Supporting Information

Cobalt-Catalyzed Highly α -Selective Hydrostannylation of Terminal Alkynes $\mbox{Yufeng Sun,}^{1,\ddagger} \mbox{ Bingcheng Wang,}^{1,\ddagger} \mbox{ Cheng, Wang,}^{1,\ddagger} \mbox{ Jiajing Li,}^1 \mbox{ Jieping Chen,}^1 \mbox{ Xin Hong,}^{1*} \mbox{ and } \mbox{ Zhan Lu}^{1,2*}$

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I. General Information

THF was distilled from sodium benzophenone ketyl prior to use. Pd₂(dba)₃(98%) was purchased from Zhejiang Metallurgical Research Institute and used received. 1,1'-Bis(diphenylphosphino)ferrocene (dppf) (98%) was purchased from Energy Chemical and used as received. HSnBu₃ (97%) and Co(OAc)₂ (99.99%) was purchased from Aladdin and used as received. The other commercially available chemicals were used as received. NMR spectra were recorded on a Bruker-400 instrument, a Bruker-500 instrument and a Wuhan Zhongke-Niujin-400 instrument. ¹H NMR chemical shifts were referenced to tetramethylsilane signal (0.0 ppm), ¹³C NMR chemical shifts were referenced to the solvent resonance (77.0 ppm, CDCl₃). ²H NMR chemical shifts were referenced to CDCl₃ signal (7.26 ppm). The following abbreviations (or combinations) were used to explain multiplicities: s = singlet, d = doublet, t = triplet, m= multiplet, brs = broad singlet, q = quadruplet. Melting points were obtained using a WRR melting point apparatus (Laboratory Devices, Shanghai Precision & Scientific Instrument Co., Ltd.). High-resolution mass spectra (HRMS) were recorded on ESI-TOF or EI. IR spectra were recorded on a Perkin-Elmer Spectrum One FTIR spectrometer with diamond ATR accessory.

II. Synthesis of Substrates and Ligands.

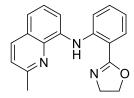
Alkynes were prepared according to Sonogashira-Coupling reaction or the previously reported procedures. L17, L2-L44, L516, L74, L817, L1017 were prepared according to the previously reported procedures.

Hept-1-yn-3-ylbenzene (**1aw**). To a 500 mL flame-dried three-necked Schlenk flask, 24.84 g (90.0 mmol) of (3,3-dibromoallyl)benzene, 250 mL (0.36 M) of THF were added in sequence under the atmosphere of nitrogen. The solution was stirred at -78 °C for a while, and then 90 mL (2.5 M in hexane, 90 mmol, 2.5 equiv.) of *n*BuLi was added into the mixture by dropwise at -78 °C. The solution was stirred at -78 °C for 5 h. After that the mixture was warmed to 0 °C slowly and quenched by saturated NH₄Cl solution at 0 °C. Then, 50 mL H₂O and 50 mL Et₂O were added into the mixture and the organic layer was separated. The aqueous layer was extracted with Et₂O (3 × 150 mL). The combined organic layers were washed with brine, dried over Na₂SO₄ and concentrated *in vacuo* to give a crude oil. And the residue was purified by flash column chromatography using PE as the eluent to give 4.60 g (26.7 mmol, 30% yield) of the title compound as a yellow oil. IR (cm⁻¹): 3304, 3063, 2957, 2862, 1494, 1455. ¹H NMR: (400 MHz, CDCl₃) δ 7.40-7.28 (m, 4H), 7.26-7.18 (m, 1H), 3.65-3.58 (m, 1H), 2.26 (d, $J_{\text{H-H}} = 2.4$ Hz, 1H), 1.80-1.70 (m, 2H), 1.45-1.25 (m, 4H), 0.89 (t, $J_{\text{H-H}} = 7.2$ Hz, 3H); ¹³C NMR: (100 MHz, CDCl₃) δ 141.7, 128.5, 127.3, 126.7, 86.2, 70.7, 38.1, 37.5, 29.4, 22.4, 13.9; HRMS (EI) calculated for [C₁₃H₁₆]⁺ [M]⁺ requires m/z 172.1252, found m/z 172.1253.

(S)-3-(4-(2-chloro-5-ethynylbenzyl)phenoxy)tetrahydrofuran (1ay). To a 50 mL flame-dried Schlenk flask, 0.0337 g (0.048 mmol, 2 mol%) of PdCl₂(PPh₃)₂, 0.0183 g (0.096 mmol, 4 mol%) of CuI, 5 (0.48)M) THF, 1.00 mL of (2.4)mmol) of (S)-3-(4-(2-chloro-5-iodobenzyl)phenoxy)tetrahydrofuran, 2.5 mL (0.73 g/mL, 18 mmol, equiv.) of Et₃N and 0.36 g (3.6 mmol, 1.5 equiv.) ethynyltrimethylsilane were added in sequence under the atmosphere of nitrogen. The solution was stirred at room temperature overnight, quenched by PE and filtered through a pad of silica gel. The schlenk flask and silica gel were washed by PE/EtOAc = 5/1 (30 mL \times 3). The combined filtrates were concentrated in vacuo. Then 20 mL (0.12 M) of MeOH and 0.0332 g (0.24 mmol, 10 mol%) of K₂CO₃ were added into the residue and the solution was stirred at room temperature for 5 h. The solution was filtered through a pad of silica gel and washed by PE/EtOAc = 20/1 (30 mL \times 3). All volatiles were removed from the solution via rotary evaporation to give an orange sticky oil. And the residue was purified by flash column chromatography using PE/EtOAc = 20/1 as the eluent to give 0.7232 g (2.3 mmol, 96% yield) of the title compound as a yellow oil. IR (cm⁻¹): 3290, 2925, 2864, 1611, 1509, 1470. ¹H NMR: (400 MHz, CDCl₃) δ 7.35-7.24 (m, 3H), 7.09 (d, J_{H-H} = 8.4 Hz, 2H), 6.79 (d, J_{H-H} = 8.4 Hz, 2H), 4.93-4.85 (m, 1H), 4.03-3.85 (m, 6H), 3.06 (s, 1H), 2.25-2.10 (m, 2H); ¹³C NMR: (100 MHz, CDCl₃) δ 156.0, 139.3, 134.9, 134.3, 131.1, 130.0, 129.5, 120.8, 115.4, 82.7, 77.9, 77.3, 73.1, 67.1, 38.1, 33.0; HRMS (EI) calculated for [C₁₉H₁₇O₂Cl]⁺ [M]⁺ requires m/z 312.0917, found m/z 312.0915.

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N-(2-(4,5-dihydrooxazol-2-yl)phenyl)quinoline-2-carboxamide (L6). To a 50 mL round-bottom flask, 1.40 g (8.0 mmol, 1.6 equiv.) of quinoline-2-carboxylic acid, 0.81 g (5.0 mmol) of 2-(4,5-dihydrooxazol-2-yl)aniline, and 20 ml (0.25 M) of DCM were added in sequence under air. The solution was stirred for 10 mins. 1.67 g (8.0 mmol, 1.6 equiv.) of DCC (dicyclohexylmethanediimine) was added in portion and 0.99 g (8.0 mmol, 1.6 equiv.) of DMAP (4-Dimethylaminopyridine) was added in sequence. The solution was stirred overnight. After that, 50 mL H₂O and 50 mL DCM were added into the mixture and the organic layer was separated. The aqueous layer was extracted with DCM (50 mL × 3). The combined organic layers were washed with brine, dried over Na₂SO₄ and concentrated in vacuo to give a crude oil. The residue was purified by flash column chromatography using PE/EtOAc = 5/1 as the eluent to give 0.95 g (3.0 mmol, 60% yield) of the title compound as a white solid. M.p. 176.5-177.8 °C. IR (cm⁻¹): 2931, 2877, 1679, 1641, 1582, 1533. ¹H NMR: (400 MHz, CDCl₃) δ 14.09 (brs, 1H), 9.09 (d, $J_{\text{H-H}}$ = 8.4 Hz, 1H), 8.43-8.32 (m, 2H), $8.22 \text{ (d, } J_{\text{H-H}} = 8.8 \text{ Hz}, 1\text{H})$, $7.95 \text{ (dd, } J_{\text{H-H}} = 7.6, 1.2 \text{ Hz}, 1\text{H})$, 7.92 (d, $J_{H-H} = 8.0$ Hz, 1H), 7.84-7.78 (m, 1H), 7.68-7.62 (m, 1H), 7.58-7.52 (m, 1H), 7.18-7.13(m, 1H), 4.55-4.38 (m, 4H); 13 C NMR: (100 MHz, CDCl₃) δ 164.3, 164.1, 150.7, 146.6, 139.5, 137.4, 132.4, 130.0, 129.9, 129.4, 129.2, 128.0, 127.7, 122.6, 119.9, 119.1, 114.6, 66.3, 55.0; HRMS (ESI) calculated for $[C_{19}H_{16}N_3O_2]^+$ [M+H]⁺ requires m/z 318.1237, found m/z 318.1236.



N-(2-(4,5-dihydrooxazol-2-yl)phenyl)-2-methylquinolin-8-amine (L9). To a 50 mL flame-dried Schlenk flask, 0.0830 g of Pd₂(dba)₃ (0.091 mmol, 2.5 mol%), 0.0998 g (0.180 mmol, 5 mol%) of dppf and 10 mL (0.36 M) of toluene were added in sequence under the atmosphere of nitrogen. The solution was stirred for 10 mins. 0.81 g (3.6 mmol) of 2-(2-bromophenyl)-4,5-dihydrooxazole, 0.57 g (3.6 mmol, 1.0 equiv.) of 2-methylquinolin-8-amine, 0.70 g (7.2 mmol, 2.0 equiv.) of sodium tert-butoxide were added in sequence under the atmosphere of nitrogen. The solution was refluxed overnight, thereafter, cooled down to room temperature. The solution was filtered through a pad of silica gel. All volatiles were removed from the solution via rotary evaporation to give a brown sticky oil. And the residue was purified by flash column chromatography using PE/EtOAc = 10/1 as the eluent to give 0.72 g (2.4 mmol, 67% yield) of the title compound as a pale yellow solid. M.p. 133.2-135.4 °C. IR (cm⁻¹): 2925, 1638, 1578, 1531, 1500, 1452. ¹H NMR: $(400 \text{ MHz}, \text{CDCl}_3) \delta 11.71 \text{ (brs, 1H)}, 8.00 \text{ (d, } J_{\text{H-H}} = 8.4 \text{ Hz}, 1\text{H)}, 7.90 \text{ (dd, } J_{\text{H-H}} = 8.0, 1.6 \text{ Hz}, 1\text{H)},$ 7.85 (d, $J_{H-H} = 8.4$ Hz, 1H), 7.78 (d, $J_{H-H} = 7.6$ Hz, 1H), 7.40-7.34 (m, 2H), 7.32-7.26 (m, 2H), 6.90-6.83 (m, 1H), 4.43-4.35 (m, 2H), 4.29-4.21 (m, 2H), 2.79 (s, 3H); ¹³C NMR: (100 MHz, CDCl₃) δ 164.4, 156.8, 143.6, 138.5, 136.1, 131.6, 130.3, 127.2, 125.8, 122.2, 118.4, 118.2, 115.2, 113.4, 111.7, 66.0, 55.2, 25.5; HRMS (ESI) calculated for [C₁₉H₁₈N₃O]⁺ [M+H]⁺ requires m/z 304.1444, found m/z 304.1445.

III. Cobalt-Catalyzed Highly α-Selective Hydrostannylation of Terminal Alkynes

Table S1. Some Phosphine Ligands for Hydrostannylation of Phenylacetylene

Entry	Changes of conditions	Yield (%) ^b	Ratio ^c (α/β)
1	Xanphos	22	0/100
2	Dpephos	17	0/100
3	dppbz	46	7/93
4	dppp	27	7/93
5	dppb	17	0/100
6	dppe	42	10/90
7	dppf	52	6/94
8	rac-BINAP	19	0/100

^a Reaction conditions: **1a** (0.6 mmol), **2a** (1.2 equiv.), Co(OAc)₂ (2 mol%), **L** (2.4 mol%) in THF (1.2 ml) at room temperature in glovebox for 1 h. ^b Yield was determined by ¹H NMR using TMSPh as an internal standard. ^c Ratio was determined by ¹H NMR of the crude reaction mixture.

General procedure:

In a nitrogen-filled glovebox, an oven-dried 25 mL vial that contained a magnetic stir bar was charged with Co(OAc)₂ (0.012 mmol, 2 mol%), **L7** (0.0144 mmol, 2.4 mol %), and THF (1.2 mL, 0.5 M). The mixture was stirred for 30 mins. Then HSnBu₃ (0.72 mmol, 1.2 equiv.) and alkynes (0.60 mmol, 1.0 equiv.) were added sequentially. The mixture was stirred at ambient temperature

for several hours, and quenched by 5 mL of petroleum ether (PE) and stirred for 5 mins until catalyst precipitated. The resulting solution was filtered through a pad of silica gel and washed by Et_2O (15 mL \times 3) (or other suitable solvent). The combined filtrates were concentrated *in vacuo*. NMR yield was monitored by 1H NMR analysis using TMSPh as internal standard. The crude mixture was purified by short flash column chromatography to give the corresponding product.

Tributyl(1-phenylvinyl)stannane (3a). Prepared according to the general procedure using 0.0022 g (0.012 mmol) of Co(OAc)₂, 0.0050 g (0.0144 mmol) of **L7**, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 66 μL (0.93 g/mL, 0.60 mmol) of phenylacetylene and 1.2 mL (0.5 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE as the eluent to give 0.2130 g (0.54 mmol, 90% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be 99/1 by the ¹H NMR analysis of the isolated mixture. ¹H NMR: (400 MHz, CDCl₃) δ 7.23-7.33 (m, 2H), 7.13-7.23 (m, 3H), 6.03 (d, $J_{\text{H-H}}$ = 2.0 Hz, $J_{\text{Sn-H}}$ = 128 Hz, 1H), 5.42 (d, $J_{\text{H-H}}$ = 2.0 Hz, $J_{\text{Sn-H}}$ = 60 Hz, 1H), 1.60-1.40 (m, 6H), 1.35-1.23 (m, 6H), 1.07-0.90 (m, 6H), 0.86 (t, $J_{\text{H-H}}$ = 7.2 Hz, 9H); ¹³C NMR: (100 MHz, CDCl₃) δ 154.7, 146.4, 128.2, 126.7, 126.3, 126.2, 29.0, 27.3, 13.6, 10.3; The spectroscopic data are in accordance with the literature. ¹⁸

Tributyl(1-(2-(trifluoromethyl)phenyl)vinyl)stannane (3b). Prepared according to the general procedure using 0.0024 g (0.014 mmol) of Co(OAc)₂, 0.0050 g (0.0144 mmol) of L7, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 0.1022 g (0.60 mmol) of 1-ethynyl-2-(trifluoromethyl)benzene and 1.2 mL (0.5 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE as the eluent to give 0.2684 g (0.58 mmol, 97% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be >99/1 by the

¹H NMR analysis of the isolated mixture. IR (cm⁻¹): 2957, 2926, 2853, 1604, 1572, 1485, 1451. ¹H NMR: (400 MHz, CDCl₃) δ 7.58 (d, $J_{\text{H-H}}$ = 8.0 Hz, 1H), 7.40 (dd, $J_{\text{H-H}}$ = 7.6, 7.2 Hz, 1H), 7.21 (dd, $J_{\text{H-H}}$ = 7.6, 7.2 Hz, 1H), 6.97 (d, $J_{\text{H-H}}$ = 8.0 Hz, 1H), 5.78 (d, $J_{\text{H-H}}$ = 2.4 Hz, $J_{\text{Sn-H}}$ = 121 Hz, 1H), 5.54 (d, $J_{\text{H-H}}$ = 2.8 Hz, $J_{\text{Sn-H}}$ = 60 Hz, 1H), 1.50-1.35 (m, 6H), 1.32-1.20 (m, 6H), 1.00-0.80 (m, 15H); ¹³C NMR: (100 MHz, CDCl₃) δ 153.5, 147.2, 131.1, 128.5 (q, J = 5.9 Hz), 128.4, 125.9 (q, J = 29.2 Hz), 125.8 (q, J = 5.1 Hz), 125.1, 124.1 (q, J = 274.8 Hz), 28.7, 27.3, 13.6, 10.3; ¹⁹F NMR: (376 MHz) δ -57.6; HRMS (EI) calculated for [C₁₇H₂₄F₃Sn]⁺[M-Bu]⁺ requires m/z 405.0852, found m/z 405.0851.

Tributyl(1-(2-methoxyphenyl)vinyl)stannane (3c). Prepared according to the general procedure using 0.0022 g (0.012 mmol) of Co(OAc)₂, 0.0050 g (0.0144 mmol) of **L7**, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 0.0793 g (0.60 mmol) of 1-ethynyl-2-methoxybenzene and 1.2 mL (0.5 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE to PE/EtOAc = 50/1 as the eluent to give 0.2324 g (0.55 mmol, 92% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be >99/1 by the ¹H NMR analysis of the isolated mixture. ¹H NMR: (400 MHz, CDCl₃) δ 7.21-7.14 (m, 1H), 7.13-7.08 (m, 1H), 6.91 (dd, $J_{\text{H-H}} = 7.6$, 7.2 Hz, 1H), 6.78 (d, $J_{\text{H-H}} = 8.0$ Hz, 1H), 5.95 (d, $J_{\text{H-H}} = 3.2$ Hz, $J_{\text{Sn-H}} = 131$ Hz, 1H), 5.39 (d, $J_{\text{H-H}} = 3.2$ Hz, $J_{\text{Sn-H}} = 62$ Hz, 1H), 3.78 (s, 3H), 1.53-1.38 (m, 6H), 1.34-1.21 (m, 6H), 0.98-0.80 (m, 15H); ¹³C NMR: (100 MHz, CDCl₃) δ 154.0, 149.2, 143.1, 126.1, 126.0, 125.2, 34.4, 31.4, 29.1, 29.0, 27.3, 13.7, 10.3; The spectroscopic data are in accordance with the literature.¹⁹

3-(1-(Tributylstannyl)vinyl)benzonitrile (3d). Prepared according to the general procedure using 0.0023 g (0.013 mmol) of Co(OAc)₂, 0.0050 g (0.0144 mmol) of **L7,** 198 μL (1.08 g/mL, 97%,

0.72 mmol) of HSnBu₃, 0.0762 g (0.60 mmol) of 3-ethynylbenzonitrile and 1.2 mL (0.5 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE to PE/EtOAc = 50/1 as the eluent to give 0.2334 g (0.56 mmol, 93% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be >99/1 by the ¹H NMR analysis of the isolated mixture. IR (cm⁻¹): 2957, 2925, 2852, 1593, 1462. ¹H NMR: (400 MHz, CDCl₃) δ 7.50-7.45 (m, 1H), 7.45-7.32 (m, 3H), 6.01 (d, $J_{\text{H-H}}$ = 2.0 Hz, $J_{\text{Sn-H}}$ = 119 Hz, 1H), 5.52 (d, $J_{\text{H-H}}$ = 2.0 Hz, $J_{\text{Sn-H}}$ = 57 Hz, 1H), 1.60-1.40 (m, 6H), 1.35-1.22 (m, 6H), 1.05-0.90 (m, 6H), 0.87 (t, $J_{\text{H-H}}$ = 7.2 Hz, 9H); ¹³C NMR: (100 MHz, CDCl₃) δ 153.1, 148.0, 130.7, 129.6, 129.5, 129.03, 129.00, 119.0, 112.3, 28.9, 27.2, 13.6, 10.3; HRMS (ESI) calculated for [C₂₁H₃₃NNaSn]⁺[M+Na]⁺ requires m/z 442.1527, found m/z 442.1529.

Tributyl(1-(3-methoxyphenyl)vinyl)stannane (3e). Prepared according to the general procedure using 0.0022 g (0.012 mmol) of Co(OAc)₂, 0.0050 g (0.0144 mmol) of **L7**, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 0.0793 g (0.60 mmol) of 1-ethynyl-3-methoxybenzene and 1.2 mL (0.5 M) of THF. After 24 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE to PE/EtOAc = 50/1 as the eluent to give 0.2227g (0.53 mmol, 88% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be >99/1 by the ¹H NMR analysis of the isolated mixture. IR (cm⁻¹): 2956, 2926, 2852, 1596, 1574, 1461. ¹H NMR: (400 MHz, CDCl₃) δ 7.20 (dd, $J_{\text{H-H}} = 8.0$, 7.6 Hz, 1H), 6.80-6.70 (m, 3H), 6.03 (d, $J_{\text{H-H}} = 2.0$ Hz, $J_{\text{Sn-H}} = 127$ Hz, 1H), 5.41 (d, $J_{\text{H-H}} = 2.4$ Hz, $J_{\text{Sn-H}} = 60$ Hz, 1H), 3.81 (s, 3H), 1.55-1.43 (m, 6H), 1.35-1.24 (m, 6H), 1.05-0.90 (m, 6H), 0.86 (t, $J_{\text{H-H}} = 7.2$ Hz, 9H); ¹³C NMR: (100 MHz, CDCl₃) δ 159.5, 154.6, 148.0, 129.2, 126.8, 118.9, 111.8, 111.5, 55.1, 29.0, 27.3, 13.7, 10.3; HRMS (ESI) calculated for [C₂₁H₃₇OSn]⁺[M+H]⁺ requires m/z 425.1861, found m/z 425.1860.

Tributyl(1-(4-fluorophenyl)vinyl)stamane (3f). Prepared according to the general procedure using 0.0022 g (0.012 mmol) of Co(OAc)₂, 0.0051 g (0.0147 mmol) of L7, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 0.0719 g (0.60 mmol) of 1-ethynyl-4-fluorobenzene and 1.2 mL (0.5 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE as the eluent to give 0.2319 g (0.56 mmol, 94% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be 98.5/1.5 by the ¹H NMR analysis of the isolated mixture. IR (cm⁻¹): 2957, 2925, 2853, 1598, 1503, 1461, 1416. ¹H NMR: (400 MHz, CDCl₃) δ 7.15-7.08 (m, 2H), 6.97 (dd, $J_{\text{H-H}} = 8.8$, 8.4 Hz, 2H), 5.98 (d, $J_{\text{H-H}} = 2.4$ Hz, $J_{\text{Sn-H}} = 126$ Hz, 1H), 5.40 (d, $J_{\text{H-H}} = 2.4$ Hz, $J_{\text{Sn-H}} = 60$ Hz, 1H), 1.55-1.42 (m, 6H), 1.35-1.23 (m, 6H), 1.05-0.90 (m, 6H), 0.86 (t, $J_{\text{H-H}} = 7.2$ Hz, 9H); ¹³C NMR: (100 MHz, CDCl₃) δ 161.7 (d, J = 244.0 Hz), 153.5, 142.5 (d, J = 2.9 Hz), 127.7 (d, J = 7.2 Hz), 126.8, 115.0 (d, J = 21.2 Hz), 29.0, 27.3, 13.6, 10.2; ¹⁹F NMR: (376 MHz) δ -117.1; HRMS (EI) calculated for [C₁₆H₂₄FSn]⁺[M-Bu]⁺ requires m/z 355.0884, found m/z 355.0890.

Tributyl(1-(4-chlorophenyl)vinyl)stannane (3g). Prepared according to the general procedure using 0.0023 g (0.013 mmol) of Co(OAc)₂, 0.0050 g (0.0144 mmol) of **L7**, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 0.0819 g (0.60 mmol) of 1-chloro-4-ethynylbenzene and 1.2 mL (0.5 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE as the eluent to give 0.2463 g (0.58 mmol, 96% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be 97.5/2.5 by the ¹H NMR analysis of the isolated mixture. IR (cm⁻¹): 2957, 2924, 2852, 1589, 1460, 1416. ¹H NMR: (400 MHz, CDCl₃) δ 7.30-7.22 (m, 2H), 7.13-7.03 (m, 2H), 6.00 (d, $J_{\text{H-H}}$ = 2.4 Hz, $J_{\text{Sn-H}}$ = 125 Hz, 1H), 5.42 (d, $J_{\text{H-H}}$ = 2.0 Hz, $J_{\text{Sn-H}}$ = 59 Hz, 1H), 1.55-1.40 (m, 6H), 1.35-1.23 (m, 6H), 1.05-0.90 (m, 6H), 0.86 (t, $J_{\text{H-H}}$ = 7.2 Hz, 9H); ¹³C

NMR: (100 MHz, CDCl₃) δ 153.5, 145.0, 131.9, 128.4, 127.5, 127.4, 29.0, 27.3, 13.6, 10.2; HRMS (EI) calculated for $[C_{16}H_{24}ClSn]^+[M-Bu]^+$ requires m/z 371.0589, found m/z 371.0593.

4-(1-(Tributylstannyl)vinyl)benzaldehyde (3h). Prepared according to the general procedure using 0.0022 g (0.012 mmol) of Co(OAc)₂, 0.0050 g (0.0144 mmol) of **L7**, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 0.0781 g (0.60 mmol) of 4-ethynylbenzaldehyde and 1.2 mL (0.5 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE as the eluent to give 0.2446 g (0.58 mmol, 97% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be >99/1 by the ¹H NMR analysis of the isolated mixture. ¹H NMR: (400 MHz, CDCl₃) δ 9.98 (s, 1H), 7.81 (d, $J_{\text{H-H}}$ = 8.4 Hz, 2H), 7.28 (d, $J_{\text{H-H}}$ = 8.0 Hz, 2H), 6.07 (d, $J_{\text{H-H}}$ = 2.4 Hz, $J_{\text{Sn-H}}$ = 120 Hz, 1H), 5.54 (d, $J_{\text{H-H}}$ = 2.4 Hz, $J_{\text{Sn-H}}$ = 58 Hz, 1H), 1.55-1.40 (m, 6H), 1.35-1.23 (m, 6H), 1.05-0.90 (m, 6H), 0.86 (t, $J_{\text{H-H}}$ = 7.2 Hz, 9H); ¹³C NMR: (100 MHz, CDCl₃) δ 191.8, 154.3, 153.5, 134.3, 129.9, 128.9, 126.8, 28.9, 27.2, 13.6, 10.3; The spectroscopic data are in accordance with the literature. ¹⁸

1-(4-(1-(Tributylstannyl)vinyl)phenyl)ethan-1-one (3i). Prepared according to the general procedure using 0.0022 g (0.012 mmol) of $Co(OAc)_2$, 0.0050 g (0.0144 mmol) of L7, 198 μ L (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 0.0866 g (0.60 mmol) of 1-(4-ethynylphenyl)ethan-1-one and 1.2 mL (0.5 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE to PE/EtOAc = 50/1 as the eluent to give 0.2545 g (0.58 mmol, 97% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be

99.5/0.5 by the ¹H NMR analysis of the isolated mixture. IR (cm⁻¹): 2957, 2925, 2871, 1684, 1600, 1557, 1460. ¹H NMR: (400 MHz, CDCl₃) δ 7.90 (d, $J_{\text{H-H}}$ = 8.4 Hz, 2H), 7.22 (d, $J_{\text{H-H}}$ = 8.4 Hz, 2H), 6.06 (d, $J_{\text{H-H}}$ = 2.4 Hz, $J_{\text{Sn-H}}$ = 122 Hz, 1H), 5.52 (d, $J_{\text{H-H}}$ = 2.4 Hz, $J_{\text{Sn-H}}$ = 58 Hz, 1H), 2.59 (s, 3H), 1.55-1.43 (m, 6H), 1.35-1.23 (m, 6H), 1.05-0.95 (m, 6H), 0.86 (t, $J_{\text{H-H}}$ = 7.2 Hz, 9H); ¹³C NMR: (100 MHz, CDCl₃) δ 197.6, 154.2, 151.8, 134.9, 128.5, 128.4, 126.3, 28.9, 27.2, 26.5, 13.6, 10.3; HRMS (ESI) calculated for [C₂₂H₃₇OSn]⁺[M+H]⁺ requires m/z 437.1861, found m/z 437.1862.

Methyl 4-(1-(tributylstannyl)vinyl)benzoate (3j). Prepared according to the general procedure using 0.0022 g (0.012 mmol) of Co(OAc)₂, 0.0050 g (0.0144 mmol) of L7, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 0.0962 g (0.60 mmol) of methyl 4-ethynylbenzoate and 1.2 mL (0.5 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE to PE/EtOAc = 50/1 as the eluent to give 0.2500 g (0.55 mmol, 92% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be >99/1 by the ¹H NMR analysis of the isolated mixture. ¹H NMR: (400 MHz, CDCl₃) δ 7.97 (d, $J_{\text{H-H}}$ = 9.2 Hz, 2H), 7.19 (d, $J_{\text{H-H}}$ = 8.8 Hz, 2H), 6.05 (d, $J_{\text{H-H}}$ = 2.4 Hz, $J_{\text{Sn-H}}$ = 123 Hz, 1H), 5.50 (d, $J_{\text{H-H}}$ = 2.4 Hz, $J_{\text{Sn-H}}$ = 58 Hz, 1H), 3.90 (s, 3H), 1.55-1.40 (m, 6H), 1.35-1.23 (m, 6H), 1.07-0.90 (m, 6H), 0.86 (t, $J_{\text{H-H}}$ = 7.2 Hz, 9H); ¹³C NMR: (100 MHz, CDCl₃) δ 167.1, 154.3, 151.6, 129.7, 128.3, 127.7, 126.2, 51.9, 28.9, 27.2, 13.6, 10.3; The spectroscopic data are in accordance with the literature.¹⁹

Tributyl(1-(4-(tert-butyl)phenyl)vinyl)stannane (**3k**). Prepared according to the general procedure using 0.0022 g (0.012 mmol) of Co(OAc)₂, 0.0050 g (0.0144 mmol) of **L7**, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 0.0949 g (0.60 mmol) of

1-(*tert*-butyl)-4-ethynylbenzene and 1.2 mL (0.5 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE as the eluent to give 0.2480 g (0.55 mmol, 92% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be 99/1 by the ¹H NMR analysis of the isolated mixture. IR (cm⁻¹): 2958, 2927, 2853, 1506, 1462. ¹H NMR: (400 MHz, CDCl₃) δ 7.31 (d, $J_{\text{H-H}}$ = 8.4 Hz, 2H), 7.12 (d, $J_{\text{H-H}}$ = 8.0 Hz, 2H), 6.05 (d, $J_{\text{H-H}}$ = 2.4 Hz, $J_{\text{Sn-H}}$ = 130 Hz, 1H), 5.38 (d, $J_{\text{H-H}}$ = 2.4 Hz, $J_{\text{Sn-H}}$ = 62 Hz, 1H), 1.55-1.43 (m, 6H), 1.35-1.23 (m, 15H), 1.05-0.90 (m, 6H), 0.86 (t, $J_{\text{H-H}}$ = 7.2 Hz, 9H); ¹³C NMR: (100 MHz, CDCl₃) δ 154.0, 149.2, 143.1, 126.1, 126.0, 125.2, 34.4, 31.4, 29.0, 27.3, 13.7, 10.3; HRMS (ESI) calculated for [C₂₄H₄₃Sn]⁺[M+H]⁺ requires m/z 451.2381, found m/z 451.2379.

4-(1-(Tributylstannyl)vinyl)aniline (3l). Prepared according to the general procedure using 0.0027 g (0.015 mmol) of Co(OAc)₂, 0.0062 g (0.0180 mmol) of **L7**, 99 μL (1.08 g/mL, 97%, 0.36 mmol) of HSnBu₃, 0.0351 g (0.30 mmol) of 4-ethynylaniline and 1.2 mL (0.25 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE to PE/EtOAc = 5/1 as the eluent to give 0.1163 g (0.29 mmol, 95% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be >99/1 by the ¹H NMR analysis of the isolated mixture. IR (cm⁻¹): 3377, 2956, 2925, 2850, 1619, 1510, 1460. ¹H NMR: (400 MHz, CDCl₃) δ 7.03 (d, $J_{\text{H-H}}$ = 8.4 Hz, 2H), 6.62 (d, $J_{\text{H-H}}$ = 8.4 Hz, $J_{\text{Sn-H}}$ = 132 Hz, 2H), 5.98 (d, $J_{\text{H-H}}$ = 2.0 Hz, $J_{\text{Sn-H}}$ = 62 Hz, 1H), 5.26 (d, $J_{\text{H-H}}$ = 2.0 Hz, 1H), 3.61 (brs, 2H), 1.58-1.42 (m, 6H), 1.37-1.24 (m, 6H), 1.05-0.90 (m, 6H), 0.86 (t, $J_{\text{H-H}}$ = 7.2 Hz, 9H); ¹³C NMR: (100 MHz, CDCl₃) δ 153.6, 145.0, 136.4, 127.4, 123.9, 115.0, 29.0, 27.3, 13.6, 10.2; HRMS (ESI) calculated for [C₂₀H₃₆NSn]⁺[M+H]⁺ requires m/z 410.1864, found m/z 410.1866.

Tributyl(1-(4-methoxyphenyl)vinyl)stannane (3m). Prepared according to the general procedure using 0.0023 g (0.013 mmol) of Co(OAc)₂, 0.0050 g (0.0144 mmol) of **L7**, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 0.0794 g (0.60 mmol) of 1-ethynyl-4-methoxybenzene and 1.2 mL (0.5 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE as the eluent to give 0.2481 g (0.59 mmol, 98% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be >99/1 by the ¹H NMR analysis of the isolated mixture. ¹H NMR: (400 MHz, CDCl₃) δ 7.13 (d, $J_{\text{H-H}}$ = 8.8 Hz, 2H), 6.84 (d, $J_{\text{H-H}}$ = 8.8 Hz, 2H), 6.00 (d, $J_{\text{H-H}}$ = 2.4 Hz, $J_{\text{Sn-H}}$ = 61 Hz, 1H), 3.79 (s, 3H), 1.57-1.43 (m, 6H), 1.37-1.23 (m, 6H), 1.05-0.90 (m, 6H), 0.86 (m, $J_{\text{H-H}}$ = 7.2 Hz, 9H); ¹³C NMR: (100 MHz, CDCl₃) δ 158.3, 153.5, 138.7, 127.4, 125.2, 113.7, 55.2, 29.0, 27.3, 13.7, 10.2; The spectroscopic data are in accordance with the literature. ¹⁸

Tributyl(1-(4-(methylthio)phenyl)vinyl)stannane (3n). Prepared according to the general procedure using 0.0027 g (0.015 mmol) of Co(OAc)₂, 0.0063 g (0.0180 mmol) of **L7**, 99 μL (1.08 g/mL, 97%, 0.36 mmol) of HSnBu₃, 0.0443 g (0.30 mmol) of (4-ethynylphenyl)(methyl)sulfane and 1.2 mL (0.25 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE as the eluent to give 0.1194 g (0.27 mmol, 91% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be 99.5/0.5 by the ¹H NMR analysis of the isolated mixture. IR (cm⁻¹): 2956, 2923, 2851, 1592, 1548, 1460. ¹H NMR: (400 MHz, CDCl₃) δ 7.20 (d, J_{H-H} = 8.4 Hz, 2H), 7.10 (d, J_{H-H} = 8.8 Hz, 2H), 6.02 (d, J_{H-H} = 2.8 Hz, J_{Sn-H} = 128 Hz, 1H), 5.39 (d, J_{H-H} = 2.4 Hz, J_{Sn-H} = 60 Hz, 1H), 2.48 (s, 3H), 1.54-1.42 (m, 6H), 1.35-1.23 (m, 6H), 1.05-0.92 (m, 6H), 0.86 (t, J_{H-H} = 7.2 Hz, 9H); ¹³C NMR: (100 MHz, CDCl₃) δ 153.8, 143.4, 136.0, 126.8, 126.4, 29.0,

27.3, 16.1, 13.6, 10.3; HRMS (ESI) calculated for $[C_{21}H_{37}SSn]^+[M+H]^+$ requires m/z 441.1632, found m/z 441.1633.

Tributyl(1-(4-vinylphenyl)vinyl)stannane (3o). Prepared according to the general procedure using 0.0021 g (0.012 mmol) of Co(OAc)₂, 0.0051 g (0.0147 mmol) of L7, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 0.0773 g (0.60 mmol) of 1-ethynyl-4-vinylbenzene and 1.2 mL (0.5 M) of THF. After 3 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE as the eluent to give 0.1786 g (0.43 mmol, 71% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be 97/3 by the ¹H NMR analysis of the isolated mixture. IR (cm⁻¹): 2957, 2925, 2852, 1597, 1460. ¹H NMR: (400 MHz, CDCl₃) δ 7.34 (d, $J_{\text{H-H}}$ = 8.0 Hz, 2H), 7.13 (d, $J_{\text{H-H}}$ = 7.6 Hz, 2H), 6.70 (dd, $J_{\text{H-H}}$ = 19.6, 10.8 Hz, 1H), 6.04 (d, $J_{\text{H-H}}$ = 2.4 Hz, $J_{\text{Sn-H}}$ = 128 Hz, 1H), 5.72 (d, $J_{\text{H-H}}$ = 19.6 Hz, 1H), 5.41 (d, $J_{\text{H-H}}$ = 2.0 Hz, $J_{\text{Sn-H}}$ = 60 Hz, 1H), 5.20 (d, $J_{\text{H-H}}$ = 10.8 Hz, 1H), 1.53-1.40 (m, 6H), 1.34-1.25 (m, 6H), 1.05-0.95 (m, 6H), 0.86 (t, $J_{\text{H-H}}$ = 7.2 Hz, 9H); ¹³C NMR (100 MHz, CDCl₃) δ 154.2, 145.9, 136.6, 135.6, 126.7, 126.5, 126.2, 113.1, 29.0, 27.3, 13.7, 10.3; HRMS (EI) calculated for [C₁₈H₂₇Sn]⁺[M-Bu]⁺ requires m/z 363.1135, found m/z 363.1132.

Tributyl(1-(naphthalen-2-yl)vinyl)stannane (3p). Prepared according to the general procedure using 0.0024 g (0.013 mmol) of Co(OAc)₂, 0.0050 g (0.0144 mmol) of L7, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 0.0900 g (0.59 mmol) of 2-ethynylnaphthalene and 1.2 mL (0.5 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE as the eluent to give 0.2473 g (0.56 mmol, 93% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be >99/1 by the ¹H NMR analysis of the isolated mixture. ¹H NMR: (400 MHz,

CDCl₃) δ 7.83-7.72 (m, 3H), 7.60-7.54 (m, 1H), 7.47-7.34 (m, 3H), 6.16 (d, $J_{\text{H-H}} = 2.4 \text{ Hz}$, $J_{\text{Sn-H}} = 127 \text{ Hz}$, 1H), 5.51 (d, $J_{\text{H-H}} = 2.0 \text{ Hz}$, $J_{\text{Sn-H}} = 60 \text{ Hz}$, 1H), 1.58-1.46 (m, 6H), 1.37-1.25 (m, 6H), 1.10-0.95 (m, 6H), 0.86 (t, $J_{\text{H-H}} = 7.2 \text{ Hz}$, 9H); ¹³C NMR: (100 MHz, CDCl₃) δ 154.6, 143.8, 133.6, 132.2, 127.9, 127.8, 127.6, 127.2, 126.0, 125.3, 125.1, 124.9, 29.0, 27.3, 13.7, 10.4; The spectroscopic data are in accordance with the literature.¹⁸

Tributyl(1-(naphthalen-1-yl)vinyl)stannane (3q). Prepared according to the general procedure using 0.0024 g (0.013 mmol) of Co(OAc)₂, 0.0051 g (0.0147 mmol) of L7, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 0.0913 g (0.60 mmol) of 1-ethynylnaphthalene and 1.2 mL (0.5 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE as the eluent to give 0.2207 g (0.50 mmol, 83% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be 98/2 by the ¹H NMR analysis of the isolated mixture. IR (cm⁻¹): 2956, 2926, 2851, 1576, 1460, 1419. ¹H NMR: (400 MHz, CDCl₃) δ 7.97-7.90 (m, 1H), 7.85-7.78 (m, 1H), 7.65 (d, $J_{\text{H-H}} = 8.4$ Hz, 1H), 7.48-7.30 (m, 3H), 7.08-7.02 (m, 1H), 5.95 (d, $J_{\text{H-H}} = 2.8$ Hz, $J_{\text{Sn-H}} = 124$ Hz, 1H), 5.72 (d, $J_{\text{H-H}} = 2.8$ Hz, $J_{\text{Sn-H}} = 60$ Hz, 1H), 1.48-1.30 (m, 6H), 1.28-1.15 (m, 6H), 0.95-0.72 (m, 15H); ¹³C NMR: (100 MHz, CDCl₃) δ 154.9, 145.6, 133.6, 130.5, 128.8, 128.2, 125.9, 125.7, 125.6, 125.4, 125.1, 122.7, 28.9, 27.3, 13.6, 10.4; HRMS (EI) calculated for [C₂₀H₂₈Sn]⁺[M-C₄H₈]⁺ requires m/z 388.1213, found m/z 388.1208.

2-(1-(Tributylstannyl)vinyl)pyridine (**3r**). Prepared according to the general procedure using 0.0022 g (0.012 mmol) of Co(OAc)₂, 0.0050 g (0.0144 mmol) of **L7**, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 0.0616 g (0.60 mmol) of 2-ethynylpyridine and 1.2 mL (0.5 M) of THF. After 3 h, the resulting solution was quenched. The combined filtrate was concentrated and the

crude mixture was purified by short flash column chromatography using PE to PE/EtOAc = 20/1 as the eluent to give 0.1438 g (0.37 mmol, 61% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be >99/1 by the ¹H NMR analysis of the isolated mixture. IR (cm⁻¹): 2955, 2924, 2851, 1583, 1461, 1429. ¹H NMR: (400 MHz, CDCl₃) δ 8.52-8.43 (m, 1H), 7.63-7.54 (m, 1H), 7.50-7.43 (m, 1H), 7.10-7.00 (m, 1H), 6.46 (d, $J_{\text{H-H}}$ = 2.0 Hz, $J_{\text{Sn-H}}$ = 132 Hz, 1H), 5.67 (d, $J_{\text{H-H}}$ = 2.0 Hz, $J_{\text{Sn-H}}$ = 63 Hz, 1H), 1.60-1.40 (m, 6H), 1.35-1.23 (m, 6H), 1.08-0.90 (m, 6H), 0.86 (t, $J_{\text{H-H}}$ = 7.2 Hz, 9H); ¹³C NMR: (100 MHz, CDCl₃) δ 161.9, 157.0, 148.7, 136.0, 127.0, 121.2, 117.9, 29.1, 27.3, 13.7, 10.6; HRMS (ESI) calculated for [C₁₉H₃₄NSn]⁺[M+H]⁺ requires m/z 396.1708, found m/z 396.1709.

$$\mathsf{N} = \mathsf{SnBu}_3$$

3-(1-(Tributylstannyl)vinyl)pyridine (3s). Prepared according to the general procedure using 0.0023 g (0.013 mmol) of Co(OAc)₂, 0.0051 g (0.0147 mmol) of L7, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 0.0619 g (0.60 mmol) of 3-ethynylpyridine and 1.2 mL (0.5 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE to PE/EtOAc = 50/1 as the eluent to give 0.2223 g (0.56 mmol, 94% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be 99/1 by the ¹H NMR analysis of the isolated mixture. IR (cm⁻¹): 2957, 2926, 2851, 1561, 1464, 1406. ¹H NMR: (400 MHz, CDCl₃) δ 8.48-8.38 (m, 2H), 7.50-7.40 (m, 1H), 7.21 (dd, $J_{\text{H-H}}$ = 7.6, 4.8 Hz, 1H), 6.06 (d, $J_{\text{H-H}}$ = 2.0 Hz, $J_{\text{Sn-H}}$ = 121 Hz, 1H), 5.53 (d, $J_{\text{H-H}}$ = 2.4 Hz, $J_{\text{Sn-H}}$ = 58 Hz, 1H), 1.58-1.40 (m, 6H), 1.37-1.24 (m, 6H), 1.08-0.95 (m, 6H), 0.86 (t, $J_{\text{H-H}}$ = 7.2 Hz, 9H); ¹³C NMR: (100 MHz, CDCl₃) δ 151.1, 147.6, 147.4, 133.2, 128.9, 123.1, 28.9, 27.2, 13.6, 10.2; HRMS (ESI) calculated for [C₁₉H₃₄NSn]⁺[M+H]⁺ requires m/z 396.1708, found m/z 396.1710.

$$N$$
 SnBu₃

2-(1-(TributyIstannyl)vinyl)pyrimidine (3t). Prepared according to the general procedure using 0.0023 g (0.013 mmol) of Co(OAc)₂, 0.0050 g (0.0144 mmol) of **L7**, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 0.0622 g (0.60 mmol) of 2-ethynylpyrimidine and 1.2 mL (0.5 M) of THF. After 3 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE/EtOAc = 5/1 as the eluent to give 0.1216 g (0.31 mmol, 52% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be >99/1 by the ¹H NMR analysis of the isolated mixture. IR (cm⁻¹): 2956, 2924, 2851, 1564, 1460. ¹H NMR: (400 MHz, CDCl₃) δ 8.66 (d, J_{H-H} = 4.8 Hz, 2H), 7.13 (d, J_{H-H} = 2.0 Hz, J_{Sn-H} = 123 Hz, 1H), 7.05 (t, J_{H-H} = 4.8 Hz, 1H), 5.90 (d, J_{H-H} = 2.0 Hz, J_{Sn-H} = 58 Hz, 1H), 1.59-1.41 (m, 6H), 1.35-1.25 (m, 6H), 1.08-0.91 (m, 6H), 0.86 (t, J_{H-H} = 7.6 Hz, 9H); ¹³C NMR (100 MHz, CDCl₃) δ 156.7, 154.7, 133.3, 118.2, 29.1, 27.3, 13.7, 10.4; HRMS (ESI) calculated for [C₁₄H₂₃N₂Sn]⁺[M-Bu]⁺ requires m/z 339.0883, found m/z 339.0877.

Tributyl(1-(thiophen-2-yl)vinyl)stannane (**3u**). Prepared according to the general procedure using 0.0027 g (0.015 mmol) of Co(OAc)₂, 0.0062 g (0.0180 mmol) of **L7**, 99 μL (1.08 g/mL, 97%, 0.36 mmol) of HSnBu₃, 0.0328 g (0.30 mmol) of 2-ethynylthiophene and 1.2 mL (0.25 M) of THF. After 12 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE as the eluent to give 0.1104 g (0.28 mmol, 92% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be >99/1 by the ¹H NMR analysis of the isolated mixture. ¹H NMR: (400 MHz, CDCl₃) δ 7.12 (dd, $J_{\text{H-H}}$ = 4.8, 0.8 Hz, 1H), 6.94 (dd, $J_{\text{H-H}}$ = 5.2, 3.6 Hz, 1H), 6.79 (dd, $J_{\text{H-H}}$ = 3.6, 1.2 Hz, 1H), 6.15 (d, $J_{\text{H-H}}$ = 2.0 Hz, $J_{\text{Sn-H}}$ = 132 Hz, 1H), 5.28 (d, $J_{\text{H-H}}$ = 1.6 Hz, $J_{\text{Sn-H}}$ = 58 Hz, 1H), 1.58-1.45 (m, 6H), 1.38-1.25 (m, 6H), 1.12-0.95 (m, 6H), 0.88 (t, $J_{\text{H-H}}$ = 7.2 Hz, 9H); ¹³C NMR: (100 MHz, CDCl₃) δ 150.2, 145.0, 127.1, 125.1, 124.7, 123.7, 29.0, 27.3, 13.6, 10.3; The spectroscopic data are in accordance with the literature.¹⁸

(1-(Benzo[*b*]thiophen-5-yl)vinyl)tributylstannane (3v). Prepared according to the general procedure using 0.0023 g (0.013 mmol) of Co(OAc)₂, 0.0050 g (0.0144 mmol) of L7, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 0.0950 g (0.60 mmol) of 5-ethynylbenzo[*b*]thiophene and 1.2 mL (0.5 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE as the eluent to give 0.2468 g (0.55 mmol, 92% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be >99/1 by the ¹H NMR analysis of the isolated mixture. IR (cm⁻¹): 2956, 2924, 2850, 1583, 1460. ¹H NMR: (400 MHz, CDCl₃) δ 7.78 (d, $J_{\text{H-H}}$ = 8.4 Hz, 1H), 7.59 (d, $J_{\text{H-H}}$ = 5.6 Hz, 1H), 7.39 (d, $J_{\text{H-H}}$ = 5.2 Hz, 1H), 7.29 (d, $J_{\text{H-H}}$ = 5.2 Hz, 1H), 7.19 (dd, $J_{\text{H-H}}$ = 8.0, 1.6 Hz, 1H), 6.09 (d, $J_{\text{H-H}}$ = 2.4 Hz, $J_{\text{Sn-H}}$ = 128 Hz, 1H), 5.46 (d, $J_{\text{H-H}}$ = 2.4 Hz, $J_{\text{Sn-H}}$ = 60 Hz, 1H), 1.58-1.43 (m, 6H), 1.35-1.25 (m, 6H), 1.10-0.94 (m, 6H), 0.86 (t, $J_{\text{H-H}}$ = 7.2 Hz, 9H); ¹³C NMR: (100 MHz, CDCl₃) δ 154.6, 142.9, 139.9, 137.7, 126.8, 126.5, 123.9, 123.3, 122.1, 120.9, 29.0, 27.3, 13.7, 10.3; HRMS (EI) calculated for [C₂₂H₃₄SSn]⁺[M]⁺ requires m/z 450.1403, found m/z 450.1404.

Tributyl(1-(dibenzo[b,d]thiophen-2-yl)vinyl)stannane (3w). Prepared according to the general procedure using 0.0022 g (0.012 mmol) of Co(OAc)₂, 0.0050 g (0.0144 mmol) of L7, 198 µL 97%. (1.08)g/mL, 0.72 mmol) of HSnBu₃, 0.1250 (0.60)mmol) of 2-ethynyldibenzo[b,d]thiophene and 1.2 mL (0.5 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE as the eluent to give 0.2756 g (0.55 mmol, 92% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be 99.5/0.5 by the ¹H NMR analysis of the isolated mixture. IR (cm⁻¹): 2955, 2924, 2851, 1544, 1462. ¹H NMR: (400 MHz, CDCl₃) δ 8.16-8.08 (m, 1H), 7.94 (d, $J_{\text{H-H}}$ = 1.6 Hz, 1H), 7.86-7.80 (m, 1H), 7.76 (d, $J_{\text{H-H}}$ =

8.4 Hz, 1H), 7.48-7.40 (m, 2H), 7.30 (dd, $J_{\text{H-H}} = 8.4$, 1.6 Hz, 1H), 6.15 (d, $J_{\text{H-H}} = 2.4$ Hz, $J_{\text{Sn-H}} = 127$ Hz, 1H), 5.51 (d, $J_{\text{H-H}} = 2.0$ Hz, $J_{\text{Sn-H}} = 60$ Hz, 1H), 1.63-1.48 (m, 6H), 1.38-1.25 (m, 6H), 1.10-0.95 (m, 6H), 0.87 (t, $J_{\text{H-H}} = 7.2$ Hz, 9H); ¹³C NMR: (100 MHz, CDCl₃) δ 154.5, 143.1, 139.9, 137.3, 135.7, 135.6, 127.0, 126.6, 125.4, 124.3, 122.9, 122.5, 121.4, 119.1, 29.1, 27.3, 13.7, 10.4; HRMS (EI) calculated for $[C_{26}H_{36}SSn]^+[M]^+$ requires m/z 500.1560, found m/z 500.1557.

1,4-Bis(1-(tributylstannyl)vinyl)benzene (3x). Prepared according to the general procedure using 0.0022 g (0.012 mmol) of Co(OAc)₂, 0.0050 g (0.0144 mmol) of **L7**, 396 μL (1.08 g/mL, 97%, 1.44 mmol) of HSnBu₃, 0.0757 g (0.60 mmol) of 1,4-diethynylbenzene and 1.2 mL (0.5 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE as the eluent to give 0.3954 g (0.56 mmol, 93% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be 98/2 by the ¹H NMR analysis of the isolated mixture. IR (cm⁻¹): 2957, 2926, 2852, 1599, 1500, 1460. ¹H NMR: (400 MHz, CDCl₃) δ 7.11 (s, 4H), 6.05 (d, $J_{\text{H-H}}$ = 2.4 Hz, $J_{\text{Sn-H}}$ = 129 Hz, 2H), 5.39 (d, $J_{\text{H-H}}$ = 2.4 Hz, $J_{\text{Sn-H}}$ = 61 Hz, 2H), 1.55-1.43 (m, 12H), 1.35-1.24 (m, 12H), 1.05-0.94 (m, 12H), 0.86 (t, $J_{\text{H-H}}$ = 7.2 Hz, 18H); ¹³C NMR: (100 MHz, CDCl₃) δ 154.2, 144.3, 126.3, 126.2, 29.0, 27.3, 13.7, 10.3; HRMS (ESI) calculated for [C₃₄H₆₃Sn₂]⁺[M+H]⁺ requires m/z 711.2968, found m/z 711.2977.

Tributyl(prop-1-en-2-yl)stannane (**3y).** Prepared according to the general procedure using 0.0022 g (0.012 mmol) of Co(OAc)₂, 0.0050 g (0.0144 mmol) of **L7**, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 600 μL (1 M in THF, 0.60 mmol) of prop-1-yne and 1.2 mL (0.5 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE as the eluent to give 0.1917 g (0.58 mmol, 96% yield) of the title compound as a colorless oil. The ratio of α/β

was determined to be 98/2 by the ¹H NMR analysis of the isolated mixture. IR (cm⁻¹): 2957, 2927, 2851, 1458. ¹H NMR: (400 MHz, CDCl₃) δ 5.73-5.63 (m, J_{Sn-H} = 138 Hz, 1H), 5.12-5.03 (m, J_{Sn-H} = 62 Hz, 1H), 2.05-1.88 (m, J_{Sn-H} = 42 Hz, 3H), 1.58-1.40 (m, 6H), 1.38-1.25 (m, 6H), 1.00-0.80 (m, 15H); ¹³C NMR: (100 MHz, CDCl₃) δ 150.4, 125.5, 29.1, 27.4, 27.3, 13.7, 9.1; HRMS (EI) calculated for [C₁₁H₂₄Sn]⁺[M-C₄H₈]⁺ requires m/z 276.0900, found m/z 276.0900.

Tributyl(hex-1-en-2-yl)stamnane (3z). Prepared according to the general procedure using 0.0022 g (0.012 mmol) of Co(OAc)₂, 0.0050 g (0.0144 mmol) of **L7**, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 70 μL (0.72 g/mL, 0.60 mmol) of hex-1-yne and 1.2 mL (0.5 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE as the eluent to give 0.2239 g (0.60 mmol, >99% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be 98/2 by the ¹H NMR analysis of the isolated mixture. ¹H NMR: (400 MHz, CDCl₃) δ 5.86-5.45 (m, J_{Sn-H} = 141 Hz, 1H), 5.20-4.98 (m, J_{Sn-H} = 64 Hz, 1H), 2.24 (t, J_{H-H} = 7.2 Hz, J_{Sn-H} = 48 Hz, 2H), 1.60-1.40 (m, 6H), 1.38-1.25 (m, 10H), 0.95-0.80 (m, 18H); ¹³C NMR: (100 MHz, CDCl₃) δ 155.7, 124.5, 41.1, 31.9, 29.1, 27.4, 22.3, 13.9, 13.7, 9.5; The spectroscopic data are in accordance with the literature. ¹⁸

Tributyl(hept-1-en-2-yl)stannane (3aa). Prepared according to the general procedure using 0.0021 g (0.012 mmol) of Co(OAc)₂, 0.0050 g (0.0144 mmol) of **L7**, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 0.0578 g (0.60 mmol) of 1-heptyne and 1.2 mL (0.5 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE as the eluent to give 0.1915 g (0.49 mmol, 82% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be 98/2 by the ¹H NMR analysis of the isolated mixture. IR (cm⁻¹): 2958, 2926, 2853, 1461. ¹H

NMR: (400 MHz, CDCl₃) δ 5.65 (d, $J_{\text{H-H}} = 2.8$ Hz, $J_{\text{Sn-H}} = 142$ Hz, 1H), 5.09 (d, $J_{\text{H-H}} = 2.8$ Hz, $J_{\text{Sn-H}} = 63$ Hz, 1H), 2.23 (t, $J_{\text{H-H}} = 6.4$ Hz, $J_{\text{Sn-H}} = 48$ Hz, 2H), 1.54-1.45 (m, 6H), 1.38-1.25 (m, 12H), 0.96-0.80 (m, 18H); ¹³C NMR (100 MHz, CDCl₃) δ 155.8, 124.5, 41.4, 31.6, 29.4, 29.2, 27.4, 22.6, 14.1, 13.7, 9.6; HRMS (EI) calculated for $[C_{15}H_{31}Sn]^+[M-Bu]^+$ requires m/z 331.1448, found m/z 331.1449.

Tributyl(oct-1-en-2-yl)stannane (3ab). Prepared according to the general procedure using 0.0022 g (0.012 mmol) of Co(OAc)₂, 0.0051 g (0.0147 mmol) of **L7**, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 0.0661 g (0.60 mmol) of oct-1-yne and 1.2 mL (0.5 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE as the eluent to give 0.2251 g (0.56 mmol, 93% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be 98/2 by the ¹H NMR analysis of the isolated mixture. ¹H NMR: (400 MHz, CDCl₃) δ 5.85-5.45 (m, $J_{Sn-H} = 141$ Hz, 1H), 5.20-4.98 (m, $J_{Sn-H} = 64$ Hz, 1H), 2.23 (t, $J_{H-H} = 7.2$ Hz, $J_{Sn-H} = 48$ Hz, 2H), 1.55-1.43 (m, 6H), 1.38-1.23 (m, 14H), 1.00-0.80 (m, 18H); ¹³C NMR: (100 MHz, CDCl₃) δ 155.8, 124.5, 41.5, 31.8, 29.7, 29.2, 29.0, 27.4, 22.7, 14.1, 13.7, 9.6; The spectroscopic data are in accordance with the literature.²⁰

Tributyl(1-cyclopropylvinyl)stannane (3ac). Prepared according to the general procedure using 0.0022 g (0.012 mmol) of Co(OAc)₂, 0.0050 g (0.0144 mmol) of L7, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 51 μL (0.78 g/mL, 0.60 mmol) of ethynylcyclopropane and 1.2 mL (0.5 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE as the eluent to give 0.2143 g (0.60 mmol, >99% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be >99/1 by the ¹H NMR analysis of the isolated mixture. ¹H NMR: (400 MHz,

CDCl₃) δ 5.84-5.42 (m, $J_{\text{Sn-H}}$ = 136 Hz, 1H), 5.13-4.92 (m, $J_{\text{Sn-H}}$ = 62 Hz, 1H), 1.60-1.40 (m, 7H), 1.38-1.28 (m, 6H), 1.00-0.80 (m, 15H), 0.70-0.60 (m, 2H), 0.50-0.35 (m, 2H); ¹³C NMR: (100 MHz, CDCl₃) δ 157.0, 121.6, 29.1, 27.4, 20.3, 13.7, 9.7, 6.9; The spectroscopic data are in accordance with the literature.²¹

Tributyl(1-(cyclohex-1-en-1-yl)vinyl)stannane (3ad). Prepared according to the general procedure using 0.0023 g (0.013 mmol) of Co(OAc)₂, 0.0050 g (0.0144 mmol) of L7, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 0.0620 g (0.58 mmol) of 1-ethynylcyclohex-1-ene and 1.2 mL (0.5 M) of THF. After 3 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE as the eluent to give 0.1359 g (0.34 mmol, 59% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be >99/1 by the ¹H NMR analysis of the isolated mixture. ¹H NMR: (400 MHz, CDCl₃) δ 5.81 (d, $J_{\text{H-H}}$ = 2.0 Hz, $J_{\text{Sn-H}}$ = 140 Hz, 1H), 5.56 (t, $J_{\text{H-H}}$ = 4.0 Hz, 1H), 5.12 (d, $J_{\text{H-H}}$ = 2.0 Hz, $J_{\text{Sn-H}}$ = 67 Hz, 1H), 2.22-2.07 (m, 4H), 1.72-1.63 (m, 2H), 1.62-1.53 (m, 2H), 1.52-1.42 (m, 6H), 1.37-1.24 (m, 6H), 1.00-0.80 (m, 15H); ¹³C NMR: (100 MHz, CDCl₃) δ 155.7, 141.0, 128.5, 121.4, 29.1, 27.3, 26.2, 26.0, 22.9, 22.5, 13.7, 10.3; The spectroscopic data are in accordance with the literature. ¹⁸

Trimethyl(1-(tributylstannyl)vinyl)silane (3ae). Prepared according to the general procedure using 0.0027 g (0.015 mmol) of Co(OAc)₂, 0.0062 g (0.0180 mmol) of L7, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 87 μL (0.695 g/mL, 0.60 mmol) of ethynyltrimethylsilane and 1.2 mL (0.5 M) of THF. After 24 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE as the eluent to give 0.1873 g (0.48 mmol, 80% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be 97/3 by the ¹H NMR analysis of the isolated mixture. IR (cm⁻¹):

2956, 2925, 2853, 1461. ¹H NMR: (400 MHz, CDCl₃) δ 6.57 (d, $J_{\text{H-H}}$ = 4.4 Hz, $J_{\text{Sn-H}}$ = 178 Hz, 1H), 6.30 (d, $J_{\text{H-H}}$ = 4.8 Hz, $J_{\text{Sn-H}}$ = 107 Hz, 1H), 1.62-1.50 (m, 6H), 1.45-1.35 (m, 6H), 1.05-0.90 (m, 15H), 0.15 (s, 9H); ¹³C NMR: (100 MHz, CDCl₃) δ 156.7, 140.5, 29.1, 27.4, 13.7, 9.8, -0.8; HRMS (EI) calculated for [C₁₃H₃₁SiSn]⁺[M-C₄H₇]⁺ requires m/z 335.1217, found m/z 335.1221.

Tributyl(**4-phenylbut-1-en-2-yl)stannane** (**3af**). Prepared according to the general procedure using 0.0022 g (0.012 mmol) of Co(OAc)₂, 0.0050 g (0.0144 mmol) of **L7**, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 0.0781 g (0.60 mmol) of but-3-yn-1-ylbenzene and 1.2 mL (0.5 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE as the eluent to give 0.2376 g (0.56 mmol, 94% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be 99/1 by the ¹H NMR analysis of the isolated mixture. ¹H NMR: (400 MHz, CDCl₃) δ 7.32-7.24 (m, 2H), 7.22-7.13 (m, 3H), 5.95-5.53 (m, J_{Sn-H} = 139 Hz, 1H), 5.26-5.05 (m, J_{Sn-H} = 63 Hz, 1H), 2.73-2.63 (m, 2H), 2.60-2.43 (m, 2H), 1.58-1.43 (m, 6H), 1.38-1.28 (m, 6H), 0.98-0.85 (m, 15H); ¹³C NMR: (100 MHz, CDCl₃) δ 154.7, 142.2, 128.4, 128.3, 125.8, 125.2, 43.2, 36.2, 29.2, 27.4, 13.7, 9.6; The spectroscopic data are in accordance with the literature.²²

Tributyl(4-(naphthalen-2-yl)but-1-en-2-yl)stannane (3ag). Prepared according to the general procedure using 0.0022 g (0.012 mmol) of Co(OAc)₂, 0.0051 g (0.0147 mmol) of L7, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 0.1082 g (0.60 mmol) of 2-(but-3-yn-1-yl)naphthalene and 1.2 mL (0.5 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE as the eluent to give 0.2432 g (0.52 mmol, 86% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be 99/1 by the ¹H NMR analysis of the isolated mixture. IR (cm⁻¹): 3051, 2956, 2924, 2850, 1600, 1458. ¹H NMR: (400 MHz, CDCl₃) δ 7.82-7.72 (m, 3H),

7.61 (s, 1H), 7.47-7.37 (m, 2H), 7.33 (dd, $J_{\text{H-H}} = 8.4$, 1.6 Hz, 1H), 5.95-5.55 (m, $J_{\text{Sn-H}} = 138$ Hz, 1H), 5.28-5.08 (m, $J_{\text{Sn-H}} = 64$ Hz, 1H), 2.90-2.80 (m, 2H), 2.72-2.55 (m, 2H), 1.63-1.40 (m, 6H), 1.40-1.28 (m, 6H), 1.05-0.85 (m, 15H); 13 C NMR: (100 MHz, CDCl₃) δ 154.6, 139.7, 133.6, 132.0, 127.8, 127.6, 127.4, 127.3, 126.3, 125.9, 125.3, 125.1, 43.1, 36.4, 29.2, 27.4, 13.7, 9.6; HRMS (EI) calculated for $[C_{26}H_{40}Sn]^+[M]^+$ requires m/z 472.2152, found m/z 472.2156.

(4-([1,1'-Biphenyl]-4-yl)but-1-en-2-yl)tributylstannane (3ah). Prepared according to the general procedure using 0.0022 g (0.012 mmol) of Co(OAc)₂, 0.0050 g (0.0144 mmol) of L7, 198 μL 97%, 0.72 mmol) of HSnBu₃, 0.1240 4-(but-3-yn-1-yl)-1,1'-biphenyl and 1.2 mL (0.5 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE as the eluent to give 0.2577 g (0.52 mmol, 86% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be 99/1 by the ¹H NMR analysis of the isolated mixture. IR (cm⁻¹): 3029, 2956, 2925, 2850, 1601, 1456. ¹H NMR: (400 MHz, CDCl₃) δ 7.60-7.55 (m, 2H), 7.52 (d, $J_{\text{H-H}}$ = 8.0 Hz, 2H), 7.45-7.38 (m, 2H), 7.34-7.28 (m, 1H), 7.26 (d, $J_{\text{H-H}} = 8.0 \text{ Hz}$, 2H), 5.96-5.55 (m, $J_{\text{Sn-H}} = 138 \text{ Hz}$, 1H), 5.30-5.05 (m, $J_{\text{Sn-H}} = 63 \text{ Hz}$, 1H), 2.78-2.68 (m, 2H), 2.65-2.50 (m, 2H), 1.60-1.45 (m, 6H), 1.40-1.28 (m, 6H), 1.05-0.85 (m, 15H); 13 C NMR: (100 MHz, CDCl₃) δ 154.6, 141.4, 141.1, 138.7, 128.8, 128.7, 127.05, 126.98, 125.2, 43.1, 35.8, 29.2, 27.4, 13.7, 9.6; HRMS (EI) calculated for [C₂₈H₄₂Sn]⁺[M]⁺ requires m/z 498.2308, found m/z 498.2307.

Tributyl(4-(thiophen-2-yl)but-1-en-2-yl)stannane (**3ai).** Prepared according to the general procedure using 0.0022 g (0.012 mmol) of Co(OAc)₂, 0.0052 g (0.0150 mmol) of **L7**, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 0.0817 g (0.60 mmol) of 2-(but-3-yn-1-yl)thiophene and 1.2 mL (0.5 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate

was concentrated and the crude mixture was purified by short flash column chromatography using PE to PE/EtOAc = 50/1 as the eluent to give 0.2393 g (0.56 mmol, 93% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be 99/1 by the ¹H NMR analysis of the isolated mixture. IR (cm⁻¹): 2956, 2926, 2849, 1456. ¹H NMR: (400 MHz, CDCl₃) δ 7.10 (dd, $J_{\text{H-H}}$ = 5.2, 1.2 Hz, 1H), 6.91 (dd, $J_{\text{H-H}}$ = 5.2, 3.6 Hz, 1H), 6.83-6.78 (m, 1H), 5.95-5.55 (m, $J_{\text{Sn-H}}$ = 137 Hz, 1H), 5.28-5.08 (m, $J_{\text{Sn-H}}$ = 63 Hz, 1H), 2.95-2.85 (m, 2H), 2.70-2.55 (m, 2H), 1.60-1.40 (m, 6H), 1.38-1.28 (m, 6H), 1.05-0.80 (m, 15H); ¹³C NMR: (100 MHz, CDCl₃) δ 153.9, 145.0, 126.6, 125.6, 124.0, 122.9, 43.2, 30.1, 29.1, 27.4, 13.7, 9.6; HRMS (EI) calculated for [C₂₀H₃₇SSn]⁺[M+H]⁺ requires m/z 429.1632, found m/z 429.1635.

Tributyl(3-phenoxyprop-1-en-2-yl)stannane (3aj). Prepared according to the general procedure using 0.0022 g (0.012 mmol) of Co(OAc)₂, 0.0050 g (0.0144 mmol) of **L7**, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 0.0794 g (0.60 mmol) of (prop-2-yn-1-yloxy)benzene and 1.2 mL (0.5 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE to PE/EtOAc = 50/1 as the eluent to give 0.2470 g (0.58 mmol, 97% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be >99/1 by the ¹H NMR analysis of the isolated mixture. ¹H NMR: (400 MHz, CDCl₃) δ 7.30-7.20 (m, 2H), 6.95-6.85 (m, 3H), 5.97 (d, $J_{\text{H-H}} = 2.0 \text{ Hz}$, $J_{\text{Sn-H}} = 126 \text{ Hz}$, 1H), 5.35 (d, $J_{\text{H-H}} = 2.0 \text{ Hz}$, $J_{\text{Sn-H}} = 60 \text{ Hz}$, 1H), 4.65 (t, $J_{\text{H-H}} = 1.6 \text{ Hz}$, 2H), 1.60-1.40 (m, 6H), 1.36-1.24 (m, 6H), 1.05-0.80 (m, 15H); ¹³C NMR: (100 MHz, CDCl₃) δ 158.7, 151.6, 129.3, 125.1, 120.5, 114.6, 74.8, 29.1, 27.3, 13.7, 9.7; The spectroscopic data are in accordance with the literature.²³

(4-(Benzyloxy)but-1-en-2-yl)tributylstannane (3ak). Prepared according to the general procedure using 0.0020 g (0.011 mmol) of Co(OAc)₂, 0.0050 g (0.0144 mmol) of L7, 198 μL

(1.08)g/mL, 97%, 0.72 mmol) of HSnBu₃, 0.0878 (0.60)((but-3-yn-1-yloxy)methyl)benzene and 1.2 mL (0.5 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE to PE/EtOAc = 50/1 as the eluent to give 0.2282 g (0.52 mmol, 87% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be >99/1 by the ¹H NMR analysis of the isolated mixture. ¹H NMR: (400 MHz, CDCl₃) δ 7.38-7.31 (m, 4H), 7.30-7.23 (m, 1H), 5.95-5.55 (m, J_{Sn-H} = 136 Hz, 1H), 5.19 (d, J_{H-H} = 2.4 Hz, $J_{\text{Sn-H}} = 61 \text{ Hz}, 1\text{H}, 4.51 \text{ (s, 2H)}, 3.48 \text{ (t, } J_{\text{H-H}} = 7.2 \text{ Hz}, 2\text{H}), 2.57 \text{ (t, } J_{\text{H-H}} = 7.2 \text{ Hz}, J_{\text{Sn-H}} = 45 \text{ Hz},$ 2H), 1.55-1.40 (m, 6H), 1.35-1.24 (m, 6H), 1.00-0.80 (m, 15H); 13 C NMR: (100 MHz, CDCl₃) δ 151.5, 138.4, 128.3, 127.7, 127.5, 126.9, 73.0, 70.2, 41.3, 29.1, 27.4, 13.7, 9.6; The spectroscopic data are in accordance with the literature.²⁴

Tributyl(3-(4-(methylthio)benzyl)oxy)prop-1-en-2-yl)stannane (3al). Prepared according to the general procedure using 0.0023 g (0.013 mmol) of Co(OAc)₂, 0.0051 g (0.0147 mmol) of L7, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 0.1154 g (0.60 mmol) of methyl(4-(prop-2-yn-1-yloxy)phenyl)sulfane and 1.2 mL (0.5 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE to PE/EtOAc = 50/1 as the eluent to give 0.2697 g (0.56 mmol, 93% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be >99/1 by the ¹H NMR analysis of the isolated mixture. IR (cm⁻¹): 2955, 2923, 2848, 1602, 1494, 1459. ¹H NMR: (400 MHz, CDCl₃) δ 7.30-7.20 (m, 4H), 6.05-5.68 (m, J_{Sn-H} = 130 Hz, 1H), 5.40-5.15 (m, J_{Sn-H} = 62 Hz, 1H), 4.43 (s, 2H), 4.13 (s, 2H), 2.47 (s, 3H), 1.55-1.35 (m, 6H), 1.35-1.23 (m, 6H), 1.00-0.80 (m, 15H); ¹³C NMR: (100 MHz, CDCl₃) δ 152.8, 137.4, 135.4, 128.3, 126.6, 124.8, 76.7, 71.6, 29.1, 27.3, 16.0, 13.7, 9.5; HRMS (ESI) calculated for [C₂₃H₄₀NaOSSn]+[M+Na]+ requires m/z 507.1714, found m/z 507.1717.

5-(TributyIstannyI)hex-5-enenitrile (3am). Prepared according to the general procedure using 0.0022 g (0.012 mmol) of Co(OAc)₂, 0.0051 g (0.0147 mmol) of **L7**, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 0.0560 g (0.60 mmol) of hex-5-ynenitrile and 1.2 mL (0.5 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE to PE/EtOAc = 50/1 as the eluent to give 0.2167 g (0.56 mmol, 94% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be >99/1 by the ¹H NMR analysis of the isolated mixture. ¹H NMR: (400 MHz, CDCl₃) δ 5.95-5.53 (m, J_{Sn-H} = 134 Hz, 1H), 5.31-5.12 (m, J_{Sn-H} = 61 Hz, 1H), 2.39 (t, J_{H-H} = 7.2 Hz, J_{Sn-H} = 45 Hz, 2H), 2.32 (t, J_{H-H} = 7.2 Hz, 2H), 1.80-1.70 (m, 2H), 1.55-1.43 (m, 6H), 1.36-1.26 (m, 6H), 1.00-0.80 (m, 15H); ¹³C NMR: (100 MHz, CDCl₃) δ 152.7, 126.9, 119.6, 39.6, 29.0, 27.3, 24.8, 16.3, 13.6, 9.5; The spectroscopic data are in accordance with the literature.²¹

$$\operatorname{\mathsf{Et}}_2\mathsf{N}$$
 $\operatorname{\mathsf{SnBu}}_3$

N,*N*-diethyl-6-(tributylstannyl)hept-6-enamide (3an). Prepared according to the general procedure using 0.0022 g (0.012 mmol) of Co(OAc)₂, 0.0050 g (0.0144 mmol) of L7, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 0.0910 g (0.59 mmol) of *N*,*N*-diethylhept-6-ynamide and 1.2 mL (0.5 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE to PE/EtOAc = 20/1 as the eluent to give 0.2078 g (0.47 mmol, 79% yield) of the title compound as a colorless oil. The ratio of α /β was determined to be >99/1 by the ¹H NMR analysis of the isolated mixture. IR (cm⁻¹): 2958, 2928, 2873, 1648, 1458, 1426. ¹H NMR: (400 MHz, CDCl₃) δ 5.90-5.45 (m, J_{Sn-H} = 140 Hz, 1H), 5.10 (d, J_{H-H} = 2.4 Hz, J_{Sn-H} = 63 Hz, 1H), 3.37 (q, J_{H-H} = 7.2 Hz, 2H), 3.30 (q, J_{H-H} = 7.2 Hz, 2H), 2.35-2.20 (m, 4H), 1.70-1.59 (m, 2H), 1.56-1.40 (m, 8H), 1.35-1.25 (m, 6H), 1.17 (t, J_{H-H} = 7.2 Hz, 3H), 1.11 (t, J_{H-H} = 7.2 Hz, 3H), 1.00-0.80 (m, 15H); ¹³C NMR: (100 MHz, CDCl₃) δ 172.1, 155.1, 124.8, 41.9, 41.0, 40.0, 32.9, 29.3, 29.1, 27.3,

25.1, 14.4, 13.6, 13.1, 9.5; HRMS (ESI) calculated for $[C_{23}H_{48}NOSn]^+[M+H]^+$ requires m/z 474.2752, found m/z 474.2760.

Tributyl(6-chlorohex-1-en-2-yl)stannane (3ao). Prepared according to the general procedure using 0.0022 g (0.012 mmol) of Co(OAc)₂, 0.0049 g (0.0142 mmol) of L7, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 0.0695 g (0.60 mmol) of 6-chlorohex-1-yne and 1.2 mL (0.5 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE as the eluent to give 0.2299 g (0.56 mmol, 94% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be 98/2 by the ¹H NMR analysis of the isolated mixture. ¹H NMR: (400 MHz, CDCl₃) δ 5.67 (d, $J_{\text{H-H}}$ = 1.2 Hz, $J_{\text{Sn-H}}$ = 138 Hz, 1H), 5.12 (d, $J_{\text{H-H}}$ = 1.6 Hz, $J_{\text{Sn-H}}$ = 63 Hz, 1H), 3.54 (t, $J_{\text{H-H}}$ = 6.8 Hz, 2H), 2.27 (t, $J_{\text{H-H}}$ = 7.2 Hz, $J_{\text{Sn-H}}$ = 46 Hz, 2H), 1.80-1.73 (m, 2H), 1.54-1.45 (m, 8H), 1.34-1.29 (m, 6H), 0.98-0.87 (m, 15H); ¹³C NMR (100 MHz, CDCl₃) δ 154.8, 125.3, 44.9, 40.4, 32.1, 30.6, 29.1, 27.4, 26.7, 13.7, 9.6; The spectroscopic data are in accordance with the literature.²¹

3-(TributyIstannyI)but-3-en-1-ol (**3ap**). Prepared according to the general procedure using 0.0019 g (0.011 mmol) of Co(OAc)₂, 0.0049 g (0.0142 mmol) of **L7**, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 0.0417 g (0.59 mmol) of but-3-yn-1-ol and 1.2 mL (0.5 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE/EtOAc = 40/1 as the eluent to give 0.1693 g (0.47 mmol, 80% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be >99/1 by the ¹H NMR analysis of the isolated mixture. ¹H NMR: (400 MHz, CDCl₃) δ 5.80 (d, $J_{\text{H-H}}$ = 0.8 Hz, $J_{\text{Sn-H}}$ = 134 Hz, 1H), 5.29 (d, $J_{\text{H-H}}$ = 2.4 Hz, $J_{\text{Sn-H}}$ = 61 Hz, 1H), 3.63 (t, $J_{\text{H-H}}$ = 6.4 Hz, 2H), 2.52 (t, $J_{\text{H-H}}$ = 6.4 Hz, $J_{\text{Sn-H}}$ = 47 Hz, 2H), 1.58-1.43 (m, 7H),

1.36-1.27 (m, 6H), 1.00-0.85 (m, 15H); 13 C NMR (100 MHz, CDCl₃) δ 151.5, 128.4, 61.3, 44.2, 29.0, 27.3, 13.6, 9.6; The spectroscopic data are in accordance with the literature. 25

N,N-dimethyl-2-(tributylstannyl)prop-2-en-1-amine (3aq). Prepared according to the general procedure using 0.0020 g (0.011 mmol) of Co(OAc)₂, 0.0053 g (0.0154 mmol) of L7, 198 μL (1.08)g/mL. 97%. 0.72 mmol) of HSnBu₃, 0.0500 (0.60)mmol) N,N-dimethylprop-2-yn-1-amine and 1.2 mL (0.5 M) of THF. After 3 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE/EtOAc = 20/1 as the eluent to give 0.1841 g (0.50 mmol, 82% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be >99/1 by the ¹H NMR analysis of the isolated mixture. IR (cm⁻¹): 2956, 2926, 2852, 2815, 2769, 1459. ¹H NMR: (400 MHz, CDCl₃) δ 5.79-5.77 (m, J_{Sn-H} = 134 Hz, 1H), 5.19-5.18 (m, J_{Sn-H} = 61 Hz, 1H), 2.96 (s, $J_{Sn-H} = 46$ Hz, 2H), 2.12 (s, 6H), 1.53-1.45 (m, 6H), 1.36-1.27 (m, 6H), 0.97-0.80 (m, 15H); 13 C NMR (100 MHz, CDCl₃) δ 156.0, 124.8, 70.0, 45.4, 29.2, 27.5, 13.7, 9.6; The spectroscopic data are in accordance with the literature.²³

Tributyl(3-((tetrahydro-2*H*-pyran-2-yl)oxy)prop-1-en-2-yl)stannane (3ar). Prepared according to the general procedure using 0.0022 g (0.012 mmol) of Co(OAc)₂, 0.0049 g (0.0142 mmol) of L7, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 0.0851 g (0.61 mmol) of 2-(prop-2-yn-1-yloxy)tetrahydro-2*H*-pyran and 1.2 mL (0.5 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE as the eluent to give 0.1585 g (0.37 mmol, 61% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be 97/3 by the ¹H NMR analysis of the isolated mixture. IR (cm⁻¹): 2954, 2927, 2872, 2850, 1459. ¹H NMR: (400 MHz, CDCl₃) δ 5.88-5.86 (m, $J_{Sn-H} = 131$ Hz, 1H), 5.25 (d, $J_{H-H} = 2.4$ Hz, $J_{Sn-H} = 63$

Hz, 1H), 4.65-4.63 (m, 1H), 4.58-4.34 (m, $J_{Sn-H} = 46$ Hz, 1H), 4.11-3.99 (m, $J_{Sn-H} = 46$ Hz, 1H), 3.89-3.83 (m, 1H), 3.53-3.49 (m, 1H), 1.89-1.82 (m, 1H), 1.75-1.68 (m, 1H), 1.55-1.48 (m, 8H), 1.35-1.29 (m, 6H), 0.97-0.80 (m, 17H); 13 C NMR (100 MHz, CDCl₃) δ 152.5, 1242, 97.9, 74.2, 61.7, 30.5, 29.1, 27.4, 25.5, 19.2, 13.7, 9.6; HRMS (ESI) calculated for [C₂₀H₄₀NaO₂Sn]⁺[M+Na]⁺ requires m/z 455.1942, found m/z 455.1946.

9-(2-(Tributylstannyl)allyl)-9*H***-carbazole (3as).** Prepared according to the general procedure using 0.0023 g (0.013 mmol) of Co(OAc)₂, 0.0052 g (0.0150 mmol) of **L7**, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 0.1231 g (0.60 mmol) of 9-(prop-2-yn-1-yl)-9*H*-carbazole and 1.2 mL (0.5 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE as the eluent to give 0.2838 g (0.57 mmol, 95% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be >99/1 by the ¹H NMR analysis of the isolated mixture. IR (cm⁻¹): 2955, 2925, 2850, 1628, 1599, 1486. ¹H NMR: (400 MHz, CDCl₃) δ 8.09 (d, $J_{\text{H-H}}$ = 7.6 Hz, 2H), 7.45-7.38 (m, 2H), 7.30 (d, $J_{\text{H-H}}$ = 8.0 Hz, 2H), 7.25-1.17 (m, 2H), 5.51 (d, $J_{\text{H-H}}$ = 2.0 Hz, $J_{\text{Sn-H}}$ = 124 Hz, 1H), 5.25 (d, $J_{\text{H-H}}$ = 2.0 Hz, $J_{\text{Sn-H}}$ = 59 Hz, 1H), 5.00 (s, $J_{\text{Sn-H}}$ = 22 Hz, 2H), 1.45-1.32 (m, 6H), 1.30-1.18 (m, 6H), 0.85 (t, $J_{\text{H-H}}$ = 7.2 Hz, 9H), 0.81-0.70 (m, 6H); ¹³C NMR: (100 MHz, CDCl₃) δ 148.8, 140.6, 125.5, 122.8, 120.2, 118.9, 109.1, 51.4, 29.0, 27.3, 13.7, 9.2; HRMS (EI) calculated for [C₂₇H₃₉NSn]+[M]+ requires m/z 497.2104, found m/z 497.2098.

2-Methyl-3-(tributylstannyl)but-3-en-2-ol (3at). Prepared according to the general procedure using 0.0022 g (0.012 mmol) of Co(OAc)₂, 0.0050 g (0.0144 mmol) of **L7**, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 0.0506 g (0.60 mmol) of 2-methylbut-3-yn-2-ol and 1.2 mL (0.5 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated

and the crude mixture was purified by short flash column chromatography using PE to PE/EtOAc = 50/1 as the eluent to give 0.1975 g (0.53 mmol, 88% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be >99/1 by the ¹H NMR analysis of the isolated mixture. IR (cm⁻¹): 3609, 3479, 2958, 2926, 2870, 1599, 1459. ¹H NMR: (400 MHz, CDCl₃) δ 5.72 (d, $J_{\text{H-H}}$ = 1.6 Hz, $J_{\text{Sn-H}}$ = 138 Hz, 1H), 5.14 (d, $J_{\text{H-H}}$ = 1.6 Hz, $J_{\text{Sn-H}}$ = 68 Hz, 1H), 1.55-1.45 (m, 6H), 1.35-1.25 (m, 12H), 0.95-0.85 (m, 15H); ¹³C NMR: (100 MHz, CDCl₃) δ 164.9, 120.8, 75.7, 30.6, 29.1, 27.4, 13.7, 10.6; HRMS (EI) calculated for [C₁₃H₂₅Sn]⁺[M-Bu-H₂O]⁺ requires m/z 301.0978, found m/z 301.0974.

1-(1-(Tributylstannyl)vinyl)cyclohexan-1-ol (3au). Prepared according to the general procedure using 0.0022 g (0.012 mmol) of Co(OAc)₂, 0.0050 g (0.0144 mmol) of **L7**, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 0.0745 g (0.60 mmol) of 1-ethynylcyclohexan-1-ol and 1.2 mL (0.5 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE to PE/EtOAc = 50/1 as the eluent to give 0.2292 g (0.55 mmol, 92% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be >99/1 by the ¹H NMR analysis of the isolated mixture. IR (cm⁻¹): 3608, 3479, 2927, 2853, 1457. ¹H NMR: (400 MHz, CDCl₃) δ 5.76 (d, $J_{\text{H-H}}$ = 1.2 Hz, $J_{\text{Sn-H}}$ = 141 Hz, 1H), 5.17 (d, $J_{\text{H-H}}$ = 1.2 Hz, $J_{\text{Sn-H}}$ = 71 Hz, 1H), 1.70-1.65 (m, 1H), 1.62-1.52 (m, 7H), 1.52-1.40 (m, 8H), 1.35-1.27 (m, 6H), 1.24-1.10 (m, 1H), 1.00-0.80 (m, 15H); ¹³C NMR: (100 MHz, CDCl₃) δ 165.6, 120.9, 76.2, 37.8, 29.2, 27.4, 25.5, 22.1, 13.7, 10.8; HRMS (EI) calculated for [C₁₆H₂₉Sn]⁺[M-Bu-H₂O]⁺ requires m/z 341.1291, found m/z 341.1290.

3,7-Dimethyl-2-(tributylstannyl)octa-1,6-dien-3-ol (3av). Prepared according to the general procedure using 0.0023 g (0.013 mmol) of $Co(OAc)_2$, 0.0052 g (0.0150 mmol) of L7, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of $HSnBu_3$, 0.0913 g (0.60 mmol) of S33

3,7-dimethyloct-6-en-1-yn-3-ol and 1.2 mL (0.5 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE to PE/EtOAc = 50/1 as the eluent to give 0.1942 g (0.44 mmol, 73% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be >99/1 by the ¹H NMR analysis of the isolated mixture. IR (cm⁻¹): 3609, 3477, 2957, 2924, 2854, 1457. ¹H NMR: (400 MHz, CDCl₃) δ 5.68 (d, $J_{\text{H-H}}$ = 1.6 Hz, $J_{\text{Sn-H}}$ = 140 Hz, 1H), 5.21 (d, $J_{\text{H-H}}$ = 1.6 Hz, $J_{\text{Sn-H}}$ = 67 Hz, 1H), 5.15-5.07 (m, 1H), 2.10-1.90 (m, 2H), 1.68 (s, 3H), 1.63 (s, 1H), 1.60 (s, 3H), 1.55-1.43 (m, 8H), 1.38-1.28 (m, 6H), 1.26 (s, 3H), 1.00-0.85 (m, 15H); ¹³C NMR: (100 MHz, CDCl₃) δ 164.0, 131.8, 124.4, 121.5, 77.9, 42.3, 29.1, 29.0, 27.4, 25.7, 22.8, 17.7, 13.7, 10.6; HRMS (EI) calculated for [C₁₈H₃₃Sn]⁺[M-Bu-H₂O]⁺ requires m/z 369.1604, found m/z 369.1602.

Tributyl(3-phenylhept-1-en-2-yl)stannane (3aw). Prepared according to the general procedure using 0.0020 g (0.011 mmol) of Co(OAc)₂, 0.0049 g (0.0141 mmol) of L7, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 0.0517 g (0.60 mmol) of hept-1-yn-3-ylbenzene and 1.2 mL (0.5 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE as the eluent to give 0.1223 g (0.26 mmol, 44% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be >99/1 by the ¹H NMR analysis of the isolated mixture. IR (cm⁻¹): 2956, 2926, 2857, 1599, 1459. ¹H NMR: (400 MHz, CDCl₃) δ 7.30-7.22 (m, 2H), 7.20-7.10 (m, 3H), 6.00-5.55 (m, J_{Sn-H} = 139 Hz, 1H), 5.32-5.10 (m, J_{Sn-H} = 65 Hz, 1H), 3.42 (t, J_{H-H} = 7.6 Hz, J_{Sn-H} = 48 Hz, 1H), 1.85-1.65 (m, 2H), 1.38-1.15 (m, 16H), 0.90-0.80 (m, 12H), 0.75-0.55 (m, 6H); ¹³C NMR: (100 MHz, CDCl₃) δ 159.0, 144.1, 128.2, 128.1, 126.0, 123.5, 55.2, 33.6, 30.2, 28.9, 27.4, 22.8, 14.1, 13.7, 9.8; HRMS (EI) calculated for [C₂₅H₄₄Sn]⁺[M]⁺ requires m/z 464.2465, found m/z 464.2469.

Ethyl 2-(tributylstannyl)acrylate (3ax). Prepared according to the general procedure using 0.0055 g (0.031 mmol) of Co(OAc)₂, 0.0126 g (0.037 mmol) of **L7**, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 0.0575 g (0.59 mmol) of ethyl propiolate and 1.2 mL (0.5 M) of THF. After 3 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE/EtOAc = 50/1 as the eluent to give 0.1761 g (0.45 mmol, 76% yield) of the title compound as a colorless oil. The ratio of α /β was determined to be 97/3 by the ¹H NMR analysis of the isolated mixture. IR (cm⁻¹): 2957, 2926, 2871, 1716, 1591, 1460. ¹H NMR: (400 MHz, CDCl₃) δ 6.91 (d, $J_{\text{H-H}}$ = 2.4 Hz, $J_{\text{Sn-H}}$ = 110 Hz, 1H), 5.92 (d, $J_{\text{H-H}}$ = 2.4 Hz, $J_{\text{Sn-H}}$ = 53 Hz, 1H), 4.19 (q, $J_{\text{H-H}}$ = 6.8 Hz, 2H), 1.59-1.41 (m, 6H), 1.35-1.26 (m, 9H), 1.06-0.85 (m, 15H); ¹³C NMR (100 MHz, CDCl₃) δ 170.5, 146.1, 139.7, 60.5, 28.9, 27.2, 14.2, 13.6, 10.0; HRMS (ESI) calculated for [C₁₇H₃₄NaO₂Na]⁺ [M+Na]⁺ requires m/z 413.1473, found m/z 413.1475.

(R) - tributyl (1 - (4 - chloro - 3 - (4 - ((tetrahydrofuran - 3 - yl)oxy)benzyl) phenyl) vinyl) stannane ~~(3ay).

Prepared according to the general procedure using 0.0027 g (0.015 mmol) of Co(OAc)₂, 0.0062 g (0.0180 mmol) of L7, 99 μL (1.08 g/mL, 97%, 0.36 mmol) of HSnBu₃, 0.0920 g (0.30 mmol) of (R)-3-(4-(2-chloro-5-ethynylbenzyl)phenoxy)tetrahydrofuran and 1.2 mL (0.25 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE to PE/EtOAc = 20/1 as the eluent to give 0.0807 g (0.14 mmol, 45% yield) of the title compound as a colorless oil. The ratio of α /β was determined to be >99/1 by the ¹H NMR analysis of the isolated mixture. IR (cm⁻¹): 2956, 2925, 2856, 1613, 1509, 1466. ¹H NMR: (400 MHz, CDCl₃) δ 7.30-7.23 (m, 1H), 7.10 (d, $J_{\text{H-H}}$ = 8.8 Hz, 2H), 6.99 (dd, $J_{\text{H-H}}$ = 8.4, 2.4 Hz, 1H), 6.86 (d, $J_{\text{H-H}}$ = 2.0 Hz, 1H), 6.79 (d, $J_{\text{H-H}}$ = 8.4 Hz, 2H), 5.98 (d, $J_{\text{H-H}}$ = 2.4 Hz, $J_{\text{Sn-H}}$ = 126 Hz, 1H), 5.38 (d, $J_{\text{H-H}}$ = 2.0 Hz, $J_{\text{Sn-H}}$ = 59 Hz, 1H), 4.92-4.85 (m, 1H), 4.05-3.85 (m, 6H), 2.24-2.08 (m, 2H), 1.47-1.35 (m, 6H), 1.32-1.20 (m, 6H),

0.95-0.80 (m, 15H); 13 C NMR: (100 MHz, CDCl₃) δ 155.9, 153.5, 145.0, 138.6, 131.9, 131.8, 130.1, 129.3, 129.0, 127.1, 125.0, 115.3, 77.2, 73.1, 67.2, 38.3, 33.0, 28.9, 27.2, 13.6, 10.2; HRMS (ESI) calculated for $[C_{31}H_{46}ClO_2Sn]^+[M+H]^+$ requires m/z 605.2203, found m/z 605.2206.

$$\operatorname{SnBu}_3$$

(*R*)-*N*-(2-(tributylstannyl)allyl)-2,3-dihydro-1*H*-inden-1-amine (3az). Prepared according to the general procedure using 0.0027 g (0.015 mmol) of Co(OAc)₂, 0.0062 g (0.0180 mmol) of L7, 99 μL (1.08 g/mL, 97%, 0.36 mmol) of HSnBu₃, 0.0514 g (0.30 mmol) of (*R*)-*N*-(prop-2-yn-1-yl)-2,3-dihydro-1*H*-inden-1-amine and 1.2 mL (0.25 M) of THF. After 3 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE to PE/EtOAc = 20/1 as the eluent to give 0.1234 g (0.27 mmol, 89% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be >99/1 by the ¹H NMR analysis of the isolated mixture. IR (cm⁻¹): 2955, 2925, 2851, 1458. ¹H NMR: (400 MHz, CDCl₃) δ 7.40-7.30 (m, 1H), 7.25-7.15 (m, 3H), 6.05-5.65 (m, $J_{Sn-H} = 136$ Hz, 1H), 5.30-5.10 (m, $J_{Sn-H} = 63$ Hz, 1H), 4.20 (t, $J_{H-H} = 6.4$ Hz, 1H), 3.65-3.35 (m, 2H), 3.05-2.90 (m, 1H), 2.85-2.72 (m, 1H), 2.50-2.38 (m, 1H), 1.83-1.70 (m, 1H), 1.55-1.40 (m, 6H), 1.35-1.23 (m, 6H), 0.95-0.80 (m, 15H); ¹³C NMR: (100 MHz, CDCl₃) δ 155.4, 145.7, 143.5, 127.2, 126.1, 124.6, 124.2, 63.0, 57.1, 34.2, 30.3, 29.2, 27.4, 13.7, 9.8; HRMS (EI) calculated for [C₂₀H₃₀NSn]⁺[M-C₄H₁₁]⁺ requires m/z 404.1400, found m/z 404.1405.

3-(Tributylstannyl)but-3-en-1-yl (S)-2-(6-methoxynaphthalen-2-yl)propanoate (3aaa). Prepared according to the general procedure using 0.0023 g (0.013 mmol) of Co(OAc)₂, 0.0050 g (0.0144 mmol) of L7, 198 μL (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃, 0.1697 g (0.60 mmol) of but-3-yn-1-yl (S)-2-(6-methoxynaphthalen-2-yl)propanoate and 1.2 mL (0.5 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude

mixture was purified by short flash column chromatography using PE to PE/EtOAc = 20/1 as the eluent to give 0.3440 g (0.60 mmol, >99% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be >99/1 by the ¹H NMR analysis of the isolated mixture. IR (cm⁻¹): 2956, 2927, 2850, 1735, 1607, 1484, 1459. ¹H NMR: (400 MHz, CDCl₃) δ 7.72-7.64 (m, 3H), 7.40 (dd, $J_{\text{H-H}}$ = 8.4, 1.6 Hz, 1H), 7.16-7.07 (m, 2H), 5.85-5.45 (m, $J_{\text{Sn-H}}$ = 133 Hz, 1H), 5.25-5.03 (m, $J_{\text{Sn-H}}$ = 60 Hz, 1H), 4.18-4.03 (m, 2H), 3.89 (s, 3H), 3.82 (q, $J_{\text{H-H}}$ = 7.2 Hz, 1H), 2.49 (t, $J_{\text{H-H}}$ = 7.2 Hz, $J_{\text{Sn-H}}$ = 44 Hz, 2H), 1.56 (d, $J_{\text{H-H}}$ = 7.2 Hz, 3H), 1.50-1.40 (m, 6H), 1.34-1.23 (m, 6H), 0.95-0.80 (m, 15H); ¹³C NMR: (100 MHz, CDCl₃) δ 174.5, 157.5, 150.0, 135.7, 133.6, 129.2, 128.9, 127.7, 127.0, 126.3, 125.9, 118.9, 105.5, 64.0, 55.2, 45.4, 39.8, 29.0, 27.3, 18.5, 13.6, 9.5; HRMS (ESI) calculated for [C₃₀H₄₆NaO₃Sn]⁺[M+Na]⁺ requires m/z 597.2361, found m/z 597.2366.

6,7-Bis(2-methoxyethoxy)-*N***-(3-(1-(tributylstannyl)vinyl)phenyl)quinazolin-4-amine** (3aab). Prepared according to the general procedure using 0.0027 g (0.015 mmol) of Co(OAc)₂, 0.0062 g (0.0180 mmol) of L7, 99 μL (1.08 g/mL, 97%, 0.36 mmol) of HSnBu₃, 0.1170 g (0.30 mmol) of *N*-(3-ethynylphenyl)-6,7-bis(2-methoxyethoxy)quinazolin-4-amine and 1.2 mL (0.25 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using EtOAc as the eluent to give 0.1547 g (0.23 mmol, 76% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be >99/1 by the ¹H NMR analysis of the isolated mixture. IR (cm⁻¹): 3390, 2955, 2925, 1622, 1576, 1507, 1433. ¹H NMR: (400 MHz, CDCl₃) δ 8.65 (s, 1H), 7.75-7.60 (m, 2H), 7.51 (d, $J_{\text{H-H}}$ = 8.0 Hz, 1H), 7.32-7.25 (m, 2H), 7.19 (s, 1H), 6.95 (d, $J_{\text{H-H}}$ = 7.6 Hz, 1H), 6.06 (d, $J_{\text{H-H}}$ = 2.4 Hz, $J_{\text{Sn-H}}$ = 126 Hz, 1H), 5.44 (d, $J_{\text{H-H}}$ = 2.4 Hz, $J_{\text{Sn-H}}$ = 60 Hz, 1H), 4.25-4.15 (m, 4H), 3.85-3.70 (m, 4H), 3.41 (d, $J_{\text{H-H}}$ = 1.6 Hz, 6H), 1.60-1.45 (m, 6H), 1.35-1.22 (m, 6H), 1.10-0.95 (m, 6H), 0.90 (t, $J_{\text{H-H}}$ = 7.2 Hz, 9H); ¹³C NMR: (100 MHz, CDCl₃) δ 156.4, 154.33,

154.31, 153.7, 148.6, 147.2, 138.7, 128.7, 127.0, 122.2, 119.45, 119.41, 109.2, 108.6, 102.7, 70.8, 70.3, 69.0, 68.2, 59.2, 59.1, 29.0, 27.2, 13.6, 10.2; HRMS (ESI) calculated for [C₃₄H₅₂N₃O₄Sn]⁺[M+H]⁺ requires m/z 686.2974, found m/z 686.2984.

$(3S,8S,9S,10R,13R,14S,17R)-10,13-dimethyl-17-((R)-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12\\,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-yl$

4-(tributylstannyl)pent-4-enoate (3aac). Prepared according to the general procedure using 0.0027 g (0.015 mmol) of Co(OAc)₂, 0.0062 g (0.0180 mmol) of L7, 99 μL (1.08 g/mL, 97%, 0.36 mmol) of HSnBu₃, 0.1410 g (0.30)mmol) of (3*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-10,13-dimethyl-17-((*R*)-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,1 3,14,15,16,17-tetradecahydro-1*H*-cyclopenta[a]phenanthren-3-yl pent-4-ynoate and 1.2 mL (0.25 M) of THF. After 1 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE to PE/EtOAc = 20/1 as the eluent to give 0.2273 g (0.30 mmol, >99% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be >99/1 by the ¹H NMR analysis of the isolated mixture. IR (cm⁻¹): 2953, 2869, 1735, 1463. ¹H NMR: (400 MHz, CDCl₃) δ 5.70 (d, $J_{\text{H-H}}$ = 2.0 Hz, $J_{\text{Sn-H}}$ = 136 Hz, 1H), 5.37 (d, $J_{H-H} = 4.0$ Hz, 1H), 5.25-5.05 (m, $J_{Sn-H} = 55$ Hz, 1H), 4.70-4.55 (m, 1H), 2.65-2.45 (m, 2H), 2.42-2.25 (m, 4H), 2.05-1.92 (m, 2H), 1.90-1.78 (m, 3H), 1.65-1.40 (m, 12H), 1.38-1.25 (m, 11H), 1.20-1.06 (m, 6H), 1.05-0.95 (m, 6H), 0.94-0.80 (m, 25H), 0.68 (s, 3H); ¹³C NMR: $(100 \text{ MHz}, \text{CDCl}_3) \delta 172.6, 153.1, 139.7, 125.3, 122.6, 73.8, 56.7, 56.1, 50.0, 42.3, 39.7,$ 39.5, 38.1, 37.0, 36.6, 36.2, 35.8, 34.2, 31.9, 31.8, 29.1, 28.2, 28.0, 27.8, 27.4, 24.3, 23.8, 22.8, 22.5, 21.0, 19.3, 18.7, 13.7, 11.8, 9.5; HRMS (ESI) calculated for $[C_{44}H_{78}NaO_2Sn]^+[M+Na]^+$ requires m/z 781.4916, found m/z 781.4924.

Tributyl(1-(3,5,5,8,8-pentamethyl-5,6,7,8-tetrahydronaphthalen-2-yl)vinyl)stannane (3aad). Prepared according to the general procedure using 0.0027 g (0.015 mmol) of Co(OAc)₂, 0.0062 g (0.0180 mmol) of L7, 99 μL (1.08 g/mL, 97%, 0.36 mmol) of HSnBu₃, 0.0679 g (0.30 mmol) of 6-ethynyl-1,1,4,4,7-pentamethyl-1,2,3,4-tetrahydronaphthalene and 1.2 mL (0.25 M) of THF. After 24 h, the resulting solution was quenched. The combined filtrate was concentrated and the crude mixture was purified by short flash column chromatography using PE as the eluent to give 0.1390 g (0.27 mmol, 90% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be >99/1 by the ¹H NMR analysis of the isolated mixture. IR (cm⁻¹): 2958, 2927, 2868, 1493, 1460. ¹H NMR: (400 MHz, CDCl₃) δ 7.02 (s, 1H), 6.77 (s, 1H), 5.78 (d, $J_{\text{H-H}}$ = 2.0 Hz, $J_{\text{Sn-H}}$ = 136 Hz, 1H), 5.50 (d, $J_{\text{H-H}}$ = 2.0 Hz, $J_{\text{Sn-H}}$ = 63 Hz, 1H), 2.16 (s, 3H), 1.65 (s, 4H), 1.48-1.35 (m, 6H), 1.30-1.20 (m, 18H), 0.95-0.80 (m, 15H); ¹³C NMR: (100 MHz, CDCl₃) δ156.0, 144.0, 141.73, 141.68, 130.0, 127.6, 127.5, 124.7, 35.3, 33.78, 33.76, 31.9, 28.9, 27.3, 20.1, 13.7, 10.3; HRMS (EI) calculated for [C₂₉H₅₀Sn]+[M]⁺ requires m/z 518.2934, found m/z 518.2932.

IV. Gram-Scale Reaction and Efficinecy Tests

Figure S1. Gram-Scale Reaction.

In a nitrogen-filled glovebox, an oven-dried 25 mL vial that contained a magnetic stir bar was charged with 0.0045 g (0.025 mmol, 0.5 mol%) of $Co(OAc)_2$, 0.0103 g (0.030 mmol, 0.6 mol %) of L7, and 1 mL (5 M) of THF. The mixture was stirred for 1 hour. Then 1650 μ L (1.08 g/mL, 97%, 6.0 mmol, 1.2 equiv.) of HSnBu₃ and 550 μ L (0.93 g/mL, 5.0 mmol) alkynes were added sequentially. The mixture was stirred at ambient temperature for 1 minute, and quenched by 5 mL of petroleum ether (PE) and stirred for 5 minutes. The resulting solution was filtered through a pad of silica gel and the vial and silica gel were washed by Et₂O (20 mL \times 3). The combined filtrates

were concentrated *in vacuo*. The residue was purified by short flash column chromatography using PE as the eluent to give 1.7104 g (4.35 mmol, 87% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be 96/4 by the ¹H NMR analysis of the isolated mixture.

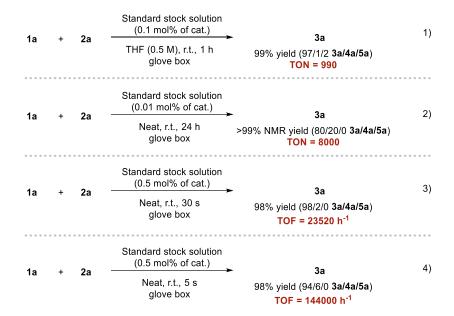


Figure S2. Efficiency Tests of Cobalt-Catalyzed Hydrostannylation of Alkynes.

Preparation of standard stock solution: Co(OAc)₂ (0.1 mmol), **L7** (0.12 mmol) in THF (4 mL) in glove box at room temperature for 4 h until no precipitate remains. The standard stock solution can be used according to the need (0.025 M).

Figure S2, Eq. 1. In a nitrogen-filled glovebox, an oven-dried 25 mL vial that contained a magnetic stir bar was charged with 24 μL of standard stock solution (0.1 mol% catalyst loading) and 1.2 mL (0.5 M) of THF. Then 198 μL (1.08 g/mL, 97%, 0.72 mmol, 1.2 equiv.) of HSnBu₃ and 66 μL (0.93 g/mL, 0.60 mmol) of phenylacetylene were added sequentially. The mixture was stirred at ambient temperature for 1 h, and quenched by 5 mL of petroleum ether (PE) and stirred for 5 minutes. The resulting solution was filtered through a pad of silica gel and the vial and silica gel were washed by Et_2O (20 mL × 3). The combined filtrates were concentrated *in vacuo*. The residue was purified by short flash column chromatography using PE as the eluent to give 0.2336 g (0.594 mmol, 99% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be 97/3 by the ¹H NMR analysis of the isolated mixture.

Figure S2, Eq. 2. In a nitrogen-filled glovebox, an oven-dried 25 mL vial that contained a magnetic stir bar was charged with 24 μL of standard stock solution (0.01 mol% catalyst loading).

Then 1980 μ L (1.08 g/mL, 97%, 7.2 mmol, 1.2 equiv.) of HSnBu₃ and 660 μ L (0.93 g/mL, 6.0 mmol) of phenylacetylene were added sequentially. The mixture was stirred at ambient temperature for 24 h, and quenched by 5 mL of petroleum ether (PE) and stirred for 5 minutes. The resulting solution was filtered through a pad of silica gel and the vial and silica gel were washed by Et₂O (20 mL × 3). The combined filtrates were concentrated *in vacuo*. The NMR yield and the ratio of α/β were determined to be >99% and 80/20 by the ¹H NMR analysis of the mixture, respectively.

Figure S2, Eq. 3. In a nitrogen-filled glovebox, an oven-dried 25 mL vial that contained a magnetic stir bar was charged with 120 μL of standard stock solution (0.5 mol% catalyst loading). Then 1980 μL (1.08 g/mL, 97%, 7.2 mmol, 1.2 equiv.) of HSnBu₃ and 660 μL (0.93 g/mL, 0.60 mmol) of phenylacetylene were added sequentially. The mixture was stirred at ambient temperature for 30 s, and quenched by 10 mL of quenching solution (the quenching solution was consisted of 10 ml of THF, 3 ml of DCM, and 0.6 ml of H₂O) and stirred for 5 minutes. The resulting solution was filtered through a pad of silica gel and the vial and silica gel were washed by Et₂O (20 mL × 3). The combined filtrates were concentrated *in vacuo*. The combined filtrates were concentrated *in vacuo*. The residue was purified by short flash column chromatography using PE as the eluent to give 0.2312 g (0.588 mmol, 98% yield) of the title compound as a colorless oil. The ratio of α/β was determined to be 98/2 by the ¹H NMR analysis of the isolated mixture.

Figure S2, Eq. 4. In a nitrogen-filled glovebox, an oven-dried 25 mL vial that contained a magnetic stir bar was charged with 300 μL of standard stock solution (0.5 mol% catalyst loading). Then 395 μL (1.08 g/mL, 97%, 1.8 mmol, 1.2 equiv.) of HSnBu₃ and 165 μL (0.93 g/mL, 1.5 mmol) of phenylacetylene were added sequentially. The mixture was stirred at ambient temperature for 5 s, and quenched by 10 mL of quenching solution (the quenching solution was consisted of 10 ml of THF, 3 ml of DCM, and 0.6 ml of H₂O) and stirred for 5 minutes. The resulting solution was filtered through a pad of silica gel and the vial and silica gel were washed by Et₂O (20 mL × 3). The combined filtrates were concentrated *in vacuo*. The combined filtrates were concentrated *in vacuo*. The ratio of α/β was determined to be 94/6 by the ¹H NMR analysis of the isolated mixture.

V. Further Derivatizations

1-Methyl-4-(1-phenylvinyl)benzene (6). Prepared according to the previously reported procedure.²⁶ A 25 mL Schlenk flask equipped with a magnetic stirrer and a flanging rubber plug was dried with flame under vacuum. When cooled to ambient temperature, it was vacuumed and flushed with N₂. This degassing procedure was repeated for three times. To the flame-dried Schlenk flask, 0.0119 g (0.01 mmol, 10 mol%) of Pd(PPh₃)₄, 0.0504 g (0.51 mmol, 5.0 equiv.) of CuCl, 0.0265 g of LiCl (0.63 mmol, 6.0 equiv.), 0.5 mL (0.2 M) of DMSO, 0.0218 g (0.10 mmol) of 1-iodo-4-methylbenzene, and 0.0471 g (0.12 mmol, 1.2 equiv.) of 3a were added in sequence. The resulting mixture was stirred at 60 °C for 24 h. After that, the reaction was quenched by addition of H₂O (10 mL) and Et₂O (10 mL). The mixture was washed with NH₃•H₂O (30 mL) and the organic layer was separated. The aqueous layer was extracted with Et_2O (20 mL \times 3). The combined organic layers were washed with brine, dried over Na₂SO₄ and concentrated in vacuo to give a crude oil. The residue was purified by short flash column chromatography using PE as the eluent to give 0.0131 g (0.07 mmol, 67% yield) of the title compound as a colorless oil. ¹H NMR: (400 MHz, CDCl₃) δ 7.35-7.30 (m, 5H), 7.24 (d, J_{H-H} = 8.0 Hz, 2H), 7.14 (d, J_{H-H} = 8.0 Hz, 2H), 5.43-5.40 (m, 2H), 2.36 (s, 3H); 13 C NMR (100 MHz, CDCl₃) δ 149.8, 141.6, 138.6, 137.5, 128.8, 128.3, 128.12, 128.08, 127.6, 113.6, 21.2; The spectroscopic data are in accordance with the literature.²⁷

1-Methoxy-4-(1-phenylvinyl)benzene (7). Prepared according to the previously reported procedure.²⁶ A 25 mL Schlenk flask equipped with a magnetic stirrer and a flanging rubber plug was dried with flame under vacuum. When cooled to ambient temperature, it was vacuumed and flushed with N₂. This degassing procedure was repeated for three times. To the flame-dried

Schlenk flask, 0.0108 g (0.01 mmol, 10 mol%) of Pd(PPh₃)₄, 0.0496 g (0.50 mmol, 5.0 equiv.) of CuCl, 0.0257 g of LiCl (0.60 mmol, 6.0 equiv.), 0.5 mL (0.2 M) of DMSO, 0.0228 g (0.10 mmol) of 1-iodo-4-methoxybenzene, and 0.0470 g (0.12 mmol, 1.2 equiv.) of **3a** were added in sequence. The resulting mixture was stirred at 60 °C for 24 h. After that, the reaction was quenched by addition of H₂O (10 mL) and Et₂O (10 mL). The mixture was washed with NH₃•H₂O (30 mL) and the organic layer was separated. The aqueous layer was extracted with Et₂O (20 mL × 3). The combined organic layers were washed with brine, dried over Na₂SO₄ and concentrated *in vacuo* to give a crude oil. The residue was purified by short flash column chromatography using PE as the eluent to give 0.0191 g (0.09 mmol, 91% yield) of the title compound as a colorless oil. ¹H NMR: (400 MHz, CDCl₃) δ 7.34-7.30 (m, 5H), 7.27 (d, $J_{\text{H-H}}$ = 8.8 Hz, 2H), 6.86 (d, $J_{\text{H-H}}$ = 8.8 Hz, 2H), 5.40-5.35 (m, 2H), 3.82 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 159.3, 149.5, 141.8, 139.9, 129.4, 128.3, 128.1, 127.6, 113.4, 113.0, 55.3; The spectroscopic data are in accordance with the literature.²⁷

Buta-1,3-diene-2,3-diyldibenzene (8). Prepared according to the previously reported procedure. ²⁸ To a 25 mL Schlenk flask covered with aluminum foil to exclude light and equipped with a magnetic stirrer, 0.0495 g (0.5 mmol, 2.5 equiv.) of CuCl and 0.5 mL of DMF were added in sequence, and then 0.0786 g (0.2 mmol, 1.0 equiv.) of **3a** in 0.5 mL of DMF were added. The resulting mixture was stirred at ambient temperature for 2 h. After that, the reaction was quenched by addition of H₂O (10 mL) and Et₂O (10 mL) and stirred for an additional hour. The mixture was then washed with NH₃•H₂O (30 mL) and the organic layer was separated. The aqueous layer was extracted with Et₂O (20 mL × 3). The combined organic layers were washed with H₂O, brine, dried over Na₂SO₄ and concentrated *in vacuo* to give a crude oil. The residue was purified by short flash column chromatography using PE as the eluent to give 0.0127 g (0.12 mmol, 62% yield) of the title compound as a white solid. ¹H NMR: (400 MHz, CDCl₃) δ 7.39 (s, $J_{\text{H-H}}$ = 7.6 Hz, 4H), 7.30-7.18 (m, 6H), 5.54 (s, 2H), 5.31 (s, 2H); ¹³C NMR: (100 MHz, CDCl₃) δ 149.8, 140.1, 128.2, 127.5, 116.4. The spectroscopic data are in accordance with the literature.²⁹

(1-Iodovinyl)benzene (9). Prepared according to the previously reported procedure.³⁰ A 25 mL Schlenk flask equipped with a magnetic stirrer and a flanging rubber plug was dried with flame under vacuum. When cooled to ambient temperature, it was vacuumed and flushed with N_2 . This degassing procedure was repeated for three times. To the flame-dried Schlenk flask, 0.0786 g (0.20 mmol) of 3a, 1 mL (0.2 M) of DCM, and 0.0507 g (0.20 mmol, 1.0 equiv.) of I_2 were added in sequence. The resulting mixture was stirred at ambient temperature for 4 h. After that, the reaction was quenched by addition of Et_2O . The resulting solution was filtered through a pad of silica gel and washed by Et_2O (20 mL × 3). The combined filtrate was concentrated *in vacuo* and the crude mixture was purified by short flash column chromatography using PE as the eluent to give 0.0423 (0.18 mmol, 92% yield) of the title compound as a faint yellow oil. 1 H NMR: (400 MHz, CDCl₃) δ 7.55-7.45 (m, 2H), 7.35-7.25 (m, 3H), 6.46 (s, 1H), 6.08 (s, 1H); 13 C NMR: (100 MHz, CDCl₃) δ 141.6, 128.8, 128.2, 128.1, 127.3, 107.4. The spectroscopic data are in accordance with the literature. 31

1-(Hex-1-en-2-yl)-4-methylbenzene (10). Prepared according to the previously reported procedure. A 25 mL Schlenk flask equipped with a magnetic stirrer and a flanging rubber plug was dried with flame under vacuum. When cooled to ambient temperature, it was vacuumed and flushed with N₂. This degassing procedure was repeated for three times. To the flame-dried Schlenk flask, 0.0230 g (0.02 mmol, 10 mol%) of Pd(PPh₃)₄, 0.0990 g (1.00 mmol, 5.0 equiv.) of CuCl, 0.0256 g of LiCl (0.60 mmol, 3.0 equiv.), 1.0 mL (0.2 M) of DMSO, 0.0441 g (0.20 mmol) of 1-iodo-4-methylbenzene, and 0.0895 g (0.24 mmol, 1.2 equiv.) of 3z were added in sequence. The resulting mixture was stirred at 80 °C for 24 h. After that, the reaction was quenched by addition of H₂O (10 mL) and Et₂O (10 mL). The mixture was washed with NH₃•H₂O (30 mL) and the organic layer was separated. The aqueous layer was extracted with Et₂O (20 mL × 3). The

combined organic layers were washed with brine, dried over Na₂SO₄ and concentrated *in vacuo* to give a crude oil. The residue was purified by short flash column chromatography using PE as the eluent to give 0.0255 g (0.14 mmol, 72% yield) of the title compound as a colorless oil. IR (cm⁻¹): 2957, 2928, 2865, 1626, 1513, 1461. ¹H NMR: (400 MHz, CDCl₃) δ 7.30 (d, $J_{\text{H-H}}$ = 8.0 Hz, 2H), 7.13 (d, $J_{\text{H-H}}$ = 8.0 Hz, 2H), 5.22 (s, 1H), 5.00 (s, 1H), 2.48 (t, $J_{\text{H-H}}$ = 6.8 Hz, 2H), 2.34 (s, 3H), 1.48-1.38 (m, 2H), 1.37-1.27 (m, 2H), 0.89 (t, $J_{\text{H-H}}$ = 7.2 Hz, 3H); ¹³C NMR: (100 MHz, CDCl₃) δ 148.5, 138.5, 137.2, 136.9, 131.2, 128.9, 126.0, 111.2, 35.1, 30.5, 22.4, 21.1, 13.9; HRMS (EI) calculated for [C₁₃H₁₈]⁺[M]⁺ requires m/z 174.1409, found m/z 174.1409.

Methyl 4-(hex-1-en-2-yl)benzoate (11). Prepared according to the previously reported procedure.²⁶ A 25 mL Schlenk flask equipped with a magnetic stirrer and a flanging rubber plug was dried with flame under vacuum. When cooled to ambient temperature, it was vacuumed and flushed with N₂. This degassing procedure was repeated for three times. To the flame-dried Schlenk flask, 0.0231 g (0.02 mmol, 10 mol%) of Pd(PPh₃)₄, 0.0992 g (1.00 mmol, 5.0 equiv.) of CuCl, 0.0257 g of LiCl (0.60 mmol, 3.0 equiv.), 1.0 mL (0.2 M) of DMSO, 0.0524 g (0.20 mmol) of methyl 4-iodobenzoate, and 0.0895 g (0.24 mmol, 1.2 equiv.) of 3z were added in sequence. The resulting mixture was stirred at 80 °C for 24 h. After that, the reaction was quenched by addition of H₂O (10 mL) and Et₂O (10 mL). The mixture was washed with NH₃•H₂O (30 mL) and the organic layer was separated. The aqueous layer was extracted with Et₂O (20 mL \times 3). The combined organic layers were washed with brine, dried over Na₂SO₄ and concentrated in vacuo to give a crude oil. The residue was purified by short flash column chromatography using PE to PE/EtOAc = 100/1 as the eluent to give 0.0349 g (0.16 mmol, 80% yield) of the title compound as a colorless oil. IR (cm⁻¹): 2956, 2866, 1725, 1609, 1436. ¹H NMR: (400 MHz, CDCl₃) δ 7.91 (d, J $= 8.4 \text{ Hz}, 2\text{H}, 7.38 \text{ (d, } J_{\text{H-H}} = 8.4 \text{ Hz}, 2\text{H}), 5.27 \text{ (s, 1H)}, 5.07 \text{ (s, 1H)}, 3.83 \text{ (s, 3H)}, 2.43 \text{ (t, } J_{\text{H-H}} = 8.4 \text{ Hz}, 2\text{H})$ 7.2 Hz, 2H), 1.40-1.22 (m, 4H), 0.82 (t, J_{H-H} = 7.2 Hz, 3H); ¹³C NMR: (100 MHz, CDCl₃) δ 167.0, 147.9, 146.0, 129.6, 128.8, 126.1, 113.9, 52.0, 34.8, 30.3, 22.3, 13.9; HRMS (EI) calculated for $[C_{14}H_{18}O_2]^+[M]^+$ requires m/z 218.1307, found m/z 218.1308.

2-Methyl-3-phenylbut-3-en-2-ol (12). Prepared according to the previously reported procedure.³² A 25 mL Schlenk flask equipped with a magnetic stirrer and a flanging rubber plug was dried with flame under vacuum. When cooled to ambient temperature, it was vacuumed and flushed with N₂. This degassing procedure was repeated for three times. To the flame-dried Schlenk flask, 0.0786 g (0.20 mmol) of **3a**, 2 mL (0.1 M) of anhydrous THF were added, and 125 μL (1.6 M in diethoxymethane, 0.20 mmol, 1.0 equiv.) of MeLi were added dropwise at 0 °C. The resulting mixture was stirred at 0 °C for 0.5 h, and the color of mixture would intensify gradually. Then, 0.0120 g (0.20 mmol) of acetone was added dropwise at 0 °C. The mixture was taken back to ambient temperature and stirred for 16 hrs. The reaction was quenched by addition of Et₂O. The resulting solution was filtered through a pad of silica gel and washed by Et₂O (20 mL × 3). The combined filtrate was concentrated *in vacuo* and the crude mixture was purified by short flash column chromatography using PE to PE/EtOAc = 10/1 as the eluent to give 0.0171 (0.11 mmol, 53% yield) of the title compound as a colorless oil. ¹H NMR: (400 MHz, CDCl₃) δ 7.30 (m, 5H), 5.43 (s, 1H), 4.97 (s, 1H), 1.42 (s, 6H); ¹³C NMR: (100 MHz, CDCl₃) δ 157.0, 141.5, 128.8, 127.8, 127.0, 112.5, 73.0, 29.6. The spectroscopic data are in accordance with the literature.³³

Figure S3. Azidation of Tributyl(1-phenylvinyl)stannane

(1-Azidovinyl)benzene (13). To a 25 mL Schlenk flask equipped with a magnetic stirrer, 0.0786 g (0.20 mmol) of 3a, 2 mL (0.1 M) of MeOH, 0.0399 g (0.20 mmol, 1.0 equiv.) of Cu(OAc)₂•H₂O, and 0.0262 g (0.40 mmol, 2.0 equiv.) of sodium azide were added in sequence. The resulting mixture was stirred at ambient temperature for 16 h. After that, the reaction was quenched with Et₂O. The resulting solution was filtered through a pad of silica gel and washed by Et₂O (20 mL ×

3). The combined filtrate was concentrated *in vacuo* and the crude mixture was purified by short flash column chromatography using PE as the eluent to give 0.0264 g (0.18 mmol, 91% yield) of the title compound as a colorless oil. 1 H NMR: (400 MHz, CDCl₃) δ 7.60-7.52 (m, 2H), 7.40-7.30 (m, 3H), 5.43 (d, $J_{\text{H-H}}$ = 2.0 Hz, 1H), 4.96 (d, $J_{\text{H-H}}$ = 2.0 Hz, 1H); 13 C NMR: (100 MHz, CDCl₃) δ 145.0, 134.2, 129.1, 128.4, 125.5, 98.0. The spectroscopic data are in accordance with those of the literature.³⁴

VI. Mechanistic Studies and Control Experiments

A) Radical Trapping Experiment

Figure S4. Radical Trapping Experiments.

The experiment was conducted according to the general procedure using 0.0022 g (0.012 mmol) of $Co(OAc)_2$, 0.0050 g (0.0144 mmol) of L7, 1.2 mL (0.5 M) of THF, 0.2680 g (1.20 mmol), 2.0 equiv.) of BHT or 0.2163 g (1.20 mmol), 2.0 equiv.) of 1,1-diphenylethylene, $198 \mu L$ (1.08 g/mL), 97%, 0.72 mmol of HSnBu₃, and $66 \mu L$ (0.93 g/mL), 0.60 mmol of phenylacetylene were added in sequence. (The radical scavengers were added before HSnBu₃, considering the reaction could finish with in 1 min) After 1 h, the reaction was quenched with Et_2O . The resulting solution was filtered through a pad of silica gel and washed by Et_2O $(20 \text{ mL} \times 3)$. The combined filtrate was concentrated in *vacuo* and TMSPh was added as the internal standard. The aiming product tributyl(1-phenylvinyl)stannane was observed by 1H NMR in high yield indicating that radical mechanism may be ruled out.

B) H-D Exchange Experiment

Figure S5. H-D Exchange Experiment.

The experiment was conducted according to the general procedure using 0.0022 g (0.012 mmol) of $Co(OAc)_2$, 0.0050 g (0.0144 mmol) of L7, and 1.2 mL (0.5 M) of THF were added in sequence. The mixture was stirred for 30 mins at ambient temperature. Then 0.0309 g (0.30 mmol) of deuterium-phenylacetylene and 39 μ L (1.02 g/mL, 0.30 mmol) of 1-ethynyl-4-methoxybenzene were added sequentially. After 1 h, the reaction was quenched. The resulting solution was filtered through a pad of silica gel and washed by Et_2O (20 mL \times 3). The combined filtrate was concentrated *in vacuo* and the crude mixture was purified by short flash column chromatography using PE as the eluent to give 0.0337 g (0.25 mmol, 85% recovery) of 1-ethynyl-4-methoxybenzene as a colorless oil. There is no hydrogen-hdeuterium exchange in 1-ethynyl-4-methoxybenzene indicating that alkynyl cobalt mechanism may be ruled out.

C) Isotopic Labeling Experiment

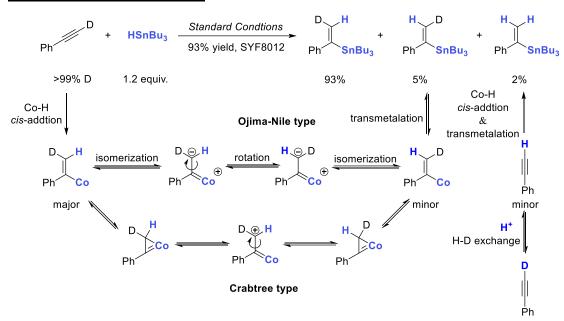


Figure S6. Isotopic Labeling Experiments using Deuterium-phenylacetylene.

The experiment was conducted according to the general procedure using 0.0022 g (0.012 mmol) of $Co(OAc)_2$, 0.0050 g (0.0144 mmol) of **L7**, and 1.2 mL (0.5 M) of THF were added in sequence. The mixture was stirred for 30 mins at ambient temperature. Then 198 μ L (1.08 g/mL, 97%, 0.72 mmol) of HSnBu₃ and 0.0619 g (0.60 mmol) of deuterium-phenylacetylene were added in sequence. After 1 h, the reaction was quenched. The resulting solution was filtered through a pad

of silica gel and washed by Et₂O (20 mL × 3). The combined filtrate was concentrated *in vacuo* and the crude mixture was purified by short flash column chromatography using PE as the eluent to give 0.2200 g (0.56 mmol, 93% yield) of title compound as a colorless oil. Quantitative deuterium spectrum was prepared with 0.0701 g title compound, 15 μ L (1.50 g/mL) CDCl₃ as internal standard (integral: 1.05), and 0.5 mL CHCl₃ as solvent. IR (cm⁻¹): 2957, 2927, 2852, 1597, 1461. ¹H NMR: (400 MHz, CDCl₃) δ 7.35-7.25 (m, 2H), 7.22-7.13 (m, 3H), 6.03 (d, $J_{\text{H-H}}$ = 1.6 Hz, $J_{\text{Sn-H}}$ = 128 Hz, 0.02H), 6.02 (s, $J_{\text{Sn-H}}$ = 127 Hz, 0.05H), 5.40 (s, $J_{\text{Sn-H}}$ = 60 Hz, 1H), 1.55-1.40 (m, 6H), 1.35-1.22 (m, 6H), 0.97 (t, $J_{\text{H-H}}$ = 8.4 Hz, 6H), 0.86 (t, $J_{\text{H-H}}$ = 8.4 Hz, 9H); ²H NMR: (77 MHz, CDCl₃) δ 6.09 (s, 0.93H), 5.49 (s, 0.05H).

D) M-H Species Observation Experiments

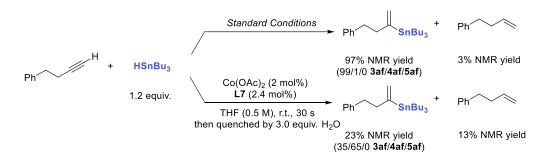
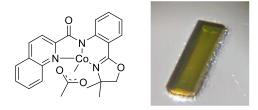


Figure S7. Quench Experiment Using 4-Phenyl-1-Butyne as the Substrate.

In a nitrogen-filled glovebox, an oven-dried 25 mL vial that contained a magnetic stir bar was charged with 0.0022 g (0.012 mmol) of $Co(OAc)_2$, 0.0051 g (0.0147 mmol) of L7, and THF (1.2 mL, 0.5 M). The mixture was stirred for 30 mins. Then 198 μ L (1.08 g/mL, 97%, 0.72 mmol, 1.2 equiv.) of HSnBu₃ and 84 μ L (0.93 g/mL, 0.60 mmol) of 4-phenyl-1-butyne were added sequentially. The mixture was stirred at ambient temperature for 30 s, and immediately quenched by 32.4 μ L of H₂O and stirred for 5 minutes. The resulting solution was filtered through a pad of silica gel and the vial and silica gel were washed by Et₂O (20 mL \times 3). The combined filtrates were concentrated *in vacuo* and 5 μ L of TMSPh was added as an internal standard. The NMR yield and ratio of α/β were determined to be 23% NMR yield and 35/65 by the ¹H NMR analysis of the mixture, respectively. 13% of 4-phenyl-1-butene was observed, indicating that Co-H species might exist in the catalytic system.

E) Preparation and X-ray Diffraction of L7•Co(OAc), (L7)2•Co, and L7•Co(OAc)(Py)



L7•Co(OAc). In a nitrogen-filled glovebox, an oven-dried 25 mL vial that contained a magnetic stir bar was charged with 0.0177 g (0.10 mmol) of Co(OAc)₂, 0.0351 g (0.10 mmol, 1.0 equiv.) of **L7**, and 1 mL (0.1 M) of THF. The mixture was stirred for 30 mins. After that, 27.5 μL of HSnBu₃ (0.10 mmol, 1.0 equiv.) were added. The mixture was stirred at ambient temperature for 4 h and then filtered through a syringe filter with 0.45 μm Nylon membrane. 1 mL of hexane was then added into the solution sequentially. The dark green crystals were obtained in 0.0120 g (0.026 mmol, 26% yield) by using THF/hexane (1/1, 0.05 M) as the solvents in the vial. The vial was sealed with a parafilm with small holes. The solvent evaporates naturally and the green crystals were separated out after about three days. IR (cm⁻¹): 2959, 2925, 1678, 1618, 1555, 1485, 1434. HRMS (ESI) calculated for [C₂₃H₂₁CoN₃NaO₄]⁺[M+Na]⁺ requires m/z 485.0756, found m/z 485.0758.

CCDC Number: 2042974

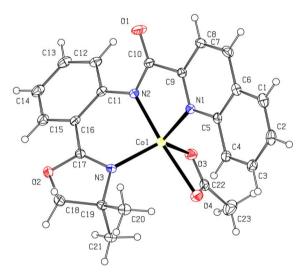


Figure S8. X-ray Diffraction of L7•Co(OAc)

Table S2. Crystal data and structure refinement for L7•Co(OAc).

Identification code	mo_201030_SYF7121_hex_0m
Empirical formula	$C_{23}H_{21}CoN_3O_4\\$
Formula weight	462.36
Temperature/K	170.0

Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	9.9487(6)
b/Å	21.9186(12)
c/Å	10.2914(6)
α/°	90
β/°	114.546(2)
γ/°	90
$Volume/\mathring{A}^3$	2041.3(2)
Z	4
$\rho_{calc}g/cm^3$	1.504
μ /mm ⁻¹	0.877
F(000)	956.0
Crystal size/mm ³	$0.23\times0.07\times0.05$
Radiation	$MoK\alpha (\lambda = 0.71073)$
2θ range for data collection/°	3.716 to 54.254
Index ranges	$\text{-}12 \leq h \leq 12, \text{-}28 \leq k \leq 27, \text{-}13 \leq l \leq 13$
Reflections collected	32929
Independent reflections	$4501 \; [R_{int} = 0.0471, R_{sigma} = 0.0246]$
Data/restraints/parameters	4501/1/283
Goodness-of-fit on F ²	1.041
Final R indexes [I>= 2σ (I)]	$R_1 = 0.0316$, $wR_2 = 0.0868$
Final R indexes [all data]	$R_1 = 0.0402$, $wR_2 = 0.0914$
Largest diff. peak/hole / e Å-3	0.43/-0.40

(**L7**)₂-Co Crystal Growing Solvent: THF/Hex = 1/1, after 7 d Orange Crystal

(L7)₂•Co. In a nitrogen-filled glovebox, an oven-dried 25 mL vial that contained a magnetic stir bar was charged with 0.0180 g (0.10 mmol) of Co(OAc)₂, 0.0350 g (0.10 mmol, 1.0 equiv.) of L7, and 2 mL (0.05 M) of THF. The mixture was stirred for 30 mins. After that, 275 μL of HSnBu₃ (0.10 mmol, 1.0 equiv.) were added. The mixture was stirred at ambient temperature for 4 h and then filtered through a syringe filter with 0.45 μm Nylon membrane. 1 mL of hexane was then added into the solution sequentially. The orange solid were obtained by using THF/hexane (1/1,

0.05 M) as the solvents in the vial. The vial was sealed with a parafilm with small holes. The solvent evaporates naturally and the orange crystals were separated out after about seven days. HRMS (ESI) calculated for $[C_{42}H_{37}CoN_6O_4]^+[M+H]^+$ requires m/z 748.2203, found m/z 748.2198.

CCDC Number: 2095773

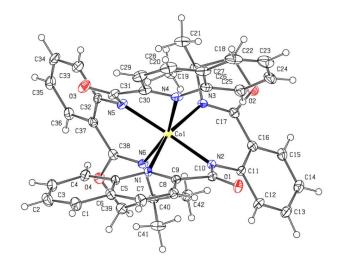


Figure S9. X-ray Diffraction of (L7)₂•Co

Table S3. Crystal data and structure refinement for (L7)2•Co

\ /=
mo_210524_SYF9163_0m_tw
$C_{42}H_{36}CoN_6O_4$
747.70
170.0
monoclinic
P2 ₁ /c
10.4657(19)
19.413(3)
18.184(3)
90
106.225(6)
90
3547.2(10)
4
1.400
0.537
1556.0
$0.09 \times 0.06 \times 0.05$
$MoK\alpha (\lambda = 0.71073)$
4.196 to 54.454

Index ranges $-13 \le h \le 13$, $-24 \le k \le 24$, $-11 \le l \le 23$ 7759 Reflections collected Independent reflections 7759 [$R_{int} = ?, R_{sigma} = 0.0499$] 7759/0/483 Data/restraints/parameters Goodness-of-fit on F² 1.157 Final R indexes [I>= 2σ (I)] $R_1 = 0.0971$, $wR_2 = 0.2812$ Final R indexes [all data] $R_1 = 0.1041, wR_2 = 0.2870$ Largest diff. peak/hole / e Å⁻³ 0.78/-1.00

L7•Co(OAc)(Py)
Crystal Growing Solvent: THF/Hex = 1/1, after 2 d
Red Crystal

L7•Co(OAc)(Py) In a nitrogen-filled glovebox, an oven-dried 25 mL vial that contained a magnetic stir bar was charged with 0.0088 g (0.05 mmol) of $Co(OAc)_2$, 0.0172 g (0.05 mmol, 1.0 equiv.) of **L7**, and 2 mL (0.025 M) of THF. The mixture was stirred for 30 mins. After that, 27.5 μ L of HSnBu₃ (0.10 mmol, 1.0 equiv.) and 42 μ L of pyridine (0.0525 mmol, 1.05 equiv.) were added in sequence. The mixture was stirred at ambient temperature for 4 h and then filtered through a syringe filter with 0.45 μ m Nylon membrane. 1 mL of hexane was then added into the solution sequentially. The red crystals were obtained by using THF/hexane (1/1, 0.05 M) as the solvents in the vial. The vial was sealed with a parafilm with small holes. The solvent evaporates naturally and the red crystals were separated out after about two days.

CCDC Number: 2165238

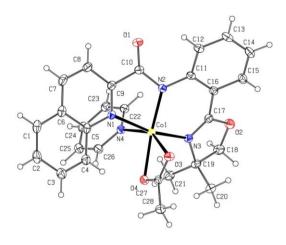


Figure S10. X-ray Diffraction of L7•Co(OAc)(Py)

Table S4. Crystal data and structure refinement for L7•Co(OAc)(Py)

Table 54. Ci ystai uata anu su	ucture refinement for L7-Co(OAC)(1 y)
Identification code	mo_220304_SYF12101_0m
Empirical formula	$C_{28}H_{26}CoN_4O_4$
Formula weight	541.46
Temperature/K	170.0
Crystal system	triclinic
Space group	P-1
a/Å	9.6488(5)
b/Å	11.3292(6)
c/Å	11.5795(6)
$lpha/\circ$	90.599(2)
β/°	97.306(2)
γ/°	101.688(2)
Volume/Å ³	1228.63(11)
Z	2
$\rho_{calc}g/cm^3$	1.464
μ/mm^{-1}	0.742
F(000)	562.0
Crystal size/mm ³	$0.4\times0.29\times0.23$
Radiation	$MoK\alpha (\lambda = 0.71073)$
2Θ range for data collection/°	4.348 to 54.334
Index ranges	$-12 \le h \le 12$, $-14 \le k \le 14$, $-14 \le l \le 14$
Reflections collected	51954
Independent reflections	5431 [$R_{int} = 0.0245$, $R_{sigma} = 0.0128$]
Data/restraints/parameters	5431/0/337
Goodness-of-fit on F ²	1.039
Final R indexes [I>= 2σ (I)]	$R_1 = 0.0234$, $wR_2 = 0.0605$
	S54

Final R indexes [all data]	$R_1 = 0.0255, wR_2 = 0.0617$
Largest diff. peak/hole / e Å-3	0.30/-0.27

F) L7•Co(OAc) Catalyzed Hydrostannylation of alkyne.

Figure S11. L7•Co(OAc) Catalyzed Hydrostannylation of alkyne.

The experiment was conducted according to the general procedure using 0.0028 g (0.006 mmol) of L7•Co(OAc), and 0.6 mL (0.5 M) of THF were added in sequence. The mixture was stirred for 30 mins at ambient temperature. Then 99 μ L (1.08 g/mL, 97%, 0.36 mmol) of HSnBu₃ and 33 μ L (0.93 g/mL, 0.30 mmol) of phenylacetylene were added in sequence. After 1 h, the reaction was quenched. The resulting solution was filtered through a pad of silica gel and washed by Et₂O (20 mL × 3). The combined filtrate was concentrated *in vacuo* and the crude mixture was purified by short flash column chromatography using PE as the eluent to give 0.1144 g (0.29 mmol, 97% yield) of title compound as a colorless oil. The ratio of α/β was determined to be 99.5/0.5 by the ¹H NMR analysis of the isolated mixture.

G) Proposed Detailed Mechanism

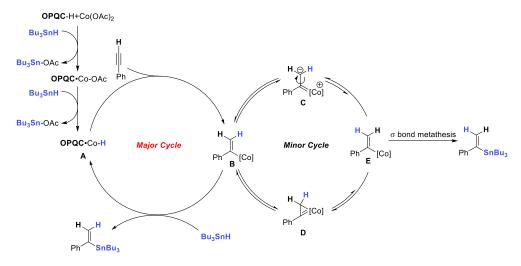


Figure S12. Proposed Detailed Mechanism of Cobalt-Catalyzed Hydrostannylation of Alkynes.

H) DFT Details

All density functional theory (DFT) calculation results are obtained with Gaussian 16 program.³⁵ Default G16 SCF convergence criteria (scf=tight), optimization convergence criteria and integral grid parameters (int=(ultrafine, acc2e=12)) for Gaussian 16 are applied unless

otherwise stated. Geometry optimizations are conducted with B3LYP functional, ³⁶⁻³⁷ employing the D3 version of Grimme's dispersion corrections ³⁸ with Becke-Johnson damping ³⁹ and def2-SVP ⁴⁰basis set was used for all atoms basis set for all atoms. The solvation effects were induced with a self-consistent reaction field (SCRF) using the PCM solvent model in THF⁴¹⁻⁴². MECP (minimum energy crossing point) was acquired using Gaussian 16 and sobMECP⁴³⁻⁴⁴ software. Single-point energies and solvent effects at THF are also evaluated with the same functional as optimization and def2-TZVPP⁴⁵ basis set for all atoms, in a self-consistent reaction field (SCRF) using the SMD implicit solvent model ⁴⁶. Frequency analysis is also performed at the same level of theory as geometry optimization using harmonic oscillator model to confirm whether optimized stationary points are either local minimum or transition state, as well as to evaluate zero-point vibrational energies and thermal corrections for enthalpies and free energies at 298.15 K.

To correct the Gibbs free energies under 1 atm to the standard state in solution (1 mol/L), a correction of $RT\ln(c_s/c_g)$ is added to energies of all species. c_s stands for the standard molar concentration in solution (1 mol/L), c_g stands for the standard molar concentration in gas phase (about 0.040876 mol/L), and R is the gas constant. For calculated intermediates at the standard state of 1 mol/L at 298.15 K, the correction value equaling to 1.89 kcal/mol is used.

Energy decomposition analysis (EDA) was conducted with sobEDA⁴⁷ and Multiwfn⁴⁸ software. The 3D diagrams of optimized structures shown in this supplementary information for computations are generated with CYLview software.⁴⁹

Discussion on Spin Multiplicity

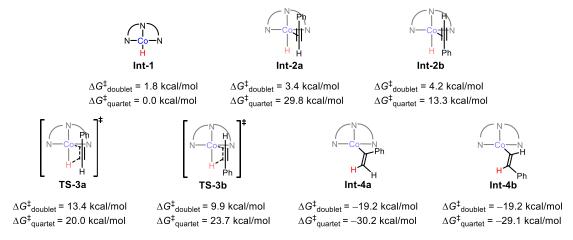


Fig S13. Gibbs free energy of spices in the free energy diagram at doublet state and quartet state.

Energy Decomposition Analysis

Energy decomposition analysis (Figure S12.) suggested that distortion of ligand dominated the regionselectivity of the reaction, consistent with the results obtained from distortion/interaction analysis. The corresponding decomposition equations are as follows:

$$\Delta E_{+}^{\dagger} = \Delta E_{\mathrm{dist}} + \Delta E_{\mathrm{int}}$$

$$\Delta E_{\mathrm{int}} = \Delta E_{\mathrm{els}} + \Delta E_{\mathrm{xrep}} + \Delta E_{\mathrm{orb}} + \Delta E_{\mathrm{disp}}$$

$$\Delta E_{\mathrm{xrep}} = \Delta E_{\mathrm{ex}} + \Delta E_{\mathrm{rep}}$$

 $\Delta E_{\rm dist}$: distortion energy. $\Delta E_{\rm int}$: interaction energy. $\Delta E_{\rm els}$: electrostatic interaction energy. $\Delta E_{\rm orb}$: orbital interaction energy. $\Delta E_{\rm disp}$: dispersion energy. $\Delta E_{\rm ex}$: exchange energy. $\Delta E_{\rm rep}$: Pauli repulsion energy.

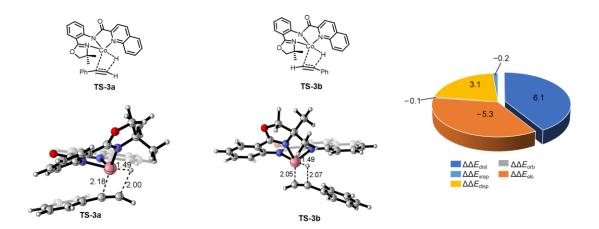


Fig S14. Energy Decomposition Analysis. EDA of $\Delta\Delta E^{\ddagger}$ (TS-3b-TS-3a) with optimized key structures of TS-3a and TS-3b

Table of Energies

Table S5 Energies in Fig S13 and Fig S14. Zero-point correction (*ZPE*), thermal correction to enthalpy (*TCH*), thermal correction to Gibbs free energy (*TCG*), energies (*E*), enthalpies (*H*), and Gibbs free energies (*G*) (in Hartree) of the structures calculated at B3LYP-D3(BJ)/def2-TZVPP-SMD(THF)//B3LYP-D3(BJ)/def2SVP-PCM(THF) level of theory.

Structure	ZPE	ТСН	TCG	E	Н	G	Imaginary Frequency
1a	0.109758	0.117072	0.079347	-308.547202	-308.430130	-308.467855	

2a	0.369624	0.391311	0.315489	-688.782568	-688.391257	-688.467079	
3a	0.486228	0.515309	0.419695	-997.394469	-996.879160	-996.974774	
Int-1(quartet)	0.357677	0.381400	0.304597	-2509.856865	-2509.475465	-2509.552268	
Int-1	0.360211	0.383359	0.308197	-2509.857673	-2509.474314	-2509.549476	
Int1(MECP)				-2509.846289			
Int-2a(quartet)	0.469528	0.500780	0.407245	-2818.376902	-2817.876122	-2817.969657	
Int-2a	0.471848	0.502910	0.410560	-2818.422308	-2817.919398	-2818.011748	
Int-2b(quartet)	0.468065	0.500371	0.400701	-2818.396600	-2817.896229	-2817.995899	
Int-2b	0.471706	0.502902	0.409318	-2818.419700	-2817.916798	-2818.010382	
TS-3a(quartet)	0.467499	0.498810	0.403853	-2818.389117	-2817.890307	-2817.985264	557.3i
TS-3a	0.471749	0.502044	0.410469	-2818.411725	-2817.909681	-2818.001256	47.9 <i>i</i>
TS-3b(quartet)	0.467798	0.498946	0.404214	-2818.383486	-2817.884540	-2817.979272	427.8i
TS-3b	0.471600	0.501767	0.410994	-2818.406755	-2817.904988	-2817.995761	23.4 <i>i</i>
Int-4a(MECP)				-2818.458773			
Int-4a(quartet)	0.474453	0.505528	0.411409	-2818.476652	-2817.971124	-2818.065243	
Int-4a	0.476061	0.506338	0.415860	-2818.463633	-2817.957295	-2818.047773	
Int-4b(quartet)	0.474964	0.506114	0.409303	-2818.472794	-2817.96668	-2818.063491	
Int-4b	0.476500	0.506880	0.414623	-2818.461944	-2817.955064	-2818.047321	

Cartesian Coordinates of Computed Species

1a Charge = 0, Multiplicity = 1

C	2.02698000	-0.00007900	-0.00004700
C	0.59431500	-0.00003600	-0.00001600
C	-0.12056200	-1.21546500	0.00002300
C	-0.12049100	1.21543500	-0.00002300
C	-1.51526000	-1.21063500	0.00005200
Н	0.42892700	-2.15865700	0.00003000
C	-1.51519000	1.21068700 S58	0.00000500

Н	0.42905200	2.15859600	-0.00005300
C	-2.21632900	0.00004700	0.00004300
Н	-2.05900500	-2.15811000	0.00008200
Н	-2.05887900	2.15819400	-0.00000200
Н	-3.30873400	0.00007800	0.00006600
C	3.24187200	-0.00004400	-0.00006100
Н	4.31663500	0.00044000	0.00001700

2a

Sn	0.00000300	-0.91912500	-0.47667600
Н	0.00008100	-1.99805100	-1.83961200
C	-1.80162800	-1.22727400	0.71571200
Н	-1.90308300	-2.30674800	0.91638600
Н	-1.62487300	-0.73953300	1.68941800
C	-3.06739700	-0.67274400	0.05838100
Н	-3.22392700	-1.15243300	-0.92554700
Н	-2.93907000	0.40444700	-0.15486100
C	-4.33140200	-0.85860200	0.90484900
Н	-4.17796300	-0.37733600	1.88779400
Н	-4.46873700	-1.93491700	1.11416500
C	-5.58969500	-0.29566500	0.24543900
Н	-5.78306100	-0.78352900	-0.72471500
Н	-6.48084100	-0.44233100	0.87642800
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C	1.80160400	-1.22714300	0.71578800
Н	1.90301100	-2.30658400	0.91666200
Н	1.62485900	-0.73921400	1.68940200

C	3.06740200	-0.67278600	0.05836700
Н	2.93911700	0.40436800	-0.15508400
Н	3.22392700	-1.15267200	-0.92546600
C	4.33139000	-0.85852600	0.90488700
Н	4.46868600	-1.93480600	1.11441000
Н	4.17795400	-0.37706700	1.88773800
C	5.58971100	-0.29575700	0.24538600
Н	5.48914800	0.78605900	0.05492900
Н	6.48084300	-0.44232800	0.87641600
Н	5.78307500	-0.78381600	-0.72467000
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Н	0.88500900	1.29654000	-1.81028600
Н	-0.88517600	1.29652100	-1.81019000
C	0.0000100	2.14502600	-0.00660000
Н	-0.88020500	1.96948000	0.63954300
Н	0.88027200	1.96948900	0.63945600
C	-0.00002800	3.61188100	-0.44985200
Н	-0.88172100	3.79224600	-1.09110900
Н	0.88157700	3.79224200	-1.09122800
C	0.00005700	4.59737100	0.71790800
Н	0.00004800	5.64249700	0.36935700
Н	-0.88855300	4.45788600	1.35635700
Н	0.88874300	4.45786600	1.35624800

3a

C	-0.95042100	0.57463300	1.34092300
С	-2.32458400	0.77474100	0.82693500

C	-2.54434200	1.38018100	-0.42608000
C	-3.45028400	0.33575900	1.55250100
С	-3.83564000	1.56204800	-0.92456000
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С	-4.74192400	0.50915100	1.05148200
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Н	-5.59867100	0.15261300	1.62902200
Н	-5.95231700	1.25621900	-0.58241900
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Н	0.36758500	0.53015200	3.02297000
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Н	4.92034400	-1.31419700	1.62731000
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Н	-1.23745000	-4.13319800	-2.02447600
Н	-2.62086500	-3.04193900	-2.10535200
C	-2.79537800	-4.57203300	-0.58134700
Н	-3.55103800	-4.04624800	0.02619600
Н	-3.32555700	-5.29185900	-1.22528900
Н	-2.15933900	-5.14840700	0.11146900
C	1.27632900	1.65625400	-1.21962400
Н	0.57079900	1.82710900	-2.05003300
Н	2.24056000	1.37786000	-1.67745800
C	1.42392600	2.91393000	-0.36166600
Н	2.11727900	2.71831500	0.47737000
Н	0.45560400	3.16038800	0.11082200
C	1.92210200	4.13630800	-1.13971800
Н	2.89468100	3.89488000	-1.60557600
Н	1.22811200	4.33509700	-1.97649400
C	2.05981200	5.38845300	-0.27472600
Н	2.41790200	6.25067400	-0.85966900
Н	1.09298200	5.66830900	0.17632300
Н	2.77270200	5.22527000	0.55099000

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C	-5.54718300	-0.22020800	0.23923400
Н	-6.38864800	-0.84725900	0.54203900
C	-5.74245500	1.09440800	-0.12729500
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C	-4.64081900	1.89630200	-0.51934500
Н	-4.81120100	2.93261300	-0.82020700
C	-3.36058500	1.38264600	-0.53090500
Н	-2.50193400	1.97436300	-0.84896100
C	-3.13200000	0.03416100	-0.15252500
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C	-3.98796800	-2.13738200	0.57660900
Н	-4.82035100	-2.78394400	0.86525600
C	-2.69891200	-2.61653600	0.54532300
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C	-1.64853700	-1.74123900	0.18655800
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C	3.93232100	-3.15574500	-0.39389500
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C	4.86831600	-2.12313400	-0.26147600
Н	5.93975200	-2.32805800	-0.29960000
C	4.40658400	-0.82736900	-0.08467500
Н	5.11425100	-0.00479700	0.01432000
C	3.02685700	-0.53252900	-0.03505300

C	2.67072200	0.86936100	0.17003900
C	3.10481300	2.98826500	0.80625000
Н	3.70387200	3.74680600	0.28546400
Н	3.16340000	3.15841600	1.89200800
C	1.64407700	2.89317400	0.29291500
C	0.62949000	3.32828200	1.35186900
Н	-0.39781600	3.16747100	0.99098900
Н	0.74651200	4.39955900	1.57971500
Н	0.76492000	2.75450800	2.28118700
C	1.45000000	3.66827000	-1.01354900
Н	2.18135100	3.34350200	-1.76911600
Н	1.58470800	4.74637700	-0.83533700
Н	0.44312900	3.48595300	-1.41284100
Co	-0.12655500	0.50135100	-0.48548500
Н	-0.58568400	1.42826100	-1.68959700

Int-1(quartet)

Charge = 0, Multiplicity = 4				
O	0.23295200	-3.38766600	0.59988000	
O	3.34752900	1.87596200	0.89678600	
N	-1.76526900	-0.57247000	-0.20663900	
N	0.81480800	-1.27963700	-0.22239500	
N	1.37688900	1.47871400	-0.06400700	
C	-5.42189000	-0.40366300	0.42353100	
Н	-6.22208700	-1.03583000	0.81526800	
C	-5.68091600	0.88363400	0.00231100	
Н	-6.69520700	1.28467400	0.05640300	
C	-4.63372500	1.69268600	-0.50811800	
Н	-4.85419100	2.70744200 S64	-0.84675300	

C	-3.34421400	1.21013100	-0.58776800
Н	-2.53427900	1.81351900	-0.99891800
C	-3.04911500	-0.10812700	-0.15139300
C	-4.10468000	-0.93155400	0.35720500
C	-3.77458400	-2.24621100	0.78058500
Н	-4.56272100	-2.89644700	1.16815700
C	-2.47183700	-2.68028800	0.70593600
Н	-2.15924300	-3.67383600	1.02420000
C	-1.48073700	-1.79857800	0.21076500
C	-0.03148100	-2.25117800	0.19460800
C	2.19180400	-1.45504400	-0.19625700
C	2.81071100	-2.71359800	-0.39016000
Н	2.17566400	-3.57918500	-0.55594700
C	4.19356800	-2.85592800	-0.36193400
Н	4.62996500	-3.84429500	-0.52850400
C	5.02798600	-1.75535200	-0.12312600
Н	6.11310200	-1.87195500	-0.09806700
C	4.45053300	-0.50929500	0.08004100
Н	5.07606800	0.36331100	0.27003100
C	3.05220000	-0.33595000	0.03763400
C	2.53385100	1.00895800	0.27385400
C	2.67206900	3.15050100	0.97172000
Н	3.24801900	3.87654500	0.37982100
Н	2.65850000	3.46774000	2.02331200
C	1.25713400	2.88265000	0.38800100
C	0.15292000	2.96021000	1.44695000
Н	-0.80442900	2.62830500	1.01455200
Н	0.03145300	3.99250800	1.80971400
Н	0.38613900	2.30941000	2.30308300

C	0.94486400	3.79210100	-0.80122300
Н	1.71398100	3.69142600	-1.58134900
Н	0.90476100	4.84407100	-0.47875700
Н	-0.02728600	3.52562800	-1.24053600
Co	-0.06534600	0.40971600	-1.00404000
Н	-0.70947400	0.82536700	-2.46764300

Int-1

Charge $= 0$,	Multiplicity = 2
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N	-1.56686400	1.39368000	0.09153000
C	5.55402300	-0.15502400	-0.21837500
Н	6.42770200	-0.79492200	-0.07493300
C	5.69600500	1.15180300	-0.63216400
Н	6.68973200	1.56433700	-0.81917200
C	4.54988500	1.96491900	-0.81896000
Н	4.67118400	2.99793500	-1.15273800
C	3.28482000	1.47015800	-0.58128000
Н	2.39228000	2.08167600	-0.70106300
C	3.10861500	0.12902700	-0.15270900
C	4.26451200	-0.70179600	0.02295500
C	4.07337400	-2.04894400	0.42384600
Н	4.94349700	-2.69190500	0.57565500
C	2.79585100	-2.52944300	0.59360000
Н	2.57952300	-3.55933800	0.87464900

C	1.70458300	-1.66040300	0.38357400
C	0.29547800	-2.20140900	0.45252900
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C	-3.69184400	-3.30898600	-0.63506400
Н	-3.95410300	-4.35629800	-0.80716600
C	-4.68504200	-2.32143500	-0.67565600
Н	-5.72711600	-2.58044300	-0.87271300
C	-4.31666700	-1.00162800	-0.46506000
Н	-5.06687100	-0.21279400	-0.49859200
C	-2.97518600	-0.63723600	-0.21135700
C	-2.70769000	0.78410200	-0.02164500
C	-3.33974200	2.94589900	0.02672900
Н	-3.88563700	3.49290400	0.80670700
Н	-3.57457200	3.38432700	-0.95585600
C	-1.81737100	2.85260300	0.28760500
C	-1.02917800	3.68254200	-0.72302800
Н	0.04767300	3.57829200	-0.53803900
Н	-1.30675100	4.74497000	-0.63605100
Н	-1.24378900	3.34887400	-1.74987100
C	-1.46894000	3.24132000	1.72688900
Н	-2.06128000	2.65051900	2.44286600
Н	-1.68307100	4.30875300	1.89354000
Н	-0.40329600	3.05454200	1.91493900
Co	0.14417400	0.54915700	0.08927300
Н	0.79708000	1.85186800	0.48743000

Int-2a(quartet)

Charge =	0,	Multi	plicity	= 4
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O	0.22595000	-3.36735500	-0.31088800
O	-3.00660400	2.13828600	-0.82352700
N	2.31478800	-0.45826100	-0.34142300
N	-0.22911800	-1.10109200	-0.75758900
N	-0.85488200	1.66126800	-0.51304700
C	5.99033300	-0.59340000	0.22782500
Н	6.75348000	-1.34621900	0.44276000
C	6.34322800	0.74962600	0.10589900
Н	7.38339300	1.06078500	0.22485400
C	5.34635500	1.69209700	-0.17511200
Н	5.60426200	2.74870600	-0.28207100
C	4.01759900	1.29734900	-0.32673400
Н	3.24922100	2.03595300	-0.55486400
C	3.63108900	-0.05383700	-0.19734500
C	4.65701600	-1.02197800	0.07996700
C	4.28451500	-2.40823200	0.19719100
Н	5.05655500	-3.14898000	0.41581900
C	2.97137800	-2.77467900	0.02253400
Н	2.63799200	-3.81065000	0.09311000
C	1.99319700	-1.80428500	-0.26125800
C	0.60151700	-2.19245800	-0.45217800
C	-1.53520100	-1.25532600	-1.14935600
C	-2.07193700	-2.50731700	-1.57549600
Н	-1.41158300	-3.36689900	-1.57875700
C	-3.39605100	-2.64747400	-1.94761600
Н	-3.75282500	-3.62995500	-2.26822600
С	-4.28401000	-1.55655000	-1.91467000

Н	-5.33213000	-1.67742900	-2.19436000
C	-3.79735300	-0.32370500	-1.52945900
Н	-4.45644500	0.54267300	-1.50633400
C	-2.43994100	-0.13891800	-1.16479100
C	-2.04459400	1.20240400	-0.81640400
C	-2.45169300	3.36518400	-0.32181100
Н	-2.82763300	3.51555300	0.70201200
Н	-2.79547600	4.18888900	-0.96013400
C	-0.92368400	3.14547400	-0.36401100
C	-0.28775800	3.79074300	-1.59891000
Н	0.76613400	3.48787000	-1.68009800
Н	-0.33285700	4.88795400	-1.52258900
Н	-0.81170800	3.48046900	-2.51583300
C	-0.26229200	3.63579900	0.92090300
Н	-0.63866900	3.08722500	1.79501100
Н	-0.47495300	4.70726700	1.05790800
Н	0.82719300	3.50343700	0.87784400
Co	0.69931300	0.57435200	-0.36392300
Н	1.43989600	1.83505300	-0.15675900
C	-0.17518000	0.06375600	2.23768700
C	-1.54394300	-0.34395000	2.18681700
C	-2.56636700	0.61205100	2.35846200
C	-1.88706400	-1.67951000	1.89935300
C	-3.90208800	0.24266800	2.21997800
Н	-2.30005900	1.64462000	2.58844900
C	-3.22687800	-2.03942700	1.76765100
Н	-1.10337900	-2.41878500	1.73274300
C	-4.23461500	-1.08251500	1.91824100
Н	-4.68678400	0.99274300	2.33888000

Н	-3.48319200	-3.07071200	1.51864700
Н	-5.28134900	-1.36824600	1.79447000
C	0.98061800	0.45313400	2.23250600
Н	2.00198500	0.76997600	2.34399500

Int-2a

Charge = 0, Multiplicity =	2
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O	0.30276300	-3.28380800	-0.12390600
O	-3.07519200	2.05147700	-0.84245800
N	2.36435300	-0.41483000	-0.26443500
N	-0.15507300	-1.07186900	-0.74970700
N	-0.90884200	1.65919700	-0.46522200
C	6.06296400	-0.55866900	0.17108600
Н	6.83304900	-1.29842800	0.40154500
C	6.39477800	0.75923700	-0.05685700
Н	7.43719900	1.08097900	-0.00597900
C	5.38058500	1.70044600	-0.36382500
Н	5.65180300	2.74164600	-0.55311500
C	4.05635600	1.32032600	-0.42714600
Н	3.25713100	2.02573200	-0.64848600
C	3.68275100	-0.02842800	-0.19090000
C	4.70964100	-0.98720900	0.10321200
C	4.33352600	-2.33879700	0.30975600
Н	5.10084800	-3.07900600	0.54854800
C	3.01183000	-2.69659900	0.18883700
Н	2.65685400	-3.71860800	0.31406900
C	2.05746700	-1.70265700	-0.11546500
C	0.61894000	-2.10602700	-0.33304200

C	-1.45540100	-1.27455200	-1.18578700
C	-1.91739400	-2.53492800	-1.64616600
Н	-1.22804600	-3.37263700	-1.63027100
C	-3.22107300	-2.72391600	-2.08370900
Н	-3.52613800	-3.71479200	-2.43085600
C	-4.14187500	-1.66809000	-2.07652600
Н	-5.17225600	-1.81860800	-2.40452700
C	-3.71611300	-0.42051300	-1.64720700
Н	-4.40921500	0.41911800	-1.63780800
C	-2.39052100	-0.19477400	-1.21760100
C	-2.05620300	1.16611500	-0.81595400
C	-2.59598100	3.28565000	-0.28789100
Н	-3.01255200	3.39069500	0.72654900
Н	-2.95418900	4.11349300	-0.91385600
C	-1.05898200	3.13344100	-0.28072300
C	-0.41079000	3.83710400	-1.47703100
Н	0.65014700	3.55617600	-1.52873300
Н	-0.49112400	4.93039500	-1.37192200
Н	-0.90007100	3.53835600	-2.41729600
C	-0.46136500	3.62102200	1.03582200
Н	-0.84321800	3.03497000	1.88301700
Н	-0.72427500	4.67942000	1.19188100
Н	0.63051900	3.51923500	1.01867000
Co	0.72809700	0.67329900	-0.34151700
Н	1.46611800	1.95800900	-0.06170100
С	-0.25111300	-0.01017200	2.28918300
C	-1.62135400	-0.40219100	2.16731600
C	-2.64352800	0.55825500	2.30823200
C	-1.96717000	-1.73049500	1.85243900

С	-3.97609000	0.20331200	2.10990000
Н	-2.37946800	1.58591200	2.55972300
C	-3.30350300	-2.07759500	1.66146500
Н	-1.18429000	-2.47581200	1.71187000
C	-4.30936900	-1.11460400	1.78029200
Н	-4.75739700	0.96074800	2.20384800
Н	-3.55747400	-3.10416100	1.39033900
Н	-5.35262000	-1.38918500	1.60974600
C	0.90601600	0.35828600	2.36957300
Н	1.92424500	0.67057600	2.50447700

Int-2b(quartet)

0	1.82649900	-3.79382600	-0.18253300
0	3.86218000	1.88841000	1.06910600
N	-1.10997500	-1.85949300	0.15371900
N	1.53406900	-1.47881500	-0.18846000
N	1.76599000	1.10976200	1.07640900
C	-4.48807900	-3.34433400	0.60200100
Н	-4.94600600	-4.32603300	0.74382200
С	-5.26202300	-2.20420700	0.55051000
Н	-6.34702600	-2.27276200	0.65467700
C	-4.65388500	-0.93734700	0.35769800
Н	-5.27625500	-0.04072500	0.31212300
C	-3.28607500	-0.82355500	0.22942500
Н	-2.80801300	0.14141800	0.09368400
С	-2.46490000	-1.97909300	0.28449100
С	-3.07612700	-3.26238600	0.46568000

C	-2.23012400	-4.40211600	0.49290200
Н	-2.67045300	-5.39218100	0.63494100
C	-0.87362600	-4.24751600	0.32895200
Н	-0.17863400	-5.08588800	0.32141200
C	-0.34950300	-2.94276300	0.15871700
C	1.13748800	-2.77514000	-0.08681600
C	2.78958900	-1.17880400	-0.70632100
C	3.41344700	-2.01429900	-1.66963300
Н	2.90794400	-2.92881300	-1.96718900
C	4.64433900	-1.70190000	-2.22919300
Н	5.07635600	-2.37441900	-2.97489300
C	5.33076900	-0.54037100	-1.84848900
Н	6.30292100	-0.29607300	-2.28093900
C	4.74600400	0.30037800	-0.91454300
Н	5.25426100	1.21353000	-0.60737800
С	3.48488300	0.01424600	-0.34435200
C	2.96827600	0.98362600	0.62066900
С	3.20858300	2.69990700	2.06028800
Н	3.39963900	3.75612600	1.82638200
Н	3.64713700	2.45982300	3.04120800
C	1.71270600	2.30482800	1.96025400
C	1.12946500	1.94878800	3.32639300
Н	0.08985100	1.61533900	3.21097400
Н	1.15983000	2.82683800	3.99100300
Н	1.70763500	1.13695700	3.79382400
C	0.88895400	3.39359000	1.26724300
Н	1.32824600	3.65287100	0.29133000
Н	0.85596000	4.30200600	1.88900800
Н	-0.13609800	3.04171400	1.10184800

Co	0.13792100	-0.10150800	0.52933700
Н	-0.95736300	0.62636300	1.53673800
С	-0.92395900	1.44611600	-1.63320800
С	-1.90402700	2.46883100	-1.40807400
С	-2.45484800	2.70150500	-0.13237500
С	-2.34285800	3.24414900	-2.50188000
С	-3.42586500	3.68794200	0.03935000
Н	-2.10347600	2.09597400	0.70711700
С	-3.31417700	4.22732700	-2.31829100
Н	-1.91790400	3.06449300	-3.49102400
C	-3.85881800	4.45197000	-1.04894400
Н	-3.84694200	3.86062300	1.03244100
Н	-3.64886200	4.82145700	-3.17152400
Н	-4.62028400	5.22272300	-0.90952500
C	-0.11576100	0.58514200	-1.93581000
Н	0.58453800	-0.16458900	-2.25626000

Int-2b

0	-0.98020800	-3.54737700	0.71426200
O	-4.11680700	2.01278900	-0.27007800
N	1.06543900	-0.99529700	-0.62969500
N	-1.51637500	-1.39836500	-0.06432400
N	-1.96593200	1.41685200	-0.35430300
C	4.66642700	-1.55363700	-1.42647300
Н	5.40317600	-2.35783900	-1.36338000
C	5.01432500	-0.31225500	-1.91069300
Н	6.03729600	-0.11538800	-2.23868700

C	4.04068700	0.71418500	-1.98080100
Н	4.32225500	1.69820100	-2.36238700
C	2.74456300	0.49246700	-1.56872600
Н	1.98289100	1.26937000	-1.59687500
C	2.35564800	-0.77209000	-1.05751300
C	3.34013500	-1.81477800	-0.98973500
C	2.95764300	-3.07343900	-0.46500400
Н	3.69812100	-3.87363700	-0.39360600
C	1.66006700	-3.26548100	-0.05543900
Н	1.29717500	-4.20812200	0.35113100
C	0.73863900	-2.20177800	-0.16814800
C	-0.70110300	-2.45118200	0.21735700
C	-2.89408700	-1.49042900	0.06968800
C	-3.57583600	-2.72750600	0.24281400
Н	-2.98068700	-3.63101100	0.30795800
C	-4.95831100	-2.80337200	0.34267600
Н	-5.42572300	-3.78371100	0.46917700
C	-5.75047100	-1.64960100	0.28833900
Н	-6.83715300	-1.70651900	0.37633900
C	-5.12141200	-0.42694800	0.11606200
Н	-5.71238900	0.48604400	0.06347400
C	-3.71671200	-0.31785300	-0.00212300
C	-3.19394200	1.02848400	-0.21024100
C	-3.41793400	3.26671800	-0.29659000
Н	-3.52109500	3.73892900	0.69353200
Н	-3.88285100	3.90988800	-1.05532200
C	-1.95547500	2.88601400	-0.61761700
C	-1.61855300	3.12010800	-2.09326700
Н	-0.63455200	2.68475100	-2.31400600

Н	-1.59717600	4.19846500	-2.31581500
Н	-2.36808700	2.64329100	-2.74414700
C	-0.97957300	3.61575600	0.30048900
Н	-1.16943700	3.35870200	1.35288600
Н	-1.09137800	4.70446900	0.17525600
Н	0.05010300	3.32792300	0.05566900
Co	-0.43337600	0.26322800	-0.40601800
Н	0.40168400	1.45551700	-0.76320300
C	0.69584200	0.63912300	2.02789100
C	2.08428800	0.94017900	1.86569300
C	3.04138800	-0.09064300	1.93512900
C	2.50978700	2.25710300	1.60479600
C	4.39161300	0.19060200	1.73409000
Н	2.71205900	-1.11315200	2.12672400
C	3.86209000	2.52977900	1.40718300
Н	1.76936000	3.05535600	1.54710200
C	4.80566900	1.49842100	1.46603800
Н	5.12289800	-0.61923900	1.77162000
Н	4.18215800	3.55299200	1.19755600
Н	5.86331000	1.71362300	1.29824100
C	-0.47924300	0.35570800	2.17670200
Н	-1.50354100	0.11639100	2.39257000

Int-4a(MECP)

O	0.02312800	-3.17913600	-1.23560000
O	-3.78359400	2.06992300	-0.49030000
N	1.75766300	-0.12050100	-0.88500800

N	-0.78433200	-0.99257700	-0.93540600
N	-1.62751900	1.66772800	-0.11797600
C	5.45171700	0.17046400	-1.07950100
Н	6.32589700	-0.47448900	-1.19530600
C	5.59234400	1.53815800	-0.97020500
Н	6.58563800	1.99042500	-0.99797300
C	4.44997800	2.36621600	-0.82592900
Н	4.57644700	3.44823200	-0.74651200
C	3.18459400	1.81920500	-0.78594300
Н	2.30127800	2.44882400	-0.67361800
C	3.01388700	0.41687600	-0.90372900
C	4.16177000	-0.42379300	-1.05441200
C	3.94861800	-1.82303200	-1.18081500
Н	4.80957400	-2.48738500	-1.28584400
C	2.66697600	-2.32287300	-1.18065100
Н	2.44355700	-3.38326000	-1.28776600
C	1.58194700	-1.42827900	-1.03456300
C	0.16223800	-1.96394500	-1.07404000
C	-2.14001400	-1.23697200	-1.08148600
C	-2.66223200	-2.50732800	-1.45307900
Н	-1.95815300	-3.32227500	-1.57728400
C	-4.01891700	-2.72080500	-1.65497300
Н	-4.36065300	-3.71954900	-1.94094900
C	-4.94496900	-1.68111700	-1.49841700
Н	-6.01201900	-1.84641800	-1.65957500
C	-4.47560300	-0.43100900	-1.13120900
Н	-5.17399700	0.39437500	-0.99963700
C	-3.10104500	-0.18054400	-0.90919100
C	-2.76770000	1.18073100	-0.50485600

C	-3.20917000	3.37171900	-0.26001600
Н	-3.88475700	3.93842200	0.39226300
Н	-3.11412400	3.88203800	-1.23261200
C	-1.84433600	3.05389000	0.37725600
C	-0.72582500	3.97591400	-0.09242800
Н	0.22657500	3.67843900	0.37091400
Н	-0.93426500	5.01549100	0.20346500
Н	-0.61682500	3.93754600	-1.18639300
C	-1.94506000	3.02349000	1.90736500
Н	-2.78434500	2.38617800	2.22649100
Н	-2.11606400	4.04024000	2.29410900
Н	-1.01874100	2.62236200	2.33767300
Co	0.05854600	0.69593100	-0.18792000
C	0.79212300	0.75520300	1.67007200
C	0.47108600	-0.56997400	2.22952300
C	1.48083600	-1.52894800	2.44819800
C	-0.86956100	-0.96830400	2.42372600
C	1.16375400	-2.83059500	2.84812400
Н	2.52176400	-1.24464300	2.27663900
C	-1.18400800	-2.26351900	2.83066600
Н	-1.66661500	-0.24773800	2.22876200
C	-0.16848800	-3.20529300	3.04177100
Н	1.96361500	-3.55970800	3.00119500
Н	-2.22985600	-2.54757700	2.97100300
Н	-0.41684600	-4.22543100	3.34467900
C	1.56869300	1.64766100	2.30253700
Н	1.85393200	2.60310500	1.84607900
Н	1.95949800	1.47463800	3.31718500

Int-4a(quartet)

Charge $= 0, N$	Iultiplicity = 4
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O	-0.67365000	-3.20608600	-1.59524900
O	-4.27414700	1.63716300	-0.36246100
N	1.09615300	-0.19274100	-1.00274000
N	-1.25982600	-1.30736200	-0.36696800
N	-2.07837500	1.41083600	-0.06074200
C	4.66372500	0.33676900	-1.87097800
Н	5.50337900	-0.21853700	-2.29507700
C	4.81422700	1.64821100	-1.47117100
Н	5.78104500	2.14501100	-1.57579900
C	3.71866100	2.35923500	-0.91823700
Н	3.85493300	3.39415100	-0.59725700
C	2.49074600	1.75154100	-0.76926400
Н	1.64788100	2.27575100	-0.31824400
C	2.30995400	0.40517300	-1.17398500
C	3.41010400	-0.31688800	-1.73457200
C	3.18765700	-1.66449900	-2.12034500
Н	4.01071700	-2.23924500	-2.55171100
C	1.94686400	-2.23266900	-1.94078600
Н	1.72417600	-3.26250200	-2.21678300
C	0.91691600	-1.46071500	-1.35619400
C	-0.44355800	-2.09679500	-1.10744200
C	-2.57883600	-1.63459600	-0.09131000
C	-3.02665200	-2.96974800	0.04185100
Н	-2.30665400	-3.76946700	-0.10952400
C	-4.34925500	-3.26347700	0.35440700
Н	-4.65154200	-4.30818400	0.46464500

C	-5.29087700	-2.24067500	0.53062400
Н	-6.32868000	-2.47394200	0.77614300
C	-4.88485100	-0.92089000	0.38487000
Н	-5.60273000	-0.10951900	0.50576400
C	-3.54677600	-0.59363700	0.08243800
C	-3.23326400	0.82527000	-0.10435200
C	-3.77922100	2.99244000	-0.39752000
Н	-4.14013400	3.51093200	0.50383800
Н	-4.18689500	3.48385400	-1.29037600
C	-2.23723100	2.83968100	-0.41842200
C	-1.64706700	3.05247800	-1.81729800
Н	-0.57935700	2.78623300	-1.82121300
Н	-1.74778000	4.10497500	-2.12409600
Н	-2.16057800	2.41953400	-2.55692800
C	-1.55360800	3.73316800	0.61313700
Н	-1.95972500	3.55013200	1.61836500
Н	-1.70574600	4.79376500	0.36077300
Н	-0.47264600	3.53503800	0.64064400
Co	-0.40263600	0.37470000	0.32358800
C	0.61206700	0.66433700	2.04108600
C	1.86860400	-0.11632500	2.09999300
C	3.11862900	0.50577400	2.29374000
C	1.86286500	-1.50596100	1.85593400
C	4.30803400	-0.22540700	2.24037200
Н	3.14867200	1.58544800	2.45628000
C	3.04824200	-2.24005700	1.81175100
Н	0.90599400	-2.00730100	1.68848600
C	4.28061500	-1.60222500	1.99732600
Н	5.26448800	0.28613500	2.37870900

Н	3.01188000	-3.31558200	1.61938200	
Н	5.21108200	-2.17290500	1.94543600	
С	0.28711400	1.51924000	3.02946000	
Н	-0.61783500	2.13583800	2.98874000	
Н	0.90096200	1.63724800	3.93705500	

Int-4a

O	-0.07149500	-3.24848100	-0.93716100
O	-3.67867700	2.11393000	-0.53158000
N	1.72297600	-0.22342400	-0.78067200
N	-0.79653400	-1.01298500	-0.95369200
N	-1.54924400	1.61684900	-0.10076500
C	5.41134600	0.04775000	-1.08876100
Н	6.27790400	-0.60598300	-1.21072500
C	5.56331400	1.41553800	-1.01054100
Н	6.55882000	1.86087900	-1.06573200
C	4.42790100	2.25365800	-0.86599600
Н	4.56039300	3.33660600	-0.81768800
C	3.16125300	1.71587700	-0.78384200
Н	2.28585100	2.35499000	-0.67690400
C	2.97940600	0.31149200	-0.85492600
C	4.11857000	-0.53930700	-1.02209400
C	3.89957200	-1.93825000	-1.12188400
Н	4.75644100	-2.60629400	-1.23609600
C	2.61488300	-2.43190900	-1.08860500
Н	2.38339800	-3.49250300	-1.17641100
C	1.54156600	-1.53070000	-0.92729600

C	0.11410700	-2.03027700	-0.93588700
C	-2.15799300	-1.24180500	-1.07643900
C	-2.70451800	-2.50015600	-1.44811900
Н	-2.02102400	-3.33060300	-1.58457000
C	-4.06923700	-2.68762400	-1.62259500
Н	-4.43420700	-3.67795500	-1.90791900
C	-4.97365200	-1.63364900	-1.43855900
Н	-6.04667100	-1.78238100	-1.57364900
C	-4.47563200	-0.39136000	-1.07955000
Н	-5.15504900	0.44709900	-0.93204300
C	-3.09289300	-0.17145800	-0.88568000
C	-2.70555500	1.17869900	-0.50053700
C	-3.04525400	3.39228800	-0.34017500
Н	-3.70098200	4.01808200	0.27746900
Н	-2.90858000	3.85980600	-1.32931400
C	-1.70710400	3.03678900	0.33335100
C	-0.55016100	3.89299100	-0.16779600
Н	0.38541100	3.59689600	0.32493400
Н	-0.73303600	4.95386000	0.06335400
Н	-0.42757200	3.78880100	-1.25624600
C	-1.83775000	3.08588300	1.86024700
Н	-2.70806400	2.49793600	2.19076000
Н	-1.97773600	4.12734300	2.18981400
Н	-0.93684200	2.67702300	2.33271900
Co	0.08278100	0.66330600	-0.27233300
C	0.77875100	0.86367600	1.52809200
C	0.42505600	-0.42924200	2.15473600
C	1.42600000	-1.37672000	2.44775800
C	-0.91910400	-0.80571200	2.35641500

C	1.09731300	-2.65233400	2.91476900
Н	2.47096000	-1.10766200	2.27622400
C	-1.24653100	-2.07447400	2.83299200
Н	-1.70991200	-0.09385000	2.11478000
C	-0.24033400	-3.00931700	3.10692000
Н	1.89167100	-3.37474800	3.12081900
Н	-2.29618500	-2.34310400	2.97760800
Н	-0.49927500	-4.00989400	3.46139900
C	1.55502200	1.76570400	2.14664800
Н	1.88091300	2.69584800	1.66989400
Н	1.89921500	1.61756700	3.18046600

Int-4b(quartet)

Chargo -	Λ	Multiplicity = 4
Charge =	v.	MuluDliCliv = 4

O	-2.25520300	2.74636000	-2.18441300
O	-3.71719500	-1.80075700	1.82893700
N	0.35195900	1.80863300	0.03566000
N	-1.88762700	0.75916500	-1.01118600
N	-1.75450600	-0.88597500	1.30425200
C	3.16042700	4.05123300	0.96866500
Н	3.53989600	5.04574800	0.72331900
C	3.80768700	3.25595100	1.89058600
Н	4.71157300	3.61604000	2.38632700
C	3.30614300	1.96567200	2.20030900
Н	3.83105100	1.34464300	2.92931300
C	2.16827500	1.48585400	1.58691400
Н	1.78867200	0.48710000	1.80251500
С	1.48216400	2.28550300	0.63579500

1.98399300	3.58884600	0.31976900
1.26976200	4.35931400	-0.63476400
1.63341900	5.35590400	-0.89669200
0.13033200	3.84842900	-1.21357800
-0.46062600	4.40109400	-1.94260100
-0.30548900	2.55376300	-0.84741200
-1.59867600	2.00999800	-1.44383700
-3.09085700	0.12468500	-1.28213600
-3.84474400	0.37338800	-2.45324100
-3.47034400	1.11320200	-3.15527600
-5.03365200	-0.30118900	-2.70856600
-5.57785100	-0.09101100	-3.63303100
-5.53471700	-1.24254600	-1.80020000
-6.46810500	-1.77154300	-2.00206000
-4.82641300	-1.49290600	-0.63222500
-5.20397900	-2.21374900	0.09271100
-3.61160200	-0.83330400	-0.35264100
-2.96550700	-1.14423900	0.92678600
-2.93125400	-1.98122100	3.02486100
-2.92366300	-3.05140600	3.27331500
-3.41776000	-1.42328900	3.83817200
-1.52669000	-1.42377300	2.66313900
-1.09146300	-0.29142300	3.59562900
-0.13055700	0.13071000	3.26585300
-0.96875300	-0.66523500	4.62397600
-1.83825600	0.51651700	3.60139600
-0.46717700	-2.52768200	2.59948500
-0.78872700	-3.33607200	1.92557100
-0.29626200	-2.95164900	3.60104600
	1.26976200 1.63341900 0.13033200 -0.46062600 -0.30548900 -1.59867600 -3.09085700 -3.84474400 -3.47034400 -5.03365200 -5.57785100 -5.53471700 -6.46810500 -4.82641300 -5.20397900 -3.61160200 -2.96550700 -2.93125400 -2.92366300 -3.41776000 -1.52669000 -1.09146300 -0.13055700 -0.96875300 -1.83825600 -0.46717700 -0.78872700	1.269762004.359314001.633419005.355904000.130332003.84842900-0.460626004.40109400-0.305489002.55376300-1.598676002.00999800-3.090857000.12468500-3.844744000.37338800-3.470344001.11320200-5.03365200-0.30118900-5.57785100-0.09101100-5.53471700-1.24254600-6.46810500-1.77154300-4.82641300-1.49290600-5.20397900-2.21374900-3.61160200-0.83330400-2.96550700-1.14423900-2.93125400-1.98122100-2.92366300-3.05140600-3.41776000-1.42328900-1.52669000-1.42377300-1.09146300-0.29142300-0.130557000.13071000-0.96875300-0.66523500-1.838256000.51651700-0.46717700-2.52768200-0.78872700-3.33607200

Н	0.48263500	-2.12679400	2.21727100
Co	-0.40585200	-0.12866300	0.01409800
C	3.47035800	-1.95567600	-1.06040000
C	3.35434400	-3.35628700	-1.17695300
C	4.74684100	-1.38873800	-1.24853600
C	4.46372700	-4.14924700	-1.46673100
Н	2.37799600	-3.82592900	-1.03839000
C	5.86036100	-2.18033300	-1.53865000
Н	4.85914100	-0.30407200	-1.16132600
C	5.72520700	-3.56734700	-1.64953300
Н	4.34623000	-5.23281500	-1.55260400
Н	6.83826700	-1.71222500	-1.67892800
Н	6.59297400	-4.19124200	-1.87695000
C	1.04690700	-1.40771700	-0.48002900
Н	0.82435000	-2.48956000	-0.51971900
C	2.33014800	-1.07189000	-0.74572400
Н	2.61646700	-0.01076700	-0.72181800

Int-4b

0	-1.96283000	2.78005300	-2.22407900
O	-3.40071400	-2.40696500	1.39625600
N	0.44960200	1.86832400	0.17497200
N	-1.96446600	1.10655300	-0.57204100
N	-1.52696500	-1.30277800	0.91086700
C	3.41434900	3.92003700	1.05561000
Н	3.90791200	4.83785600	0.72829100
C	3.91800800	3.18346400	2.10640200

Н	4.82406900	3.51026900	2.62076100
C	3.25673800	2.00361100	2.53381900
Н	3.65584700	1.43758300	3.37815600
C	2.11714000	1.56438600	1.89416700
Н	1.60191800	0.66065400	2.21895200
C	1.58677000	2.29719100	0.80201200
C	2.23177700	3.50552500	0.38500100
C	1.64443400	4.24569300	-0.67402200
Н	2.12846500	5.16235800	-1.01872200
C	0.46225200	3.81447300	-1.23324700
Н	-0.05194400	4.35724200	-2.02543200
C	-0.11862000	2.61763900	-0.76300200
С	-1.46503600	2.16239400	-1.28095700
C	-3.25228800	0.62513900	-0.76159700
C	-4.22977200	1.30630100	-1.53642000
Н	-3.93171300	2.21602900	-2.04559600
C	-5.52969500	0.83391300	-1.66239700
Н	-6.24016400	1.39858700	-2.27205600
C	-5.93535600	-0.34536300	-1.02477400
Н	-6.95638200	-0.71795400	-1.12667500
C	-5.00937200	-1.03298700	-0.25629800
Н	-5.29809300	-1.95056500	0.25461100
C	-3.67785800	-0.58143000	-0.11383600
C	-2.80837600	-1.39842300	0.72338800
C	-2.43351500	-2.92389100	2.32804200
Н	-2.53755800	-4.01506500	2.37006300
Н	-2.64826300	-2.49292800	3.31974300
C	-1.08183900	-2.44867100	1.75990100
C	-0.11886300	-1.98219600	2.84631200

Н	0.82965700	-1.65647200	2.39683800
Н	0.09874800	-2.80844700	3.54091800
Н	-0.54828900	-1.14781600	3.42096100
C	-0.44836400	-3.53422500	0.88091300
Н	-1.14984100	-3.85849200	0.09694700
Н	-0.19293700	-4.40742600	1.50120800
Н	0.46693800	-3.16397800	0.40437200
Co	-0.46575400	0.18634800	0.38937500
C	3.20072500	-1.84336700	-0.96869900
C	2.76906900	-2.79405200	-1.91793000
C	4.58595700	-1.75586900	-0.72058000
C	3.68004100	-3.61006400	-2.58747100
Н	1.70260900	-2.89488600	-2.13029300
C	5.50035100	-2.57181200	-1.39018600
Н	4.94431300	-1.02787800	0.01312100
C	5.05303600	-3.50560900	-2.32983400
Н	3.31654800	-4.33839800	-3.31742300
Н	6.56852600	-2.47829300	-1.17677300
Н	5.76444000	-4.14729600	-2.85521700
C	0.94561500	-0.85270800	-0.38806800
Н	0.50265600	-1.49282600	-1.17053800
C	2.28080200	-0.95825200	-0.22919700
Н	2.79039000	-0.34775900	0.52432900

TS-3a(quartet)

O	0.20285400	-2.38795600	-2.42481000
O	-3.16114600	2.62050600	-0.93475800

N	2.22064300	-0.24143300	-0.44473500
N	-0.41492500	-0.61994900	-1.03561100
N	-1.08291300	2.07897500	-0.32123000
C	5.90905400	-0.66985500	-0.18614600
Н	6.68873100	-1.33542700	-0.56386200
C	6.21953600	0.37607000	0.65658900
Н	7.25452700	0.54951000	0.95902900
C	5.19553400	1.23564400	1.12820100
Н	5.45401600	2.06827100	1.78660100
C	3.88013900	1.03787500	0.76362600
Н	3.07925600	1.69651300	1.09992300
C	3.52880200	-0.03825600	-0.09345200
C	4.56482600	-0.90054700	-0.58316000
C	4.19374800	-1.95495400	-1.45639800
Н	4.96474700	-2.62478400	-1.84535200
C	2.87385600	-2.11891700	-1.80128400
Н	2.52931300	-2.90774200	-2.46772900
C	1.90522000	-1.23621600	-1.26301700
C	0.44784400	-1.47133200	-1.63252900
C	-1.78767500	-0.81201700	-1.11493900
C	-2.36650000	-2.08949800	-1.31108900
Н	-1.70477500	-2.93934900	-1.44144500
C	-3.74106500	-2.27649900	-1.32104200
Н	-4.13889400	-3.28656800	-1.44860900
C	-4.61587500	-1.19409500	-1.15926600
Н	-5.69769200	-1.34090900	-1.17112800
C	-4.08120600	0.07282000	-0.97959500
Н	-4.73890400	0.93196000	-0.85035600
C	-2.68656300	0.28545400	-0.94184800

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TS-3a Charge = 0, Multiplicity = 2

Ciluigo	o, manipuoti =		
O	0.07902900	2.19245700	-2.15218300
O	3.85428200	-2.11243700	-0.61335400
N	-1.51256900	-0.48575200	-0.45351100
N	0.85563500	0.73110000	-0.51288000
N	1.76004100	-1.77725100	0.08962000
C	-5.08209000	-1.39996500	-0.95779600
Н	-5.94485800	-1.07191300	-1.54259400
C	-5.18256800	-2.46937800	-0.09201800
Н	-6.13091700	-3.00027600	0.01612500
C	-4.05619700	-2.88292600	0.66307900
Н	-4.14835700	-3.72863600	1.34843100
C	-2.84860200	-2.22713800	0.54285700
Н	-1.97054300	-2.51651400	1.12010000
C	-2.71549700	-1.12568500	-0.34283400
C	-3.85347800	-0.70245500	-1.10445700
C	-3.69333400	0.40778800	-1.97712100
Н	-4.54492100	0.75010100	-2.57033500
C	-2.47528200	1.03698500	-2.05323700
Н	-2.29112400	1.89962800	-2.69195600
C	-1.40082900	0.56125700	-1.26057800
C	-0.06524500	1.26673400	-1.34356700
C	2.17621500	1.14808100	-0.53148200
C	2.56545600	2.49396600	-0.71264400
Н	1.78849100	3.23700700	-0.87020000
C	3.90793600	2.86130100	-0.68867300

Н	4.17504100	3.91431500	-0.81138800
C	4.91580700	1.90305200	-0.51077800
Н	5.96693900	2.19784600	-0.49558300
C	4.55978200	0.56656100	-0.36418600
Н	5.32637400	-0.20059700	-0.24727300
C	3.20787600	0.17759700	-0.36347100
C	2.88158900	-1.24536800	-0.27836300
C	3.26254600	-3.42808500	-0.64168700
Н	3.94530200	-4.12710500	-0.14184000
Н	3.14363100	-3.72278900	-1.69602500
C	1.90361200	-3.25663900	0.08251100
C	0.74780400	-3.89295100	-0.68478900
Н	-0.20193300	-3.69750400	-0.16797700
Н	0.88890800	-4.98247300	-0.75999000
Н	0.67959000	-3.47510000	-1.70021700
C	1.97499600	-3.77441300	1.52283700
Н	2.81939200	-3.31474700	2.05958000
Н	2.11248500	-4.86679700	1.52507000
Н	1.04872000	-3.53193200	2.06116500
Co	0.26884000	-0.68241400	0.79913200
Н	-0.14569100	-1.86949700	1.59197000
C	-0.56739800	0.83486800	2.11703200
C	-0.91184100	2.14010400	1.64464100
C	-2.20867500	2.39661100	1.15453500
C	0.05335800	3.16664300	1.59458100
C	-2.52738600	3.64865300	0.62953900
Н	-2.95569700	1.60177100	1.17895200
С	-0.27477600	4.41406200	1.06840700
Н	1.06419900	2.96675300	1.95252100

C	-1.56329400	4.65996300	0.57955500
Н	-3.53373200	3.83053500	0.24544500
Н	0.48495500	5.19812800	1.02746800
Н	-1.81298300	5.63620100	0.15803800
С	-0.36945100	-0.24031100	2.72184500
Н	-0.37637500	-0.85153700	3.61321400

TS-3b(quartet)

О	-2.15507700	3.62804600	-0.19047400
O	-3.61557800	-2.06430600	1.36612700
N	0.91652000	1.88623500	0.14527000
N	-1.71189500	1.34225400	-0.24545000
N	-1.57729000	-1.22633900	0.98453400
C	4.15221900	3.64939000	0.68170400
Н	4.51979500	4.66742500	0.83049400
C	5.02280600	2.58070200	0.65263700
Н	6.09545300	2.74189100	0.77986200
C	4.52627700	1.26750100	0.45696900
Н	5.22062100	0.42435100	0.43443700
C	3.17620800	1.03832000	0.29599900
Н	2.78430900	0.03648100	0.15885000
C	2.25555600	2.11760300	0.31871900
C	2.75595700	3.44738100	0.51410400
C	1.82158900	4.51462400	0.52429400
Н	2.17687900	5.53687600	0.67619300
C	0.48721500	4.24879400	0.33419100
Н	-0.27565200	5.02546400	0.31701500

C	0.07207300	2.90819800	0.14066700
C	-1.40097900	2.65081200	-0.12292800
C	-2.98011100	0.95211500	-0.65434700
C	-3.76098000	1.72729000	-1.54733800
Н	-3.36483900	2.68038300	-1.88748500
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Н	-5.56755100	1.92334100	-2.68899600
C	-5.54827000	0.08463000	-1.54389800
Н	-6.53031300	-0.24827600	-1.88547400
C	-4.81152000	-0.69134600	-0.66016100
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C	-2.84049800	-1.17064400	0.71941700
C	-2.78325800	-2.74197700	2.32561500
Н	-2.98452100	-3.81949400	2.26266900
Н	-3.05489600	-2.37780800	3.32885000
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C	-0.51131200	-1.89890300	3.12134600
Н	0.48735500	-1.58115100	2.79081700
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Н	-1.26091300	-3.82262700	0.31171400
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Н	1.01006000	-0.84798400	0.70498900
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C	2.12821300	-2.23029300	-1.14430900

C	2.81108600	-2.55967300	0.03688300
C	2.55797900	-2.80992000	-2.35695200
C	3.89422100	-3.43976800	0.01271900
Н	2.47275600	-2.10785400	0.97137300
C	3.63909700	-3.68903100	-2.37928100
Н	2.03202100	-2.55807600	-3.28009600
C	4.31289000	-4.00762600	-1.19389600
Н	4.41309300	-3.68363300	0.94270800
Н	3.95976400	-4.12830200	-3.32686500
Н	5.16081600	-4.69626100	-1.21260800
C	0.11804400	-0.75264400	-1.91505700
Н	-0.40479700	-0.52590700	-2.83421600

TS-3b

Charge = 0, Multiplicity = 2				
O	1.86115600	3.42519500	-0.16195200	
O	3.72924900	-2.04589200	-1.25736900	
N	-0.73256000	1.07106800	-0.70569400	
N	1.72140600	1.15484200	0.33189500	
N	1.69491800	-1.41394800	-0.57844800	
C	-4.08241000	1.93536600	-2.05729700	
Н	-4.64528600	2.81492800	-2.37917200	
C	-4.65446100	0.68038300	-2.09223200	
Н	-5.68150600	0.55686400	-2.44285000	
C	-3.91641200	-0.45583000	-1.67149900	
Н	-4.38449100	-1.44231200	-1.69413600	
C	-2.62032600	-0.32341400	-1.22266800	
Н	-2.03711600	-1.17232400	-0.86999000	

C	-2.00859300	0.95678800	-1.17036000
C	-2.74965000	2.10690600	-1.59558200
C	-2.10471900	3.37070600	-1.52257600
Н	-2.64411500	4.26630900	-1.84119800
C	-0.81660300	3.45036100	-1.04685700
Н	-0.27313300	4.39124200	-0.96623500
C	-0.16045400	2.26322300	-0.63349800
C	1.25821200	2.34529400	-0.10641600
C	3.04959100	0.97233000	0.68412400
C	3.81999300	1.93308300	1.37418700
Н	3.35699000	2.88392400	1.62758300
C	5.14436400	1.67456700	1.71939600
Н	5.70977800	2.43138300	2.26954900
C	5.75825100	0.46345600	1.37126600
Н	6.79745300	0.26905700	1.64377800
C	5.02839500	-0.48699300	0.66436700
Н	5.48992400	-1.42813800	0.36216100
C	3.68461800	-0.25280700	0.32379400
C	2.97377300	-1.23855300	-0.49037000
C	2.84155100	-2.99194600	-1.88696300
Н	2.99070800	-3.97194900	-1.40734100
Н	3.10694400	-3.06136400	-2.94990900
C	1.42265600	-2.42190500	-1.63667400
C	0.86684000	-1.68232700	-2.85899700
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Н	0.64793100	-2.39084700	-3.67305600
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C	0.46506900	-3.51513600	-1.17133600
Н	0.80283400	-3.95190500	-0.22009500

Н	0.42012500	-4.31358300	-1.92877200	
Н	-0.54725900	-3.11599500	-1.02696100	
Co	0.42453100	-0.38017600	0.53998500	
Н	-0.47252500	-1.56941500	0.52135000	
C	-1.08380700	-0.28316500	2.01791800	
C	-2.44062300	-0.78633300	2.06022100	
C	-2.76789200	-2.12077400	1.76392600	
С	-3.47438200	0.11310000	2.38598700	
С	-4.09486100	-2.54637100	1.79694400	
Н	-1.97010800	-2.81237300	1.48931300	
С	-4.80270300	-0.31365200	2.40277500	
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С	-5.11821300	-1.64382800	2.10862400	
Н	-4.33488300	-3.58703400	1.56656200	
Н	-5.59603400	0.39833800	2.64213400	
Н	-6.15883900	-1.97618900	2.11826600	
C	-0.13544200	0.47418700	2.31670900	
Н	0.45325000	1.20760900	2.84658700	

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