

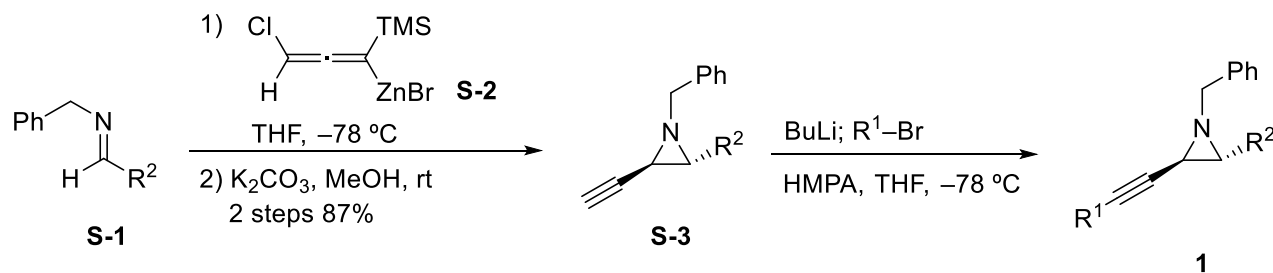
Supporting Information for
Diastereoselective Synthesis of 5-Iodoalkenyl-2-Oxazolines by Electrophilic
Cyclization of Allenyl Amides

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Preparation of *N*-benzylpropargylaziridines **1.**

N-Benzylpropargylaziridines **1** were prepared from the corresponding benzylimines **S-1** according to the procedure described in the literature^{1,2} (Scheme S-1).



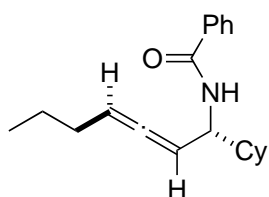
Scheme S-1

General procedure for the synthesis of *N*-benzoylallenylamine **2 from propargylaziridine **1**.**

To a solution of propargylaziridine **1a** (300 mg, 1.07 mmol) in toluene (2.0 mL) was stirred for 4 days at 110 °C in air. The reaction mixture was cooled to room temperature and then BzCl (752 mg, 5.35 mmol), 18-crown-6 (28.3 mg, 0.107 mmol) and 3 M aq. KOH (2.0 mL, 2.14 mmol) was added to the reaction

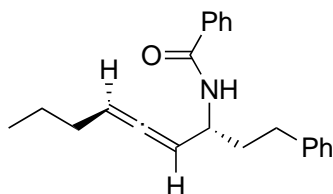
mixture. After further stirring at 90 °C for 24 h, the mixture was poured directly into a separatory funnel charged with Et₂O and 1M aq. NaOH. The organic layer was washed with brine, dried over MgSO₄, and the solvent was evaporated under reduced pressure. The crude product was purified by column chromatography (SiO₂, hexane/AcOEt = 50/1 to 10/1) to afford *N*-benzoylallenylamine **2a** (227 mg, 0.760 mmol, 71% yield) as a colorless oil.

(±)-*N*-((1*R,*aR**)-1-cyclohexylhepta-2,3-dien-1-yl)benzamide (2a).**



Pale yellow oil; IR (neat) 3320, 2923, 2851, 2022, 1634, 1534, 1324, 690 cm⁻¹; ¹H-NMR (500 MHz, CDCl₃) δ 0.85 (3H, t, *J* = 7.3 Hz), 1.04–1.28 (5H, m), 1.36 (2H, sext, *J* = 7.3 Hz), 1.59–1.68 (2H, m), 1.75–1.84 (4H, m), 1.94–1.98 (2H, m), 4.57 (1H, dddd, *J* = 1.6, 2.8, 4.4, 8.9 Hz), 5.25–5.35 (2H, m), 6.18 (1H, d, *J* = 8.9 Hz), 7.41–7.50 (3H, m), 7.75–7.77 (2H, m); ¹³C-NMR (100 MHz, CDCl₃) δ 13.7 (CH₃), 22.5 (CH₂), 26.2 (CH₂), 26.3 (CH₂), 26.5 (CH₂), 29.0 (CH₂), 29.3 (CH₂), 31.0 (CH₂), 42.9 (CH), 52.3 (CH), 91.9 (CH), 94.8 (CH), 126.9 (CH×2), 128.7 (CH×2), 131.4 (CH), 135.2 (Cq), 166.8 (Cq), 202.7 (Cq); HRMS (EI) *m/z* calcd for C₂₀H₂₇NO (M⁺) 297.2093, found 297.2095.

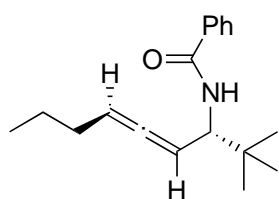
(±)-*N*-((3*R,*aR**)-1-phenylnona-4,5-dien-3-yl)benzamide (2b)**



Pale yellow oil; IR (neat) 3710, 3292, 2927, 2856, 1633, 1526, 1488, 1455, 1336, 1276 cm⁻¹; ¹H-NMR (500 MHz, CDCl₃) δ 0.87 (3H, t, *J* = 7.3 Hz), 1.39 (2H, sext, *J* = 7.3 Hz), 1.70 (1H, br s), 1.93–2.09 (4H,

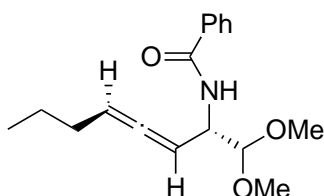
m), 2.71–2.08 (2H, m), 4.27–4.79 (1H, m), 5.30–5.39 (2H, m), 6.13(1H, br d, $J = 6.7$ Hz), 7.16–7.29 (5H, m), 7.41 (2H, d, $J = 7.6$ Hz), 7.47–7.50 (1H, m), 7.68–7.70 (1H, m); ^{13}C -NMR (100 MHz, CDCl_3) δ 13.8 (CH_3), 22.5 (CH_2), 31.0 (CH_2), 32.3 (CH_2), 37.0 (CH_2), 48.1 (CH), 93.3 (CH), 95.3 (CH), 126.0 (CH), 126.9 ($\text{CH}\times 2$), 128.5 ($\text{CH}\times 2$), 128.6 ($\text{CH}\times 2$), 128.6 ($\text{CH}\times 2$), 131.5 (CH), 134.9 (Cq), 141.8 (Cq), 166.8 (Cq), 202.6 (Cq); HRMS (EI) m/z calcd for $\text{C}_{22}\text{H}_{25}\text{NO}$ (M^+) 319.1936, found 319.1941.

(\pm)-*N*-((3*R,*aR**)-2,2-dimethylnona-4,5-dien-3-yl)benzamide (2c)**



Pale yellow oil; IR (neat) 3296, 2961, 2931, 2870, 1961, 1628, 1537, 1331, 1064, 692 cm^{-1} ; ^1H -NMR (500 MHz, CDCl_3) δ 0.81 (3H, t, $J = 7.3$ Hz), 1.00 (9H, s), 1.31 (2H, sext, $J = 7.3$ Hz), 1.93 (2H, m), 4.53–4.57 (1H, m), 5.28–5.34 (2H, m), 6.21 (1H, br d, $J = 9.8$ Hz), 7.40–7.50 (3H, m), 7.75–7.77 (2H, m); ^{13}C -NMR (100 MHz, CDCl_3) δ 13.7 (CH_3), 22.4 (CH_2), 26.4 ($\text{CH}_3\times 3$), 30.8 (CH_2), 35.7 (Cq), 55.9 (CH), 90.9 (CH), 94.4 (CH), 126.8 ($\text{CH}\times 2$), 128.6 ($\text{CH}\times 2$), 131.3 (CH), 135.2 (Cq), 167.0 (Cq), 203.2 (Cq); HRMS (EI) m/z calcd for $\text{C}_{18}\text{H}_{25}\text{NO}$ (M^+) 271.1936, found 271.1937.

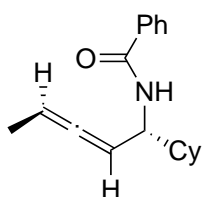
(\pm)-*N*-((2*R,*aR**)-1,1-dimethoxyocta-3,4-dien-2-yl)benzamide (2d)**



Pale yellow oil; IR (neat) 3324, 2961, 2959, 2932, 2871, 1967, 1726, 1640, 1533, 1323, 1069, 694 cm^{-1} ; ^1H -NMR (500 MHz, CDCl_3) δ 0.85 (3H, t, $J = 7.3$ Hz), 1.37 (2H, sext, $J = 7.3$ Hz), 1.93 (2H, m), 3.47

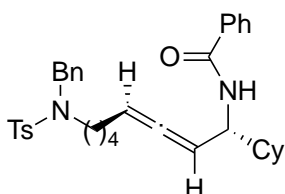
(3H, s), 3.50 (3H, s), 4.23 (1H, d, $J = 3.7$ Hz), 4.89–4.93 (1H, m), 5.34–5.40 (2H, m), 6.41 (1H, d, $J = 8.5$ Hz), 7.42–7.52 (3H, m), 7.77–7.79 (2H, m); ^{13}C -NMR (100 MHz, CDCl_3) δ 13.6 (CH_3), 22.3 (CH_2), 30.7 (CH_2), 49.7 (O), 55.9 (CH_3), 56.3 (CH_3), 88.8 (CH), 94.9 (CH), 105.5 (CH), 127.0 ($\text{CH}\times 2$), 128.5 ($\text{CH}\times 2$), 131.5 (Cq), 134.6 (Cq), 166.8 (Cq), 203.4 (Cq); HRMS (EI) m/z calcd for $\text{C}_{17}\text{H}_{23}\text{NO}_3$ (M^+) 289.1678, found 289.1673.

(±)-*N*-((1*R,*aR**)-1-cyclohexylpenta-2,3-dien-1-yl)benzamide (2e)**



Pale yellow oil; IR (neat) 3280, 2928, 2949, 2932, 2871, 1969, 1632, 1528, 1333, 1073, 693 cm^{-1} ; ^1H -NMR (500 MHz, CDCl_3) δ 1.02–1.28 (5H, m), 1.58–1.83 (9H, m), 4.57 (1H, dddd, $J = 2.0, 2.4, 4.8, 9.2$ Hz), 5.24 (2H, ddd, $J = 2.4, 4.8, 9.2$ Hz), 5.30 (1H, ddq, $J = 3.1, 6.7, 6.7$ Hz), 6.24 (1H, br d, $J = 7.9$ Hz), 7.41–7.50 (3H, m), 7.75–7.77 (2H, m); ^{13}C -NMR (100 MHz, CDCl_3) δ 14.4 (CH_3), 26.2 (CH_2), 26.3 (CH_2), 26.5 (CH_2), 29.0 (CH_2), 29.3 (CH_2), 42.7 (CH), 52.7 (CH), 89.3 (CH), 91.3 (CH), 126.9 ($\text{CH}\times 2$), 128.6 ($\text{CH}\times 2$), 131.4 (CH), 135.2 (Cq), 166.9 (Cq), 203.6 (Cq); HRMS (EI) m/z calcd for $\text{C}_{18}\text{H}_{23}\text{NO}$ (M^+) 269.1780, found 269.1782.

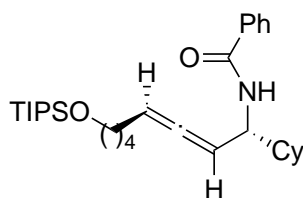
(±)-*N*-((1*R,*aR**)-8-(*N*-benzyl-toluenesulfonamido-1-cyclohexylocta-2,3-dien-1-yl)benzamide (2f)**



White solid ; IR (neat) 3334, 2925, 2851, 1973, 1637, 1525, 1489, 1449, 1336, 1156, 1024 cm^{-1} ; ^1H -NMR (500 MHz, CDCl_3) δ 1.03–1.31 (8H, m), 1.64–1.81 (9H, m), 2.44 (3H, s), 2.97–3.00 (2H, m),

4.25 (2H, s), 4.50–4.55 (1H, m), 5.15–5.23 (2H, m), 6.14 (1H, d, $J = 8.9$ Hz), 7.23–7.31 (7H, m), 7.38–7.41 (2H, m), 7.45–7.48 (1H, m), 7.68–7.73 (4H, m); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 21.7 (CH_3), 26.2 (CH_2), 26.3 (CH_2), 26.5 (CH_2), 27.6 (CH_2), 28.3 (CH_2), 29.0 (CH_2), 29.4 (CH_2), 42.7 (CH), 48.1 (CH_2), 52.2 (CH_2), 52.5 (CH), 92.3 (CH), 94.3 (CH), 126.9 ($\text{CH}\times 2$), 127.3 ($\text{CH}\times 2$), 127.8 (CH), 128.4 ($\text{CH}\times 2$), 128.6 ($\text{CH}\times 2$), 128.7 ($\text{CH}\times 2$), 129.8 ($\text{CH}\times 2$), 131.5 (CH), 135.1 (Cq), 136.7 (Cq), 137.1 (Cq), 143.3 (Cq), 166.8 (Cq), 202.6 (Cq); HRMS (EI) m/z calcd for $\text{C}_{35}\text{H}_{42}\text{N}_2\text{O}_3\text{S}$ (M^+) 570.2916, found. 570.2919

(±)-*N*-((1*R,*aR**)-8-(*N*-benzyl-toluenesulfonamido-1-cyclohexylocta-2,3-dien-1-yl)benzamide (2g)**



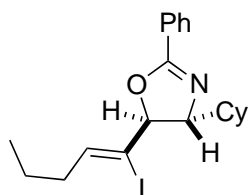
Pale yellow oil; IR (neat) 3309, 2924, 2863, 2794, 1962, 1634, 1537, 1462, 1107, 681 cm^{-1} ; $^1\text{H-NMR}$ (500 MHz, CDCl_3) δ 1.00–1.28 (25H, m), 1.37–1.53 (4H, m), 1.60–1.83 (7H, m), 1.97–2.05 (2H, m), 3.58 (2H, t, $J = 6.4$ Hz), 4.54–4.59 (1H, m), 5.25–5.35 (2H, m), 6.18 (1H, d, $J = 8.9$ Hz), 7.40–7.50 (3H, m), 7.75 (2H, m); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 12.1 ($\text{CH}\times 3$), 18.2 ($\text{CH}_3\times 6$), 25.7 (CH_2), 26.2 (CH_2), 26.3 (CH_2), 26.5 (CH_2), 28.8 (CH_2), 29.0 (CH_2), 29.3 (CH_2), 32.6 (CH_2), 42.9 (CH), 52.6 (CH), 63.3 (CH_2), 92.0 (CH), 94.9 (CH), 126.9 ($\text{CH}\times 2$), 128.7 ($\text{CH}\times 2$), 131.4 (CH), 135.1 (Cq), 166.7 (Cq), 202.7 (Cq); HRMS (EI) m/z calcd for $\text{C}_{30}\text{H}_{49}\text{NO}_2\text{Si}$ (M^+) 483.3533, found. 483.3530.

General procedure for the synthesis of oxazoline 3 from *N*-benzoylallenylamine 2.

A mixture of *N*-benzoylallenylamine **2a** (30 mg, mmol), K_2CO_3 (29.3 mg, 0.212 mmol) and I_2 (51.3 mg, 0.202 mmol) in toluene (1.0 mL) was stirred for 1 h at room temperature in air. The reaction mixture was quenched with 10% aq. $\text{Na}_2\text{S}_2\text{O}_3$. The mixture was extracted with Et_2O . The organic layer was

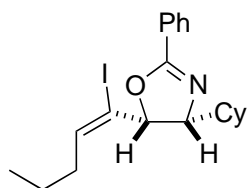
successively washed with water and brine, dried over MgSO₄, and then the solvent was evaporated under reduced pressure. The crude product was purified by column chromatography (SiO₂, hexane/AcOEt = 50/1 to 10/1) to afford oxazoline **3a** (39.8 mg, 0.940 mmol, 93% yield) as a colorless oil.

(±)-(4R*, 5S*)-4-cyclohexyl-(Z)-5-(1-iodopent-1-en-1-yl)- 2-phenyl-2-oxazoline (3a)



Colorless oil; IR (neat) 2924, 2853, 1652, 1580, 1495, 1323, 1061, 755 cm⁻¹; ¹H-NMR (500 MHz, CDCl₃) δ 0.95 (3H, t, *J* = 7.3 Hz), 1.07–1.30 (7H, m), 1.48 (2H, sext, *J* = 7.3 Hz), 1.59–1.79 (4H, m), 1.88–1.91 (1H, m), 2.16–2.21 (2H, m), 3.92 (1H, t, *J* = 5.8 Hz), 4.61 (1H, d, *J* = 5.8 Hz), 6.01 (1H, t, *J* = 7.0 Hz), 7.40–7.49 (3H, m), 7.97–7.99 (2H, m); ¹³C-NMR (100 MHz, CDCl₃) δ 13.7 (CH₃), 21.4 (CH₂), 26.1 (CH₂), 26.1 (CH₂), 26.5 (CH₂), 29.1 (CH₂), 29.3 (CH₂), 37.5 (CH₂), 42.7 (CH), 78.2 (CH), 86.8 (CH), 109.9 (Cq), 127.7 (Cq), 128.3 (CH×2), 128.3 (CH×2), 131.3 (CH), 137.6 (CH), 161.9 (Cq); HRMS (EI) *m/z* calcd for C₂₀H₂₇INO (M⁺+H) 424.1137, found. 424.1141.

(±)-(4R*, 5R*)-4-cyclohexyl-(Z)-5-(1-iodopent-1-en-1-yl)- 2-phenyl-2-oxazoline (4a)

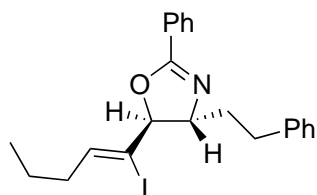


Colorless oil

Pale yellow oil; IR (neat) 2923, 2851, 1659, 1449, 1328, 1057, 972, 692 cm⁻¹; ¹H-NMR (500 MHz, CDCl₃) δ 0.97 (3H, t, *J* = 7.3 Hz), 1.05–1.33 (5H, m), 1.43–1.51 (2H, m), 1.65–1.80 (1H, m), 1.65–1.80 (5H, m), 2.06–2.15 (2H, m), 2.24–2.35 (2H, m), 4.09 (1H, t, *J* = 9.8 Hz), 5.28 (1H, d, *J* = 9.8 Hz), 6.46 (1H, t, *J* = 7.3 Hz), 7.40–7.49 (3H, m), 7.99–8.00 (2H, m); ¹³C-NMR (100 MHz, CDCl₃) δ 13.8 (CH₃),

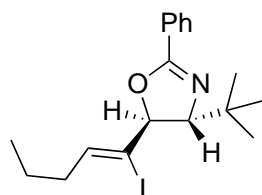
22.3 (CH₂), 26.1 (CH₂), 26.1 (CH₂), 26.6 (CH₂), 31.6 (CH₂), 32.3 (CH₂), 34.1 (CH₂), 37.4 (CH), 76.0 (CH), 79.0 (CH), 96.4 (Cq), 128.1 (Cq), 128.4 (CH×2), 128.6 (CH×2), 131.4 (CH), 146.4 (CH), 162.1 (Cq); HRMS (EI) *m/z* calcd for C₂₀H₂₇INO (M⁺+H) 424.1137, found. 424.1141.

(±)-(4R*, 5S*)-(Z)-5-(1-iodopent-1-en-1-yl)-4-phenylethyl-2-phenyl-oxazoline (3b)



Pale yellow oil; IR (neat) 3062, 2957, 2927, 1652, 1450, 1326, 1060, 958, 692 cm⁻¹; ¹H-NMR (500 MHz, CDCl₃) δ 0.96 (3H, t, *J* = 7.6 Hz), 1.48 (2H, sextet, *J* = 7.6 Hz), 2.00–2.07 (2H, m), 2.17–2.22 (2H, m), 2.76–2.92 (2H, m), 4.15 (1H, dt, *J* = 6.4, 6.7 Hz), 4.54 (1H, d, *J* = 6.4 Hz), 6.02 (1H, t, *J* = 7.0 Hz), 7.17–7.30 (5H, m), 7.41–7.51 (3H, m), 8.00 (2H, d, *J* = 7.3 Hz); ¹³C-NMR (100 MHz, CDCl₃) δ 13.9 (CH₃), 21.6 (CH₂), 32.3 (CH₂), 37.6 (CH₂), 37.6 (CH₂), 73.3 (CH), 89.6 (CH), 108.6 (Cq), 126.1 (CH), 127.7 (Cq), 128.5 (CH×4), 128.5 (CH×4), 131.6 (CH), 137.9 (CH), 141.8 (Cq), 162.5 (Cq); HRMS (EI) *m/z* calcd for C₂₂H₂₄INO (M⁺+H) 445.0903, found. 445.0900.

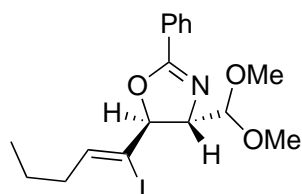
(±)-(4R*, 5S*)-(Z)-4-(*tert*-butyl)-5-(1-iodopent-1-en-1-yl)-2-phenyl-oxazoline (3c)



Pale yellow oil; IR (neat) 2956, 2930, 1656, 1450, 1323, 1063, 958, 691 cm⁻¹; ¹H-NMR (500 MHz, CDCl₃) δ 0.95 (3H, t, *J* = 7.3 Hz), 0.99 (9H, s), 1.44–1.52 (2H, m), 2.17–2.22 (2H, m), 3.83 (1H, d, *J* = 6.1 Hz), 4.62 (1H, d, *J* = 6.1 Hz), 6.01 (1H, t, *J* = 6.7 Hz), 7.40–7.50 (3H, m), 7.98–8.01 (2H, m); ¹³C-NMR (100 MHz, CDCl₃) δ 13.8 (CH₃), 21.5 (CH₂), 26.4 (CH₃×3), 34.6 (Cq), 37.6 (CH₂), 82.6 (CH),

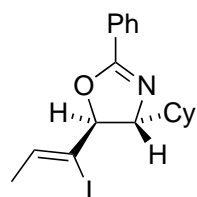
85.5 (CH), 110.8 (Cq), 127.8 (Cq), 128.4 (CH \times 2), 128.5 (CH \times 2), 131.4 (CH), 138.2 (CH), 162.2 (Cq); HRMS (EI) m/z calcd for C₁₈H₂₄INO (M⁺) 397.0903, found. 397.0904.

(±)-(4R*, 5S*)-(Z)-4-(dimethoxymethyl)-5-(1-iodopent-1-en-1-yl)-2-phenyl-2-oxazoline (3d)



Pale yellow oil; IR (neat) 2957, 2930, 2870, 1650, 1450, 1324, 1131, 1064, 967, 692 cm⁻¹; ¹H-NMR (500 MHz, CDCl₃) δ 0.96 (3H, t, J = 7.3 Hz), 1.49 (2H, sext, J = 7.3 Hz), 2.19 (2H, m), 3.43 (3H, s), 3.47 (3H, s), 4.27 (1H, dd, J = 4.3, 6.1 Hz), 4.52 (1H, d, J = 4.3 Hz), 4.89 (1H, d, J = 6.4 Hz), 6.09 (1H, t, J = 6.7 Hz), 7.40–7.43 (2H, m), 7.47–7.51 (1H, m), 7.99–8.01 (2H, m); ¹³C-NMR (100 MHz, CDCl₃) δ 13.9 (CH₃), 21.5 (CH₂), 37.7 (CH₂), 55.4 (CH₃), 56.1 (CH₃), 75.3 (CH), 85.2 (CH), 105.5 (CH), 109.0 (Cq), 127.6 (Cq), 128.4 (CH \times 2), 128.7 (CH \times 2), 131.7 (CH), 139.2 (CH), 164.3 (Cq); HRMS (EI) m/z calcd for C₁₇H₂₂INO₃ (M⁺) 415.0644, found. 415.0632.

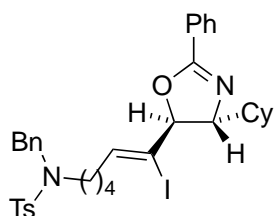
(±)-(4R*, 5S*)-(Z)-4-cyclohexyl-5-(1-iodoprop-1-en-1-yl)-2-phenyl-2-oxazoline (3e)



Pale yellow oil; IR (neat) 2921, 2850, 1654, 1448, 1321, 1060, 960, 691 cm⁻¹; ¹H-NMR (500 MHz, CDCl₃) δ 1.06–1.31 (5H, m), 1.58–1.79 (5H, m), 1.83 (3H, d, J = 6.4 Hz), 6.10 (1H, t, J = 6.1 Hz), 4.63 (1H, d, J = 6.1 Hz), 6.10 (1H, q, J = 6.4 Hz), 7.40–7.43 (2H, m), 7.46–7.50 (1H, m), 7.97–7.99 (2H, m); ¹³C-NMR (100 MHz, CDCl₃) δ 21.6 (CH₃), 26.3 (CH₂), 26.3 (CH₂), 26.6 (CH₂), 29.3 (CH₂), 29.3 (CH₂), 42.8 (CH), 78.3 (CH), 86.9 (CH), 111.4 (Cq), 127.8 (Cq), 128.5 (CH \times 2), 128.5 (CH \times 2), 131.4 (CH),

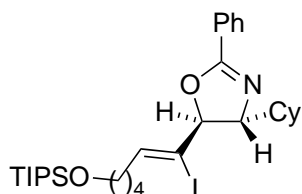
132.6 (CH), 162.0 (Cq); HRMS (EI) m/z calcd for $C_{18}H_{22}INO$ (M^+) 395.0746, found. 395.0740.

(±)-(4*R, 5*S**)-(*Z*)-4-cyclohexyl-5-(6-*N*-benzyltoluenesulfonamido -1-iodohex-1-en-1-yl)-2-phenyl-2-oxazoline (3f)**



Pale yellow oil; IR (neat) 2923, 2852, 1654, 1449, 1336, 1157, 694 cm^{-1} ; 1H -NMR (500 MHz, $CDCl_3$) δ 1.07–1.38 (10H, m), 1.57–1.88 (5H, m), 2.01 (2H, q, $J = 7.0$ Hz), 2.44 (3H, s), 3.08–3.11 (2H, m), 3.87 (1H, t, $J = 5.8$ Hz), 4.29 (2H, s), 4.55 (1H, d, $J = 5.8$ Hz), 5.81 (1H, t, $J = 7.0$ Hz), 7.26–7.33 (7H, m), 7.40–7.43 (2H, m), 7.47–7.50 (1H, m), 7.73 (2H, d, $J = 7.9$ Hz), 7.97 (2H, d, $J = 7.3$ Hz); ^{13}C -NMR (100 MHz, $CDCl_3$) δ 21.7 (CH_3), 25.1 (CH_2), 26.3 (CH_2), 26.6 (CH_2), 27.8 (CH_2), 29.3 (CH_2), 29.3 (CH_2), 35.1 (CH_2), 42.8 (CH), 48.3 (CH_2), 52.4 (CH_2), 78.3 (CH), 86.7 (CH), 110.4 (Cq), 127.3 ($CH \times 2$), 127.8 (Cq), 127.9 (CH), 128.4 ($CH \times 2$), 128.5 ($CH \times 4$), 128.7 ($CH \times 2$), 129.9 ($CH \times 2$), 131.5 (CH), 136.7 (Cq), 137.0 (Cq), 137.1 (CH), 143.4 (Cq), 162.0 (Cq); HRMS (EI) m/z calcd for $C_{35}H_{41}IN_2O_3S$ (M^+) 696.1883, found. 696.1880.

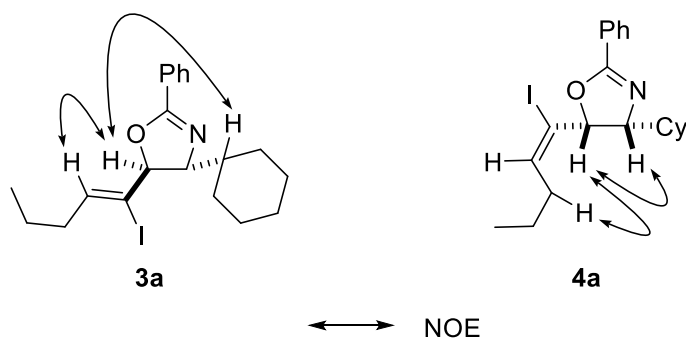
(±)-(4*R, 5*S**)-(*Z*)-4-cyclohexyl-5-(1-iodopent-6-(triisopropylsilyloxy)hex-1-en-1-yl)-2-phenyl-2-oxazoline (3g)**



Pale yellow oil; IR (neat) 2923, 2863, 1656, 1449, 1323, 1103, 881, 776, 690 cm^{-1} ; 1H -NMR (500 MHz, $CDCl_3$) δ 1.03–1.27 (25H, m), 1.52–1.88 (11H, m), 2.22–2.26 (2H, m), 3.70 (2H, t, $J = 6.1$ Hz), 3.92 (1H,

t, $J = 6.1$ Hz), 4.60 (1H, d, $J = 5.8$ Hz), 6.02 (1H, t, $J = 7.0$ Hz), 7.40–7.43 (2H, m), 7.46–7.49 (1H, m), 7.97–7.98 (2H, m); ^{13}C -NMR (100 MHz, CDCl_3) δ 12.2 ($\text{CH}\times 3$), 18.2 ($\text{CH}_3\times 6$), 24.6 (CH_2), 26.3 (CH_2), 26.3 (CH_2), 26.6 (CH_2), 29.3 (CH_2), 29.4 (CH_2), 32.6 (CH_2), 35.5 (CH_2), 42.8 (CH), 63.2 (CH_2), 78.3 (CH), 86.9 (CH), 110.1 (Cq), 127.8 (Cq), 128.4 ($\text{CH}\times 2$), 128.5 ($\text{CH}\times 2$), 131.4 (CH), 137.9 (CH), 162.0 (Cq); HRMS (EI) m/z calcd for $\text{C}_{30}\text{H}_{48}\text{INO}_2\text{Si}$ (M^+) 609.2499, found. 609.2499.

Figure SI-1. NOESY correlations of 3a and 4a.



References

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