3	6332	4619	14104	26
H5	6915	5000	10574	24
H6	3970	5388	10868	29
H8A	6402	3977	13177	24
H8B	6776	3596	12402	24
H9A	3704	4174	11852	27
H9B	3257	3729	11924	27
H10E	3897	4011	9769	27
H10F	5011	3615	10075	27
H11	6939	4336	9971	20
H12	10014	4045	9323	18
H13C	8129	3339	9916	21
H13D	10222	3515	10535	21
H14	12098	3446	8667	20
H16	10635	3811	7139	17
H17C	6376	3761	8024	20
H17D	7591	4146	7739	20
H18C	7011	3595	5697	24
H18D	8284	3982	5549	24
H19C	11335	3657	4877	25
H19D	9360	3543	4012	25
H20	8835	2994	5203	20
H21C	12534	3213	6580	20
H21D	11335	2821	6756	20
H22D	7953	2774	7757	31
H22E	6809	3056	6809	31
H22F	6715	3135	8268	31
H23D	12340	2953	10067	39
H23E	12426	2786	8691	39
H23F	10282	2755	9480	39
H24	11799	2630	4622	24
H25D	9116	2749	3134	49
H25E	11375	2690	2484	49
H25F	10425	3104	2640	49
H26D	13801	3300	3757	41

H26E	14691	2883	3554	41
H26F	14610	3058	4919	41
H1BA	13318	4326	6271	71
H1BB	13497	4292	7747	71
H1BC	14724	4621	7036	71
H2B	12073	4866	8972	43
H3B	9221	5281	9153	36
H5B	7490	5048	5604	27
H6B	10381	4637	5441	32
H8BA	8759	5984	8660	39
H8BB	8302	6386	8031	39
H8BC	9393	5925	8363	39
H8BD	7940	6294	8439	39
H9BA	11372	5843	7278	30
H9BB	11744	6288	7465	30
H10A	11126	6055	5260	29
H10B	9925	6435	5667	29
H10C	11235	5981	5697	29
H10D	10175	6361	5200	29
H11B	8185	5699	5432	23
H12B	5019	5977	4823	22
H13A	6848	6690	5384	26
H13B	4762	6513	5993	26
H14B	2896	6572	4123	24
H16B	4346	6199	2625	22
H17A	8616	6256	3496	25
H17B	7397	5869	3239	25
H18A	7948	6405	1165	30
H18B	6645	6021	1034	30
H19A	3606	6349	356	32
H19B	5571	6456	-517	32
H20B	6150	7009	660	25
H21A	2449	6798	2019	25
H21B	3647	7191	2185	25
H22A	8263	6881	3738	39
H22B	7044	7239	3187	39
H22C	8186	6949	2272	39
H23A	2701	7074	5513	45
H23B	2510	7229	4124	45
H23C	4700	7272	4872	45
H24B	3237	7379	57	29
H25A	5899	7226	-1425	55
H25B	3657	7322	-2059	55
H25C	4412	6894	-1931	55

H26A	1120	6715	-767	46
H26B	284	7134	-986	46
H26C	379	6964	387	46
H0AA	11769	6299	7456	28
H0AB	9994	6609	7106	28

(*S*)-2-((3*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-10,13-Dimethyl-17-((*R*)-6-methylheptan-2-yl)-2,3,4,7,8,-9,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[a]phenanthren-3-yl)-1-tosylpyrrolidine (Table 2, entry 6). This compound was synthesized under the standard cross-coupling conditions from (3*R*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-3-iodo-10,13-dimethyl-17-((*R*)-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[a]-phenanthrene and the organozinc reagent, using (*S*,*S*)-**1**, then using procedure mentioned in optimization of reaction conditions (0.1 mmol) to synthesize this compound with TsCl.

A suitable crystal of $C_{38}H_{59}NO_2S$ was selected for analysis. All measurements were made on a Bruker AXS KAPPA APEX II diffractometer coupled to an APEX II CCD detector with graphite monochromated Cu K_α radiation (λ = 1.54178 Å) for the structure of compound P15185. The structure was solved by direct methods using SHELXS[6] and refined against F^2 on all data by full-matrix least squares with SHELXL-2014[7] using established refinement techniques.[8]

Table S-1. Crystal data and structure refinement for P15185.

Identification code	P15185	
Empirical formula	$C_{38}H_{59}NO_2S$	
Formula weight	593.92	
Temperature	100(2) K	
Crystal system	orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 7.5862(2) Å	α = 90°
	b = 9.5375(3) Å	β = 90°
	c = 46.8778(13) Å	γ = 90°
Volume	3391.77(17) $Å^3$	
Z	4	
Density(calculated)	1.163 Mg/m^3	
Absorption coefficient	1.086 mm^{-1}	
F(000)	1304.0	
Crystal size	0.200 × 0.200 × 0.040 mm^3	
Radiation	CuKα (λ = 1.54178)	
Theta range for data collection	7.544° to 148.736°	
Index ranges	$-8 \leq h \leq 9$, $-11 \leq k \leq 11$, $-57 \leq l \leq 58$	
Reflections collected	34014	
Independent reflections	6843 [Rint = 0.0505]	
Data/restraints/parameters	6843/468/494	
Goodness-of-fit on F^2	1.022	
R indexes [I>=2sigma (I)]	R1 = 0.0389, wR2 = 0.0945	
R indexes [all data]	R1 = 0.0418, wR2 = 0.0964	
Largest diff. peak/hole	0.21/-0.35 e/$Å^{-3}$	
Flack parameter	0.075(7)	

Table S-2. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for P15185. Ueq is defined as 1/3 of of the trace of the orthogonalised UIJ tensor.

Atom	x	y	z	U(eq)
S(1)	2709.3(7)	1778.5(6)	8916.3(2)	23.46(14)
C(24)	2600(20)	2147(13)	9289(2)	18(2)
C(25)	2990(30)	3500(15)	9376(3)	29(3)
C(26)	2810(20)	3859(14)	9661(2)	33(2)
C(27)	2200(13)	2878(15)	9858.5(17)	33(2)
C(28)	1800(12)	1535(14)	9763.9(14)	34(2)
C(29)	1973(14)	1159(12)	9479.1(17)	27.5(19)
C(30)	1986(12)	3262(16)	10169.8(16)	46(3)
C(24A)	2490(20)	2516(13)	9267(2)	20(2)
C(25A)	3140(20)	3831(14)	9335(3)	27(2)
C(26A)	2990(20)	4319(14)	9614(2)	37(2)
C(27A)	2207(14)	3512(15)	9825.5(19)	38(2)
C(28A)	1557(11)	2215(15)	9752.5(14)	38(2)
C(29A)	1730(13)	1697(13)	9474.5(17)	31.1(19)
C(30A)	2007(15)	4060(17)	10130.2(17)	57(3)
O(1)	2268(2)	2956.9(19)	8741.8(3)	29.4(4)
O(2)	1705(2)	511(2)	8899.7(4)	34.9(4)
N(1)	4736(3)	1370(2)	8853.7(4)	21.6(4)
C(1)	6088(3)	2422(2)	8765.2(5)	20.0(4)
C(2)	7545(3)	2171(3)	8986.4(4)	24.3(5)
C(3)	7505(3)	581(3)	9030.1(5)	27.1(5)
C(4)	5539(4)	220(3)	9021.7(6)	30.1(6)
C(5)	6654(3)	2160(2)	8454.7(4)	19.0(4)
C(6)	8055(3)	3214(2)	8357.2(4)	19.3(4)
C(7)	8578(3)	3035(2)	8047.0(4)	16.9(4)
C(8)	7078(3)	2957(2)	7830.6(4)	15.7(4)
C(9)	5662(3)	1931(2)	7944.5(4)	17.7(4)
C(10)	5081(3)	2227(2)	8250.3(4)	19.4(4)
C(11)	7776(3)	2400(2)	7541.0(4)	16.1(4)

C(12)	9497(3)	3115(2)	7447.4(4)	16.2(4)
C(13)	10933(3)	2860(2)	7671.9(4)	18.3(4)
C(14)	10268(3)	2979(2)	7973.2(4)	18.9(4)
C(15)	6376(3)	2450(2)	7303.9(5)	19.3(4)
C(16)	7038(3)	1887(2)	7016.2(4)	19.8(4)
C(17)	8684(3)	2669(2)	6915.4(4)	17.8(4)
C(18)	10061(3)	2536(2)	7157.4(4)	16.8(4)
C(19)	11754(3)	3094(3)	7022.6(4)	22.1(5)
C(20)	11644(3)	2561(3)	6711.7(5)	23.7(5)
C(21)	9737(3)	1982(2)	6668.4(4)	20.0(4)
C(22)	6264(3)	4423(2)	7797.1(5)	19.0(4)
C(23)	8245(4)	4205(2)	6844.3(5)	25.1(5)
C(31)	9089(4)	2174(3)	6359.0(5)	27.6(5)
C(32)	7169(4)	1746(3)	6314.2(5)	34.4(6)
C(33)	10277(4)	1324(3)	6156.9(5)	34.6(6)
C(34)	9880(10)	1882(9)	5846.6(13)	23.4(14)
C(35)	11107(10)	1111(8)	5643.8(13)	36.6(15)
C(36)	10980(10)	1521(7)	5329.1(14)	42.6(17)
C(37)	12052(11)	504(7)	5146.0(13)	55(2)
C(38)	11559(11)	3024(7)	5281.8(13)	58(2)
C(34A)	10614(13)	1670(9)	5846.1(16)	30.5(18)
C(35A)	11805(11)	638(7)	5680.3(13)	35.0(16)
C(36A)	12661(9)	1212(6)	5408.3(11)	39.8(16)
C(37A)	11281(12)	1727(9)	5195.6(16)	55(2)
C(38A)	14021(10)	2327(8)	5473.6(14)	51.0(19)

Table S-3. Anisotropic Displacement Parameters (Å2×103) for P15185. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11}+\ldots+2hka^*b^*U^{12}]$.

Atom	U11	U22	U33	U23	U13	U12
S(1)	14.6(3)	33.3(3)	22.5(2)	-6.2(2)	0.92(19)	-1.6(2)
C(24)	13(4)	16(5)	23(3)	-1(3)	-2(3)	5(4)
C(25)	37(4)	26(6)	25(4)	2(4)	2(3)	-13(5)
C(26)	32(4)	34(6)	32(4)	-12(4)	2(3)	-8(5)
C(27)	23(3)	53(6)	22(3)	-5(4)	-2(2)	-10(5)
C(28)	40(4)	33(5)	28(3)	6(3)	9(2)	-4(4)
C(29)	33(4)	18(4)	32(3)	0(3)	8(2)	-5(4)
C(30)	43(4)	68(7)	28(3)	-15(4)	5(3)	-9(5)
C(24A)	18(4)	22(5)	20(3)	4(3)	0(2)	9(5)
C(25A)	31(5)	26(5)	25(4)	-2(3)	1(3)	7(4)
C(26A)	36(6)	38(6)	37(4)	-13(4)	-8(3)	7(5)
C(27A)	36(4)	52(6)	25(3)	-8(4)	2(3)	15(5)
C(28A)	41(4)	45(6)	26(3)	8(3)	6(3)	13(4)
C(29A)	35(4)	26(5)	33(3)	-2(3)	5(2)	-2(4)
C(30A)	63(6)	77(7)	33(3)	-13(4)	-6(3)	31(6)
O(1)	21.7(9)	37.4(10)	28.9(8)	-3.3(7)	-2.4(7)	8.7(8)
O(2)	23.3(10)	38.8(11)	42.7(10)	-10.2(8)	4.9(8)	-10.5(8)
N(1)	15.2(10)	24.4(10)	25.1(9)	1.1(7)	2.1(7)	1.0(8)
C(1)	14.6(11)	20.8(11)	24.6(11)	0.3(8)	-0.4(8)	0.8(9)
C(2)	16.4(11)	33.8(13)	22.6(10)	0.3(8)	-2.5(8)	-0.7(9)
C(3)	22.1(13)	32.6(13)	26.5(10)	4.2(9)	-0.9(10)	5.3(10)
C(4)	25.7(14)	29.8(14)	34.8(12)	8.8(10)	0.4(10)	0.2(10)
C(5)	14.5(11)	20.1(11)	22.5(10)	0.3(8)	-0.8(8)	0.2(8)
C(6)	13.2(10)	22.6(11)	22.2(10)	-2.4(8)	-2.4(7)	-0.1(9)
C(7)	15.1(11)	13.7(10)	21.9(10)	1.1(8)	-3.7(8)	-1.0(8)
C(8)	12.1(10)	13.5(10)	21.5(9)	0.2(7)	-2.2(7)	0.0(8)
C(9)	12.6(10)	16.1(10)	24.3(10)	0.3(8)	-3.1(8)	-2.5(8)
C(10)	12.9(10)	21.2(11)	24.2(10)	1.0(8)	-1.9(8)	-2.0(8)
C(11)	14.4(10)	12.5(9)	21.4(9)	0.0(7)	-3.6(8)	0.7(8)
C(12)	13.8(10)	13.8(10)	20.9(9)	-0.2(8)	-4.0(7)	-2.0(8)

C(13)	12.5(11)	20.9(11)	21.3(10)	0.5(8)	-2.7(8)	0.4(8)
C(14)	14.8(11)	21.2(11)	20.8(10)	0.5(8)	-4.4(8)	-1.3(9)
C(15)	13.2(11)	17.4(11)	27.1(11)	-2.1(8)	-5.3(8)	-0.2(8)
C(16)	16.1(11)	19.2(11)	24.1(10)	-2.8(8)	-5.5(8)	-2.0(9)
C(17)	18.7(11)	13.9(10)	20.8(10)	1.5(8)	-5.4(8)	0.4(8)
C(18)	14.1(11)	16.1(10)	20.1(9)	1.5(8)	-2.6(8)	0.4(8)
C(19)	18.2(11)	24.7(12)	23.4(10)	1.6(9)	-0.7(8)	-4.9(9)
C(20)	24.1(13)	25.2(12)	21.7(10)	3.0(9)	0.6(8)	-3.5(10)
C(21)	24.2(12)	16.3(11)	19.6(9)	2.6(8)	-3.0(8)	-2.9(9)
C(22)	15.6(12)	16.0(11)	25.3(11)	-0.9(8)	-2.5(8)	2.9(8)
C(23)	31.9(14)	16.0(11)	27.4(11)	1.4(9)	-9.6(9)	3.3(10)
C(31)	39.9(15)	20.7(12)	22.1(11)	3.1(9)	-7.8(10)	-3.7(10)
C(32)	39.3(15)	33.7(14)	30.3(12)	-3.4(10)	-16.1(10)	2.3(13)
C(33)	44.8(17)	38.3(15)	20.6(11)	-0.3(10)	1.5(10)	-10.4(12)
C(34)	25(4)	27(3)	18(2)	-1(2)	3(3)	-3(3)
C(35)	42(4)	37(4)	30(3)	-2(3)	8(3)	8(3)
C(36)	64(4)	39(4)	25(3)	-2(3)	12(3)	3(3)
C(37)	74(5)	53(4)	40(3)	-10(3)	21(3)	4(3)
C(38)	87(6)	52(4)	35(3)	-2(3)	19(3)	-14(4)
C(34A)	37(5)	28(4)	26(3)	3(2)	8(3)	2(4)
C(35A)	54(5)	25(4)	25(3)	-4(2)	7(3)	9(3)
C(36A)	57(4)	35(3)	27(3)	-4(2)	6(3)	2(3)
C(37A)	82(6)	53(5)	29(4)	4(4)	1(4)	8(4)
C(38A)	59(5)	49(4)	45(4)	-3(3)	16(3)	-4(3)

Table S-4. Bond Lengths for P15185.

Atom	Atom	Length/Å
S(1)	O(1)	1.4300(18)
S(1)	O(2)	1.4309(19)
S(1)	N(1)	1.613(2)
S(1)	C(24)	1.782(10)
S(1)	C(24A)	1.794(10)
C(24)	C(29)	1.383(11)
C(24)	C(25)	1.385(11)
C(25)	C(26)	1.386(12)
C(26)	C(27)	1.396(10)
C(27)	C(28)	1.389(10)
C(27)	C(30)	1.513(9)
C(28)	C(29)	1.389(10)
C(24A)	C(29A)	1.376(11)
C(24A)	C(25A)	1.385(12)
C(25A)	C(26A)	1.393(11)
C(26A)	C(27A)	1.389(10)
C(27A)	C(28A)	1.375(11)
C(27A)	C(30A)	1.528(10)
C(28A)	C(29A)	1.400(10)
N(1)	C(4)	1.481(3)
N(1)	C(1)	1.494(3)
C(1)	C(2)	1.535(3)
C(1)	C(5)	1.538(3)
C(2)	C(3)	1.530(3)
C(3)	C(4)	1.531(4)
C(5)	C(10)	1.532(3)
C(5)	C(6)	1.533(3)
C(6)	C(7)	1.517(3)
C(7)	C(14)	1.329(3)
C(7)	C(8)	1.526(3)
C(8)	C(22)	1.537(3)
C(8)	C(9)	1.548(3)
C(8)	C(11)	1.551(3)
C(9)	C(10)	1.526(3)
C(11)	C(12)	1.537(3)
C(11)	C(15)	1.538(3)
C(12)	C(18)	1.529(3)
C(12)	C(13)	1.534(3)
C(13)	C(14)	1.504(3)
C(15)	C(16)	1.536(3)
C(16)	C(17)	1.529(3)
C(17)	C(23)	1.539(3)
C(17)	C(18)	1.547(3)
C(17)	C(21)	1.552(3)
C(18)	C(19)	1.527(3)
C(19)	C(20)	1.546(3)
C(20)	C(21)	1.561(3)
C(21)	C(31)	1.542(3)
C(31)	C(32)	1.527(4)
C(31)	C(33)	1.538(4)
C(33)	C(34A)	1.516(8)
C(33)	C(34)	1.578(7)
C(34)	C(35)	1.520(9)
C(35)	C(36)	1.529(9)
C(36)	C(38)	1.516(9)
C(36)	C(37)	1.529(8)
C(34A)	C(35A)	1.545(9)
C(35A)	C(36A)	1.532(8)
C(36A)	C(38A)	1.513(9)
C(36A)	C(37A)	1.527(9)

Table S-5. Bond Angles for P15185.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O(1)	S(1)	O(2)	120.53(12)	C(7)	C(8)	C(9)	108.61(16)
O(1)	S(1)	N(1)	108.00(11)	C(22)	C(8)	C(9)	109.34(17)
O(2)	S(1)	N(1)	107.06(11)	C(7)	C(8)	C(11)	110.12(17)
O(1)	S(1)	C(24)	113.2(4)	C(22)	C(8)	C(11)	111.05(17)
O(2)	S(1)	C(24)	101.3(5)	C(9)	C(8)	C(11)	108.80(17)
N(1)	S(1)	C(24)	105.7(6)	C(10)	C(9)	C(8)	114.04(17)
O(1)	S(1)	C(24A)	101.2(4)	C(9)	C(10)	C(5)	110.81(18)
O(2)	S(1)	C(24A)	109.4(5)	C(12)	C(11)	C(15)	111.49(17)
N(1)	S(1)	C(24A)	110.5(6)	C(12)	C(11)	C(8)	112.80(17)
C(29)	C(24)	C(25)	121.3(9)	C(15)	C(11)	C(8)	112.72(18)
C(29)	C(24)	S(1)	120.9(8)	C(18)	C(12)	C(13)	110.77(17)
C(25)	C(24)	S(1)	117.5(8)	C(18)	C(12)	C(11)	109.32(17)
C(24)	C(25)	C(26)	119.5(9)	C(13)	C(12)	C(11)	109.68(17)
C(25)	C(26)	C(27)	120.5(8)	C(14)	C(13)	C(12)	113.24(18)
C(28)	C(27)	C(26)	118.6(7)	C(7)	C(14)	C(13)	124.82(19)
C(28)	C(27)	C(30)	120.5(7)	C(16)	C(15)	C(11)	113.46(18)
C(26)	C(27)	C(30)	120.9(8)	C(17)	C(16)	C(15)	111.58(18)
C(29)	C(28)	C(27)	121.6(7)	C(16)	C(17)	C(23)	110.75(19)
C(24)	C(29)	C(28)	118.5(8)	C(16)	C(17)	C(18)	106.55(17)
C(29A)	C(24A)	C(25A)	119.8(9)	C(23)	C(17)	C(18)	112.50(18)
C(29A)	C(24A)	S(1)	117.7(8)	C(16)	C(17)	C(21)	116.43(18)
C(25A)	C(24A)	S(1)	122.4(8)	C(23)	C(17)	C(21)	110.60(18)
C(24A)	C(25A)	C(26A)	119.6(9)	C(18)	C(17)	C(21)	99.50(17)
C(27A)	C(26A)	C(25A)	121.1(8)	C(19)	C(18)	C(12)	118.50(18)
C(28A)	C(27A)	C(26A)	118.4(7)	C(19)	C(18)	C(17)	103.67(17)
C(28A)	C(27A)	C(30A)	120.3(8)	C(12)	C(18)	C(17)	115.71(17)
C(26A)	C(27A)	C(30A)	121.3(9)	C(18)	C(19)	C(20)	103.28(18)
C(27A)	C(28A)	C(29A)	121.1(7)	C(19)	C(20)	C(21)	106.81(18)
C(24A)	C(29A)	C(28A)	119.9(8)	C(31)	C(21)	C(17)	119.2(2)
C(4)	N(1)	C(1)	111.29(19)	C(31)	C(21)	C(20)	112.07(19)
C(4)	N(1)	S(1)	118.29(16)	C(17)	C(21)	C(20)	103.33(17)

C(1)	N(1)	S(1)	122.84(16)	C(32)	C(31)	C(33)	109.5(2)
N(1)	C(1)	C(2)	101.62(18)	C(32)	C(31)	C(21)	113.7(2)
N(1)	C(1)	C(5)	110.20(18)	C(33)	C(31)	C(21)	109.3(2)
C(2)	C(1)	C(5)	114.39(18)	C(34A)	C(33)	C(31)	125.2(4)
C(3)	C(2)	C(1)	103.37(19)	C(31)	C(33)	C(34)	106.2(3)
C(2)	C(3)	C(4)	103.8(2)	C(35)	C(34)	C(33)	107.3(5)
N(1)	C(4)	C(3)	104.3(2)	C(34)	C(35)	C(36)	116.2(6)
C(10)	C(5)	C(6)	109.05(17)	C(38)	C(36)	C(37)	111.3(6)
C(10)	C(5)	C(1)	111.57(18)	C(38)	C(36)	C(35)	111.4(6)
C(6)	C(5)	C(1)	111.68(18)	C(37)	C(36)	C(35)	110.3(6)
C(7)	C(6)	C(5)	113.15(18)	C(33)	C(34A)	C(35A)	116.4(6)
C(14)	C(7)	C(6)	120.44(19)	C(36A)	C(35A)	C(34A)	116.1(6)
C(14)	C(7)	C(8)	122.96(19)	C(38A)	C(36A)	C(37A)	111.9(6)
C(6)	C(7)	C(8)	116.58(18)	C(38A)	C(36A)	C(35A)	111.8(5)
C(7)	C(8)	C(22)	108.87(17)	C(37A)	C(36A)	C(35A)	111.6(7)

Table S-6. Torsion Angles for P15185.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O(1)	S(1)	C(24)	C(29)	142.1(10)	C(7)	C(8)	C(9)	C(10)	50.7(2)
O(2)	S(1)	C(24)	C(29)	11.6(13)	C(22)	C(8)	C(9)	C(10)	-68.0(2)
N(1)	S(1)	C(24)	C(29)	-99.9(12)	C(11)	C(8)	C(9)	C(10)	170.57(18)
O(1)	S(1)	C(24)	C(25)	-31.5(17)	C(8)	C(9)	C(10)	C(5)	-58.7(2)
O(2)	S(1)	C(24)	C(25)	-161.9(15)	C(6)	C(5)	C(10)	C(9)	57.5(2)
N(1)	S(1)	C(24)	C(25)	86.5(15)	C(1)	C(5)	C(10)	C(9)	-178.69(18)
C(29)	C(24)	C(25)	C(26)	2(3)	C(7)	C(8)	C(11)	C(12)	-46.3(2)
S(1)	C(24)	C(25)	C(26)	175.7(15)	C(22)	C(8)	C(11)	C(12)	74.4(2)
C(24)	C(25)	C(26)	C(27)	-1(3)	C(9)	C(8)	C(11)	C(12)	-165.19(17)
C(25)	C(26)	C(27)	C(28)	1(2)	C(7)	C(8)	C(11)	C(15)	-173.62(17)
C(25)	C(26)	C(27)	C(30)	-179.6(15)	C(22)	C(8)	C(11)	C(15)	-52.9(2)
C(26)	C(27)	C(28)	C(29)	-0.8(14)	C(9)	C(8)	C(11)	C(15)	67.4(2)
C(30)	C(27)	C(28)	C(29)	179.5(9)	C(15)	C(11)	C(12)	C(18)	-50.4(2)
C(25)	C(24)	C(29)	C(28)	-2(2)	C(8)	C(11)	C(12)	C(18)	-178.41(16)
S(1)	C(24)	C(29)	C(28)	-175.5(9)	C(15)	C(11)	C(12)	C(13)	-172.03(18)
C(27)	C(28)	C(29)	C(24)	1.5(14)	C(8)	C(11)	C(12)	C(13)	60.0(2)
O(1)	S(1)	C(24A)	C(29A)	139.9(10)	C(18)	C(12)	C(13)	C(14)	-161.83(18)
O(2)	S(1)	C(24A)	C(29A)	11.7(13)	C(11)	C(12)	C(13)	C(14)	-41.1(2)
N(1)	S(1)	C(24A)	C(29A)	-105.9(11)	C(6)	C(7)	C(14)	C(13)	-177.5(2)
O(1)	S(1)	C(24A)	C(25A)	-43.8(16)	C(8)	C(7)	C(14)	C(13)	1.2(4)
O(2)	S(1)	C(24A)	C(25A)	-172.0(14)	C(12)	C(13)	C(14)	C(7)	12.0(3)
N(1)	S(1)	C(24A)	C(25A)	70.4(15)	C(12)	C(11)	C(15)	C(16)	52.6(2)
C(29A)	C(24A)	C(25A)	C(26A)	-1(2)	C(8)	C(11)	C(15)	C(16)	-179.36(18)
S(1)	C(24A)	C(25A)	C(26A)	-177.1(13)	C(11)	C(15)	C(16)	C(17)	-56.4(2)
C(24A)	C(25A)	C(26A)	C(27A)	0(2)	C(15)	C(16)	C(17)	C(23)	-66.7(2)
C(25A)	C(26A)	C(27A)	C(28A)	-0.4(19)	C(15)	C(16)	C(17)	C(18)	55.9(2)
C(25A)	C(26A)	C(27A)	C(30A)	-178.5(13)	C(15)	C(16)	C(17)	C(21)	165.80(18)
C(26A)	C(27A)	C(28A)	C(29A)	1.9(14)	C(13)	C(12)	C(18)	C(19)	-58.7(3)
C(30A)	C(27A)	C(28A)	C(29A)	-180.0(8)	C(11)	C(12)	C(18)	C(19)	-179.62(18)
C(25A)	C(24A)	C(29A)	C(28A)	2(2)	C(13)	C(12)	C(18)	C(17)	177.29(18)
S(1)	C(24A)	C(29A)	C(28A)	178.8(9)	C(11)	C(12)	C(18)	C(17)	56.3(2)

C(27A)	C(28A)	C(29A)	C(24A)	-3.0(14)
O(1)	S(1)	N(1)	C(4)	176.66(18)
O(2)	S(1)	N(1)	C(4)	-52.2(2)
C(24)	S(1)	N(1)	C(4)	55.2(4)
C(24A)	S(1)	N(1)	C(4)	66.9(5)
O(1)	S(1)	N(1)	C(1)	29.7(2)
O(2)	S(1)	N(1)	C(1)	160.89(17)
C(24)	S(1)	N(1)	C(1)	-91.8(4)
C(24A)	S(1)	N(1)	C(1)	-80.1(5)
C(4)	N(1)	C(1)	C(2)	-22.3(2)
S(1)	N(1)	C(1)	C(2)	126.72(17)
C(4)	N(1)	C(1)	C(5)	99.4(2)
S(1)	N(1)	C(1)	C(5)	-111.63(19)
N(1)	C(1)	C(2)	C(3)	36.8(2)
C(5)	C(1)	C(2)	C(3)	-81.9(2)
C(1)	C(2)	C(3)	C(4)	-38.6(2)
C(1)	N(1)	C(4)	C(3)	-1.3(3)
S(1)	N(1)	C(4)	C(3)	-151.82(17)
C(2)	C(3)	C(4)	N(1)	24.6(2)
N(1)	C(1)	C(5)	C(10)	58.2(2)
C(2)	C(1)	C(5)	C(10)	171.93(19)
N(1)	C(1)	C(5)	C(6)	-179.48(18)
C(2)	C(1)	C(5)	C(6)	-65.7(2)
C(10)	C(5)	C(6)	C(7)	-53.3(2)
C(1)	C(5)	C(6)	C(7)	-177.06(18)
C(5)	C(6)	C(7)	C(14)	-131.1(2)
C(5)	C(6)	C(7)	C(8)	50.2(3)
C(14)	C(7)	C(8)	C(22)	-106.2(2)
C(6)	C(7)	C(8)	C(22)	72.5(2)
C(14)	C(7)	C(8)	C(9)	134.8(2)
C(6)	C(7)	C(8)	C(9)	-46.5(2)
C(14)	C(7)	C(8)	C(11)	15.8(3)
C(6)	C(7)	C(8)	C(11)	-165.54(18)

C(16)	C(17)	C(18)	C(19)	169.99(18)
C(23)	C(17)	C(18)	C(19)	-68.5(2)
C(21)	C(17)	C(18)	C(19)	48.6(2)
C(16)	C(17)	C(18)	C(12)	-58.5(2)
C(23)	C(17)	C(18)	C(12)	63.0(3)
C(21)	C(17)	C(18)	C(12)	-179.91(18)
C(12)	C(18)	C(19)	C(20)	-166.82(19)
C(17)	C(18)	C(19)	C(20)	-37.0(2)
C(18)	C(19)	C(20)	C(21)	10.9(2)
C(16)	C(17)	C(21)	C(31)	80.5(3)
C(23)	C(17)	C(21)	C(31)	-47.0(3)
C(18)	C(17)	C(21)	C(31)	-165.6(2)
C(16)	C(17)	C(21)	C(20)	-154.42(18)
C(23)	C(17)	C(21)	C(20)	78.0(2)
C(18)	C(17)	C(21)	C(20)	-40.5(2)
C(19)	C(20)	C(21)	C(31)	148.5(2)
C(19)	C(20)	C(21)	C(17)	18.9(2)
C(17)	C(21)	C(31)	C(32)	-53.9(3)
C(20)	C(21)	C(31)	C(32)	-174.6(2)
C(17)	C(21)	C(31)	C(33)	-176.5(2)
C(20)	C(21)	C(31)	C(33)	62.8(3)
C(32)	C(31)	C(33)	C(34A)	82.1(5)
C(21)	C(31)	C(33)	C(34A)	-152.8(5)
C(32)	C(31)	C(33)	C(34)	69.9(4)
C(21)	C(31)	C(33)	C(34)	-165.0(3)
C(31)	C(33)	C(34)	C(35)	177.1(4)
C(33)	C(34)	C(35)	C(36)	-178.4(5)
C(34)	C(35)	C(36)	C(38)	65.3(9)
C(34)	C(35)	C(36)	C(37)	-170.6(6)
C(31)	C(33)	C(34A)	C(35A)	-177.9(5)
C(33)	C(34A)	C(35A)	C(36A)	-159.6(7)
C(34A)	C(35A)	C(36A)	C(38A)	67.9(9)
C(34A)	C(35A)	C(36A)	C(37A)	-58.3(8)

Table S-7. Hydrogen Atom Coordinates (Å×104) and Isotropic Displacement Parameters (Å2×103) for P15185.

Atom	x	y	z	U(eq)
H(25)	3385	4176	9241	35
H(26)	3103	4779	9722	39
H(28)	1397	857	9897	40
H(29)	1668	243	9417	33
H(30A)	1136	2625	10259	70
H(30B)	1557	4228	10185	70
H(30C)	3126	3181	10267	70
H(25A)	3679	4395	9193	32
H(26A)	3443	5220	9661	44
H(28A)	983	1661	9893	45
H(29A)	1324	781	9430	37
H(30D)	759	4046	10184	86
H(30E)	2454	5022	10141	86
H(30F)	2679	3462	10261	86
H(1)	5605	3393	8786	24
H(2A)	8705	2480	8913	29
H(2B)	7288	2671	9167	29
H(3A)	8030	321	9216	33
H(3B)	8151	93	8876	33
H(4A)	5343	-697	8928	36
H(4B)	5039	188	9217	36
H(5)	7175	1199	8443	23
H(6A)	7597	4176	8385	23
H(6B)	9116	3107	8478	23
H(9A)	4617	1978	7818	21
H(9B)	6133	964	7934	21
H(10A)	4186	1529	8309	23
H(10B)	4535	3169	8260	23
H(11)	8065	1387	7571	19
H(12)	9288	4147	7430	19

H(13A)	11433	1912	7643	22
H(13B)	11893	3548	7643	22
H(14)	11119	3016	8122	23
H(15A)	5341	1893	7365	23
H(15B)	5985	3432	7279	23
H(16A)	7312	877	7035	24
H(16B)	6095	1989	6872	24
H(18)	10251	1508	7186	20
H(19A)	12808	2714	7120	26
H(19B)	11793	4131	7029	26
H(20A)	12522	1810	6679	28
H(20B)	11879	3336	6577	28
H(21)	9777	951	6707	24
H(22A)	7074	5025	7690	28
H(22B)	6054	4831	7986	28
H(22C)	5144	4349	7694	28
H(23A)	7301	4235	6702	38
H(23B)	9296	4670	6768	38
H(23C)	7858	4689	7018	38
H(31)	9206	3188	6308	33
H(32A)	6991	790	6385	52
H(32B)	6887	1781	6110	52
H(32C)	6397	2391	6418	52
H(33A)	10004	312	6171	41
H(33B)	11534	1467	6206	41
H(33C)	11450	1288	6249	41
H(33D)	9813	354	6160	41
H(34A)	8635	1697	5795	28
H(34B)	10091	2905	5836	28
H(35A)	10867	94	5660	44
H(35B)	12334	1269	5708	44
H(36)	9717	1443	5270	51
H(37A)	11649	-457	5181	83
H(37B)	11890	735	4944	83
H(37C)	13303	583	5196	83

H(38A)	10851	3650	5402	87
H(38B)	12806	3121	5332	87
H(38C)	11393	3273	5081	87
H(34C)	11156	2613	5836	37
H(34D)	9463	1722	5747	37
H(35C)	12753	316	5810	42
H(35D)	11092	-193	5628	42
H(36A)	13298	414	5316	48
H(37D)	10427	977	5159	82
H(37E)	10669	2544	5275	82
H(37F)	11861	1989	5017	82
H(38D)	14880	1958	5610	77
H(38E)	14627	2596	5297	77
H(38F)	13435	3150	5555	77

Table S-8. Atomic Occupancy for P15185.

Atom	Occupancy	Atom	Occupancy	Atom	Occupancy
C(24)	0.49(2)	C(25)	0.49(2)	H(25)	0.49(2)
C(26)	0.49(2)	H(26)	0.49(2)	C(27)	0.49(2)
C(28)	0.49(2)	H(28)	0.49(2)	C(29)	0.49(2)
H(29)	0.49(2)	C(30)	0.49(2)	H(30A)	0.49(2)
H(30B)	0.49(2)	H(30C)	0.49(2)	C(24A)	0.51(2)
C(25A)	0.51(2)	H(25A)	0.51(2)	C(26A)	0.51(2)
H(26A)	0.51(2)	C(27A)	0.51(2)	C(28A)	0.51(2)
H(28A)	0.51(2)	C(29A)	0.51(2)	H(29A)	0.51(2)
C(30A)	0.51(2)	H(30D)	0.51(2)	H(30E)	0.51(2)
H(30F)	0.51(2)	H(33A)	0.517(5)	H(33B)	0.517(5)
H(33C)	0.483(5)	H(33D)	0.483(5)	C(34)	0.517(5)
H(34A)	0.517(5)	H(34B)	0.517(5)	C(35)	0.517(5)
H(35A)	0.517(5)	H(35B)	0.517(5)	C(36)	0.517(5)
H(36)	0.517(5)	C(37)	0.517(5)	H(37A)	0.517(5)
H(37B)	0.517(5)	H(37C)	0.517(5)	C(38)	0.517(5)
H(38A)	0.517(5)	H(38B)	0.517(5)	H(38C)	0.517(5)
C(34A)	0.483(5)	H(34C)	0.483(5)	H(34D)	0.483(5)
C(35A)	0.483(5)	H(35C)	0.483(5)	H(35D)	0.483(5)
C(36A)	0.483(5)	H(36A)	0.483(5)	C(37A)	0.483(5)
H(37D)	0.483(5)	H(37E)	0.483(5)	H(37F)	0.483(5)
C(38A)	0.483(5)	H(38D)	0.483(5)	H(38E)	0.483(5)
H(38F)	0.483(5)				

V. ^{1}H NMR Spectra and HPLC/SFC Data

Table 1, Entry 1

^{1}H NMR

($CDCl_3$, 400 MHz)

Data File C:\CHEM32\1\DATA\XM\2015-02-12 17-09-30\XM-2-16-1.D
Sample Name: XM-2-16-1

Table 1, entry 1 with (S,S)-1 ligand

==========

Acq. Operator	: XM	Seq. Line :	4
Acq. Instrument	: Instrument 1	Location :	P1-B-01
Injection Date	: 2/12/2015 5:23:20 PM	Inj :	1
		Inj Volume :	5 µl

Acq. Method : C:\Chem32\1\DATA\XM\2015-02-12 17-09-30\S1C2 12MIN 10.M
Last changed : 4/26/2014 11:47:17 PM by YNJ
Analysis Method : C:\CHEM32\1\DATA\YL\2015-02-12 19-36-40\S1C4 08MIN 05_5.M
Last changed : 2/12/2015 8:09:21 PM by YL
(modified after loading)
Method Info : S1C4 08min 05_5.M: 5% MeOH, OJ-H 5 mL/min, 8 min

Data File C:\CHEM32\1\DATA\XM\2015-02-12 17-09-30\XM-2-16-1.D
Sample Name: XM-2-16-1

==========

Area Percent Report

==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=210,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.901	VB	0.1923	1.12232e4	907.19537	96.5317
2	8.075	BB	0.1585	403.24420	33.01280	3.4683
Totals :				1.16264e4	940.20818	

Signal 2: DAD1 B, Sig=235,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.901	VV	0.1911	1.47456e4	1202.09192	96.0528
2	8.076	MM	0.2233	605.94922	45.22766	3.9472
Totals :				1.53516e4	1247.31958	

Signal 3: DAD1 C, Sig=245,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.901	VV	0.1897	7142.72607	588.12457	96.1957
2	8.080	MM	0.2150	282.48016	21.89603	3.8043
Totals :				7425.20624	610.02060	

Data File C:\CHEM32\1\DATA\XM\2015-02-12 17-09-30\XM-2-16-1.D
Sample Name: XM-2-16-1

Signal 4: DAD1 D, Sig=254,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.901	VB	0.1814	2592.29321	213.83340	96.3563
2	8.084	MM	0.2142	98.02831	7.62888	3.6437
Totals :				2690.32153	221.46228	

Signal 5: DAD1 E, Sig=280,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.905	VB	0.1848	103.05167	8.08164	100.0000
Totals :				103.05167	8.08164	

*** End of Report ***

Data File C:\CHEM32\1\DATA\XM\XM-2-106.D
Sample Name: XM-2-106

Table 1, entry 1 with (R,R)-1 ligand

==========

Acq. Operator	: XM	Seq. Line :	4
Acq. Instrument	: Instrument 1	Location :	P1-B-02
Injection Date	: 5/18/2015 8:59:59 PM	Inj :	1
		Inj Volume :	5 µl

Acq. Method : C:\Chem32\1\DATA\XM\2015-05-18 20-45-49\S1C2 12MIN 10.M
Last changed : 4/26/2014 11:47:17 PM by YNJ
Analysis Method : C:\CHEM32\1\DATA\JCB\2017-02-27 15-15-35\S3C1 12MIN 3.M
Last changed : 2/27/2017 3:59:41 PM by SBJKAN
(modified after loading)
Method Info : S3C1 12min 3.M: 3% IPA, IB 2.5 mL/min, 12 min

Data File C:\CHEM32\1\DATA\XM\XM-2-106.D
Sample Name: XM-2-106

==========

Area Percent Report

==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=210,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.827	VV	0.1530	710.84296	68.51685	3.9686
2	7.666	VV	0.2722	1.72008e4	963.90472	96.0314

Totals : 1.79116e4 1032.42157

Signal 2: DAD1 B, Sig=235,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.827	VV	0.1517	888.38214	86.58187	3.7551
2	7.666	VB	0.2677	2.27694e4	1304.31189	96.2449

Totals : 2.36577e4 1390.89376

Signal 3: DAD1 C, Sig=245,8 Ref=360,100

Signal 4: DAD1 D, Sig=254,8 Ref=360,100

Signal 5: DAD1 E, Sig=280,8 Ref=360,100

Table 1, Entry 2

^{1}H NMR

($CDCl_3$, 400 MHz)

Data File C:\CHEM32\1\DATA\XM\XM-2-30-RE.D
Sample Name: XM-2-30-RE

with (S,S)-1 ligand

==========

Acq. Operator	: XM	Seq. Line :	5
Acq. Instrument	: Instrument 1	Location :	P1-B-02
Injection Date	: 2/26/2015 10:57:18 AM	Inj :	1
		Inj Volume :	5 µl

Acq. Method : C:\Chem32\1\DATA\XM\2015-02-26 10-29-39\S1C2 12MIN 10.M
Last changed : 4/26/2014 11:47:17 PM by YNJ
Analysis Method : C:\CHEM32\1\DATA\JCB\2017-02-27 15-15-35\S3C1 12MIN 3.M
Last changed : 2/27/2017 3:59:41 PM by SBJKAN
(modified after loading)
Method Info : S3C1 12min 3.M: 3% IPA, IB 2.5 mL/min, 12 min

Data File C:\CHEM32\1\DATA\XM\XM-2-30-RE.D
Sample Name: XM-2-30-RE

==========

Area Percent Report

==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=210,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.400	MM	0.2563	7916.74512	514.82910	96.0429
2	10.843	MM	0.3209	326.18243	16.94343	3.9571
Totals :				8242.92755	531.77253	

Signal 2: DAD1 B, Sig=235,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.399	BV	0.2430	1.02436e4	667.79437	96.0468
2	10.850	MM	0.3353	421.61572	20.95412	3.9532
Totals :				1.06652e4	688.74849	

Signal 3: DAD1 C, Sig=245,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.400	MM	0.2559	4983.22021	324.61368	96.4409
2	10.846	MM	0.3173	183.90131	9.66001	3.5591
Totals :				5167.12152	334.27369	

Data File C:\CHEM32\1\DATA\XM\2015-03-16 20-39-15\XM-2-41-RENEW1.D
Sample Name: XM-2-41

with (R,R)-1 ligand

==========

Acq. Operator	: XM	Seq. Line :	6
Acq. Instrument	: Instrument 1	Location :	P1-B-03
Injection Date	: 3/16/2015 9:19:23 PM	Inj :	1
		Inj Volume :	5 µl

Acq. Method : C:\Chem32\1\DATA\XM\2015-03-16 20-39-15\S1C2 12MIN 10.M
Last changed : 4/26/2014 11:47:17 PM by YNJ
Analysis Method : C:\CHEM32\1\METHODS\S1C2\S1C2 EQUIL 40.M
Last changed : 3/16/2015 11:36:30 PM by XM
(modified after loading)
Method Info : S1C2 EQUIL 40.M: 40% MeOH (2.5 min), AD-H 3 mL/min

Data File C:\CHEM32\1\DATA\XM\2015-03-16 20-39-15\XM-2-41-RENEW1.D
Sample Name: XM-2-41

==========

Area Percent Report

==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=210,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.315	BV	0.1918	456.57434	34.19200	4.0766
2	10.501	BB	0.3277	1.07433e4	486.32562	95.9234

Totals : 1.11998e4 520.51762

Signal 2: DAD1 B, Sig=235,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.308	MM	0.2188	580.97711	44.24936	4.0101
2	10.498	MM	0.3667	1.39069e4	632.04791	95.9899

Totals : 1.44879e4 676.29727

Signal 3: DAD1 C, Sig=245,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.307	MM	0.2038	257.63766	21.07265	3.6689
2	10.496	MM	0.3675	6764.62598	306.76483	96.3311

Totals : 7022.26364 327.83748

Data File C:\CHEM32\1\DATA\XM\2015-03-16 20-39-15\XM-2-41-RENEW1.D
Sample Name: XM-2-41

Signal 4: DAD1 D, Sig=254,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.307	MM	0.2117	105.79601	8.32938	4.1849
2	10.497	MM	0.3623	2422.26758	111.42914	95.8151
Totals :				2528.06358	119.75852	

Signal 5: DAD1 E, Sig=280,8 Ref=360,100

*** End of Report ***

Table 1, Entry 3

^{1}H NMR

($CDCl_3$, 400 MHz)

Data File C:\CHEM32\1\DATA\XM\2015-03-20 23-48-34\XM-2-51.D
Sample Name: XM-2-51

with (S,S)-1 ligand

==========

Acq. Operator : NCOWPER
Seq. Line : 10
Acq. Instrument : Instrument 1
Location : P1-C-03
Injection Date : 3/21/2015 12:41:02 AM
Inj : 1
Inj Volume : 5 µl
Acq. Method : C:\Chem32\1\DATA\XM\2015-03-20 23-48-34\S3C5 12MIN20.M
Last changed : 4/28/2010 3:17:04 PM by scv
Analysis Method : C:\CHEM32\1\DATA\AHCVIII\2015-03-29 16-41-23\S3C3 08MIN 3.M
Last changed : 3/30/2015 4:40:36 PM by AHC
(modified after loading)
Method Info : S3C3 08min 3.M: 3% IPA, OD-H 2.5 mL/min, 8 min

==========

==========

Area Percent Report

==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=210,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.749	FM	0.1425	940.66180	110.00637	4.7876
2	5.613	MM	0.2959	1.87072e4	1053.66833	95.2124

Totals : 1.96478e4 1163.67471

Data File C:\CHEM32\1\DATA\XM\2015-03-20 23-48-34\XM-2-51.D
Sample Name: XM-2-51

==========

Acq. Operator : NCOWPER Seq. Line : 10
Acq. Instrument : Instrument 1 Location : P1-C-03
Injection Date : 3/21/2015 12:41:02 AM Inj : 1
Inj Volume : 5 µl
Acq. Method : C:\Chem32\1\DATA\XM\2015-03-20 23-48-34\S3C5 12MIN20.M
Last changed : 4/28/2010 3:17:04 PM by scv
Analysis Method : C:\CHEM32\1\DATA\AHCVIII\2015-03-29 16-41-23\S3C3 08MIN 3.M
Last changed : 3/30/2015 4:40:36 PM by AHC
(modified after loading)
Method Info : S3C3 08min 3.M: 3% IPA, OD-H 2.5 mL/min, 8 min

==========

Signal 2: DAD1 D, Sig=254,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.749	FM	0.1529	248.43715	27.07398	4.7010
2	5.614	BB	0.2517	5036.32080	306.48572	95.2990
Totals :				5284.75795	333.55970	

==========

*** End of Report ***

Data File C:\CHEM32\1\DATA\XM\2015-03-27 21-41-38\XM-2-59.D
Sample Name: XM-2-59

with (R,R)-1 ligand

==========

Acq. Operator : XM
Seq. Line : 10
Acq. Instrument : Instrument 1
Location : P1-C-03
Injection Date : 3/27/2015 10:33:37 PM
Inj : 1
Inj Volume : 5 µl
Acq. Method : C:\Chem32\1\DATA\XM\2015-03-27 21-41-38\S3C5 12MIN20.M
Last changed : 4/28/2010 3:17:04 PM by scv
Analysis Method : C:\CHEM32\1\DATA\NTK4\2015-03-30 14-10-25\S3C5 12MIN10ALL.M
Last changed : 3/30/2015 5:19:23 PM by AHC
(modified after loading)
Method Info : S3C5 12min10.M: 10% IPA, AS-H 2.5 mL/min, 12 min, all wavelengths

==========

Area Percent Report

==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=210,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.649	FM	0.2365	1.67850e4	1183.06409	95.1693
2	5.745	MM	0.2593	851.98560	54.76173	4.8307

Totals : 1.76370e4 1237.82582

Data File C:\CHEM32\1\DATA\XM\2015-03-27 21-41-38\XM-2-59.D
Sample Name: XM-2-59

Signal 2: DAD1 D, Sig=254,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.649	FM	0.2000	4516.39307	376.32648	95.4219
2	5.743	MM	0.2616	216.68608	13.80326	4.5781
Totals :				4733.07915	390.12974	

*** End of Report ***

Table 1, Entry 4

^{1}H NMR

($CDCl_3$, 400 MHz)

Data File C:\CHEM32\1\DATA\XM\2015-03-20 23-48-34\XM-2-54.D
Sample Name: XM-2-54

with (S,S)-1 ligand

==========

Acq. Operator : NCOWPER
Seq. Line : 4
Acq. Instrument : Instrument 1
Location : P1-C-01
Injection Date : 3/21/2015 12:03:04 AM
Inj : 1
Inj Volume : 5 µl
Acq. Method : C:\Chem32\1\DATA\XM\2015-03-20 23-48-34\S1C2 12MIN 10.M
Last changed : 4/26/2014 11:47:17 PM by YNJ
Analysis Method : C:\CHEM32\1\DATA\AHCVIII\2015-03-29 16-41-23\S3C3 08MIN 3.M
Last changed : 3/30/2015 3:38:41 PM by AHC
(modified after loading)
Method Info : S3C3 08min 3.M: 3% IPA, OD-H 2.5 mL/min, 8 min

==========

Data File C:\CHEM32\1\DATA\XM\2015-03-20 23-48-34\XM-2-54.D
Sample Name: XM-2-54

==========

Acq. Operator : NCOWPER Seq. Line : 4
Acq. Instrument : Instrument 1 Location : P1-C-01
Injection Date : 3/21/2015 12:03:04 AM Inj : 1
Inj Volume : 5 µl
Acq. Method : C:\Chem32\1\DATA\XM\2015-03-20 23-48-34\S1C2 12MIN 10.M
Last changed : 4/26/2014 11:47:17 PM by YNJ
Analysis Method : C:\CHEM32\1\DATA\AHCVIII\2015-03-29 16-41-23\S3C3 08MIN 3.M
Last changed : 3/30/2015 3:38:41 PM by AHC
(modified after loading)
Method Info : S3C3 08min 3.M: 3% IPA, OD-H 2.5 mL/min, 8 min

==========

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Area Percent Report

==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=210,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.162	MM	0.2140	1.17195e4	912.86688	95.9325
2	6.400	MM	0.2329	496.89969	35.55254	4.0675

Totals : 1.22164e4 948.41942

Data File C:\CHEM32\1\DATA\XM\2015-03-20 23-48-34\XM-2-54.D
Sample Name: XM-2-54

==========

Acq. Operator : NCOWPER Seq. Line : 4
Acq. Instrument : Instrument 1 Location : P1-C-01
Injection Date : 3/21/2015 12:03:04 AM Inj : 1
Inj Volume : 5 µl
Acq. Method : C:\Chem32\1\DATA\XM\2015-03-20 23-48-34\S1C2 12MIN 10.M
Last changed : 4/26/2014 11:47:17 PM by YNJ
Analysis Method : C:\CHEM32\1\DATA\AHCVIII\2015-03-29 16-41-23\S3C3 08MIN 3.M
Last changed : 3/30/2015 3:38:41 PM by AHC
(modified after loading)
Method Info : S3C3 08min 3.M: 3% IPA, OD-H 2.5 mL/min, 8 min

==========

Signal 2: DAD1 B, Sig=235,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.162	MM	0.2092	1.58179e4	1260.20312	95.9904
2	6.400	MM	0.2353	660.73035	46.80261	4.0096
Totals :				1.64786e4	1307.00573	

Signal 3: DAD1 C, Sig=245,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.164	BV	0.1769	7075.40771	569.77557	95.3415
2	6.395	MM	0.2532	345.71423	22.75997	4.6585
Totals :				7421.12195	592.53554	

Signal 4: DAD1 D, Sig=254,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.164	BV	0.1768	2428.23438	195.61308	95.7446
2	6.412	MM	0.2441	107.92239	7.36945	4.2554
Totals :				2536.15676	202.98254	

Signal 5: DAD1 E, Sig=280,8 Ref=360,100

==========

*** End of Report ***

Data File C:\CHEM32\1\DATA\XM\2015-03-27 21-41-38\XM-2-61.D
Sample Name: XM-2-61

with (R,R)-1 ligand

==========

Acq. Operator : XM
Seq. Line : 4
Acq. Instrument : Instrument 1
Location : P1-C-01
Injection Date : 3/27/2015 9:55:21 PM
Inj : 1
Inj Volume : 5 µl

Acq. Method : C:\Chem32\1\DATA\XM\2015-03-27 21-41-38\S1C2 12MIN 10.M
Last changed : 4/26/2014 11:47:17 PM by YNJ
Analysis Method : C:\CHEM32\1\DATA\AHCVIII\2015-03-29 16-41-23\S3C3 08MIN 3.M
Last changed : 3/30/2015 3:38:41 PM by AHC
(modified after loading)
Method Info : S3C3 08min 3.M: 3% IPA, OD-H 2.5 mL/min, 8 min

==========

Data File C:\CHEM32\1\DATA\XM\2015-03-27 21-41-38\XM-2-61.D
Sample Name: XM-2-61

==========

Acq. Operator : XM
Seq. Line : 4
Acq. Instrument : Instrument 1
Location : P1-C-01
Injection Date : 3/27/2015 9:55:21 PM
Inj : 1
Inj Volume : 5 µl
Acq. Method : C:\Chem32\1\DATA\XM\2015-03-27 21-41-38\S1C2 12MIN 10.M
Last changed : 4/26/2014 11:47:17 PM by YNJ
Analysis Method : C:\CHEM32\1\DATA\AHCVIII\2015-03-29 16-41-23\S3C3 08MIN 3.M
Last changed : 3/30/2015 3:38:41 PM by AHC
(modified after loading)
Method Info : S3C3 08min 3.M: 3% IPA, OD-H 2.5 mL/min, 8 min

==========

==========

Area Percent Report

==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=210,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.300	MM	0.2301	626.35876	45.36358	4.0602
2	6.347	MM	0.2772	1.48005e4	889.92834	95.9398

Totals : 1.54269e4 935.29193

Data File C:\CHEM32\1\DATA\XM\2015-03-27 21-41-38\XM-2-61.D
Sample Name: XM-2-61

==========

Acq. Operator : XM
Seq. Line : 4
Acq. Instrument : Instrument 1
Location : P1-C-01
Injection Date : 3/27/2015 9:55:21 PM
Inj : 1
Inj Volume : 5 µl
Acq. Method : C:\Chem32\1\DATA\XM\2015-03-27 21-41-38\S1C2 12MIN 10.M
Last changed : 4/26/2014 11:47:17 PM by YNJ
Analysis Method : C:\CHEM32\1\DATA\AHCVIII\2015-03-29 16-41-23\S3C3 08MIN 3.M
Last changed : 3/30/2015 3:38:41 PM by AHC
(modified after loading)
Method Info : S3C3 08min 3.M: 3% IPA, OD-H 2.5 mL/min, 8 min

==========

Signal 2: DAD1 B, Sig=235,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.300	MM	0.2386	880.65363	61.52452	4.2122
2	6.347	MM	0.2719	2.00264e4	1227.63489	95.7878
Totals :				2.09071e4	1289.15941	

Signal 3: DAD1 C, Sig=245,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.299	MM	0.2471	414.64178	27.96679	4.3894
2	6.347	MM	0.2692	9031.87402	559.18933	95.6106
Totals :				9446.51581	587.15612	

Signal 4: DAD1 D, Sig=254,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.295	MM	0.2490	141.73151	9.48483	4.3668
2	6.348	VB	0.2336	3103.96582	191.02971	95.6332
Totals :				3245.69733	200.51453	

Signal 5: DAD1 E, Sig=280,8 Ref=360,100

==========

*** End of Report ***

Table 1, Entry 5

^{1}H NMR

($CDCl_3$, 400 MHz)

Data File C:\CHEM32\1\DATA\XM\XM-2-31.D
Sample Name: XM-2-31

with (S,S)-1 ligand

==========

Acq. Operator	: XM	Seq. Line :	10
Acq. Instrument	: Instrument 1	Location :	P1-B-03
Injection Date	: 2/26/2015 2:23:55 AM	Inj :	1
		Inj Volume :	5 µl

Acq. Method : C:\Chem32\1\DATA\XM\2015-02-26 01-30-25\S3C2 12MIN25_3PT5.M
Last changed : 8/20/2013 1:57:34 PM by VB
Analysis Method : C:\CHEM32\1\DATA\JCB\2017-02-27 15-15-35\S3C1 12MIN 3.M
Last changed : 2/27/2017 3:59:41 PM by SBJKAN
(modified after loading)
Method Info : S3C1 12min 3.M: 3% IPA, IB 2.5 mL/min, 12 min

==========

Area Percent Report

==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Data File C:\CHEM32\1\DATA\XM\XM-2-31.D
Sample Name: XM-2-31

Signal 1: DAD1 A, Sig=330,8 Ref=360,100

Signal 2: DAD1 D, Sig=254,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.811	MM	0.1676	242.83171	24.14211	5.7390
2	5.524	MM	0.2199	3988.44336	302.26990	94.2610
Totals :				4231.27507	326.41201	

Signal 3: DAD1 E, Sig=280,8 Ref=360,100

*** End of Report ***

Data File C:\CHEM32\1\DATA\XM\2015-03-16 00-50-11\XM-2-42.D
Sample Name: XM-2-42

with (R,R)-1 ligand

==========

Acq. Operator	: XM	Seq. Line	: 11
Acq. Instrument	: Instrument 1	Location	: P1-B-05
Injection Date	: 3/16/2015 2:04:15 AM	Inj	: 1
		Inj Volume	: 5 µl

Acq. Method : C:\Chem32\1\DATA\XM\2015-03-16 00-50-11\S3C2 12MIN25_3PT5.M
Last changed : 8/20/2013 1:57:34 PM by VB
Analysis Method : C:\CHEM32\1\METHODS\S1C2\S1C2 EQUIL 40.M
Last changed : 3/16/2015 11:36:30 PM by XM
(modified after loading)
Method Info : S1C2 EQUIL 40.M: 40% MeOH (2.5 min), AD-H 3 mL/min

==========

Area Percent Report

==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Data File C:\CHEM32\1\DATA\XM\2015-03-16 00-50-11\XM-2-42.D
Sample Name: XM-2-42

Signal 1: DAD1 A, Sig=330,8 Ref=360,100

Signal 2: DAD1 D, Sig=254,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.852	VB	0.1702	1.17187e4	1050.27966	95.9148
2	7.136	BB	0.2092	499.12030	36.58693	4.0852
Totals :				1.22178e4	1086.86659	

Signal 3: DAD1 E, Sig=280,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.852	BB	0.1671	481.10571	44.17622	100.0000
Totals :				481.10571	44.17622	

==========

*** End of Report ***

Table 1, Entry 6

^{1}H NMR

($CDCl_3$, 400 MHz)

Data File C:\HPCHEM\1\DATA\GROUP\XM20752H.D Sample Name: XM20752H

```
==========================================================================
Injection Date  : 12/6/2016 4:19:13 AM          Seq. Line :  45
Sample Name     : XM20752H                       Location : Vial 1
Acq. Operator   : SES                                 Inj :   1
Acq. Instrument : Instrument 1                 Inj Volume : 5 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 2 µl
Acq. Method     : C:\HPCHEM\1\METHODS\OD-05-20.M
Last changed    : 3/20/2014 8:54:43 PM by MK
Analysis Method : C:\HPCHEM\1\METHODS\OJ-04-10.M
Last changed    : 12/6/2016 9:32:05 AM by SES
                  (modified after loading)
```

with (S,S)-1 ligand

Instrument 1 12/6/2016 10:25:54 AM SES

Data File C:\HPCHEM\1\DATA\GROUP\XM20752H.D Sample Name: XM20752H

```
==========================================================================
                          Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=250,10 Ref=360,100

Peak RetTime Type  Width     Area      Height      Area
  #   [min]        [min]   [mAU*s]     [mAU]        %
---|-------|----|-------|----------|----------|--------|
   1   8.065 BB    0.2559 2127.54517  126.72887  96.1653
   2  10.488 PB    0.3575   84.83785    3.54083   3.8347

Totals :                  2212.38302  130.26969

 Results obtained with enhanced integrator!

Signal 2: DAD1 B, Sig=254,10 Ref=360,100

Peak RetTime Type  Width     Area      Height      Area
  #   [min]        [min]   [mAU*s]     [mAU]        %
---|-------|----|-------|----------|----------|--------|
   1   8.065 MM    0.2871 1452.81287   84.32626  96.3610
   2  10.487 BB    0.3511   54.86360    2.32672   3.6390

Totals :                  1507.67647   86.65298

 Results obtained with enhanced integrator!

Signal 3: DAD1 C, Sig=210,10 Ref=360,100

Peak RetTime Type  Width     Area      Height      Area
  #   [min]        [min]   [mAU*s]     [mAU]        %
---|-------|----|-------|----------|----------|--------|
   1   8.065 MM    0.2869 5509.61523  320.06961  95.3387
   2  10.489 MM    0.4560  269.37869    9.84597   4.6613

Totals :                  5778.99393  329.91558

 Results obtained with enhanced integrator!

Signal 4: DAD1 D, Sig=230,10 Ref=360,100

Peak RetTime Type  Width     Area      Height      Area
  #   [min]        [min]   [mAU*s]     [mAU]        %
---|-------|----|-------|----------|----------|--------|
   1   8.065 BB    0.2569 5685.06104  336.89581  96.1844
   2  10.488 BB    0.3605  225.52528    9.38131   3.8156

Totals :                  5910.58632  346.27712

 Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,10 Ref=360,100

==========================================================================
                        *** End of Report ***
```

Instrument 1 12/6/2016 10:25:54 AM SES

```
==========================================================================
Injection Date  : 12/6/2016 4:40:24 AM          Seq. Line :  46
Sample Name     : XM20762H                       Location : Vial 2
Acq. Operator   : SES                                Inj :   1
Acq. Instrument : Instrument 1                 Inj Volume : 5 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 2 µl
Acq. Method     : C:\HPCHEM\1\METHODS\OD-05-20.M
Last changed    : 3/20/2014 8:54:43 PM by MK
Analysis Method : C:\HPCHEM\1\METHODS\OJ-04-10.M
Last changed    : 12/6/2016 9:32:05 AM by SES
                  (modified after loading)
```

with (R,R)-1 ligand

Instrument 1 12/6/2016 10:29:46 AM SES


```
==========================================================================
                          Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=250,10 Ref=360,100

Peak RetTime Type  Width     Area      Height      Area
  #   [min]        [min]   [mAU*s]     [mAU]        %
----|-------|----|-------|----------|----------|--------|
   1   8.152 BB    0.2522  192.52194   11.80906   4.3069
   2  10.174 MM    0.4167 4277.58301  171.07571  95.6931

Totals :                  4470.10495  182.88477

 Results obtained with enhanced integrator!

Signal 2: DAD1 B, Sig=254,10 Ref=360,100

Peak RetTime Type  Width     Area      Height      Area
  #   [min]        [min]   [mAU*s]     [mAU]        %
----|-------|----|-------|----------|----------|--------|
   1   8.152 PB    0.2526  128.06651    7.83708   4.3661
   2  10.174 MM    0.4144 2805.13843  112.82346  95.6339

Totals :                  2933.20494  120.66055

 Results obtained with enhanced integrator!

Signal 3: DAD1 C, Sig=210,10 Ref=360,100

Peak RetTime Type  Width     Area      Height      Area
  #   [min]        [min]   [mAU*s]     [mAU]        %
----|-------|----|-------|----------|----------|--------|
   1   8.150 PB    0.2573  517.46490   30.29782   4.6991
   2  10.174 BB    0.3678 1.04945e4   425.47501  95.3009

Totals :                  1.10120e4   455.77283

 Results obtained with enhanced integrator!

Signal 4: DAD1 D, Sig=230,10 Ref=360,100

Peak RetTime Type  Width     Area      Height      Area
  #   [min]        [min]   [mAU*s]     [mAU]        %
----|-------|----|-------|----------|----------|--------|
   1   8.151 BB    0.2522  516.33008   31.34383   4.4707
   2  10.174 BB    0.3648 1.10328e4   451.87842  95.5293

Totals :                  1.15491e4   483.22225

 Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,10 Ref=360,100

==========================================================================
                        *** End of Report ***
```

Instrument 1 12/6/2016 10:29:46 AM SES

Table 1, Entry 7
^{1}H NMR
($CDCl_3$, 400 MHz)

Data File C:\CHEM32\1\DATA\NTK4\2015-03-30 14-10-25\XM-2-74.D
Sample Name: XM-2-74

with (S,S)-1 ligand

==========

Acq. Operator	: NTK	Seq. Line	: 29
Acq. Instrument	: Instrument 1	Location	: P1-C-03
Injection Date	: 3/30/2015 5:06:50 PM	Inj	: 1
		Inj Volume	: 5 µl

Acq. Method : C:\Chem32\1\DATA\NTK4\2015-03-30 14-10-25\S1C2 12MIN 10.M
Last changed : 4/26/2014 11:47:17 PM by YNJ
Analysis Method : C:\CHEM32\1\DATA\NTK4\2015-03-30 14-10-25\S3C5 12MIN10ALL.M
Last changed : 3/30/2015 7:48:20 PM by AHC
(modified after loading)
Method Info : S3C5 12min10.M: 10% IPA, AS-H 2.5 mL/min, 12 min, all wavelengths

Data File C:\CHEM32\1\DATA\NTK4\2015-03-30 14-10-25\XM-2-74.D
Sample Name: XM-2-74

==========

Area Percent Report

==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=210,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.271	MM	0.1598	1.36462e4	1422.92993	95.3704
2	4.376	MM	0.1878	662.42780	58.77791	4.6296
Totals :				1.43086e4	1481.70784	

Signal 2: DAD1 B, Sig=235,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.272	MM	0.1523	1.79793e4	1967.07605	95.8142
2	4.377	MM	0.1787	785.44885	73.25290	4.1858
Totals :				1.87647e4	2040.32895	

Signal 3: DAD1 C, Sig=245,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.273	VV	0.1215	9736.96582	1165.00793	95.4306
2	4.376	MM	0.2042	466.22430	38.05719	4.5694
Totals :				1.02032e4	1203.06513	

Data File C:\CHEM32\1\DATA\NTK4\2015-03-30 14-10-25\XM-2-74.D
Sample Name: XM-2-74

Signal 4: DAD1 D, Sig=254,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.271	MM	0.1370	3720.83008	452.72186	95.1733
2	4.375	MM	0.2124	188.70302	14.81053	4.8267
Totals :				3909.53310	467.53239	

Signal 5: DAD1 E, Sig=280,8 Ref=360,100

*** End of Report ***

Data File C:\CHEM32\1\DATA\XM\2015-03-16 20-39-15\XM-2-40-RENEW1.D
Sample Name: XM-2-40

with (R,R)-1 ligand

==========

Acq. Operator	: XM	Seq. Line :	5
Acq. Instrument	: Instrument 1	Location :	P1-B-02
Injection Date	: 3/16/2015 9:06:27 PM	Inj :	1
		Inj Volume :	5 µl

Acq. Method : C:\Chem32\1\DATA\XM\2015-03-16 20-39-15\S1C2 12MIN 10.M
Last changed : 4/26/2014 11:47:17 PM by YNJ
Analysis Method : C:\CHEM32\1\METHODS\S1C2\S1C2 EQUIL 40.M
Last changed : 3/16/2015 11:36:30 PM by XM
(modified after loading)
Method Info : S1C2 EQUIL 40.M: 40% MeOH (2.5 min), AD-H 3 mL/min

Data File C:\CHEM32\1\DATA\XM\2015-03-16 20-39-15\XM-2-40-RENEW1.D
Sample Name: XM-2-40

==========

Area Percent Report

==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=210,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.254	MM	0.1059	688.15118	108.30387	4.5228
2	4.258	VB	0.1773	1.45270e4	1252.89941	95.4772

Totals : 1.52151e4 1361.20329

Signal 2: DAD1 B, Sig=235,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.253	MM	0.1155	968.10730	139.75650	4.7411
2	4.256	MM	0.1884	1.94512e4	1721.07886	95.2589

Totals : 2.04193e4 1860.83536

Signal 3: DAD1 C, Sig=245,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.252	MM	0.1069	426.59058	66.51580	4.1372
2	4.256	MM	0.1792	9884.42383	919.37872	95.8628

Totals : 1.03110e4 985.89452

Data File C:\CHEM32\1\DATA\XM\2015-03-16 20-39-15\XM-2-40-RENEW1.D
Sample Name: XM-2-40

Signal 4: DAD1 D, Sig=254,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.251	MM	0.1065	154.64348	24.19030	3.9959
2	4.256	MM	0.1786	3715.43237	346.66592	96.0041
Totals :				3870.07585	370.85622	

Signal 5: DAD1 E, Sig=280,8 Ref=360,100

*** End of Report ***

Table 1, Entry 8
^{1}H NMR
($CDCl_3$, 400 MHz)

Data File C:\CHEM32\1\DATA\XM\2017-02-27 19-26-58\XM-2-83.D
Sample Name: XM-2-83

with (S,S)-1 ligand

==========

Acq. Operator : xm
Seq. Line : 3
Acq. Instrument : Instrument 1
Location : P1-F-01
Injection Date : 2/27/2017 7:43:51 PM
Inj : 1
Inj Volume : 5 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 8 µl
Acq. Method : C:\Chem32\1\DATA\XM\2017-02-27 19-26-58\S1C2 12MIN 10.M
Last changed : 2/8/2017 1:15:35 AM by JLH
Analysis Method : C:\CHEM32\1\DATA\JCB\2017-02-27 15-15-35\S3C1 12MIN 3.M
Last changed : 2/27/2017 3:59:41 PM by SBJKAN
(modified after loading)
Method Info : S3C1 12min 3.M: 3% IPA, IB 2.5 mL/min, 12 min

Data File C:\CHEM32\1\DATA\XM\2017-02-27 19-26-58\XM-2-83.D
Sample Name: XM-2-83

==========

Area Percent Report

==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=210,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.236	MM	0.1672	1.11311e4	1109.72998	95.1893
2	4.942	MM	0.1516	562.54919	61.86582	4.8107
Totals :				1.16937e4	1171.59580	

Signal 2: DAD1 B, Sig=235,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.236	MM	0.1623	1.57427e4	1616.73511	95.0706
2	4.941	MM	0.1596	816.24841	85.22842	4.9294
Totals :				1.65589e4	1701.96352	

Signal 3: DAD1 C, Sig=245,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.237	BV	0.1428	7462.51318	815.14923	94.6996
2	4.945	MM	0.1732	417.68307	40.19280	5.3004
Totals :				7880.19626	855.34203	

Data File C:\CHEM32\1\DATA\XM\2017-02-27 19-26-58\XM-2-83.D
Sample Name: XM-2-83

Signal 4: DAD1 D, Sig=254,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.237	BV	0.1414	2624.74878	290.66962	95.2739
2	4.948	MM	0.1606	130.20035	13.51188	4.7261
Totals :				2754.94913	304.18150	

Signal 5: DAD1 E, Sig=280,8 Ref=360,100

*** End of Report ***

Data File C:\CHEM32\1\DATA\KMCHAN\2015-04-13 21-34-41\XM-2-84.D
Sample Name: XM-2-84

with (R,R)-1 ligand

==========

Acq. Operator	: KMCHAN	Seq. Line	: 43
Acq. Instrument	: Instrument 1	Location	: P1-C-04
Injection Date	: 4/14/2015 1:39:34 AM	Inj	: 1
		Inj Volume	: 5 µl

Acq. Method : C:\Chem32\1\DATA\KMCHAN\2015-04-13 21-34-41\S1C2 12MIN 10.M
Last changed : 4/26/2014 11:47:17 PM by YNJ
Analysis Method : C:\CHEM32\1\DATA\KMCHAN\2015-04-13 21-34-41\S3C2 12MIN 1.M
Last changed : 4/14/2015 2:13:59 AM by KMCHAN
(modified after loading)
Method Info : S3C2 12min 1.M: 1% IPA, AD-H 2.5 mL/min, 12 min

Data File C:\CHEM32\1\DATA\KMCHAN\2015-04-13 21-34-41\XM-2-84.D
Sample Name: XM-2-84

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Area Percent Report

==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=210,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.295	MM	0.1221	196.00064	26.75252	4.7297
2	3.857	MM	0.1419	3948.05200	463.67178	95.2703

Totals : 4144.05264 490.42430

Signal 2: DAD1 B, Sig=235,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.295	MM	0.1265	259.54041	34.19540	4.7447
2	3.857	MM	0.1405	5210.61279	618.29919	95.2553

Totals : 5470.15320 652.49459

Signal 3: DAD1 C, Sig=245,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.295	MM	0.1197	111.94508	15.59130	4.4593
2	3.857	VB	0.1286	2398.44360	278.11951	95.5407

Totals : 2510.38868 293.71080

Data File C:\CHEM32\1\DATA\KMCHAN\2015-04-13 21-34-41\XM-2-84.D
Sample Name: XM-2-84

Signal 4: DAD1 D, Sig=254,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.292	MM	0.1180	44.90385	6.34196	5.0029
2	3.857	VV	0.1338	852.64728	97.71813	94.9971
Totals :				897.55113	104.06009	

Signal 5: DAD1 E, Sig=280,8 Ref=360,100

==========

*** End of Report ***

Table 2, Entry 1

^{1}H NMR

($CDCl_3$, 400 MHz)

Data File C:\HPCHEM\1\DATA\GROUP\XM-2-722.D

```
==========================================================
Injection Date  : 4/22/2015 11:50:52 AM          Seq. Line :   5
Sample Name     :                                 Location : Vial 72
Acq. Operator   : SES                                  Inj :   1
Acq. Instrument : Instrument 1                 Inj Volume : 15 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 3 µl
Acq. Method     : C:\HPCHEM\1\METHODS\AD-10-20.M
Last changed    : 3/18/2014 8:29:19 AM by MK
Analysis Method : C:\HPCHEM\1\METHODS\OJ-10-10.M
Last changed    : 11/29/2016 9:02:30 AM by SES
                  (modified after loading)
```

with (S,S)-1 ligand

Instrument 1 11/29/2016 9:45:10 PM SES

Data File C:\HPCHEM\1\DATA\GROUP\XM-2-722.D

==========
Area Percent Report
==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=250,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.101	VV	0.1676	1.59265e4	1479.00330	96.8973
2	8.670	MF	0.2516	509.97775	33.78212	3.1027

Totals : 1.64365e4 1512.78542

Results obtained with enhanced integrator!

Signal 2: DAD1 B, Sig=254,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.101	VP	0.1617	1.05418e4	994.49957	96.8910
2	8.670	MF	0.2517	338.26172	22.39765	3.1090

Totals : 1.08801e4 1016.89723

Results obtained with enhanced integrator!

Signal 3: DAD1 C, Sig=210,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.103	VV	0.2183	3.01062e4	2191.58716	97.4909
2	8.670	VV	0.1817	774.84235	65.64034	2.5091

Totals : 3.08811e4 2257.22749

Results obtained with enhanced integrator!

Signal 4: DAD1 D, Sig=230,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.099	VV	0.2134	3.48462e4	2582.44995	97.6988
2	8.670	VV	0.1815	820.76105	69.64350	2.3012

Totals : 3.56669e4 2652.09345

Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.370	PP	0.1284	14.38663	1.74138	2.7727
2	7.102	BB	0.1605	504.47714	48.05094	97.2273

Instrument 1 11/29/2016 9:45:10 PM SES

Data File C:\HPCHEM\1\DATA\GROUP\XM-2-722.D

Totals : 518.86377 49.79232

Results obtained with enhanced integrator!

==========

*** End of Report ***

Instrument 1 11/29/2016 9:45:10 PM SES

Data File C:\HPCHEM\1\DATA\GROUP\XM-2-732.D

```
    ==========================================================
    Injection Date  : 4/22/2015 12:12:05 PM          Seq. Line :   6
    Sample Name     :                                 Location : Vial 73
    Acq. Operator   : SES                                  Inj :   1
    Acq. Instrument : Instrument 1                 Inj Volume : 15 µl
    Different Inj Volume from Sequence !     Actual Inj Volume : 3 µl
    Acq. Method     : C:\HPCHEM\1\METHODS\AD-10-20.M
    Last changed    : 3/18/2014 8:29:19 AM by MK
    Analysis Method : C:\HPCHEM\1\METHODS\OJ-10-10.M
    Last changed    : 11/29/2016 9:02:30 AM by SES
                      (modified after loading)
```

with (R,R)-1 ligand

Instrument 1 11/29/2016 9:42:49 PM SES

Data File C:\HPCHEM\1\DATA\GROUP\XM-2-732.D

```
    ==========================================================================
                                   Area Percent Report
    ==========================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=250,10 Ref=360,100

    Peak RetTime Type  Width     Area      Height      Area
     #   [min]        [min]   [mAU*s]     [mAU]        %
    ----|-------|----|-------|----------|----------|--------|
      1   7.108 VV    0.1906  535.74573   42.62881   6.8600
      2   8.629 VB    0.2008 7274.01221  562.88757  93.1400

    Totals :                   7809.75793  605.51638

     Results obtained with enhanced integrator!

    Signal 2: DAD1 B, Sig=254,10 Ref=360,100

    Peak RetTime Type  Width     Area      Height      Area
     #   [min]        [min]   [mAU*s]     [mAU]        %
    ----|-------|----|-------|----------|----------|--------|
      1   7.108 MM    0.2172  372.30045   28.56381   7.2418
      2   8.628 VB    0.2007 4768.70068  369.23962  92.7582

    Totals :                   5141.00113  397.80343

     Results obtained with enhanced integrator!

    Signal 3: DAD1 C, Sig=210,10 Ref=360,100

    Peak RetTime Type  Width     Area      Height      Area
     #   [min]        [min]   [mAU*s]     [mAU]        %
    ----|-------|----|-------|----------|----------|--------|
      1   7.107 MM    0.2177 1467.32190  112.31230   7.5284
      2   8.628 MM    0.2244 1.80233e4  1338.67163  92.4716

    Totals :                   1.94906e4  1450.98393

     Results obtained with enhanced integrator!

    Signal 4: DAD1 D, Sig=230,10 Ref=360,100

    Peak RetTime Type  Width     Area      Height      Area
     #   [min]        [min]   [mAU*s]     [mAU]        %
    ----|-------|----|-------|----------|----------|--------|
      1   7.107 MM    0.2154 1540.08752  119.14174   7.1980
      2   8.628 MM    0.2185 1.98560e4  1514.70837  92.8020

    Totals :                   2.13961e4  1633.85011

     Results obtained with enhanced integrator!

    Signal 5: DAD1 E, Sig=280,10 Ref=360,100

    Peak RetTime Type  Width     Area      Height      Area
     #   [min]        [min]   [mAU*s]     [mAU]        %
    ----|-------|----|-------|----------|----------|--------|
      1   7.109 PB    0.1853   15.90698    1.33204   6.5367
      2   8.629 PB    0.1995  227.44136   17.74785  93.4633
```

Instrument 1 11/29/2016 9:42:49 PM SES

Data File C:\HPCHEM\1\DATA\GROUP\XM-2-732.D

Totals : 243.34834 19.07989

Results obtained with enhanced integrator!

==========

*** End of Report ***

Instrument 1 11/29/2016 9:42:49 PM SES

Ar = 4-BrC$_6$H$_4$

Table 2, Entry 2

^{1}H NMR

($CDCl_3$, 400 MHz)

with (S,S)-1 ligand

```
==================================================================
Injection Date  : 5/19/2015 1:42:53 AM          Seq. Line :   3
Sample Name     : XM-2-122                       Location : Vial 51
Acq. Operator   : XM                                 Inj :   1
Acq. Instrument : Instrument 1                 Inj Volume : 15 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 2 µl
Acq. Method     : C:\HPCHEM\1\METHODS\AD-03-15.M
Last changed    : 4/18/2014 7:45:58 PM by MK
Analysis Method : C:\HPCHEM\1\METHODS\OD-08-10.M
Last changed    : 3/1/2017 7:57:39 AM by JLH
```

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=250,10 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   5.169 BB    0.1161  190.81052   24.71057  93.8232
   2   6.350 PB    0.1624   12.56189    1.14147   6.1768

Totals :                   203.37240   25.85204

 Results obtained with enhanced integrator!

Signal 2: DAD1 B, Sig=254,10 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   5.169 MM    0.1326  171.17365   21.51041  92.8996
   2   6.347 MM    0.2047   13.08299    1.06506   7.1004

Totals :                   184.25663   22.57547

 Results obtained with enhanced integrator!

Signal 3: DAD1 C, Sig=210,10 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   5.170 MM    0.1260 5725.72070  757.33978  93.7212
   2   6.352 MM    0.1829  383.59216   34.95875   6.2788

Totals :                  6109.31287  792.29853

 Results obtained with enhanced integrator!

Signal 4: DAD1 D, Sig=230,10 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   5.170 VV    0.1140 4581.42822  607.28485  94.0686
   2   6.352 BB    0.1606  288.87833   27.48623   5.9314

Totals :                  4870.30655  634.77108

 Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,10 Ref=360,100

==================================================================
                        *** End of Report ***
```

with (R,R)-1 ligand

```
==================================================================
Injection Date  : 5/19/2015 1:59:07 AM          Seq. Line :   4
Sample Name     : XM-2-123                       Location : Vial 52
Acq. Operator   : XM                                  Inj :   1
Acq. Instrument : Instrument 1                  Inj Volume : 15 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 2 µl
Acq. Method     : C:\HPCHEM\1\METHODS\AD-03-15.M
Last changed    : 4/18/2014 7:45:58 PM by MK
Analysis Method : C:\HPCHEM\1\METHODS\OD-08-10.M
Last changed    : 3/1/2017 7:57:39 AM by JLH
```

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=250,10 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   5.249 MM    0.1489   19.57143    2.19030   7.7502
   2   6.340 MM    0.1884  232.95741   20.61187  92.2498

Totals :                   252.52884   22.80217

 Results obtained with enhanced integrator!

Signal 2: DAD1 B, Sig=254,10 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   5.250 MM    0.1509   20.17203    2.22801   9.1490
   2   6.340 MM    0.1886  200.31168   17.69848  90.8510

Totals :                   220.48370   19.92650

 Results obtained with enhanced integrator!

Signal 3: DAD1 C, Sig=210,10 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   5.249 MM    0.1785  519.96698   48.54576   7.3606
   2   6.340 MM    0.1748 6544.18506  623.82068  92.6394

Totals :                  7064.15204  672.36644

 Results obtained with enhanced integrator!

Signal 4: DAD1 D, Sig=230,10 Ref=360,100


Signal 5: DAD1 E, Sig=280,10 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   3.383 BP    0.0856   18.08247    2.86576  15.5054
   2   6.340 BB    0.1582   98.53800    9.56592  84.4946

Totals :                   116.62047   12.43168

 Results obtained with enhanced integrator!
==================================================================
                        *** End of Report ***
```

Table 2, Entry 3
^{1}H NMR
($CDCl_3$, 400 MHz)

with (S,S)-1 ligand

```
==================================================================
Injection Date  : 4/17/2015 2:43:45 PM          Seq. Line :  14
Sample Name     : XM-2-93                        Location : Vial 72
Acq. Operator   : SES                                 Inj :   1
Acq. Instrument : Instrument 1                  Inj Volume : 15 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 4 µl
Acq. Method     : C:\HPCHEM\1\METHODS\IC-10-20.M
Last changed    : 4/7/2015 7:37:44 AM by SES
Analysis Method : C:\HPCHEM\1\METHODS\OD-08-10.M
Last changed    : 3/1/2017 7:57:39 AM by JLH
```

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=250,10 Ref=360,100


Signal 2: DAD1 B, Sig=254,10 Ref=360,100


Signal 3: DAD1 C, Sig=210,10 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  10.006 MM    0.3068  140.88203    7.65231   4.1051
   2  12.000 MM    0.3249 3291.00391  168.83461  95.8949

Totals :                  3431.88594  176.48692

 Results obtained with enhanced integrator!

Signal 4: DAD1 D, Sig=230,10 Ref=360,100


Signal 5: DAD1 E, Sig=280,10 Ref=360,100

==================================================================
                        *** End of Report ***
```

with (R,R)-1 ligand

```
==================================================================
Injection Date  : 4/17/2015 3:04:58 PM          Seq. Line :  15
Sample Name     : XM-2-94                        Location : Vial 73
Acq. Operator   : SES                                 Inj :   1
Acq. Instrument : Instrument 1                  Inj Volume : 15 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 4 µl
Acq. Method     : C:\HPCHEM\1\METHODS\IC-10-20.M
Last changed    : 4/7/2015 7:37:44 AM by SES
Analysis Method : C:\HPCHEM\1\METHODS\OD-08-10.M
Last changed    : 3/1/2017 7:57:39 AM by JLH
```

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=250,10 Ref=360,100


Signal 2: DAD1 B, Sig=254,10 Ref=360,100


Signal 3: DAD1 C, Sig=210,10 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  10.001 MM    0.2754 4380.17871  265.06342  93.8384
   2  12.036 MM    0.3082  287.61264   15.55151   6.1616

Totals :                  4667.79135  280.61492

 Results obtained with enhanced integrator!

Signal 4: DAD1 D, Sig=230,10 Ref=360,100


Signal 5: DAD1 E, Sig=280,10 Ref=360,100

==================================================================
                        *** End of Report ***
```

Ar = 4-ClC$_6$H$_4$

Table 2, Entry 4

^{1}H NMR

(CDCl$_3$, 400 MHz)

with (S,S)-1 ligand

```
==================================================================
Injection Date  : 5/1/2015 9:25:02 PM          Seq. Line :   7
Sample Name     : XM-2-101                      Location : Vial 71
Acq. Operator   : XM                                 Inj :   1
Acq. Instrument : Instrument 1                 Inj Volume : 15 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 2 µl
Acq. Method     : C:\HPCHEM\1\METHODS\AD-03-20.M
Last changed    : 9/9/2011 8:37:36 PM by NB
Analysis Method : C:\HPCHEM\1\METHODS\OD-08-10.M
Last changed    : 3/1/2017 7:57:39 AM by JLH
```

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=250,10 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  11.735 MM    0.2947   32.47197    1.83637   0.4759
   2  14.201 MM    0.3741  956.40204   42.61166  14.0162
   3  17.118 MM    0.4885 5834.67822  199.07234  85.5079

Totals :                  6823.55223  243.52036

 Results obtained with enhanced integrator!

Signal 2: DAD1 B, Sig=254,10 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  11.738 BB    0.2526   20.15431    1.16038   0.4418
   2  14.201 BB    0.3342  633.27307   28.60936  13.8833
   3  17.118 MM    0.4867 3907.96094  133.83009  85.6748

Totals :                  4561.38832  163.59983

 Results obtained with enhanced integrator!

Signal 3: DAD1 C, Sig=210,10 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.148 BP    0.2406   29.87443    1.52448   0.0995
   2  11.738 VP    0.2523   92.67373    5.45333   0.3085
   3  14.201 PB    0.3396 4053.97607  180.80489  13.4962
   4  17.118 VB    0.4384 2.58613e4   896.82465  86.0958

Totals :                  3.00378e4  1084.60733

 Results obtained with enhanced integrator!

Signal 4: DAD1 D, Sig=230,10 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  11.737 VB    0.2523   88.12701    5.03306   0.3299
   2  14.201 MM    0.3652 3687.73096  168.27452  13.8064
   3  17.118 BP    0.4380 2.29344e4   796.27490  85.8636

Totals :                  2.67103e4   969.58248

 Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,10 Ref=360,100

==================================================================
                      *** End of Report ***
```

with (R,R)-1 ligand

```
==================================================================
Injection Date  : 5/1/2015 9:46:15 PM          Seq. Line :   8
Sample Name     : XM-2-102                      Location : Vial 72
Acq. Operator   : XM                                 Inj :   1
Acq. Instrument : Instrument 1                 Inj Volume : 15 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 2 µl
Acq. Method     : C:\HPCHEM\1\METHODS\AD-03-20.M
Last changed    : 9/9/2011 8:37:36 PM by NB
Analysis Method : C:\HPCHEM\1\METHODS\OD-08-10.M
Last changed    : 3/1/2017 7:57:39 AM by JLH
```

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=250,10 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.826 MM    0.8399 1153.51147   22.88986  85.0142
   2  11.776 MM    0.2960   67.97147    3.82778   5.0095
   3  14.215 MM    0.4480   18.90322 7.03266e-1   1.3932
   4  17.188 MM    0.4563  116.46017    4.25400   8.5832

Totals :                  1356.84634   31.67490

 Results obtained with enhanced integrator!

Signal 2: DAD1 B, Sig=254,10 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.824 MM    0.8384  775.65430   15.41873  85.2351
   2  11.774 PB    0.2703   44.63988    2.52505   4.9054
   3  14.214 MM    0.4039   10.17639 4.19886e-1   1.1183
   4  17.187 MM    0.4601   79.54671    2.88140   8.7412

Totals :                   910.01728   21.24506

 Results obtained with enhanced integrator!

Signal 3: DAD1 C, Sig=210,10 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.828 VP    0.7489 5201.97314  103.75797  85.7218
   2  11.777 MM    0.3302  240.51018   12.14134   3.9633
   3  14.218 PV    0.3022   85.25111    3.47476   1.4048
   4  17.188 MM    0.4550  540.69946   19.80652   8.9100

Totals :                  6068.43390  139.18061

 Results obtained with enhanced integrator!

Signal 4: DAD1 D, Sig=230,10 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.830 MM    0.8288 4671.32422   93.93405  86.6275
   2  11.776 BB    0.2808  198.97351   10.90772   3.6899
   3  14.210 PB    0.3320   57.21024    2.43555   1.0609
   4  17.188 BB    0.4054  464.91882   17.19977   8.6217

Totals :                  5392.42679  124.47710

 Results obtained with enhanced integrator!
```

Signal 5: DAD1 E, Sig=280,10 Ref=360,100

==========

*** End of Report ***

Table 2, Entry 5

^{1}H NMR

($CDCl_3$, 400 MHz)

with (S,S)-1 ligand

```
==================================================================
Injection Date  : 4/29/2015 10:41:17 AM          Seq. Line :   3
Sample Name     : XM-2-99                         Location : Vial 71
Acq. Operator   : SES                                 Inj :   1
Acq. Instrument : Instrument 1                  Inj Volume : 15 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 2 µl
Acq. Method     : C:\HPCHEM\1\METHODS\AD-02-20.M
Last changed    : 1/26/2014 12:23:42 PM by MK
Analysis Method : C:\HPCHEM\1\METHODS\OD-08-10.M
Last changed    : 3/1/2017 7:57:39 AM by JLH
```

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=250,10 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.687 MM    0.1616   76.61696    7.90429   0.3719
   2   8.473 MM    0.1858  507.87531   45.54671   2.4653
   3   9.576 MM    0.2626 1.95542e4  1241.09253  94.9191
   4  10.558 MM    0.2752  462.22336   27.99637   2.2437

Totals :                  2.06010e4  1322.53990

 Results obtained with enhanced integrator!

Signal 2: DAD1 B, Sig=254,10 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.689 BV    0.1314   22.06115    2.58868   0.1591
   2   8.473 MM    0.2172  444.95145   34.14276   3.2094
   3   9.576 MM    0.2609 1.30861e4   835.85907  94.3895
   4  10.558 MM    0.2759  310.82675   18.77762   2.2420

Totals :                  1.38640e4   891.36813

 Results obtained with enhanced integrator!

Signal 3: DAD1 C, Sig=210,10 Ref=360,100


Signal 4: DAD1 D, Sig=230,10 Ref=360,100


Signal 5: DAD1 E, Sig=280,10 Ref=360,100

==================================================================
                        *** End of Report ***
```

with (R,R)-1 ligand

```
==========================================================================
Injection Date  : 4/29/2015 11:02:32 AM          Seq. Line :   4
Sample Name     : XM-2-100                        Location : Vial 72
Acq. Operator   : SES                                 Inj :   1
Acq. Instrument : Instrument 1                  Inj Volume : 15 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 2 µl
Acq. Method     : C:\HPCHEM\1\METHODS\AD-02-20.M
Last changed    : 1/26/2014 12:23:42 PM by MK
Analysis Method : C:\HPCHEM\1\METHODS\OD-08-10.M
Last changed    : 3/1/2017 7:57:39 AM by JLH
```

```
==========================================================================
                          Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=250,10 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]    [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.677 BB    0.1324   57.12731    6.64046   0.2422
   2   8.304 MM    0.2474 2.22443e4  1498.66785  94.2968
   3   9.590 BP    0.2185  793.03851   55.56034   3.3618
   4  10.666 BP    0.2645  495.20718   28.52632   2.0993

Totals :                  2.35897e4  1589.39497

 Results obtained with enhanced integrator!

Signal 2: DAD1 B, Sig=254,10 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]    [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.678 BV    0.1283   23.41937    2.83812   0.1517
   2   8.304 BB    0.2215 1.45192e4  1011.34692  94.0200
   3   9.590 BP    0.2185  529.96362   37.13478   3.4318
   4  10.666 MM    0.2978  370.09280   20.71576   2.3966

Totals :                  1.54426e4  1072.03559

 Results obtained with enhanced integrator!

Signal 3: DAD1 C, Sig=210,10 Ref=360,100


Signal 4: DAD1 D, Sig=230,10 Ref=360,100


Signal 5: DAD1 E, Sig=280,10 Ref=360,100

==========================================================================
                          *** End of Report ***
```

Table 2, Entry 6

^{1}H NMR

($CDCl_3$, 400 MHz)

Data File C:\HPCHEM\1\DATA\GROUP\XM-2-853.D

with (S,S)-1 ligand

```
==================================================================
Injection Date  : 4/14/2015 6:10:40 PM          Seq. Line :   3
Sample Name     :                                Location : Vial 71
Acq. Operator   : SES                                 Inj :   1
Acq. Instrument : Instrument 1                  Inj Volume : 15 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 3 µl
Acq. Method     : C:\HPCHEM\1\METHODS\AD-02-20.M
Last changed    : 1/26/2014 12:23:42 PM by MK
Analysis Method : C:\HPCHEM\1\METHODS\OD-08-10.M
Last changed    : 3/1/2017 7:57:39 AM by JLH
```

Data File C:\HPCHEM\1\DATA\GROUP\XM-2-853.D

==========
Area Percent Report
==========

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=250,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.156	BV	0.2333	195.87419	12.74635	2.5840
2	8.738	MM	0.2366	250.89896	17.67264	3.3099
3	10.058	MM	0.2350	520.85590	36.94784	6.8713
4	10.503	MM	0.3498	6612.53857	315.06055	87.2347
Totals :				7580.16762	382.42738	

Results obtained with enhanced integrator!

Signal 2: DAD1 B, Sig=254,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.157	BV	0.2345	125.91825	8.13929	2.5008
2	8.737	VB	0.2398	192.85680	12.51075	3.8303
3	10.058	BV	0.2233	348.35565	24.29834	6.9186
4	10.503	MM	0.3493	4367.93262	208.43471	86.7503
Totals :				5035.06332	253.38309	

Results obtained with enhanced integrator!

Signal 3: DAD1 C, Sig=210,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.160	MM	0.2694	615.86871	38.10742	2.7018
2	8.735	MM	0.2525	919.69788	60.69901	4.0347
3	10.058	MM	0.2281	1841.40588	134.53355	8.0783
4	10.503	MM	0.3484	1.94175e4	928.99701	85.1851
Totals :				2.27945e4	1162.33699	

Results obtained with enhanced integrator!

Signal 4: DAD1 D, Sig=230,10 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.154	PV	0.2249	577.24890	38.94510	2.9914
2	8.740	MM	0.2493	710.70947	47.50518	3.6830
3	10.058	MM	0.2307	1251.75500	90.44328	6.4867
4	10.503	MM	0.3493	1.67575e4	799.61981	86.8390
Totals :				1.92972e4	976.51336	

Results obtained with enhanced integrator!

Data File C:\HPCHEM\1\DATA\GROUP\XM-2-853.D

Signal 5: DAD1 E, Sig=280,10 Ref=360,100

==========

*** End of Report ***

Data File C:\HPCHEM\1\DATA\GROUP\XM-2-863.D

with (R,R)-1 ligand

```
==================================================================
Injection Date  : 4/14/2015 6:31:54 PM          Seq. Line :   4
Sample Name     :                                Location : Vial 72
Acq. Operator   : SES                                 Inj :   1
Acq. Instrument : Instrument 1                  Inj Volume : 15 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 4 µl
Acq. Method     : C:\HPCHEM\1\METHODS\AD-02-20.M
Last changed    : 1/26/2014 12:23:42 PM by MK
Analysis Method : C:\HPCHEM\1\METHODS\OD-08-10.M
Last changed    : 3/1/2017 7:57:39 AM by JLH
```

Data File C:\HPCHEM\1\DATA\GROUP\XM-2-863.D

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=250,10 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.283 BV    0.1982 1224.83264   96.40526  20.0833
   2   8.716 VB    0.2307 4164.40332  278.06259  68.2829
   3  10.133 PV    0.2475   72.82558    4.63011   1.1941
   4  10.762 VB    0.2813  636.68829   34.50557  10.4397

Totals :                  6098.74983  413.60353

 Results obtained with enhanced integrator!

Signal 2: DAD1 B, Sig=254,10 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.283 BV    0.1984  822.25220   64.64721  20.3324
   2   8.716 VB    0.2312 2748.95386  183.09338  67.9752
   3  10.132 PV    0.2420   49.40000    3.13219   1.2215
   4  10.762 VB    0.2816  423.44623   22.91028  10.4708

Totals :                  4044.05228  273.78307

 Results obtained with enhanced integrator!

Signal 3: DAD1 C, Sig=210,10 Ref=360,100


Signal 4: DAD1 D, Sig=230,10 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.283 BV    0.1985 3067.32715  240.90208  19.3306
   2   8.716 VB    0.2322 1.09467e4   724.92230  68.9868
   3  10.134 BV    0.2593  208.62434   12.33401   1.3148
   4  10.762 VB    0.2848 1645.14673   87.72217  10.3679

Totals :                  1.58678e4  1065.88056

 Results obtained with enhanced integrator!

Signal 5: DAD1 E, Sig=280,10 Ref=360,100

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                      *** End of Report ***
```

(1) (a) Cordier, C. J.; Lundgren, R. J.; Fu, G. C. *J. Am. Chem. Soc*. **2013**, *135*, 10946–10949. (b) Denmark, S. E.; Su, X.; Nishigaichi, Y.; Coe, D. M.; Wong, K.-T.; Winter, S. B. D.; Choi, J. Y. *J. Org. Chem.* **1999**, *64*, 1958–1967.

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