Supporting Information for

Regio-divergent Nickel Catalysis: Intramolecular [4+2] and [2+2] Cycloaddition Reactions Between Vinylallenes and Alkynes

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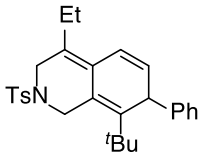
Contents

General remarks: All reactions were performed with dry solvents and reagents that were purified by the usual methods. Reactions were monitored by thin-layer chromatography carried out on 0.25 mm Merck silica gel plates (60F-254). Column chromatography was performed with Wakogel® 60N from Wako Pure Chemical Industries, or NH-silica (Fuji Silysia, DM2035). IR spectra were recorded on a JASCO FT/IR-230 Fourier transform spectrophotometer. NMR spectra were recorded on JEOL-JMN-ECS-400, -ECZ400, -ECZ600 and ECA-600 spectrometers operating at 400 and 600 MHz for ^{1}H NMR and at 100 and 150 MHz for ^{13}C NMR, with calibration using residual undeuterated solvent as an internal reference. Mass spectra were measured by The AccuTOFLC-plus JMS-T100LP (TOF) for LRMS and HRMS.

General procedure for Ni(0)-catalyzed [4+2] cycloaddition reaction

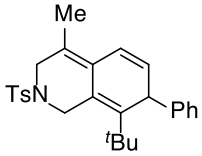
A solution of a conjugated allenene-yne **1c** (18.5 mg, 0.040 mmol) with $Ni[P(OPh)_3]_4$ (5.2 mg, 0.004 mmol) in toluene (0.4 mL, degassed by Freeze-Pump-Thaw method) was heated to 100 ℃ under an Ar atmosphere. The reaction mixture was filtered through Celite®, concentrated *in vacuo* and purified by column chromatography (*n*-Hexane/AcOEt = 50/1 to 20/1) to afford **2c** (17.8 mg, 0.038 mmol, 96%) as colorless solid.

8-(*tert*-butyl)-4-ethyl-7-phenyl-2-tosyl-1,2,3,7-tetrahydroisoquinoline (2a)



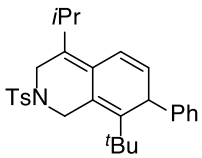
^{1}H NMR (400 MHz, $CDCl_3$) δ: 0.99 (t, *J* = 7.6 Hz, 3H), 1.15 (s, 9H), 2.07 (dq, *J* = 7.6, 14.8 Hz, 1H), 2.19 (dq, *J* = 7.6, 14.8 Hz, 1H), 2.45 (s, 3H), 3.19 (dd, *J* = 1.2, 13.6 Hz, 1H), 3.39 (d, *J* = 16.8 Hz, 1H), 4.03 (d, *J* = 16.8 Hz, 1H), 4.34 (br s, 1H), 4.99 (d, *J* = 13.6 Hz, 1H), 5.83 (dd, *J* = 5.2, 9.6 Hz, 1H), 6.26 (d, *J* = 9.6 Hz, 1H), 7.15-7.20 (m, 3H), 7.25-7.29 (m, 2H), 7.37 (d, *J* = 8.0 Hz, 2H), 7.75 (d, *J* = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 13.3, 21.6, 23.9, 31.3, 36.3, 46.3, 47.3, 48.2, 118.8, 125.6, 126.2, 126.3, 127.8, 127.9, 128.8, 129.7, 129.7, 132.7, 133.1, 141.7, 143.6, 143.8; HRMS (ESI) m/z calcd for $C_{28}H_{33}N_1Na_1O_2S_1^+$ $[M+Na]^+$ 470.2130, found 470.2137; IR (ATR) ν: 2964, 1490, 1400, 1340, 1235, 1163, 967 cm^{-1}; yellow gum (87%, 30.3 mg).

8-(*tert*-butyl)-4-methyl-7-phenyl-2-tosyl-1,2,3,7-tetrahydroisoquinoline (2b)



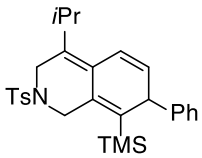
^{1}H NMR (400 MHz, $CDCl_3$) δ: 1.15 (s, 9H), 1.76 (s, 3H), 2.45 (s, 3H), 3.20 (d, *J* = 12.4 Hz, 1H), 3.36 (d, *J* = 17.6 Hz, 1H), 3.97 (d, *J* = 17.6 Hz, 1H), 4.34 (br s, 1H), 5.00 (d, *J* = 12.4 Hz, 1H), 5.82 (dd, *J* = 5.6, 9.6 Hz, 1H), 6.26 (d, *J* = 9.6 Hz, 1H), 7.15-7.20 (m, 3H), 7.26-7.29 (m, 2H), 7.37 (d, *J* = 8.4 Hz, 2H), 7.75 (d, *J* = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 16.4, 21.5, 31.3, 36.3, 46.4, 47.3, 49.9, 119.2, 123.6, 126.2, 126.3, 126.4, 127.8, 127.8, 128.8, 129.7, 132.6, 133.2, 141.5, 143.6, 143.8; HRMS (ESI) m/z calcd for $C_{27}H_{31}N_1Na_1O_2S_1^+$ $[M+Na]^+$ 456.1973, found 456.1983; IR (ATR) ν: 3023, 2956, 1488, 1399, 1337, 1238, 1164, 1026, 662 cm^{-1}; m.p. 79-80 ℃; colorless amorphous (43%, 17.5 mg)

8-(*tert*-butyl)-4-isopropyl-7-phenyl-2-tosyl-1,2,3,7-tetrahydroisoquinoline (2c)



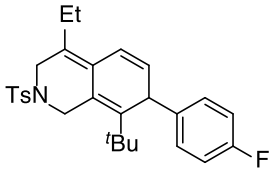
^{1}H NMR (400 MHz, $CDCl_3$) δ: 1.00 (d, *J* = 12.8 Hz, 3H), 1.02 (d, *J* = 12.8 Hz, 3H), 1.14 (s, 9H), 2.45 (s, 3H), 2.98-3.07 (m, 1H), 3.22 (d, *J* = 13.2 Hz, 1H), 3.39 (d, *J* = 17.6 Hz), 4.06 (d, *J* = 17.6 Hz, 1H), 4.34 (br s, 1H), 4.92 (d, *J* = 13.2 Hz, 1H), 5.83 (dd, *J* = 5.6, 9.6 Hz, 1H), 6.35 (d, *J* = 9.6 Hz, 1H), 7.12-7.19 (m, 3H), 7.25-7.29 (m, 2H), 7.36 (d, *J* = 8.4 Hz, 2H), 7.75 (d, *J* = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 20.3, 21.1, 21.5, 28.5, 31.3, 36.3, 44.4, 46.4, 47.1, 118.6, 124.9, 126.3, 126.4, 127.8, 127.9, 128.7, 129.7, 132.8, 133.2, 141.8, 143.6, 143.9; HRMS (ESI) m/z calcd for $C_{29}H_{35}N_1Na_1O_2S_1^+$ $[M+Na]^+$ 484.2286, found 484.2284; IR (ATR) ν: 2963, 1488, 1338, 1243, 1163, 907, 829 cm^{-1}; m.p. 62-63 ℃; colorless solid (96%, 44.4 mg)

4-isopropyl-7-phenyl-2-tosyl-8-(trimethylsilyl)-1,2,3,7-tetrahydroisoquinoline (2d)



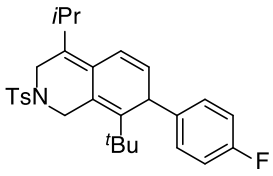
^{1}H NMR (400 MHz, $CDCl_3$) δ: 0.03 (s, 9H), 1.01 (d, *J* = 6.8 Hz, 3H), 1.03 (d, *J* = 6.8 Hz, 3H), 2.45 (s, 3H), 2.70-3.06 (m, 1H), 3.52-3.60 (m, 2H), 3.99 (d, *J* = 16.8 Hz, 1H), 4.23 (br s, 1H), 4.31 (d, *J* = 13.6 Hz, 1H), 5.86 (dd, *J* = 4.8, 9.6 Hz, 1H), 6.35 (d, *J* = 9.6 Hz, 1H), 7.10 (d, *J* = 7.2 Hz, 2H), 7.17-7.20 (m, 1H), 7.23-7.37 (m, 4H), 7.72 (d, *J* = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 0.4, 20.2, 20.7, 21.5, 28.2, 44.6, 47.9, 48.6, 118.6, 122.5, 126.4, 127.8, 128.3, 128.6, 129.7, 133.1, 133.2, 134.0, 134.4, 137.2, 143.4, 143.6; HRMS (ESI) m/z calcd for $C_{28}H_{35}N_1Na_1O_2S_1Si_1^+$ $[M+Na]^+$ 500.2056, found 500.2053; IR (ATR) ν: 2963, 1597, 1343, 1251, 1164, 1094, 843 cm^{-1}; m.p. 59-60 ℃; colorless amorphous (89%, 42.4 mg)

8-(*tert*-butyl)-4-ethyl-7-(4-fluorophenyl)-2-tosyl-1,2,3,7-tetrahydroisoquinoline (2e)



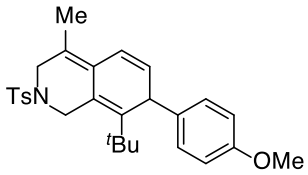
^{1}H NMR (400 MHz, $CDCl_3$) δ: 1.00 (t, *J* = 7.2 Hz, 3H), 1.14 (s, 9H), 2.02-2.12 (m, 1H), 2.16-2.25 (m, 1H), 2.45 (s, 3H), 3.15 (d, *J* = 12.8 Hz, 1H), 3.37 (d, *J* = 17.2 Hz, 1H), 4.04 (d, *J* = 17.2 Hz, 1H), 4.33 (br s, 1H), 4.98 (d, *J* = 12.8 Hz, 1H), 5.80 (dd, *J* = 5.6, 9.6 Hz, 1H), 6.27 (d, *J* = 9.6 Hz, 1H), 6.96 (d, *J* = 8.8 Hz, 1H), 6.97 (d, *J* = 8.8 Hz, 1H), 7.11 (d, *J* = 8.8 Hz, 1H), 7.12 (d, *J* = 8.8 Hz, 1H), 7.36 (d, *J* = 8.0 Hz, 2H), 7.74 (d, *J* = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 13.3, 21.5, 23.9, 31.3, 36.2, 46.3, 46.4, 48.2, 115.5 (d, *J* = 21.0 Hz), 119.0, 125.4, 126.3, 127.8, 129.3 (d, *J* = 7.7 Hz), 129.7, 130.1, 132.5, 133.0, 139.6 (d, *J* = 2.9 Hz), 141.7, 143.7, 161.4 (d, *J* = 244.1 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ: -116.5; HRMS (ESI) m/z calcd for $C_{28}H_{32}F_1N_1Na_1O_2S_1^+$ $[M+Na]^+$ 488.2036, found 488.2042; IR (ATR) ν: 2965, 1504, 1339, 1220, 1164, 832 cm^{-1}; pale yellow gum (85%, 33.0 mg)

8-(*tert*-butyl)-7-(4-fluorophenyl)-4-isopropyl-2-tosyl-1,2,3,7-tetrahydroisoquinoline (2f)



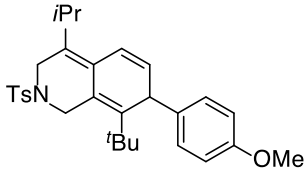
^{1}H NMR (400 MHz, $CDCl_3$) δ: 0.99 (d, *J* = 6.8 Hz, 3H), 1.03 (d, *J* = 6.8 Hz, 3H), 1.14 (s, 9H), 2.45 (s, 3H), 3.00-3.07 (m, 1H), 3.17 (d, *J* = 12.8 Hz, 1H), 3.77 (d, *J* = 17.2 Hz, 1H), 4.08 (d, *J* = 17.2 Hz, 1H), 4.32 (br s, 1H), 4.92 (d, *J* = 12.8 Hz, 1H), 5.80 (dd, *J* = 5.6, 9.6 Hz, 1H), 6.35 (d, *J* = 9.6 Hz, 1H), 6.90-7.00 (m, 2H), 7.08-7.17 (m, 2H), 7.37 (d, *J* = 7.6 Hz, 2H), 7.75 (d, *J* = 7.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 20.2, 21.2, 21.5, 28.5, 31.3, 36.3, 44.4, 46.2, 46.4, 115.5 (*J* = 21.9 Hz), 118.7, 124.7, 126.5, 127.8, 129.2 (d, *J* = 7.7 Hz), 129.7, 132.6, 133.0, 133.2, 139.6 (d, *J* = 2.9 Hz), 141.7, 143.6, 161.4 (d, *J* = 243.1 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ: -116.6; HRMS (ESI) m/z calcd for $C_{29}H_{34}F_1N_1Na_1O_2S_1^+$ $[M+Na]^+$ 502.2192, found 502.2187; IR (ATR) ν: 2963, 1503, 1338, 1221, 1163, 831 cm^{-1}; m.p. 70 ℃; colorless amorphous (87%, 74.9 mg)

8-(*tert*-butyl)-7-(4-methoxyphenyl)-4-methyl-2-tosyl-1,2,3,7-tetrahydroisoquinoline (2g)



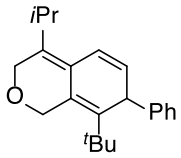
^{1}H NMR (400 MHz, $CDCl_3$) δ: 1.15 (s, 9H), 1.76 (s, 3H), 2.45 (s, 3H), 3.16 (d, *J* = 13.2 Hz, 1H), 3.33 (d, *J* = 16.4 Hz, 1H), 3.78 (s, 3H), 3.96 (d, *J* = 16.4 Hz, 1H), 4.28 (br s, 1H), 4.99 (d, *J* = 13.2 Hz, 1H), 5.82 (dd, *J* = 5.6, 9.6 Hz, 1H), 6.25 (d, *J* = 9.6 Hz, 1H), 6.82 (d, *J* = 8.4 Hz, 2H), 7.01 (d, *J* = 8.4 Hz, 2H), 7.37 (d, *J* = 8.4 Hz, 2H), 7.74 (d, *J* = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 16.4, 21.5, 31.3, 36.2, 46.3, 49.9, 55.2, 114.1, 118.9, 120.1, 125.7, 125.9, 126.2, 127.8, 128.8, 129.7, 129.8, 132.9, 133.0, 135.8, 141.8, 143.6, 158.1; HRMS (ESI) m/z calcd for $C_{28}H_{33}N_1Na_1O_3S_1^+$ $[M+Na]^+$ 486.2079, found 486.2078; IR (ATR) ν: 2957, 1807, 1507, 1339, 1249, 1164, 828 cm^{-1}; pale yellow gummy amorphous (85%, 65.7 mg)

8-(*tert*-butyl)-4-isopropyl-7-(4-methoxyphenyl)-2-tosyl-1,2,3,7-tetrahydroisoquinoline (2h)



^{1}H NMR (600 MHz, $CDCl_3$) δ: 0.99 (d, *J* = 6.6 Hz, 3H), 1.03 (d, *J* = 6.6 Hz, 3H), 1.15 (s, 9H), 2.46 (s, 3H), 3.00-3.08 (m, 1H), 3.18 (d, *J* = 13.2 Hz, 1H), 3.37 (d, *J* = 17.4 Hz, 1H), 3.78 (s, 3H), 4.06 (d, *J* = 17.4 Hz, 1H), 4.28 (br s, 1H), 4.92 (d, *J* = 13.2 Hz, 1H), 5.82 (dd, *J* = 4.8, 9.6 Hz, 1H), 6.33 (d, *J* = 9.6 Hz, 1H), 6.82 (d, *J* = 9.0 Hz, 2H), 7.06 (d, *J* = 9.0 Hz, 2H), 7.37 (d, *J* = 8.4 Hz, 2H), 7.75 (d, *J* = 8.4 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ: 20.3, 21.2, 21.6, 28.4, 31.3, 36.3, 44.4, 46.1, 46.5, 55.2, 114.1, 118.3, 124.9, 126.1, 127.8, 128.8, 129.7, 132.6, 133.1, 133.2, 135.9, 142.1, 143.6, 158.1; HRMS (ESI) m/z calcd for $C_{30}H_{37}N_1Na_1O_3S_1^+$ $[M+Na]^+$ 514.2392, found 514.2380; IR (ATR) ν: 2961, 1606, 1507, 1464, 1399, 1339, 1249, 1165, 829, 680 cm^{-1}; pale yellow gum (quant., 20.0 mg)

8-(*tert*-butyl)-4-isopropyl-7-phenyl-3,7-dihydro-1*H*-isochromene (2i)

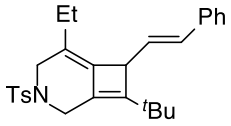


^{1}H NMR (400 MHz, $CDCl_3$) δ: 1.04 (d, *J* = 6.8 Hz, 3H), 1.09 (d, *J* = 6.8 Hz, 3H), 1.33 (s, 9H), 3.00-3.10 (m, 1H), 4.19 (d, *J* = 13.2 Hz, 1H), 4.28 (br s, 1H), 4.29-4.38 (m, 2H), 5.06 (d, *J* = 13.2 Hz, 1H), 5.83 (dd, *J* = 4.8, 9.6 Hz, 1H), 6.41 (d, *J* = 9.6 Hz, 1H), 7.15-7.30 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 20.3, 21.2, 27.7, 30.9, 31.3, 36.2, 46.9, 65.3, 67.2, 118.4, 123.5, 126.2, 127.7, 128.0, 128.6, 132.1, 135.8, 139.3, 144.3; HRMS (ESI) m/z calcd for $C_{23}H_{32}Na_1O_2^+$ $[M+MeOH+Na]^+$ 363.2300, found 363.2301; IR (ATR) ν: 2961, 1598, 1398, 1364, 1239, 1119, 1017, 732, 701 cm^{-1}; pale yellow oil (97%, 35.0 mg). This product was purified by using NH silica gel column chromatography because of its unstability for normal silica gel.

General procedure for Ni(II)-catalyzed [2+2] cycloaddition reaction

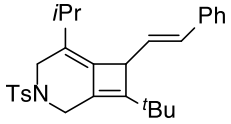
A solution of conjugated allenene-yne **1a** (46.2 mg, 0.100 mmol), $NiF_2 \cdot 4H_2O$ (1.7 mg, 0.010 mmol) in toluene (1.0 mL, degassed by Freeze-Pump-Thaw method) was heated to 150 ℃ under argon atmosphere. The reaction mixture was filtered through Celite®, concentrated *in vacuo* and purified by column chromatography (*n*-Hexane/AcOEt = 20/1 to 12/1) to afford pure **3a** (40.4 mg, 0.088 mmol, 88%) as pale yellow oil.

(*E*)-8-(*tert*-butyl)-5-ethyl-7-styryl-3-tosyl-3-azabicyclo[4.2.0]octa-1(8),5-diene (3a)



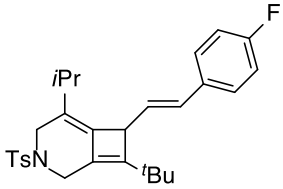
^{1}H NMR (400 MHz, $CDCl_3$) δ: 0.91 (t, *J* = 7.2 Hz, 3H), 1.05 (s, 9H), 1.90 (q, *J* = 7.2 Hz, 2H), 2.43 (s, 3H), 3.73 (d, *J* = 16.4 Hz, 1H), 3.85 (dd, *J* = 2.0, 9.2 Hz, 1H), 3.89 (d, *J* = 16.4 Hz, 1H), 3.98 (dd, *J* = 3.2, 16.4 Hz, 1H), 4.26 (dd, *J* = 2.0, 16.4 Hz, 1H), 5.77 (dd, *J* = 9.2, 16.0 Hz, 1H), 6.41 (d, *J* = 16.0 Hz, 1H), 7.20-7.35 (m, 7H), 7.69 (d, *J* = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 12.5, 21.5, 23.3, 28.6, 34.3, 42.5, 46.9, 52.7, 117.2, 126.0, 127.1, 127.6, 128.5, 129.4, 129.9, 131.2, 132.3, 132.7, 135.3, 137.5, 143.2, 153.0; HRMS (ESI) m/z calcd for $C_{28}H_{33}N_1Na_1O_2S_1^+$ $[M+Na]^+$ 470.2130, found 470.2127; IR (ATR) ν: 2961, 1598, 1342, 1158, 1091, 902, 660 cm^{-1}; yellow oil (88%, 30.7 mg)

(*E*)-8-(*tert*-butyl)-5-isopropyl-7-styryl-3-tosyl-3-azabicyclo[4.2.0]octa-1(8),5-diene (3c)



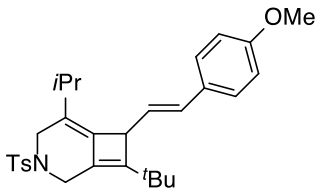
^{1}H NMR (600 MHz, $CDCl_3$) δ: 0.92 (d, *J* = 6.6 Hz, 3H), 0.94 (d, *J* = 6.6 Hz, 3H), 1.05 (s, 9H), 2.15-2.20 (m, 1H), 2.43 (s, 3H), 3.73 (d, *J* = 16.2 Hz, 1H), 3.86 (d, *J* = 10.2 Hz, 1H), 3.96 (d, *J* = 16.2 Hz, 1H), 3.97 (d, *J* = 16.2 Hz, 1H), 4.28 (d, *J* = 16.2 Hz, 1H), 5.74 (dd, *J* = 10.2, 15.6 Hz, 1H), 6.40 (d, *J* = 15.6 Hz, 1H), 7.22 (t, *J* = 7.2 Hz, 1H), 7.27-7.32 (m, 6H), 7.70 (d, *J* = 7.2 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ: 21.4, 21.5, 21.6, 28.6, 30.2, 34.3, 42.6, 45.6, 53.3, 121.7, 126.0, 127.1, 127.7, 128.5, 129.4, 130.1, 131.6, 132.0, 132.4, 135.6, 137.6, 143.2, 153.1; HRMS (ESI) m/z calcd for $C_{29}H_{35}N_1Na_1O_2S_1^+$ $[M+Na]^+$ 484.2286, found 484.2285; IR (ATR) ν: 2960, 1448, 1343, 1159, 1092, 966, 814 cm^{-1}; pale yellow oil (88%, 40.4 mg)

(*E*)-8-(*tert*-butyl)-7-(4-fluorostyryl)-5-isopropyl-3-tosyl-3-azabicyclo[4.2.0]octa-1(8),5-diene (3f)



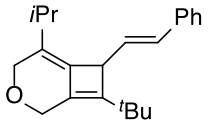
^{1}H NMR (400 MHz, $CDCl_3$) δ: 0.92 (d, *J* = 8.8 Hz, 3H), 0.94 (d, *J* = 8.8 Hz, 3H), 1.05 (s, 9H), 2.10-2.22 (m, 1H), 2.42 (s, 3H), 3.72 (d, *J* = 16.8 Hz, 1H), 3.84 (d, *J* = 9.6 Hz, 1H), 3.94 (d, *J* = 16.8 Hz, 1H), 3.95 (d, *J* = 16.8 Hz, 1H), 4.26 (d, *J* = 16.8 Hz, 1H), 5.67 (dd, *J* = 9.6, 15.6 Hz, 1H), 6.36 (d, *J* = 15.6 Hz, 1H), 6.98 (d, *J* = 8.8 Hz, 1H), 7.00 (d, *J* = 8.8 Hz, 1H), 7.21-7.25 (m, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 7.70 (d, *J* = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 21.4, 21.5, 21.5, 28.6, 30.2, 34.3, 42.5, 45.6, 53.1, 115.4 (*J* = 21.0 Hz), 121.7, 127.4 (*J* = 7.6 Hz), 127.6, 128.8, 129.4, 131.4 (*J* = 1.9 Hz), 131.9, 132.4, 133.7 (*J* = 2.9 Hz), 135.4, 143.1, 153.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ: -115.1; HRMS (ESI) m/z calcd for $C_{29}H_{34}F_1N_1Na_1O_2S_1^+$ $[M+Na]^+$ 502.2192, found 502.2205; IR (ATR) ν: 2961, 1461, 1343, 1226, 1159, 1092, 967, 830 cm^{-1}; m.p. 49 ℃; colorless amorphous (82%, 26.5 mg)

(*E*)-8-(*tert*-butyl)-5-isopropyl-7-(4-methoxystyryl)-3-tosyl-3-azabicyclo[4.2.0]octa-1(8),5-diene (3h)



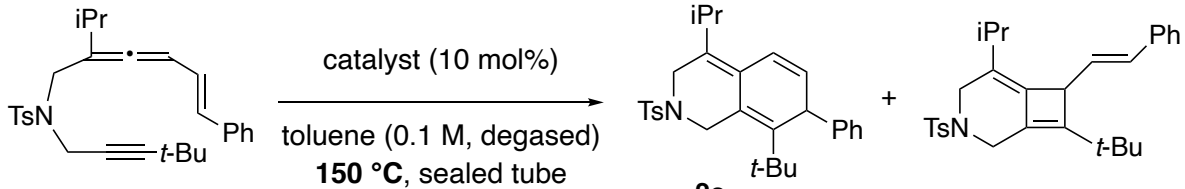
^{1}H NMR (600 MHz, $CDCl_3$) δ: 0.92 (d, *J* = 6.6 Hz, 3H), 0.94 (d, *J* = 6.6 Hz, 3H), 1.04 (s, 9H), 2.14-2.20 (m, 1H), 2.43 (s, 3H), 3.72 (d, *J* = 16.2 Hz, 1H), 3.81 (s, 3H), 3.84 (dd, *J* = 3.0, 10.2 Hz, 1H), 3.95 (d, *J* = 16.2 Hz, 1H), 3.96 (d, *J* = 16.2 Hz, 1H), 4.27 (d, *J* = 16.2 Hz, 1H), 5.60 (dd, *J* = 10.2, 16.2 Hz, 1H), 6.34 (d, *J* = 16.2 Hz, 1H), 6.85 (d, *J* = 8.4 Hz, 2H), 7.21 (d, *J* = 8.4 Hz, 2H), 7.29 (d, *J* = 8.4 Hz, 2H), 7.70 (d, *J* = 8.4 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ: 21.4, 21.5, 21.6, 28.6, 30.2, 34.3, 42.6, 45.6, 53.4, 55.3, 114.0, 121.4, 127.1, 127.7, 129.4, 129.4, 129.5, 130.4, 132.2, 132.2, 135.5, 143.1, 153.3, 158.8; HRMS (ESI) m/z calcd for $C_{30}H_{37}N_1Na_1O_3S_1^+$ $[M+Na]^+$ 514.2392, found 514.2387; IR (ATR) ν: 2959, 1511, 1464, 1343, 1250, 1160, 1092, 1032, 814 cm^{-1}; m.p. 156-157 ℃; colorless solid (70%, 8.8 mg)

(*E*)-8-(*tert*-butyl)-5-isopropyl-7-styryl-3-oxabicyclo[4.2.0]octa-1(8),5-diene (3i)



^{1}H NMR (400 MHz, $CDCl_3$) δ: 1.00 (d, *J* = 9.6 Hz, 3H), 1.03 (d, *J* = 9.6 Hz, 3H), 1.07 (s, 9H), 2.20-2.26 (m, 1H), 4.00-4.10 (m, 2H), 4.14-4.17 (m, 1H), 4.30 (dd, *J* = 3.2, 15.2 Hz, 1H), 4.41 (d, *J* = 15.2 Hz, 1H), 6.25 (ddd, *J* = 0.8, 10.0, 15.6 Hz, 1H), 6.53 (d, *J* = 15.6 Hz, 1H), 7.21 (t, *J* = 8.0 Hz, 1H), 7.31 (dd, *J* = 7.6, 8.0 Hz, 2H), 7.37 (d, *J* = 7.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 21.6, 21.7, 28.8, 29.7, 54.2, 62.5, 65.9, 125.1, 126.1, 127.0, 128.5, 129.9, 130.6, 132.3, 135.6, 137.7, 151.3; HRMS (ESI) m/z calcd for $C_{23}H_{32}Na_1O_2^+$ $[M+MeOH+Na]^+$ 363.2300, found 363.2301; IR (ATR) ν: 3025, 2960, 1495, 1361, 1258, 965, 754, 694 cm^{-1}; pale yellow oil (70%, 34.9 mg). This product was purified by using NH silica gel column chromatography because of its unstability for normal silica gel.

Table S1: Catalyst Screening for [2+2] cycloaddition of **1c**

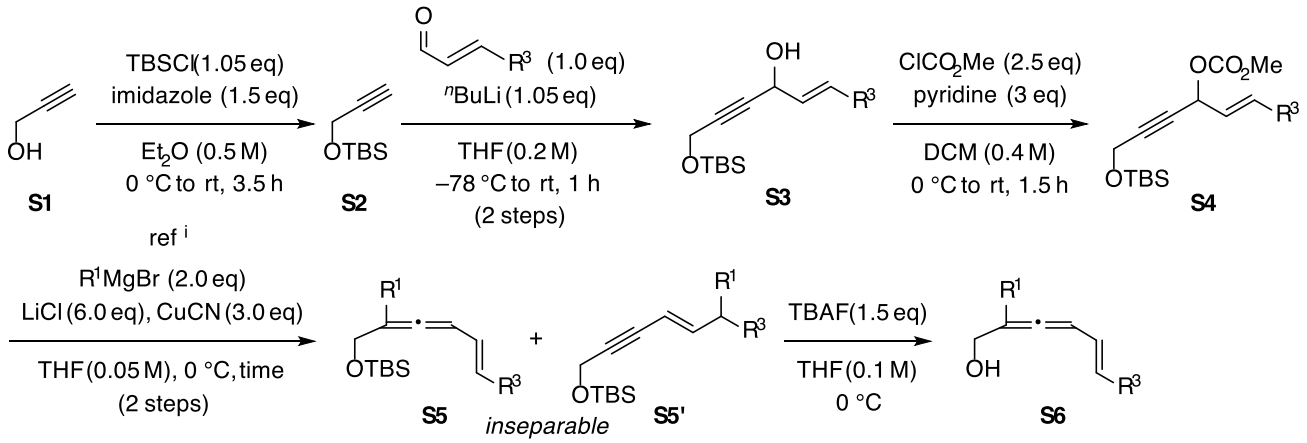


1c **2c** **3c**

entry	catalyst	conditions	**2c** (%)	**3c** (%)
1	$Ni[P(OPh)_3]_4$	15 min, under Ar	quant	0
2	$Ni[P(OPh)_3]_4$	4.5 h, under O_2	0	18
3	$Ni[P(OPh)_3]_4$ with $PhCO_2H$ (10 mol%)	7 h, under Ar	15	34
4	AcOH	6 h under Ar	0	45
5	$NiCl_2$	6 h under Ar	0	52
6	$NiCl_2 \cdot 6H_2O$	5 h, under Ar	0	45
7	$NiBr_2$	4 h, under Ar	0	49
8	$NiF_2 \cdot 4H_2O$	6 h, under Ar	0	88
9	$Ni(acac)_2$	6 h under Ar	0	65
10	$Ni(OTf)_2$	5 h under Ar	0	43
11	CuCl	6 h under Ar	0	34
12	$AlCl_3$	6 h under Ar	0	24
13	$Pd_2(dba)_3$	6 h under Ar	0	64
14	$AuCl(PPh_3)_3$	6 h under Ar	0	78

Substrate synthesis

Synthesisof the conjugated allenene alcohol S6



S1 to **S2**: TBSCl (1.58 g, 10.5 mmol) and imidazole (1.02 g, 15 mmol) were added to a solution of propargyl alcohol **S1** (0.56 g, 10 mmol) in Et_2O (20 mL) at 0 ℃. The reaction mixture was warmed up to room temperature and stirred for 3.5 h. When the reaction was complete, it was quenched with saturated aqueous solution of NH_4Cl and extracted with Et_2O, dried over anhydrous Na_2SO_4. Then, the solvent was removed under residue pressure. The crude **S2** was used in the next step without further purification.

S2 to **S3**: ^{n}BuLi (6.77 mL, 1.55 M in hexanes, 10.5 mmol) was added to a solution of crude **S2** (1.70 g, 10 mmol) in THF (50 mL) dropwise at -78 °C under argon. After being stirred for 0.5 h at the same temperature, corresponding aldehyde (10 mmol) was added dropwise, then it was allowed to warm up to room temperature and stirred for 1 h. When the reaction was complete, it was quenched with saturated aqueous solution of NH_4Cl, extracted with THF and dried over anhydrous Na_2SO_4. The organic phase was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel (*n*-Hexane/AcOEt = 20/1-5/1) to afford corresponding **S3** as pale yellow oil.

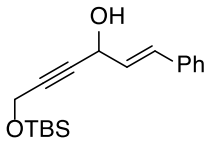
S3 to **S4**: Methyl chloroformate (1.86 g, 20.0 mmol) was added dropwise to a solution of corresponding alcohol **S3** (7.98 mmol) and pyridine (1.93 mL, 23.9 mmol) in DCM (20 mL) at 0 ℃. The reaction mixture was warmed up to room temperature and stirred for 1.5 h. It was quenched with saturated aqueous solution of NH_4Cl and extracted with DCM, dried over anhydrous Na_2SO_4. Then, the solvent was removed under residue pressure. The crude **S4** was used in the next step without further purification. **S5** was sensitive for air and unstable for normal silica gel column chromatography. It should be used for next step immediately.

S4 to **S5**[ref i]: To a stirred suspension of LiCl (2.03 g, 47.9 mmol) and CuCN (2.14 g, 23.9 mmol) in THF (80 mL) at 0 °C was slowly added a solution of R^2MgBr (16.0 mmol, 2.0 or 3.0 M in Et_2O) under argon. After the mixture was stirred for 0.5 h, a solution of **S4** (7.98 mmol) in THF (80 mL) was added. The reaction mixture was stirred for 1 h at 0 °C, and then a saturated aqueous solution of NH_4Cl was added. The organic layer was extracted with AcOEt, dried over (Na_2SO_4), concentrated *in vacuo*, and purified by flash column chromatography (eluting with *n*-Hexane), corresponding **S5** was obtained (with inseparable corresponding byproduct **S5'** frequently).

S5 to **S6**: Tetrabutylammonium fluoride (4.37 mL, 1.0 M in THF, 4.37 mmol) was added to a solution of **S5** (3.64 mmol) in THF (18 mL) dropwise at 0 °C under argon. The reaction mixture was stirred for 1 h at 0 °C, and then a saturated solution of NH_4Cl was added and the reaction was extracted with AcOEt. After drying (Na_2SO_4),

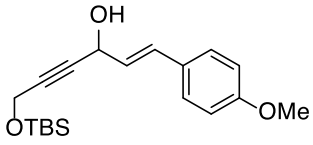
concentration, and flash column chromatography (*n*-Hexane/AcOEt = 15/1-8/1), corresponding **S6** was obtained as pale yellow oil.

(*E*)-6-((*tert*-butyldimethylsilyl)oxy)-1-phenylhex-1-en-4-yn-3-ol (S3a)



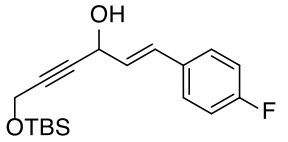
^{1}H NMR (400MHz, CDCl3) δ: 0.08 (d, *J* = 3.6 Hz, 6H), 0.90 (s, 9H), 1.05 (t, *J* = 7.6 Hz, 3H), 2.09 (ddt, *J* = 2.8, 7.6, 14.4 Hz, 2H), 4.91 (d, *J* = 2.8 Hz, 2H), 6.08 (dtt, *J* = 2.8, 2.8, 10.0 Hz, 1H), 6.48 (d, *J* = 16.0 Hz, 1H), 6.61 (dd, *J* = 10.0, 16.0 Hz, 1H), 7.18-7.38 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) d: -5.3, 12.1, 18.3, 22.2, 25.9, 64.2, 96.8, 125.6, 126.1, 127.1, 128.5, 129.8, 137.4, 204.8; ; HRMS (ESI) m/z calcd for $C_{18}H_{25}Na_1O_2Si_1^+$ $[M+Na]^+$ 325.1600, found 325.1605; IR (ATR) ν: 3339, 3028, 2119, 1254, 964, 834, 692 cm^{-1}; yellow oil (53% for 2 steps)

(*E*)-6-((*tert*-butyldimethylsilyl)oxy)-1-(4-methoxyphenyl)hex-1-en-4-yn-3-ol (S3b)



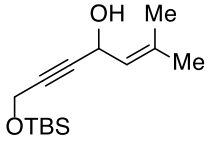
^{1}H NMR (400 MHz, $CDCl_3$) δ: 0.14 (s, 6H), 0.92 (s, 9H), 1.92 (dd, *J* = 2.4, 6.0 Hz, 1H), 3.81 (s, 3H), 4.41 (d, *J* = 2.4 Hz, 2H), 5.07 (dd, *J* = 6.0, 6.0 Hz, 1H), 6.16 (dd, *J* = 6.0, 16.0 Hz, 1H), 6.71 (d, *J* = 16.0 Hz, 1H), 6.86 (d, *J* = 8.8 Hz, 2H), 7.34 (d, *J* = 8.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: -5.2, 18.2, 25.8, 51.7, 55.2, 63.0, 83.8, 84.9, 113.9, 125.7, 127.9, 128.7, 131.4, 159.5; HRMS (ESI) m/z calcd for $C_{19}H_{28}Na_1O_3Si_1^+$ $[M+Na]^+$ 355.1705, found 355.1715; IR (ATR) ν: 3257, 2117, 1652, 1463, 1250, 1174, 1081, 965, 834 cm^{-1}; yellow gum (24% for 2 steps from **S1**)

(*E*)-6-((*tert*-butyldimethylsilyl)oxy)-1-(4-fluorophenyl)hex-1-en-4-yn-3-ol (S3c)



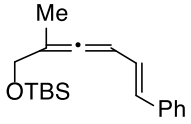
^{1}H NMR (400 MHz, $CDCl_3$) δ: 0.14 (s, 6H), 0.92 (s, 9H), 1.97 (d, *J* = 5.6 Hz, 1H), 4,41 (t, *J* = 1.6 Hz, 2H), 5.05-5.11 (m, 1H), 6.21 (dd, *J* = 10.0, 16.0 Hz, 1H), 6.74 (d, *J* = 16.0 Hz, 1H), 7.01 (d, *J* = 8.0 Hz, 1H), 7.03 (d, *J* = 8.0 Hz, 1H), 7.36 (d, *J* = 8.0 Hz, 1H), 7.38 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: -5.2, 18.3, 25.8, 51.7, 62.8, 83.6, 85.2, 115.5 (d, *J* = 21.0 Hz), 127.7, 128.3 (d, *J* = 7.6 Hz), 130.6, 132.2 (d, *J* = 2.8 Hz), 162.5 (d, *J* = 245.0 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ: -113.5; HRMS (ESI) m/z calcd for $C_{18}H_{25}F_1Na_1O_2Si_1^+$ $[M+Na]^+$ 343.1506, found 343.1492; IR (ATR) ν: 3370, 1509, 1255, 1231, 1158, 1084, 968, 835 cm^{-1}; yellow oil (78% for 2steps from **S1**)

7-((*tert*-butyldimethylsilyl)oxy)-2-methylhept-2-en-5-yn-4-ol (S3d)



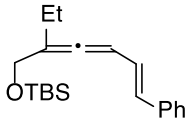
^{1}H NMR (400 MHz, $CDCl_3$) δ: 0.12 (s, 6H), 0.91 (s, 9H), 1.72 (d, *J* = 1.6 Hz, 3H), 1.73 (bd, *J* = 1.6 Hz, 1H), 1.75 (d, *J* = 1.6 Hz, 3H), 4.35 (d, *J* = 1.6 Hz, 2H), 5.10 (ddd, *J* = 8.4, 2.4, 1.6 Hz 1H), 5.36 (ddd, *J* = 8.4, 1.6, 1.6 Hz, 2H), 7.74 (d, *J* = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: -5.2, 18.0, 18.2, 25.5, 25.7, 51.7, 59.0, 83.0, 85.3, 124.6, 136.6; HRMS (ESI) m/z calcd for $C_{14}H_{26}Na_1O_2Si_1^+$ $[M+Na]^+$ 277.1600, found 277.1593; IR (ATR) ν: 3357, 2120, 1254, 998, 833, 664 cm^{-1}; yellow oil (75% for 2 steps)

(*E*)-*tert*-butyldimethyl((2-methyl-6-phenylhexa-2,3,5-trien-1-yl)oxy)silane (S5a)



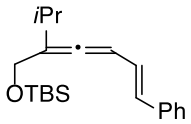
^{1}H NMR (400MHz, $CDCl_3$) δ: 0.08 (s, 3H), 0.09 (s, 3H), 0.91 (s, 9H), 3.81 (s, 3H), 4.15 (d, *J* = 2.4 Hz, 2H), 5.92-5.98 (m, 1H), 6.40-6.50 (m, 2H), 6.84 (d, *J* = 9.2 Hz, 2H), 7.28-7.31 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: -5.2, -5.1, 15.5, 18.3, 25.9, 65.1, 95.0, 101.4, 125.5, 126.1, 127.2, 128.5, 130.0, 137.4, 205.2; HRMS (ESI) m/z calcd for $C_{19}H_{28}Na_1O_1Si_1^+$ $[M+Na]^+$ 323.1807, found 323.1811; IR (ATR) ν: 2856, 1947, 1462, 1254, 1072, 963, 836, 690 cm^{-1}; pale yellow oil (51% for 2 steps)

(*E*)-*tert*-butyl((2-ethyl-6-phenylhexa-2,3,5-trien-1-yl)oxy)dimethylsilane (S5b)



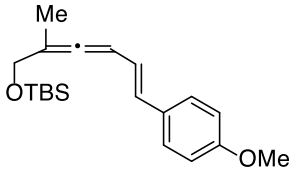
^{1}H NMR (400MHz, $CDCl_3$) δ: 0.07 (s, 3H), 0.08 (s, 3H), 0.90 (s, 9H), 1.05 (t, *J* = 7.6 Hz, 3H), 2.09 (ddt, *J* = 2.8, 7.6, 14.4 Hz, 2H), 4.91 (d, *J* = 2.8 Hz, 2H), 6.08 (dtt, *J* = 2.8, 2.8, 10.0 Hz, 1H), 6.48 (d, *J* = 16.0 Hz, 1H), 6.61 (dd, *J* = 10.0, 16.0 Hz, 1H), 7.18-7.38 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: -5.3, 12.1, 18.3, 22.2, 25.9, 64.2, 96.8, 125.6, 126.1, 127.1, 128.5, 129.8, 137.4, 204.8; IR (ATR) ν: 2929, 2856, 1942, 1254, 1073, 837, 744 cm^{-1}; pale yellow oil (98% for 2 steps from **S3a**)

(*E*)-*tert*-butyl((2-isopropyl-6-phenylhexa-2,3,5-trien-1-yl)oxy)dimethylsilane (S5c)



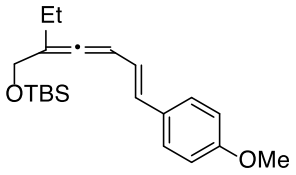
^{1}H NMR (400MHz, $CDCl_3$) δ: 0.07 (s, 3H), 0.08 (s, 3H), 0.90 (s, 9H), 1.06 (d, *J* = 6.8 Hz, 3H), 1.08 (d, *J* = 6.8 Hz, 3H), 2.32-2.39 (m, 1H), 4.23 (d, *J* = 2.4 Hz, 2H), 6.07-6.12 (m, 1H), 6.48 (d, *J* = 16.0 Hz, 1H), 6.59 (dd, *J* = 10.4, 16.0 Hz, 1H), 7.20 (t, *J* = 7.2 Hz, 1H), 7.30 (dd, *J* = 6.8, 7.2 Hz, 2H), 7.37 (d, *J* = 6.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: -5.2, 12.4, 21.7, 22.0, 25.9, 27.9, 63.1, 97.4, 113.0, 125.9, 126.1, 127.1, 128.5, 129.7, 137.5, 204.4; pale yellow oil (76% for 2 steps from **S3a**, 806.6 mg)

(*E*)-*tert*-butyl((6-(4-methoxyphenyl)-2-methylhexa-2,3,5-trien-1-yl)oxy)dimethylsilane (S5d)



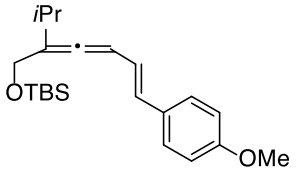
^{1}H NMR (400 MHz, $CDCl_3$) δ: 0.08 (s, 3H), 0.09 (s, 3H), 0.90 (s, 9H), 1.76 (d, *J* = 2.8 Hz, 3H), 3.80 (s, 3H), 4.15 (d, *J* = 2.8 Hz, 2H), 5.93-5.99 (m, 1H), 6.40-6.50 (m, 2H), 6.84 (d, *J* = 8.8 Hz, 2H), 7.30 (d, *J* = 8.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: -5.2, 15.6, 18.4, 25.9, 55.2, 65.2, 95.0, 101.3, 114.0, 123.3, 127.3, 129.5, 130.3, 158.9, 204.8; HRMS (ESI) m/z calcd for $C_{40}H_{60}Na_1O_4Si_2^+$ $[2M+Na]^+$ 683.3928, found 683.3913; IR (ATR) ν: 2927, 1946, 1606, 1510, 1389, 1173, 834, 775 cm^{-1}; pale yellow oil (76% for 2 steps from **S3b**)

(*E*)-*tert*-butyl((2-ethyl-6-(4-methoxyphenyl)hexa-2,3,5-trien-1-yl)oxy)dimethylsilane (S5e)



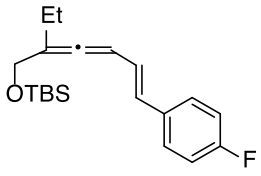
^{1}H NMR (400 MHz, $CDCl_3$) δ: 0.07 (s, 3H), 0.08 (s, 3H), 0.90 (s, 9H), 1.04 (t, *J* = 7.6 Hz, 3H), 2.07-2.10 (m, 2H), 3.80 (s, 3H), 4.19 (d, *J* = 2.4 Hz, 2H), 6.05-6.07 (m, 1H), 6.41-6.51 (m, 2H), 6.84 (d, *J* = 8.8 Hz, 2H), 7.30 (d, *J* = 8.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: -5.2, 12.1, 18.4, 22.2, 25.9, 55.2, 64.4, 96.9, 108.1, 114.0, 123.5, 127.3, 129.3, 130.3, 158.9, 204.4; HRMS (ESI) m/z calcd for $C_{42}H_{64}Na_1O_4Si_2^+$ $[2M+Na]^+$ 711.4241, found 711.4219; IR (ATR) ν: 2928, 1943, 1606, 1510, 1389, 1173, 834, 775 cm^{-1}; pale yellow oil (85% for 2 steps from **S3b**)

(*E*)-*tert*-butyl((2-isopropyl-6-(4-methoxyphenyl)hexa-2,3,5-trien-1-yl)oxy)dimethylsilane (S45)



^{1}H NMR (400 MHz, $CDCl_3$) δ: 0.07 (s, 3H), 0.08 (s, 3H), 0.90 (s, 9H), 1.06 (d, *J* = 6.8 Hz, 3H), 1.08 (d, *J* = 6.8 Hz, 3H), 2.30-2.38 (m, 1H), 3.81 (s, 3H), 4.23 (d, *J* = 2.4 Hz, 2H), 6.05-6.09 (m, 1H), 6.40-6.50 (m, 2H), 6.84 (d, *J* = 8.4 Hz, 2H), 7.31 (d, *J* = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: -5.3, 18.3, 21.7, 22.0, 25.9, 27.9, 55.2, 63.1, 97.4, 112.8, 114.0, 123.6, 127.2, 129.2, 130.3, 158.9, 203.9; HRMS (ESI) m/z calcd for $C_{22}H_{34}Na_1O_2Si_1^+$ $[M+Na]^+$ 381.2226, found 381.2231; IR (ATR) ν: 2956, 2928, 2856, 1939, 1510, 1362, 1251, 959, 835, 671 cm^{-1}; pale yellow oil (34% for 2 steps from **S3b**)

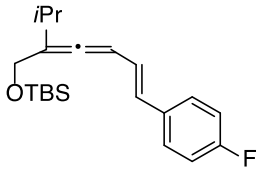
(*E*)-*tert*-butyl((2-ethyl-6-(4-fluorophenyl)hexa-2,3,5-trien-1-yl)oxy)dimethylsilane (S5g)



^{1}H NMR (400 MHz, $CDCl_3$) δ: 0.08 (s, 3H), 0.08 (s, 3H), 0.90 (s, 9H), 1.05 (t, *J* = 7.6 Hz, 3H), 2.05-2.14 (m, 2H), 4.19 (d, *J* = 2.4 Hz, 2H), 6.02-6.08 (m, 1H), 6.44 (d, *J* = 15.6 Hz, 1H), 6.52 (dd, *J* = 9.6, 15.6 Hz, 1H), 6.97-7.02 (m, 2H), 7.31-7.36 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: -5.3, 12.1, 18.3, 22.2, 25.9, 64.2, 96.7, 108.3, 115.4 (d, *J* = 22.0 Hz), 125.5, 127.5 (d, *J* = 7.7 Hz), 128.5, 133.6 (d, *J* = 2.8 Hz), 162.0 (d, *J* = 245.4 Hz), 204.8; ^{19}F NMR

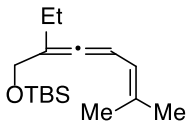
(376 MHz, $CDCl_3$) δ: -114.8; HRMS (ESI) m/z calcd for $C_{40}H_{58}F_2Na_1O_2Si_2^+$ $[2M+Na]^+$ 687.3841, found 687.3849; IR (ATR) ν: 2957, 2929, 1943, 1601, 1508, 1229, 1157, 836 cm^{-1}; colorless oil (71% for 2 steps from **S3c**)

(*E*)-*tert*-butyl((6-(4-fluorophenyl)-2-isopropylhexa-2,3,5-trien-1-yl)oxy)dimethylsilane (S5h)



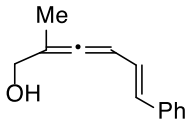
^1H NMR (400 MHz, $CDCl_3$) δ: 0.07 (s, 3H), 0.08 (s, 3H), 0.90 (s, 9H), 1.06 (d, *J* = 6.8 Hz, 3H), 1.08 (d, *J* = 6.8 Hz, 3H), 2.33-2.37 (m, 1H), 4.23 (d, *J* = 2.4 Hz, 2H), 6.05-6.10 (m, 1H), 6.44 (d, *J* = 15.6 Hz, 1H), 6.50 (dd, *J* = 9.2, 15.6 Hz, 1H), 6.96-7.02 (m, 2H), 7.30-7.35 (m, 2H);^{13}C NMR (100 MHz, $CDCl_3$) δ: -5.3, 18.3, 21.7, 22.0, 25.9, 27.9, 63.0, 97.2, 113.0, 115.4 (d, *J* = 21.1 Hz), 125,6 (d, *J* = 1.9 Hz), 127.5 (d, *J* = 7.7 Hz), 128.4, 133.7 (d, *J* = 2.9 Hz), 162.5 (d, *J* = 245.3 Hz), 204.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ: -114.9; HRMS (ESI) m/z calcd for $C_{42}H_{62}F_2Na_1O_2Si_2^+$ $[2M+Na]^+$ 715.4154, found 715.4129; IR (ATR) ν: 2958, 2928, 1942, 1602, 1230, 1157, 837 cm^{-1}; colorless oil (63% for 2 steps from **S3c**)

***tert*-butyl((2-ethyl-6-methylhepta-2,3,5-trien-1-yl)oxy)dimethylsilane (S5i)**



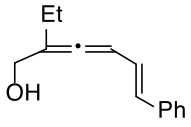
^1H NMR (400 MHz, $CDCl_3$) δ: 0.06 (s, 3H), 0.07 (s, 3H), 0.90 (s, 9H), 1.01 (t, *J* = 7.2 Hz, 3H), 2.05 (dq, *J* = 7.2, 3.2 Hz, 3H), 4.15 (d, *J* = 2.0 Hz, 2H), 5.61 (dt, *J* = 11.2, 2.0 Hz 1H), 6.03-6.09 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: -5.3, -5.2, 12.2, 18.0, 18.4, 22.2, 25.9, 26.0, 64.6, 92.5, 107.1, 120.3, 133.4, 203.3; HRMS (ESI) m/z calcd for $C_{16}H_{31}O_1Si_1^+$ $[M+H]^+$ 267.2144, found 267.2149; IR (ATR) ν: 2958, 2928, 1650, 1253, 940, 835, 665 cm^{-1}; colorless oil (66% for 2 steps from **S3d**)

(*E*)-2-methyl-6-phenylhexa-2,3,5-trien-1-ol (S6a)



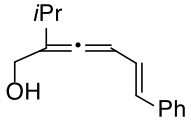
^1H NMR (400 MHz, $CDCl_3$) δ: 1.52 (bs, 1 H), 1.79 (d, *J* = 2.8 Hz, 3H), 4.05-4.13 (m, 2H), 6.11-6.15 (m, 1H), 6.51 (d, *J* = 16.0 Hz, 1H), 6.6 (dd, *J* = 10.0, 16.0 Hz, 1H), 7.21 (t, *J* = 7.6 Hz, 1H), 7.30 (dd, *J* = 7.6, 7.6 Hz, 2H), 7.37 (d, *J* = 7.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 15.6, 63.8, 97.0, 102.2, 125.0, 126.2, 127.4, 128.5, 130.7, 137.1, 203.8; HRMS (ESI) m/z calcd for $C_{13}H_{15}O_1^+$ $[M+H]^+$ 187.1123, found 187.1124; IR (ATR) ν: 3332, 1945, 1446, 1263, 1009, 961, 744, 690 cm^{-1}; pale yellow oil (82%)

(*E*)-2-ethyl-6-phenylhexa-2,3,5-trien-1-ol (S6b)



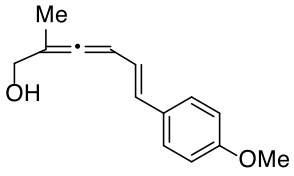
^1H NMR (400 MHz, $CDCl_3$) δ: 1.07 (t, *J* = 7.2 Hz, 3H), 1.50 (t, *J* = 5.2 Hz, 1 H), 2.09 (m, 2H), 4.11 (dd, *J* = 2.8, 12.8 Hz, 1H), 4.15 (dd, *J* = 2.8, 12.8 Hz, 1H), 6.23 (dtt, *J* = 2.8, 2.8, 10.0 Hz, 1H), 6.53 (d, *J* = 15.6 Hz, 1H), 6.61 (dd, *J* = 10.0, 15.6 Hz, 1H), 7.21 (t, *J* = 8.0 Hz, 1H), 7.31 (dd, *J* = 8.0, 8.0 Hz, 2H), 7.38 (d, *J* = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 12.0, 22.5, 62.9, 98.7, 109.1, 125.2, 126.1, 127.3, 128.5, 130.5, 137.1, 203.4; HRMS (ESI) m/z calcd for $C_{28}H_{32}Na_1O_2^+$ $[2M+Na]^+$ 423.2300, found 423.2307; IR (ATR) ν: 3320, 2964, 1942, 1451, 1013, 961, 746 cm^{-1}; colorless oil (99%)

(*E*)-2-isopropyl-6-phenylhexa-2,3,5-trien-1-ol (S6c)



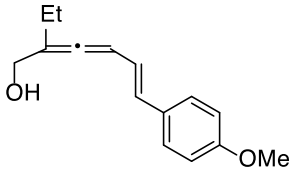
^1H NMR (400 MHz, $CDCl_3$) δ: 1.09 (d, *J* = 6.8 Hz, 3H), 1.11 (d, *J* = 6.8 Hz, 3H), 1.47 (brt, *J* = 6.0 Hz, 1H), 2.25-2.36 (m, 1H), 4.13-4.18 (m, 2H), 6.22-6.27 (m, 1H), 6.53 (d, *J* = 15.6 Hz, 1H), 6.60 (dd, *J* = 9.6, 15.6 Hz, 1H), 7.21 (t, *J* = 7.2 Hz, 1H), 7.30 (dd, *J* = 7.2, 8.0 Hz, 2H), 7.38 (d, *J* = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: -3.6, 21.7, 21.9, 25.6, 28.7, 61.7, 99.6, 114.1, 125.3, 126.2, 127.3, 128.5, 130.6, 137.2, 202.6; HRMS (ESI) m/z calcd for $C_{30}H_{37}Na_1O_2^+$ $[2M+Na]^+$ 451.2613, found 451.2602; IR (ATR) ν: 3346, 2960, 1938, 1496, 1383, 1012, 959, 746, 656 $cm^{-1;}$ m.p. 51-52 ℃; colorless solid (66%)

(*E*)-6-(4-methoxyphenyl)-2-methylhexa-2,3,5-trien-1-ol (S6d)



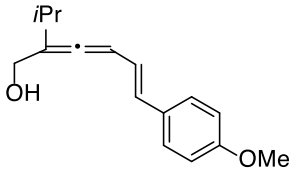
^{1}H NMR (400 MHz, $CDCl_3$) δ: 1.52 (bt, *J* = 4.0 Hz, 1H), 1.78 (d, *J* = 2.8 Hz, 3H), 3.81 (s, 3H), 4.06-4.12 (m, 2H), 6.09-6.17 (m, 1H), 6.42-6.50 (m, 2H), 6.85 (d, *J* = 9.2 Hz, 2H), 7.32 (d, *J* = 9.2 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 15.6, 55.2, 63.8, 97.2, 102.1, 113.9, 122.8, 127.3, 120.0, 130.3, 159.0, 203.2; HRMS (ESI) m/z calcd for $C_{28}H_{32}Na_1O_4^+$ $[2M+Na]^+$ 450.1807, found 450.1803; IR (ATR) ν: 3347, 2913, 1944, 1604, 1510, 1463, 1246, 803 cm^{-1}; yellow gum (95%)

(*E*)-2-ethyl-6-(4-methoxyphenyl)hexa-2,3,5-trien-1-ol (S6e)



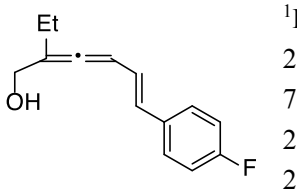
^{1}H NMR (400 MHz, $CDCl_3$) δ: 1.07 (t, *J* = 7.6 Hz, 3H), 1.52 (bs, 1H), 2.05-2.14 (m, 2H), 3.81 (s, 3H), 4.08-4.15 (m, 2H), 6.19-6.26 (m, 1H), 6.43-6.56 (m, 2H), 6.85 (d, *J* = 8.8 Hz, 2H), 7.32 (d, *J* = 8.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 12.1, 22.5, 55.2, 63.0, 99.1, 109.1, 114.0, 123.0, 127.3, 130.0, 130.1, 159.0, 202.8; HRMS (ESI) m/z calcd for $C_{30}H_{36}Na_1O_4^+$ $[2M+Na]^+$ 483.2511, found 483.2491; IR (ATR) ν: 3335, 2963, 1940, 1739, 1604, 1510, 1456, 1248, 962, 804 cm^{-1}; yellow gum (95%)

(*E*)-2-isopropyl-6-(4-methoxyphenyl)hexa-2,3,5-trien-1-ol (S6f)



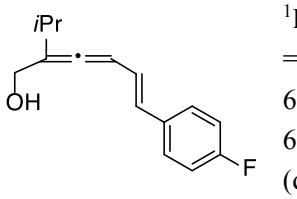
^{1}H NMR (400 MHz, $CDCl_3$) δ: 1.08 (d, *J* = 6.4 Hz, 3H), 1.12 (d, *J* = 6.4 Hz, 3H), 1.46 (t, *J* = 6.0 Hz, 1H), 2.25-2.36 (m, 1H), 3.81 (s, 3H), 4.10-4.21 (m, 2H), 6.22-6.26 (m, 1H), 6.42-6.51 (m, 2H), 6.85 (d, *J* = 8.8 Hz, 2H), 7.32 (d, *J* = 8.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 21.7, 21.0, 28.7, 55.2, 61.7, 99.8, 113.8, 113.9, 123.0, 127.3, 130.0, 130.1, 159.0, 202.1; HRMS (ESI) m/z calcd for $C_{32}H_{40}Na_1O_4^+$ $[2M+Na]^+$ 511.2824, found 511.2837; IR (ATR) ν: 3397, 2960, 1938, 1511, 1383, 1250, 1174, 1032, 963, 803 cm^{-1}; yellow oil (90%)

(*E*)-2-ethyl-6-(4-fluorophenyl)hexa-2,3,5-trien-1-ol (S6g)



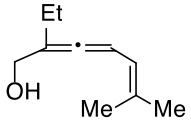
^{1}H NMR (400 MHz, $CDCl_3$) δ: 1.07 (t, *J* = 7.6 Hz, 3H), 1.49-1.53 (m, 1H), 2.05-2.13 (m, 2H), 4.07-4.17 (m, 2H), 6.17-6.23 (m, 1H), 6.46-6.56 (m, 2H), 6.97-7.02 (m, 2H), 7.32-7.37 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 12.0, 22.5, 62.9, 98.6, 109.2, 115.4 (d, *J* = 21.9 Hz), 125.0, 127.6 (d, *J* = 7.7 Hz), 129.2, 133.3 (d, *J* = 2.9 Hz), 162.0 (d, *J* = 246.0 Hz), 203.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ: -114.4; HRMS (ESI) m/z calcd for $C_{14}H_{15}F_1Na_1O_1^+$ $[M+Na]^+$ 241.1005, found 241.1006; IR (ATR) ν: 3330, 2966, 1941, 1600, 1508, 1456, 962, 805 cm^{-1}; yellow oil (31%)

(*E*)-6-(4-fluorophenyl)-2-isopropylhexa-2,3,5-trien-1-ol (S6h)



^{1}H NMR (400 MHz, $CDCl_3$) δ: 1.09 (d, *J* = 6.4 Hz, 3H), 1.10 (d, *J* = 6.4 Hz, 3H), 1.46 (t, *J* = 6.0 Hz, 1H), 2.25-2.34 (m, 1H), 4.11-4.22 (m, 2H), 6.19-6.25 (m, 1H), 6.46-6.55 (m, 2H), 6.97-7.02 (m, 2H), 7.32-7.36 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 21.5, 21.8, 28.4, 61.5, 98.9, 113.8, 115.3 (d, *J* = 21.9 Hz), 125.0, 127.5 (d, *J* = 8.6 Hz), 129.0, 133.3, 161.9 (d, *J* = 245.9 Hz), 202.9; ^{19}F NMR (376 MHz, $CDCl_3$) δ: -114.4; HRMS (ESI) m/z calcd for $C_{15}H_{17}F_1Na_1O_1^+$ $[M+Na]^+$ 255.1161, found 255.1154; IR (ATR) ν: 3353, 2962, 1939, 1601, 1508, 1228, 962, 803 cm$^{-1;}$ m.p. 53 °C; pale red solid (quant)

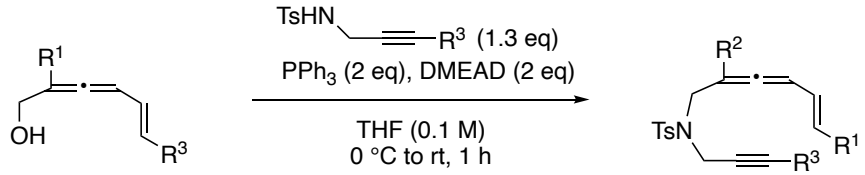
2-ethyl-6-methylhepta-2,3,5-trien-1-ol (S6i)



^{1}H NMR (400 MHz, $CDCl_3$) δ: 1.04 (t, *J* = 7.6 Hz, 3H), 1.45 (t, *J* = 6.0 Hz, 1H), 1.75 (s, 3H), 1.78 (s, 3H), 2.00-2.06 (m, 2H), 4.01-4.11 (m, 2H), 5.61 -5.65 (m, 1H), 6.21-6.27 (m, 1H); ^{13}C

NMR (100 MHz, $CDCl_3$) δ: 18.0, 22.6, 25.6, 25.9, 63.0, 95.0, 108.2, 120.0, 134.5, 201.6; HRMS (ESI) m/z calcd for $C_{10}H_{17}O_1^+$ $[M+H]^+$ 153.1279, found 153.1247; IR (ATR) ν: 3341, 2965, 1943, 1376, 1010, 821 cm^{-1}; colorless oil (84%)

Synthesis of 1

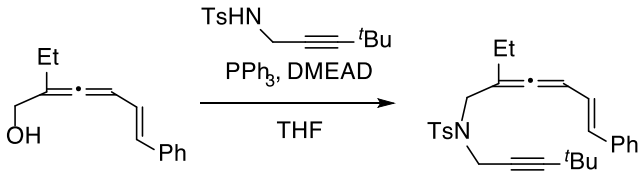


S6 **1**

General procedure of the Mitsunobu reaction

To a solution of **S6** (1.40 mmol), PPh_3 (477.3 mg, 1.820 mmol), **S7** (1.540 mmol) in THF (7.0 mL) was added bis(2-methoxyethyl) azodicarboxylate (426.2 mg, 1.820 mmol) at 0 ℃. The reaction mixture was warmed up to room temperature and stirred for 1 h. When the reaction was completed, it was quenched by H_2O and the aqueous layer was extracted with AcOEt then dried over anhydrous Na_2SO_4. The organic phase was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel (*n*-Hexane/AcOEt = 50/1-20/1) to afford **1**.

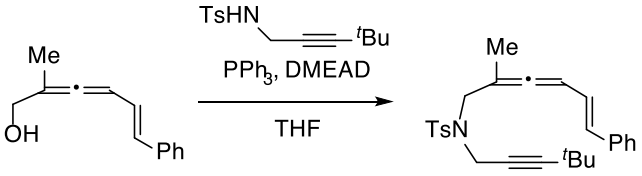
(*E*)-*N*-(4,4-dimethylpent-2-yn-1-yl)-*N*-(2-ethyl-6-phenylhexa-2,3,5-trien-1-yl)-4-methylbenzenesulfonamide (1a)



S6b general Mitsunobu reaction **XX**: 73%

^{1}H NMR (400 MHz, $CDCl_3$) δ: 0.89 (s, 9H), 1.06 (t, 3H, *J* = 7.2 Hz), 2.01-2.08 (m, 2H), 2.40 (s, 3H), 3.82 (dq, 1H, *J* = 1.6, 13.2 Hz), 3.88 (dq, 1H, 1.6, 13.2 Hz), 4.12 (d, 2H, *J* = 1.6 Hz), 6.05 (dt, 1H, *J* = 1.6, 9.6 Hz) 6.46 (d, 1H, *J* = 15.6 Hz), 6.53 (dd, 1H, *J* = 9.6, 15.6 Hz), 7.20 (t, 1H, *J* = 6.8 Hz), 7.28 (d, 2H, *J* = 8.0 Hz), 7.30 (d, 2H, *J* = 6.8 Hz), 7.36 (d, 2H, *J* = 6.8Hz), 7.73 (d, 2H, *J* = 8.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 12.0, 21.4, 22.7, 27.0, 30.5, 36.1, 48.7, 70.2, 94.9, 96.5, 102.4, 125.0, 126.1, 127.3, 127.7, 128.5, 129.4, 130.4, 136.1, 137.1, 143.2, 206.9; HRMS (ESI) m/z calcd for $C_{28}H_{33}N_1Na_1O_2S_1^+$ $[M+Na]^+$ 470.2130, found 470.2125; IR (ATR) ν: 2967, 1944, 1495, 1349, 1162, 961, 750, 673 cm^{-1}; yellow gum (73%)

(*E*)-*N*-(4,4-dimethylpent-2-yn-1-yl)-4-methyl-*N*-(2-methyl-6-phenylhexa-2,3,5-trien-1-yl)benzenesulfonamide (1b)

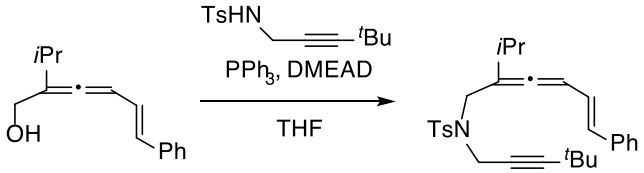


S6a general Mitsunobu reaction **XX**: 16%

^{1}H NMR (400 MHz, $CDCl_3$) δ: 0.90 (s, 9H), 1.80 (d, *J* = 2.8 Hz, 3H), 2.40 (s, 3H), 3.79 (dd, *J* = 2.0, 13.6 Hz, 1H),

3.85 (dd, *J* = 2.0, 13.6 Hz, 1H), 4.08-4.18 (m, 2H), 5.92-5.98 (m, 1H), 6.46 (d, *J* = 16.0 Hz, 1H), 6.53 (dd, *J* = 9.6, 16.0 Hz, 1H), 7.20 (t, *J* = 8.0 Hz, 1H), 7.29-7.31 (m, 4H), 7.35 (d, *J* = 7.2 Hz, 2H), 7.73 (d, *J* = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 16.1, 21.4, 27.0, 30.4, 36.0, 49.8, 70.2, 94.6, 94.8, 95.7, 124.8, 126.1, 127.3, 127.6, 128.5, 129.4, 130.6, 136.1, 137.0, 143.2, 207.4; HRMS (ESI) m/z calcd for $C_{27}H_{31}N_1Na_1O_2S_1^+$ $[M+Na]^+$ 456.1973, found 456.1977; IR (ATR) ν: 2968, 2240, 1948, 1747, 1496, 1349, 1162, 962, 749 cm^{-1}; yellow gum (16%)

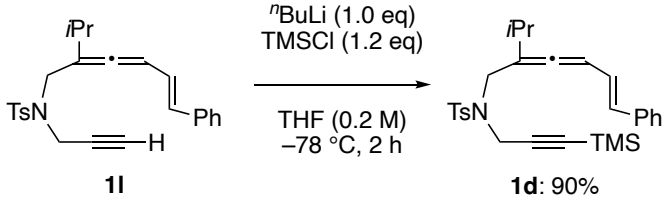
(*E*)-*N*-(4,4-dimethylpent-2-yn-1-yl)-*N*-(2-isopropyl-6-phenylhexa-2,3,5-trien-1-yl)-4-methylbenzenesulfonamide (1c)



S6c general Mitsunobu reaction **XX**: 69%

^{1}H NMR (400 MHz, $CDCl_3$) δ: 0.88 (s, 9H), 1.10 (d, *J* = 6.8 Hz, 3H), 1.11 (d, *J* = 6.8 Hz, 3H), 2.33-2.37 (m, 1H), 3.85 (dd, *J* = 2.4, 11.6 Hz, 1H), 3.94 (dd, *J* = 11.6, 2.4 Hz, 1H), 4.07-4.17 (m, 2H), 6.03-6.07 (m, 1H), 6.44-6.54 (m, 2H), 7.20 (t, *J* = 6.0 Hz, 1H), 7.26-7.36 (m, 6H), 7.73 (d, *J* = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 21.3, 21.5, 21.7, 26.9, 28.0, 30.4, 36.0, 47.4, 70.1, 94.9, 97.0, 107.0, 125.0, 126.1, 127.2, 127.6, 128.4, 129.4, 130.4, 136.0, 137.1, 143.1, 206.3; HRMS (ESI) m/z calcd for $C_{29}H_{35}N_1Na_1O_2S_1^+$ $[M+Na]^+$ 484.2286, found 484.2278; IR (ATR) ν: 2964, 1946, 1456, 1350, 1264, 1163, 1092, 960, 814 cm^{-1}; m.p. 103-104 ℃; colorless solid (69%)

(*E*)-*N*-(2-isopropyl-6-phenylhexa-2,3,5-trien-1-yl)-4-methyl-*N*-(3-(trimethylsilyl)prop-2-yn-1-yl)benzenesulfonamide (1d)



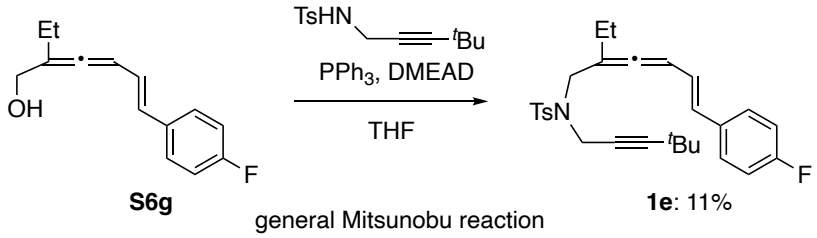
1l **1d**: 90%

1l to **1d**: ^{n}BuLi (0.25 mL, 1.55 M in hexanes, 0.380 mmol) was added to a solution of **xx** (154.0 mg, 0.380 mmol) in THF (1.9 mL) dropwise at -78 °C under argon. After being stirred for 10 minutes at same temperature, trimethylsilyl chloride (0.06 mL, 0.456 mmol) was added, and stirred for 3 h at -78 ℃. When the reaction was complete, it was quenched with saturated aqueous solution of NH_4Cl, extracted with Et_2O and dried over anhydrous Na_2SO_4. The organic phase was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel (*n*-Hexane/AcOEt = 50/1) to afford pure **1d** as colorless solid (90%, 163.0 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ: 0.09 (s, 9H), 1.10 (d, *J* = 6.8 Hz, 3H), 1.11 (d, *J* = 6.8 Hz, 3H), 2.33-2.38 (m, 1H), 2.40 (s, 3H), 3.86 (dd, *J* = 2.0, 13.6 Hz, 1H), 3.94 (dd, *J* = 2.0, 13.6 Hz, 1H), 4.15 (s, 2H), 6.04-6.07 (m, 1H), 6.44-6.54 (m, 2H), 7.18-7.22 (m, 1H), 7.27-7.31 (m, 4H), 7.36 (d, *J* = 8.4 Hz, 2H), 7.73 (d, *J* = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: -0.5, 21.5, 21.5, 21.8, 28.1, 36.6, 47.7, 91.2, 97.2, 97.2, 107.0, 124.9, 126.2, 127.3, 127.7, 128.5, 129.4, 130.5, 135.8, 137.1, 143.3, 206.3; HRMS (ESI) m/z calcd for $C_{28}H_{35}N_1Na_1O_2S_1Si_1^+$ $[M+Na]^+$ 500.2056, found 500.2057; IR (ATR) ν: 2960, 1942, 1449, 1349, 1250, 1161, 961, 814 cm^{-1}; m.p. 120-121 ℃; colorless solid (89%, 42.2 mg)

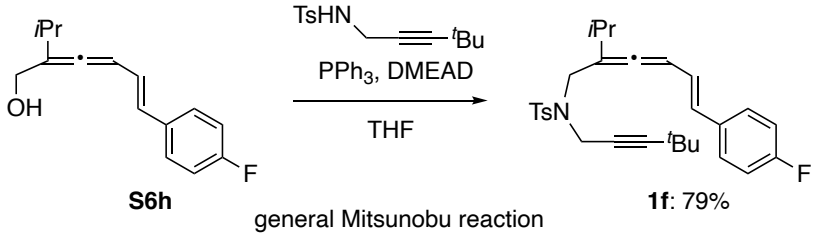
(*E*)-*N*-(4,4-dimethylpent-2-yn-1-yl)-*N*-(2-ethyl-6-(4-fluorophenyl)hexa-2,3,5-trien-1-yl)-4-

methylbenzenesulfonamide (1e)



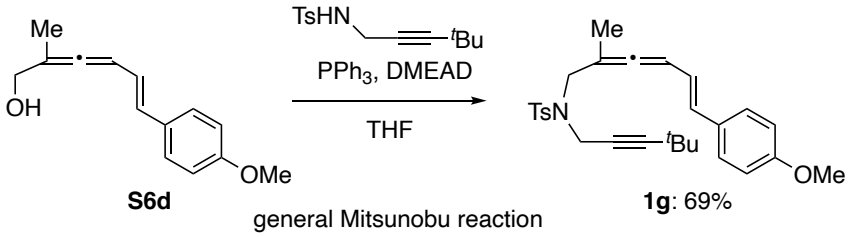
^{1}H NMR (400 MHz, $CDCl_3$) δ: 0.89 (s, 9H), 1.06 (t, *J* = 7.2 Hz, 3H), 2.05-2.17 (m, 2H), 2.40 (s, 3H), 3.81 (dd, *J* = 2.0, 12.8 Hz, 1H), 3.89 (dd, *J* = 2.0, 12.8 Hz, 1H), 4.09 (d, *J* = 18.4 Hz, 1H), 4.15 (d, *J* = 18.4 Hz, 1H), 6.00-6.05 (m, 1H), 6.40-6.48 (m, 2H), 6.96-7.01 (m, 2H), 7.27-7.33 (m, 4H), 7.73 (d, *J* = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 12.0, 21.4, 22.8, 27.0, 30.5, 36.1, 48.7, 70.2, 94.9, 96.4, 102.6, 115.4 (d, *J* = 21.0 Hz), 124.8, 127.6 (d, *J* = 10.5 Hz), 127.7, 129.2, 129.4, 133.4 (d, *J* = 2.9 Hz), 136.2, 143.2, 162.1 (d, *J* = 245.3 Hz), 206.8; ^{19}F NMR (376 MHz, $CDCl_3$) δ: -114.4; HRMS (ESI) m/z calcd for $C_{28}H_{32}F_1N_1Na_1O_2S_1^+$ $[M+Na]^+$ 488.2036, found 488.2050; IR (ATR) ν: 2968, 1945, 1455, 1349, 1227, 1162, 1093, 963, 810 cm^{-1}; colorless oil (11%)

(*E*)-*N*-(4,4-dimethylpent-2-yn-1-yl)-*N*-(6-(4-fluorophenyl)-2-isopropylhexa-2,3,5-trien-1-yl)-4-methylbenzenesulfonamide (1f)



^{1}H NMR (400 MHz, $CDCl_3$) δ: 0.88 (s, 9H), 1.10 (d, *J* = 6.4 Hz, 6H), 2.33-2.40 (m, 1H), 2.40 (s, 3H), 3.83 (d, *J* = 2.0, 13.6 Hz, 1H), 3.94 (d, *J* = 13.6 Hz, 1H), 4.08 (d, *J* = 18.4 Hz, 1H), 4.15 (d, *J* = 18.4 Hz, 1H), 6.01-6.05 (m, 1H), 6.37-6.46 (m, 2H), 6.97 (d, *J* = 8.4 Hz, 1H), 6.99 (d, *J* = 8.4 Hz, 1H), 7.27-7.32 (m, 4H), 7.73 (d, *J* = 7.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 21.4, 21.5, 21.8, 27.0, 28.1, 30.5, 36.1, 47.7, 70.2, 95.0, 96.9, 107.2, 115.4 (d, *J* = 20.9 Hz), 124.9, 127.6 (d, *J* = 7.7 Hz), 127.7, 129.1, 129.5, 133.4 (d, *J* = 2.9 Hz), 136.1, 143.2, 160.1 (d, *J* = 145.9 Hz), 206.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ: -114.4; HRMS (ESI) m/z calcd for $C_{29}H_{34}F_1N_1Na_1O_2S_1^+$ $[M+Na]^+$ 502.2192, found 502.2200; IR (ATR) ν: 2966, 1942, 1508, 1350, 1228, 1162, 834 cm^{-1}; m.p. 127 ℃; colorless solid (79%)

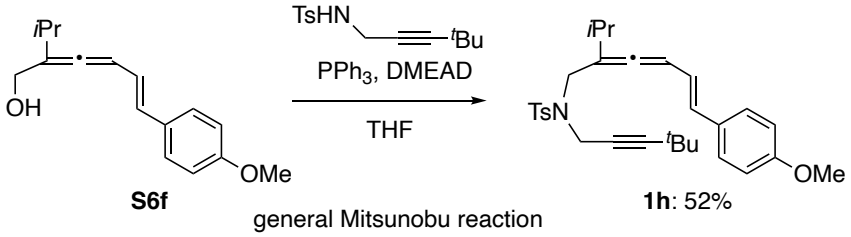
(*E*)-*N*-(4,4-dimethylpent-2-yn-1-yl)-*N*-(6-(4-methoxyphenyl)-2-methylhexa-2,3,5-trien-1-yl)-4-methylbenzenesulfonamide (1g)



^{1}H NMR (400 MHz, $CDCl_3$) δ: 0.89 (s, 9H), 1.80 (d, *J* = 2.8 Hz, 3H), 2.41 (s, 3H), 3.77-3.87 (m, 2H), 3.81 (s, 3H), 4.13 (d, *J* = 2.0 Hz, 2H), 5.91-5.95 (m, 1H), 6.35-6.44 (m, 2H), 6.84 (d, *J* = 8.8 Hz, 2H), 7.29 (d, *J* = 8.8 Hz, 1H),

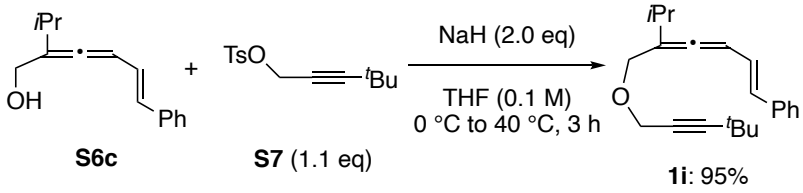
7.30 (d, J = 8.8 Hz, 2H), 7.74 (d, J = 8.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 16.2, 21.4, 27.0, 30.5, 36.0, 49.9, 55.2, 70.2, 94.8, 95.6, 113.9, 122.6, 127.3, 127.6, 127.6, 129.4, 129.9, 130.1, 136.1, 143.2, 159.0, 207.1; HRMS (ESI) m/z calcd for $C_{28}H_{33}N_1Na_1O_3S_1^+$ $[M+Na]^+$ 486.2079, found 486.2081; IR (ATR) ν: 2967, 1948, 1455, 1349, 1252, 1162, 1092, 963, 812 cm^{-1}; yellow gum (69%)

(*E*)-*N*-(4,4-dimethylpent-2-yn-1-yl)-*N*-(2-isopropyl-6-(4-methoxyphenyl)hexa-2,3,5-trien-1-yl)-4-methylbenzenesulfonamide (1h)



^{1}H NMR (400 MHz, $CDCl_3$) δ: 0.88 (s, 9H), 1.10 (d, J = 6.4 Hz, 3H), 1.10 (d, J = 6.4 Hz, 3H), 2.31-2.38 (m, 1H), 2.40 (s, 3H), 3.80 (s, 3H), 3.84 (dd, J = 2.0, 13.2 Hz, 1H), 3.94 (dd, J = 2.0, 13.2 Hz, 1H), 4.09 (d J = 18.4 Hz, 1H), 4.15 (d, J = 18.0 Hz, 1H), 6.01-6.04 (m, 1H), 6.33-6.44 (m, 2H), 6.83 (d, J = 8.4 Hz, 2H), 7.27-7.30 (m, 4H), 7.73 (d, J = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 21.4, 21.5, 21.8, 27.0, 28.1, 30.5, 36.0, 47.5, 55.3, 70.2, 94.9, 97.2, 106.9, 113.9, 122.9, 127.3, 127.7, 129.4, 129.9, 130.0, 136.1, 143.2, 159.0, 206.1; HRMS (ESI) m/z calcd for $C_{30}H_{37}N_1Na_1O_3S_1^+$ $[M+Na]^+$ 514.2392, found 514.2385; IR (ATR) ν: 2965, 1940, 1511, 1349, 1252, 1162, 813 cm^{-1}; m.p. 128 ℃; colorless solid (52%)

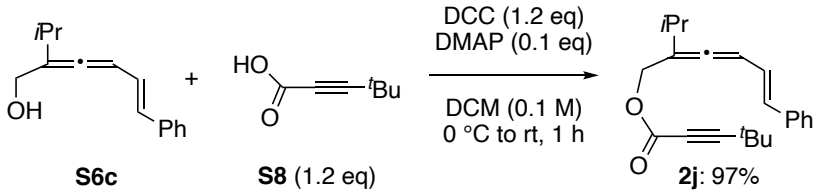
(*E*)-(5-(((4,4-dimethylpent-2-yn-1-yl)oxy)methyl)-6-methylhepta-1,3,4-trien-1-yl)benzene (1i)



To a solution of **S6c** (107.2 mg, 0.500 mmol) in THF (1.5 mL) at 0 ℃ was added sodium hydride (2.0 eq) slowly. The mixture was stirred for 10 minutes at the same temperature, then a solution of **S7** (146.5 mg, 0.550 mmol) in THF (1.0 mL) was added slowly. The reaction mixture was warmed up to 40 ℃ and stirred for 3 h. When the reaction was completed, the reaction mixture was cooled down to 0 ℃, and quenched by H_2O carefully. The aqueous layer was extracted with AcOEt then dried over anhydrous Na_2SO_4. The organic phase was concentrated under reduced pressure, and the residue was purified by column chromatography on silica gel (*n*-Hexane/AcOEt = 100/1-50/1) to afford pure **1i** as colorless oil (95%, 146.7 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ: 1.09 (dd, J = 6.4, 6.4 Hz, 6 H), 1.23 (s, 9H), 2.34-2.41 (m, 1H), 4.15 (s, 4H), 6.03-6.14 (m, 1H), 6.49 (d, J = 15.6 Hz, 1H), 6.59 (dd, J = 10.0, 15.6 Hz, 1 H), 7.20 (t, J = 7.2 Hz, 1H), 7.30 (dd, J = 7.2, 7.6 Hz, 2H), 7.38 (d, J = 7.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 21.6, 21.8, 27.4, 28.3, 30.9, 57.3, 68.8, 74.1, 95.4, 96.6, 109.1, 125.5, 126.1, 127.2, 128.5, 130.1, 137.3, 205.9; HRMS (ESI) m/z calcd for $C_{22}H_{28}Na_1O_1^+$ $[M+Na]^+$ 331.2038, found 331.2036; IR (ATR) ν: 2966, 1940, 1451, 1362, 1264, 1082, 960 cm^{-1}; colorless oil (95%, 146.7 mg)

(*E*)-2-isopropyl-6-phenylhexa-2,3,5-trien-1-yl 4,4-dimethylpent-2-ynoate (2j)

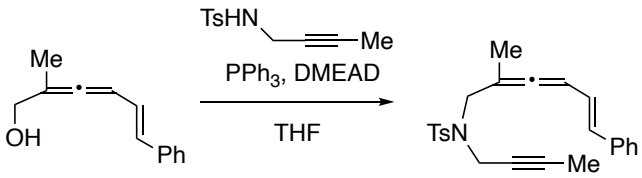


S6c **S8** (1.2 eq) **2j**: 97%

S8 (70.6 mg, 0.560 mmol) was added to a solution of **S6c** (100.9 mg, 0.467 mmol), *N,N'*-dicyclohexylcarbodiimide (115.6 mg, 0.560 mmol) and *N,N*-dimethyl-4-aminopyridine (5.6 mg, 0.047 eq) in DCM (4.67 mL) at 0 ℃ under argon. The reaction mixture was warmed up to room temperature and stirred for 1 h. When the reaction was completed, crude material was concentrated under reduced pressure and the residue was filtered. The crude material was purified by column chromatography on silica gel (*n*-Hexane/AcOEt = 50/1) to afford pure **2j** as colorless oil (97%, 146.6 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ: 1.09 (dd, *J* = 6.4, 6.4 Hz, 6 H), 1.27 (s, 9H), 2.31-2.38 (m, 1H), 4.69-4.76 (m, 2H), 6.15-6.18 (m, 1H), 6.52 (d, *J* = 15.6 Hz, 1H), 6.58 (dd, *J* = 9.2, 15.6 Hz, 1 H), 7.21 (t, *J* = 7.2 Hz, 1H), 7.31 (dd, *J* = 7.2, 8.0 Hz, 2H), 7.39 (d, *J* = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 21.5, 21.7, 27.5, 28.6, 29.9, 64.8, 71.5, 97.1, 97.9, 124.7, 128.3, 127.4, 128.5, 130.8, 137.2, 153.8, 205.9; HRMS (ESI) m/z calcd for $C_{22}H_{26}Na_1O_2^+$ $[M+Na]^+$ 345.1831, found 345.1831; IR (ATR) ν: 2967, 1943, 1709, 1383, 1362, 1210, 960, 746 cm^{-1}; colorless oil (97%, 146.6 mg)

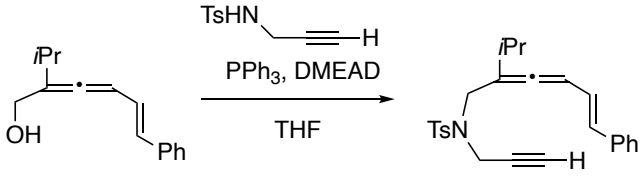
(*E*)-*N*-(but-2-yn-1-yl)-4-methyl-*N*-(2-methyl-6-phenylhexa-2,3,5-trien-1-yl)benzenesulfonamide (1k)



S6a general Mitsunobu reaction **1k**: 33%

^{1}H NMR (400 MHz, $CDCl_3$) δ: 1.47 (t, *J* = 2.0 Hz, 3H), 1.79 (d, *J* = 2.8 Hz, 3H), 2.41 (s, 3H), 3.80 (d, *J* = 2.0 Hz, 2H), 4.08 (q, *J* = 2.0 Hz, 2H), 5.94 (dtq, *J* = 2.0, 2.8, 9.6 Hz, 1H), 6.43-6.56 (m, 2H), 7.19-7.37 (m, 7H), 7.74 (d, *J* = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 207.2, 143.2, 137.1, 136.0, 130.7, 129.2, 128.5, 127.8, 127.4, 126.1, 124.7, 96.0, 94.7, 81.7, 71.2, 50.0, 36.2, 21.4, 16.2, 3.1; yellow gum (33%, 55.4 mg)

(*E*)-*N*-(2-isopropyl-6-phenylhexa-2,3,5-trien-1-yl)-4-methyl-N-(prop-2-yn-1-yl)benzenesulfonamide (1l)

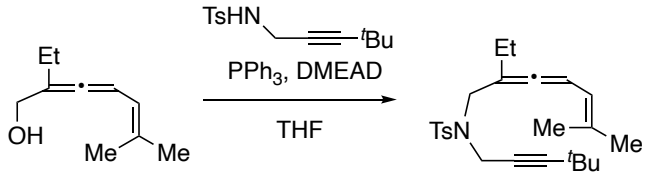


S6c general Mitsunobu reaction **1l**: 88%

^{1}H NMR (400 MHz, $CDCl_3$) δ: 1.08 (d, *J* = 6.8 Hz, 3H), 1.10 (d, *J* = 6.0 Hz, 3H), 1.96 (t, *J* = 2.4 Hz, 1H), 2.34 (qq, *J* = 6.0, 6.8 Hz, 1H), 2.41 (s, 3H), 3.87 (dd, *J* = 2.0, 13.6 Hz, 1H), 3.93 (dd, *J* = 2.0, 13.6 Hz, 1H), 4.14 (d, *J* = 2.4 Hz, 2H), 6.04-6.07 (m, 1H), 6.45-6.54 (m, 2H), 7.21 (t, *J* = 7.2 Hz, 1H), 7.27-7.32 (m, 4H), 7.36 (d, *J* = 7.2 Hz, 2H), 7.74 (d, *J* = 8.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 21.5, 21.8, 28.2, 35.7, 47.7, 73.9, 76.2, 97.4, 107.3, 124.8, 126.2, 127.4, 127.7, 128.6, 129.4, 130.7, 135.8, 137.1, 143.5, 206.2; HRMS (ESI) m/z calcd for $C_{25}H_{27}N_1Na_1O_2S_1^+$ $[M+Na]^+$ 428.1660, found 428.1657; IR (ATR) ν: 3295, 2961, 1941, 1495, 1349, 1161, 962, 749 cm^{-1}; colorless oil

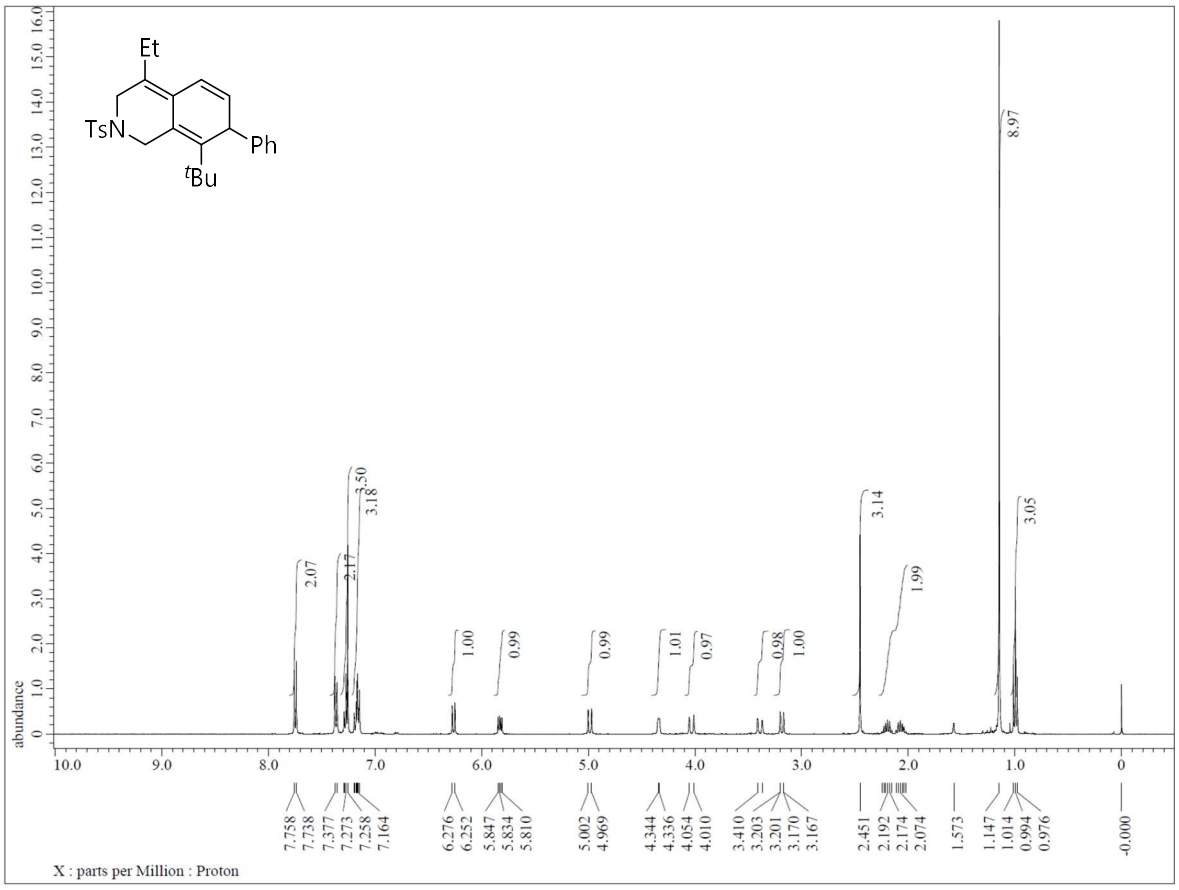
(88%)

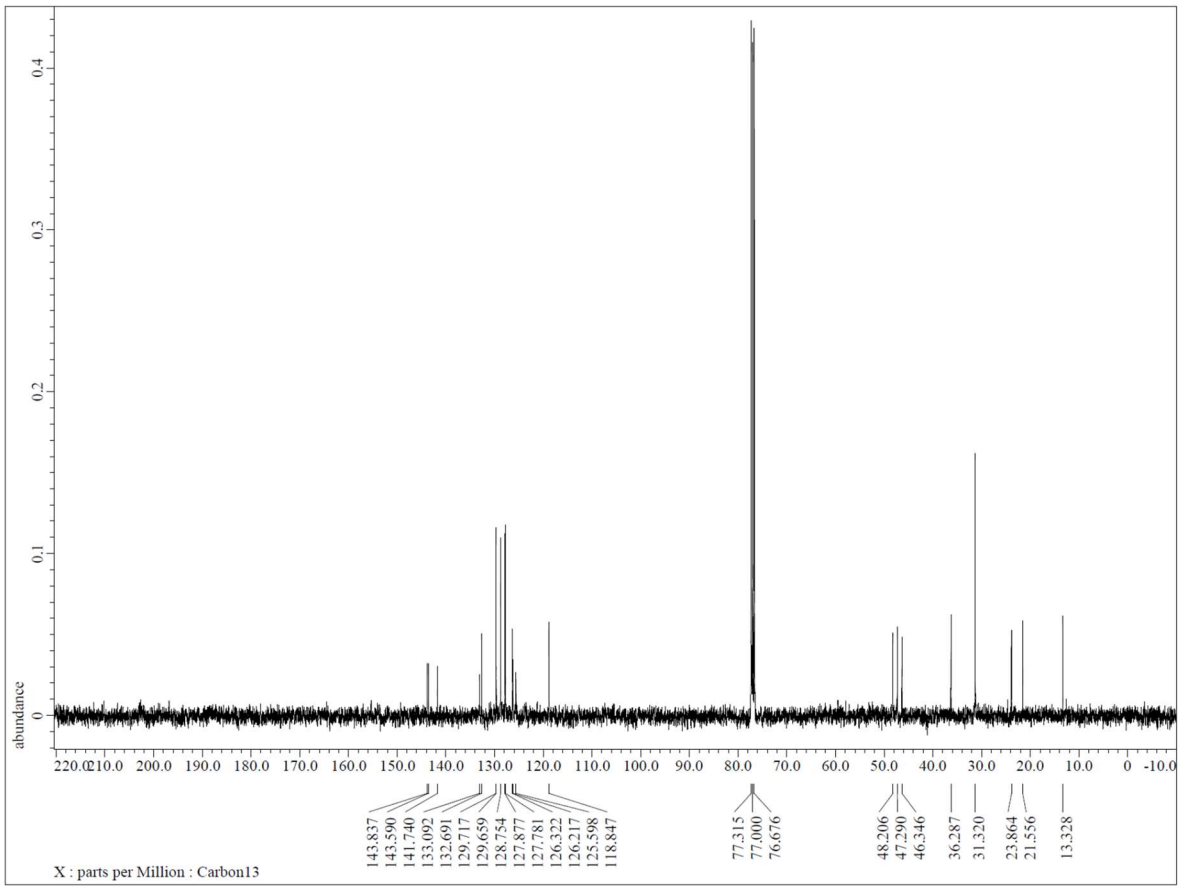
***N*-(4,4-dimethylpent-2-yn-1-yl)-*N*-(2-ethyl-6-methylhepta-2,3,5-trien-1-yl)-4-methylbenzenesulfonamide (1m)**

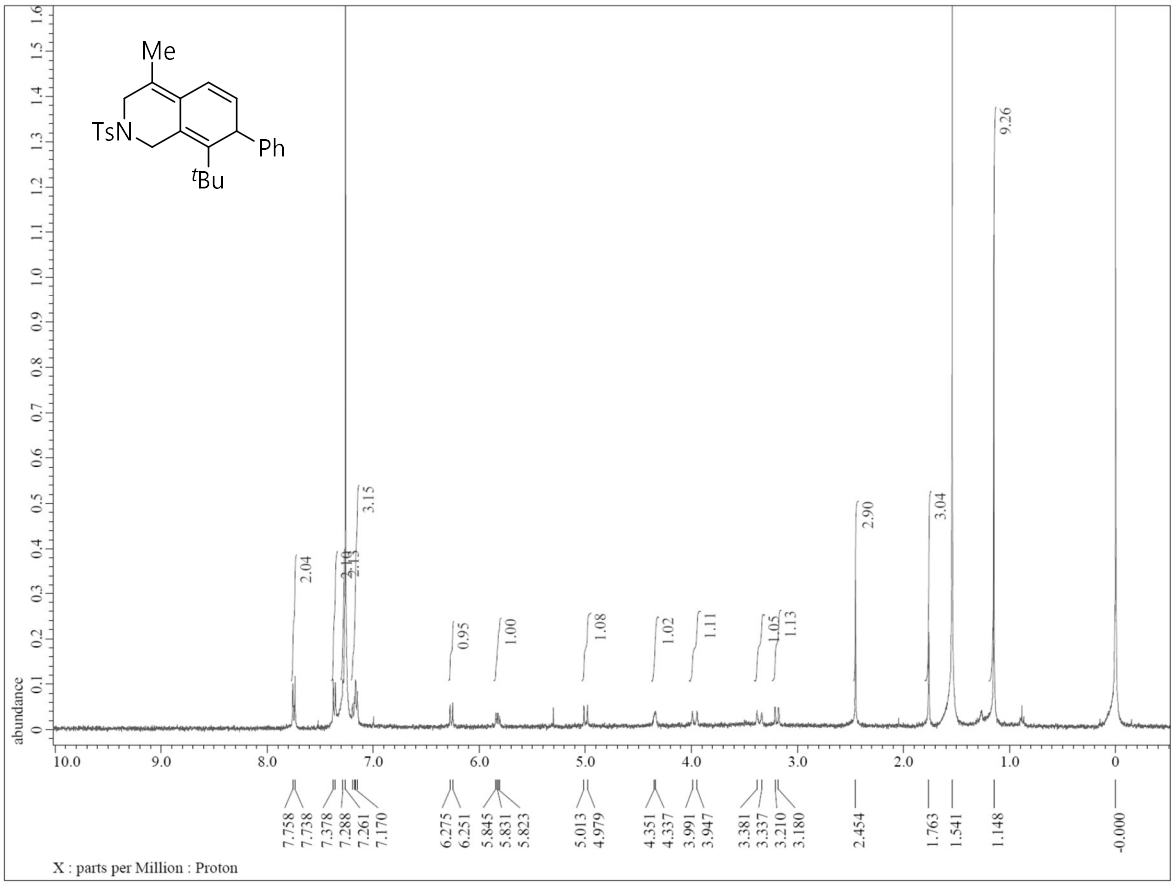


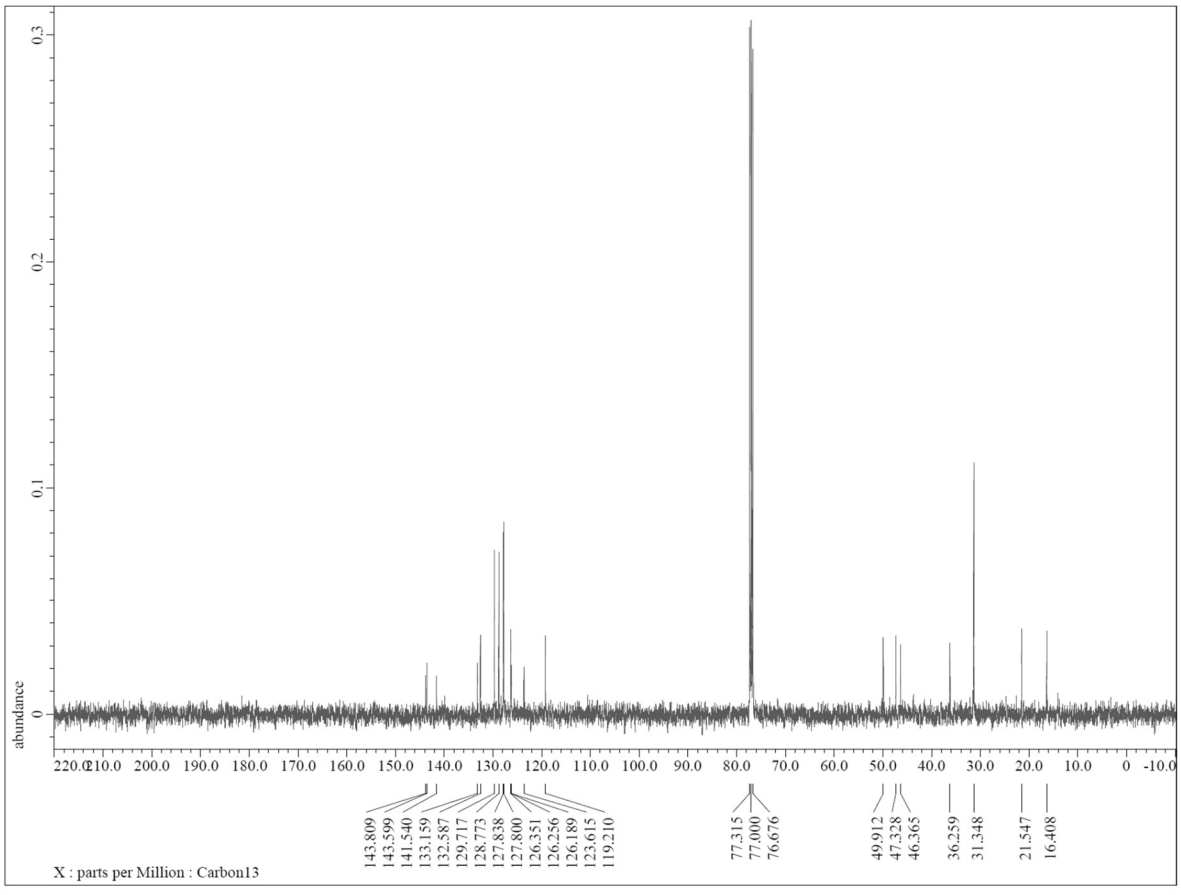
S6i general Mitsunobu reaction **1m**: 31%

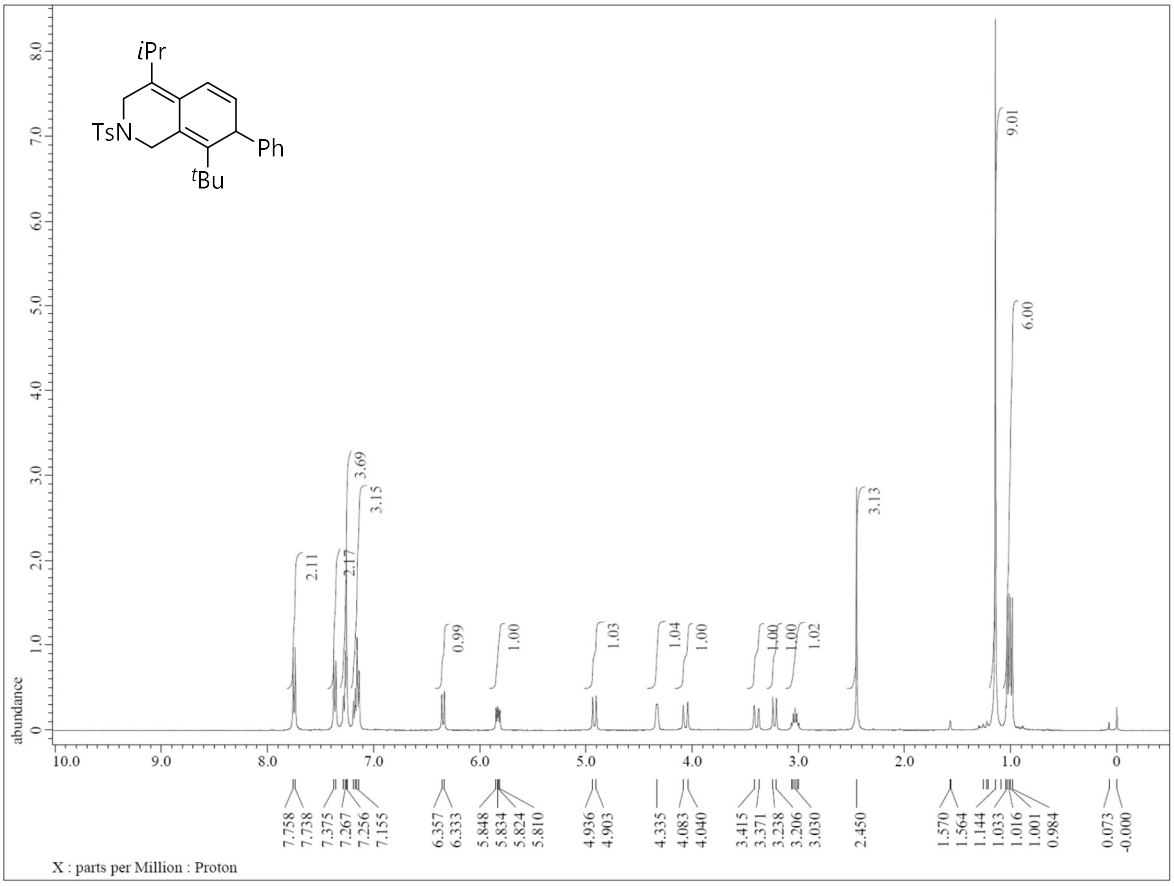
^{1}H NMR (400 MHz, $CDCl_3$) δ: 0.92 (s, 9H), 1.03 (t, *J* = 7.6 Hz, 3H), 1.67 (s, 3H), 1.74 (s, 3H), 2.00-2.10 (m, 2H), 2.40 (s, 3H), 3.76 (dd, *J* = 12.8, 1.6 Hz, 1H), 3.83 (dd, *J* = 12.8, 1.6 Hz, 1H), 4.08 (s, 2H), 5.37-5.57 (m, 1H), 6.00-6.05 (m, 1H), 7.28 (d, *J* = 8.0 Hz, 2H), 7.72 (d, *J* = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 12.3, 18.0, 21.4, 22.7, 25.9, 27.0, 30.1, 35.9, 48.9, 70.3, 92.4, 94.6, 101.2, 119.8, 127.7, 129.4, 134.1, 136.2, 143.1, 205.6; HRMS (ESI) m/z calcd for $C_{24}H_{33}N_1Na_1O_2S_1^+$ $[M+Na]^+$ 422.2130, found 422.2101; IR (ATR) ν: 2969, 1455, 1351, 1163, 835 cm^{-1}; m.p. 73 ℃; colorless solid (31%)

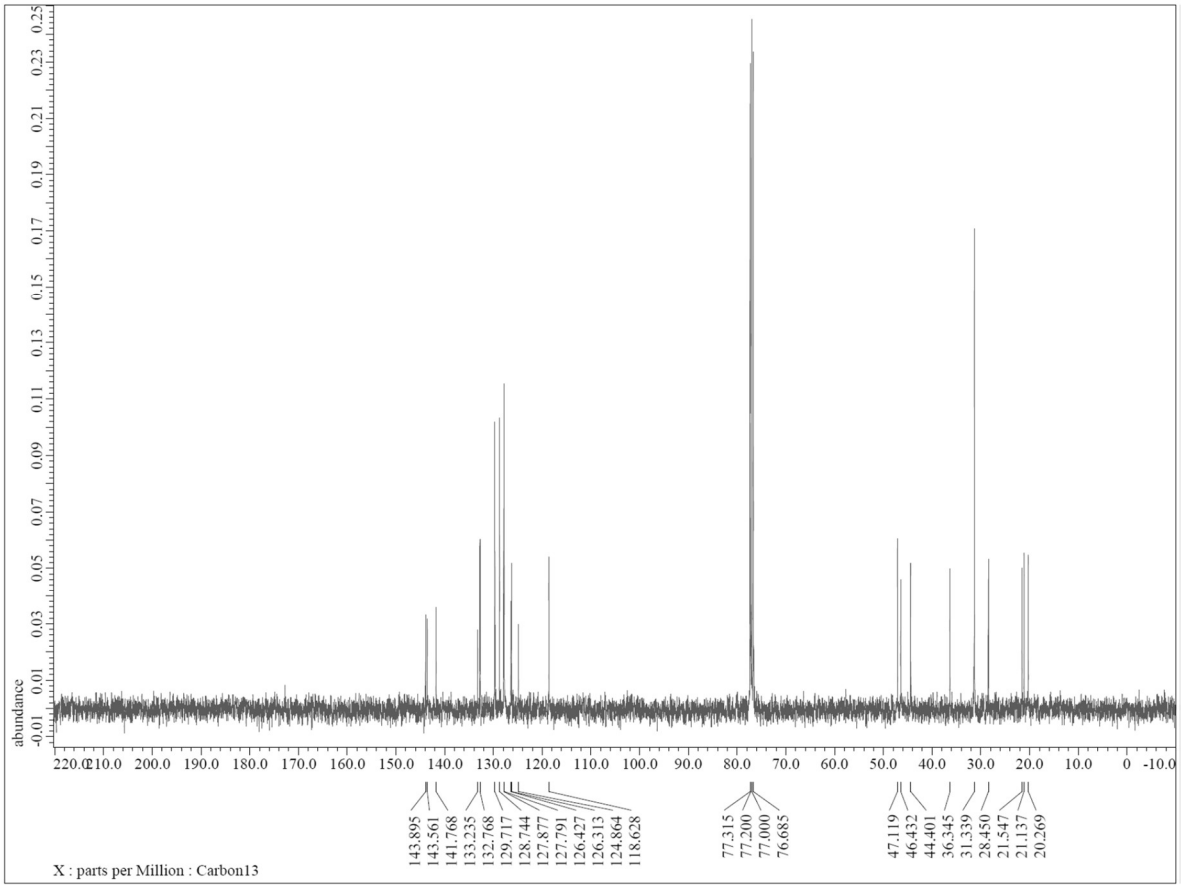

Et
TsN
Ph
tBu
abundance
X : parts per Million : Proton

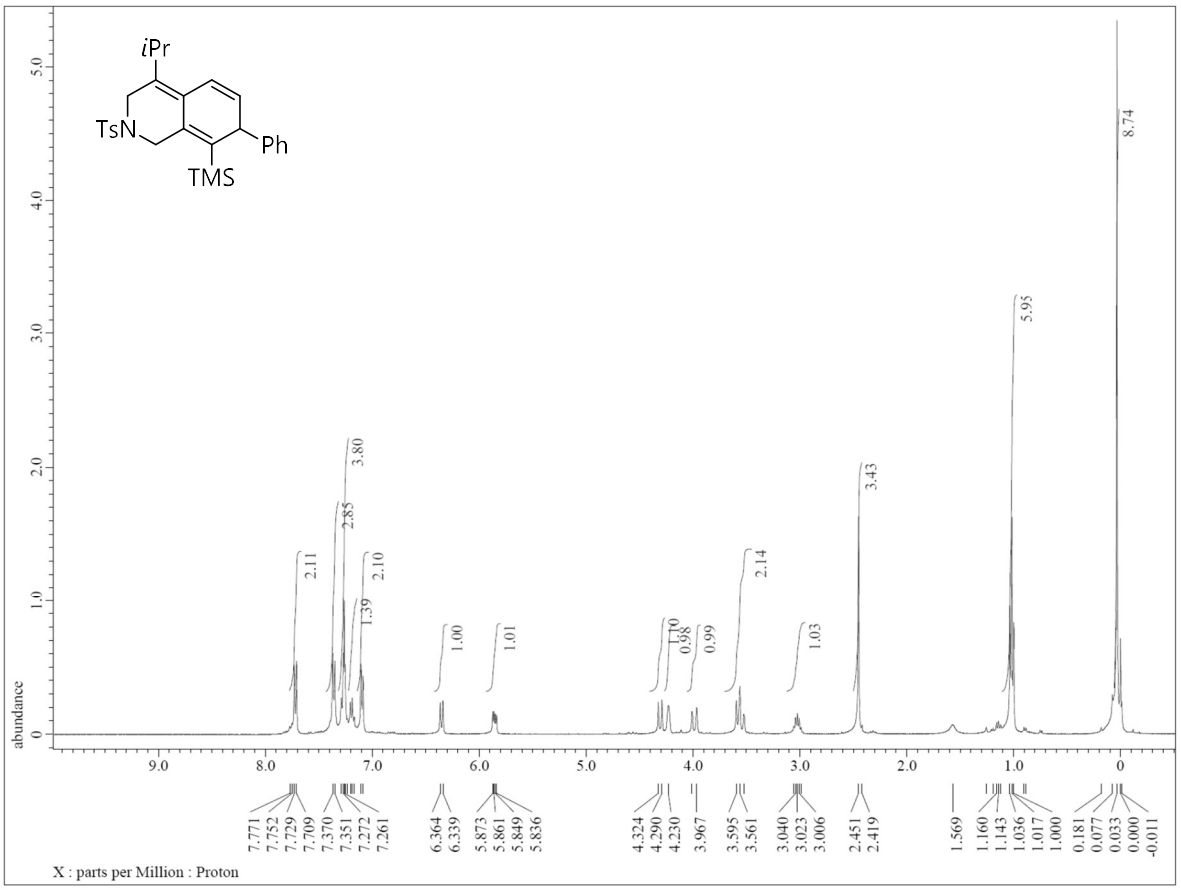

abundance
X : parts per Million : Carbon13

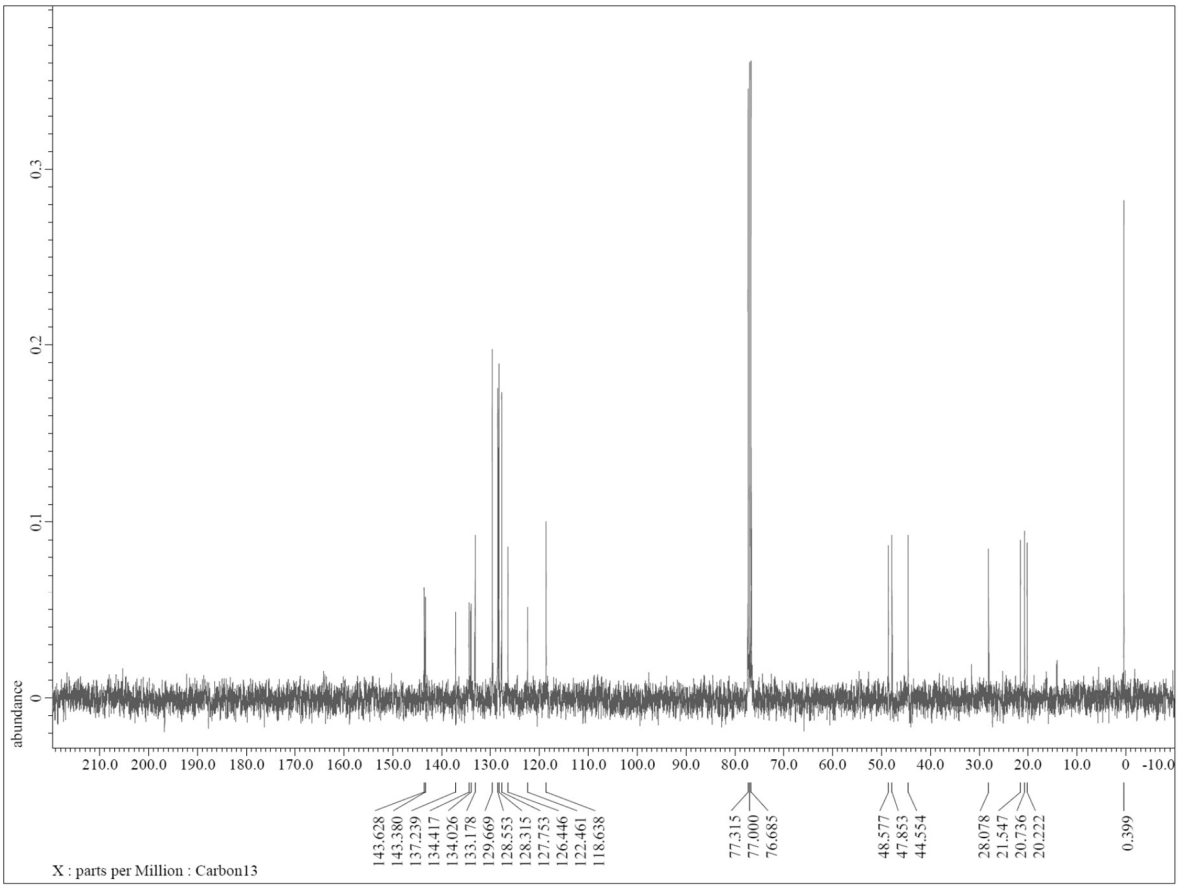

Me
TsN
Ph
tBu
abundance
2.04
3.15
0.95
1.00
1.08
1.02
1.11
1.05
1.13
2.90
3.04
9.26
7.758
7.738
7.378
7.288
7.261
7.170
6.275
6.251
5.845
5.831
5.823
5.013
4.979
4.351
4.337
3.991
3.947
3.381
3.337
3.210
3.180
2.454
1.763
1.541
1.148
-0.000
X : parts per Million : Proton

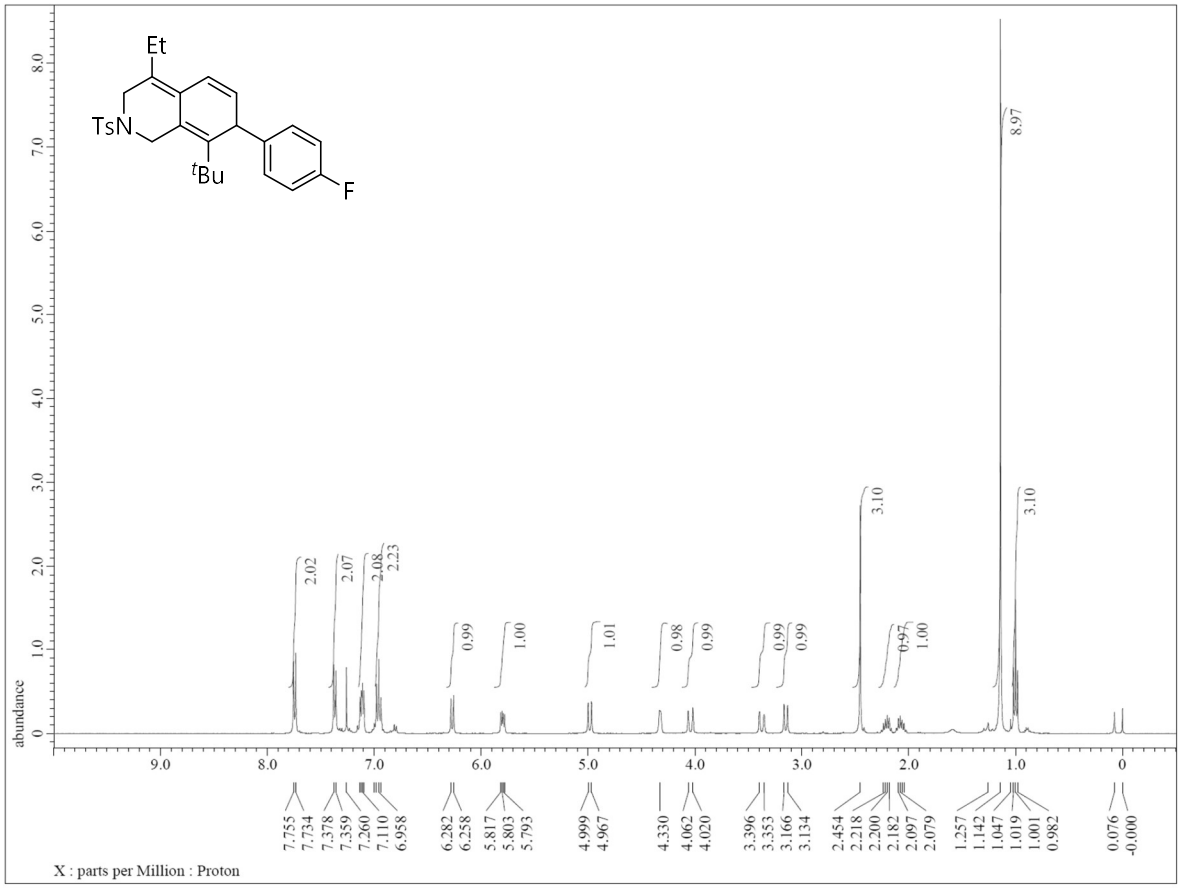

abundance
143.809
143.599
141.540
133.159
132.587
129.717
128.773
127.838
127.800
126.351
126.256
126.189
123.615
119.210
77.315
77.000
76.676
49.912
47.328
46.365
36.259
31.348
21.547
16.408
X : parts per Million : Carbon13

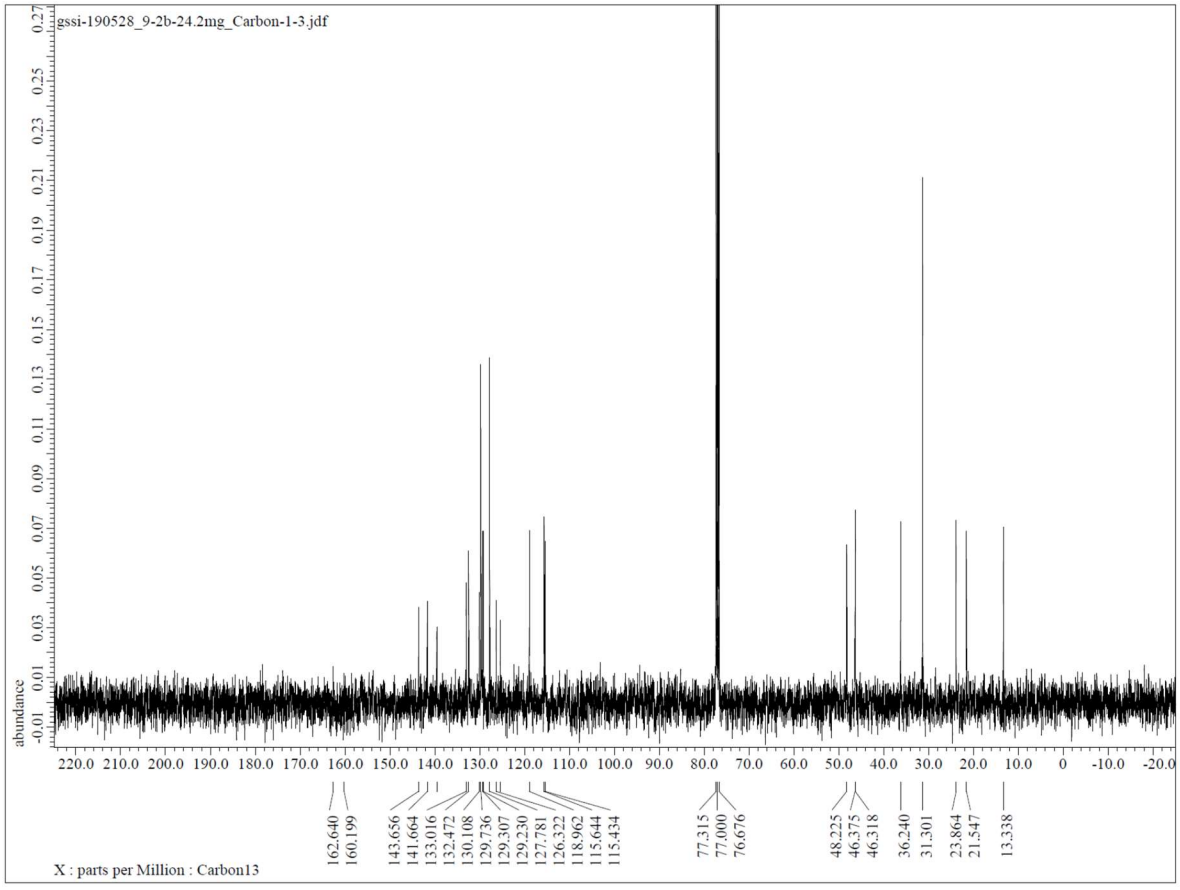

iPr
TsN
Ph
tBu
abundance
9.01
6.00
3.69
3.15
3.13
2.11
2.17
0.99
1.00
1.03
1.04
1.00
1.00
1.00
1.02
7.758
7.738
7.375
7.267
7.256
7.155
6.357
6.333
5.848
5.834
5.824
5.810
4.936
4.903
4.335
4.083
4.040
3.415
3.371
3.238
3.206
3.030
2.450
1.570
1.564
1.144
1.033
1.016
1.001
0.984
0.073
-0.000
X : parts per Million : Proton


abundance
143.895
143.561
141.768
133.235
132.768
129.717
128.744
127.877
127.791
126.427
126.313
124.864
118.628
77.315
77.200
77.000
76.685
47.119
46.432
44.401
36.345
31.339
28.450
21.547
21.137
20.269
X : parts per Million : Carbon13

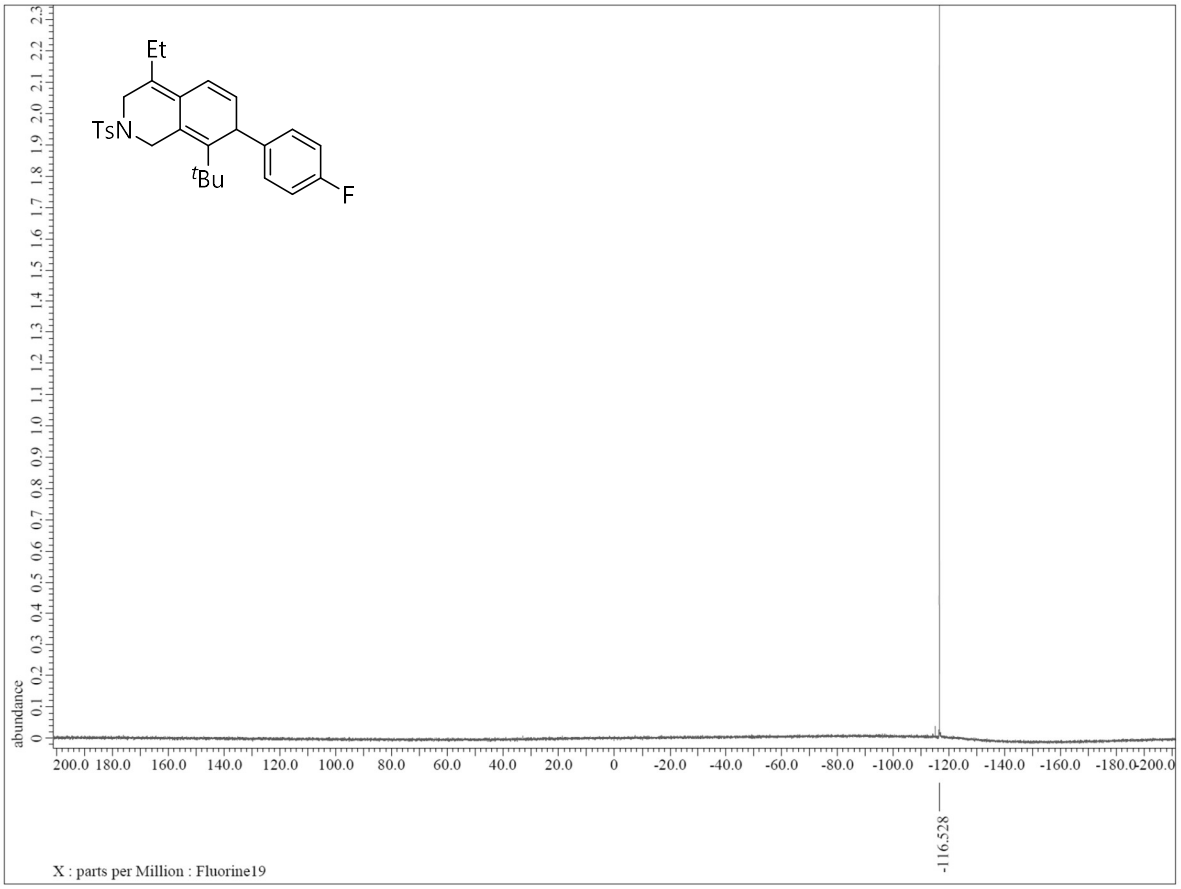

iPr
TsN
Ph
TMS
abundance
X : parts per Million : Proton

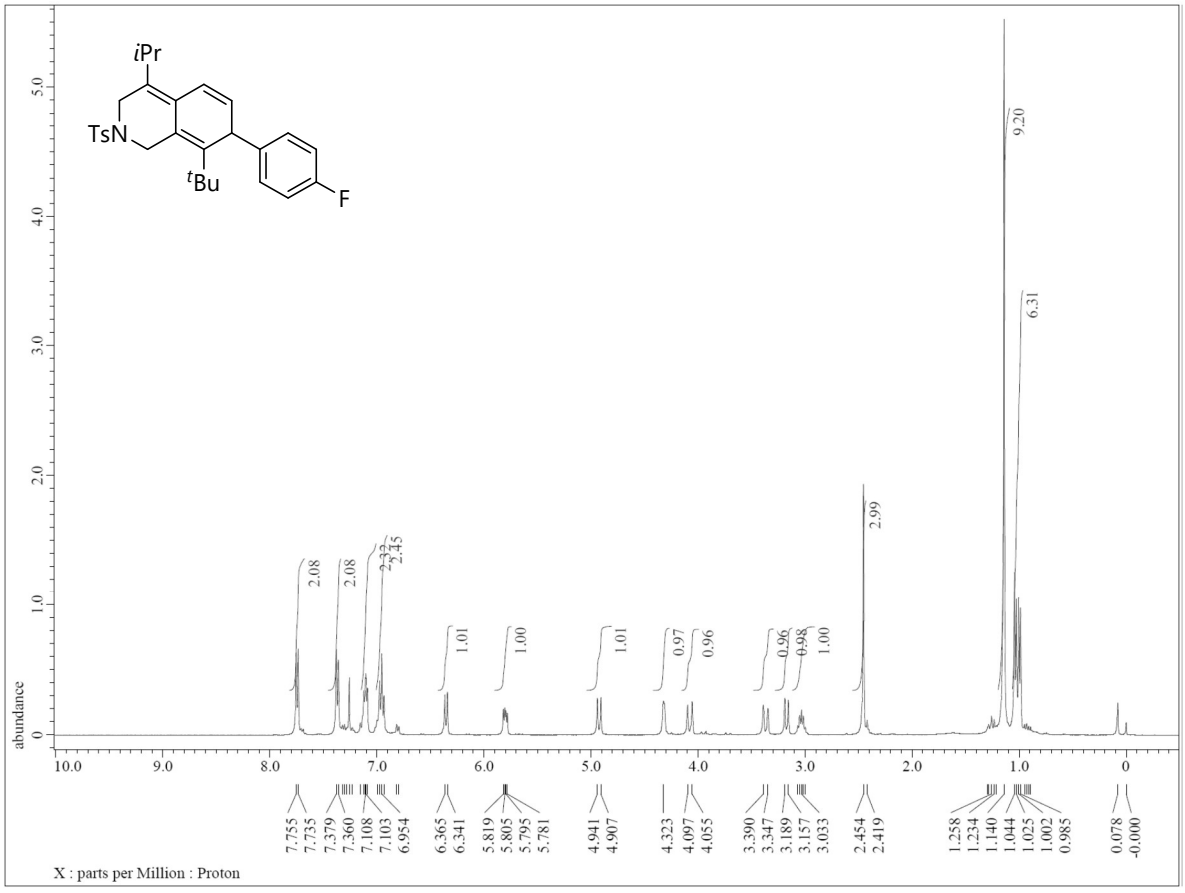

abundance
X : parts per Million : Carbon13

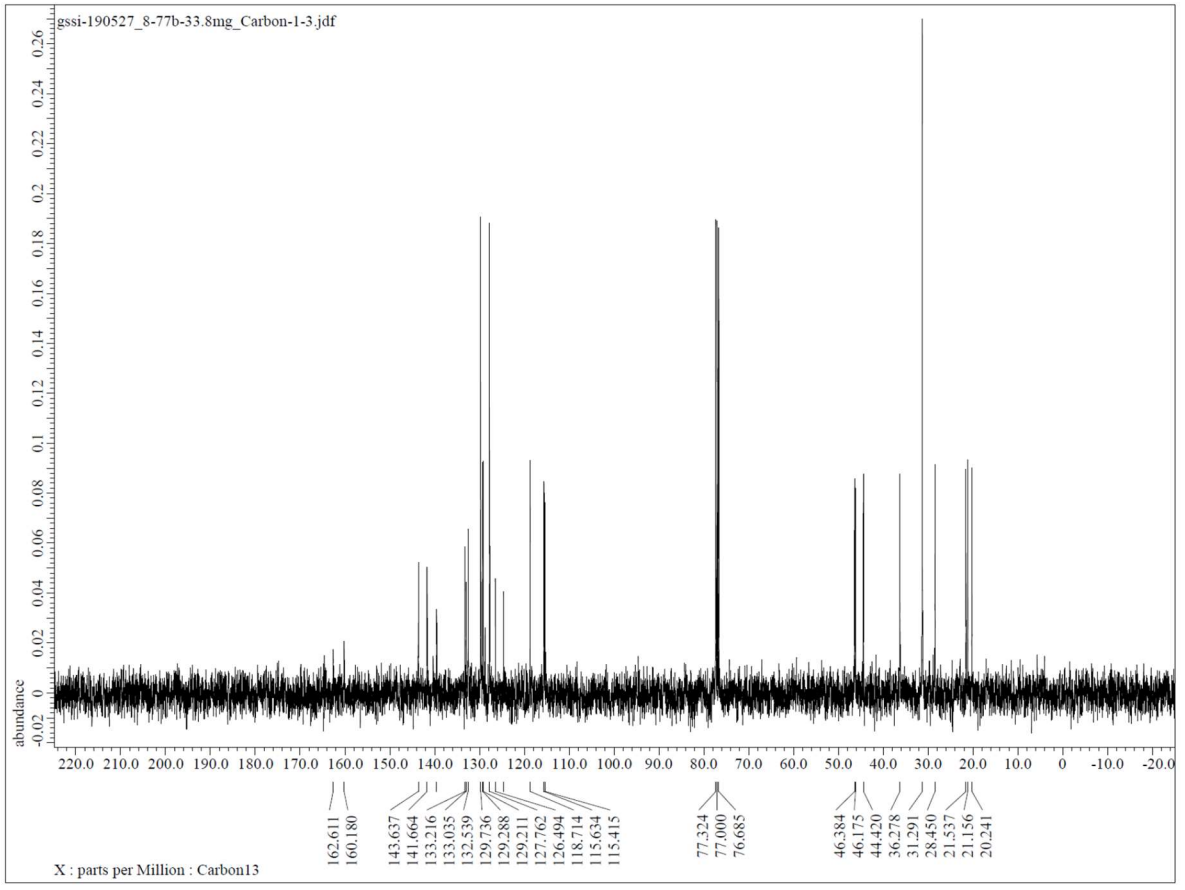

Et
TsN
tBu
F
abundance
X : parts per Million : Proton
8.97
3.10
3.10
2.02
2.07
2.08
2.23
0.99
1.00
1.01
0.98
0.99
0.99
0.99
0.97
1.00
7.755
7.734
7.378
7.359
7.260
7.110
6.958
6.282
6.258
5.817
5.803
5.793
4.999
4.967
4.330
4.062
4.020
3.396
3.353
3.166
3.134
2.454
2.218
2.200
2.182
2.097
2.079
1.257
1.142
1.047
1.019
1.001
0.982
0.076
-0.000


gssi-190528_9-2b-24.2mg_Carbon-1-3.jdf
abundance
X : parts per Million : Carbon13
162.640
160.199
143.656
141.664
133.016
132.472
130.108
129.736
129.307
129.230
127.781
126.322
118.962
115.644
115.434
77.315
77.000
76.676
48.225
46.375
46.318
36.240
31.301
23.864
21.547
13.338

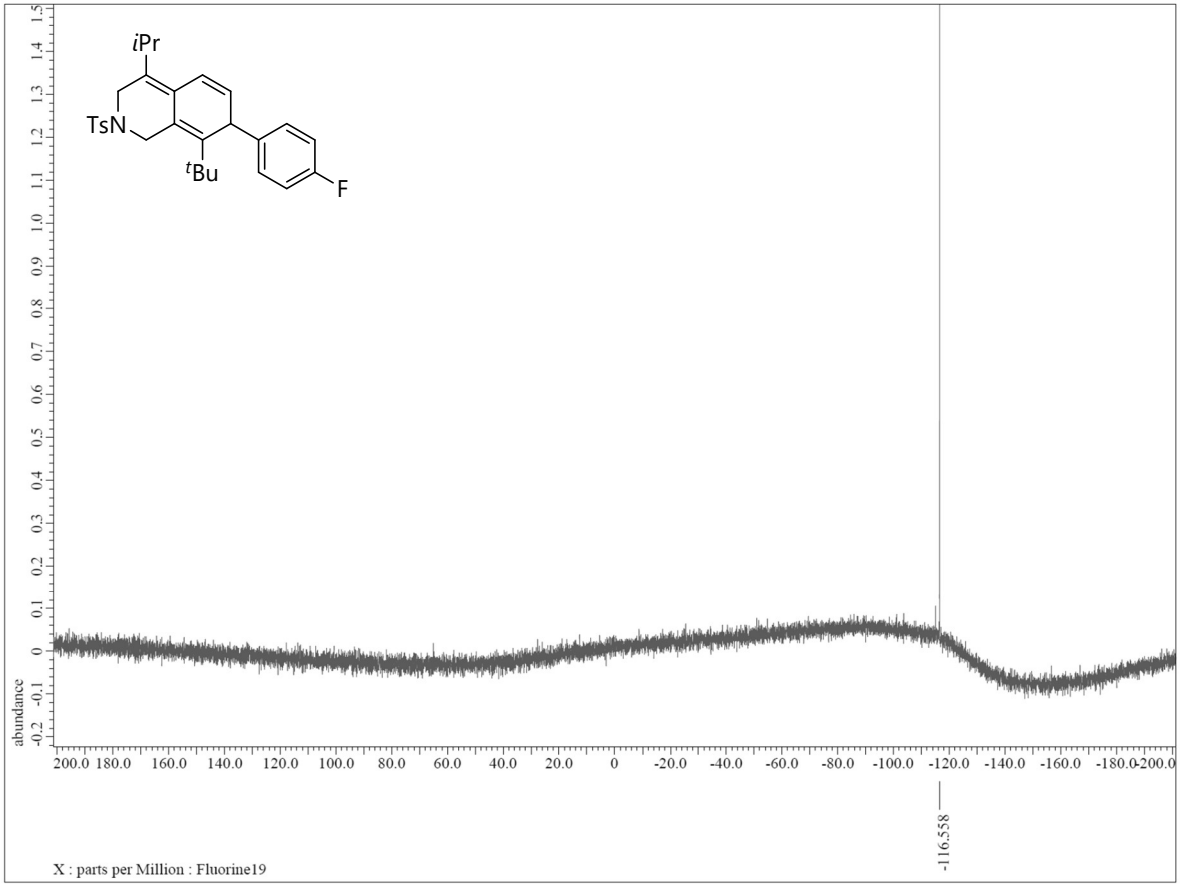
^{19}F NMR (376 MHz, $CDCl_3$)

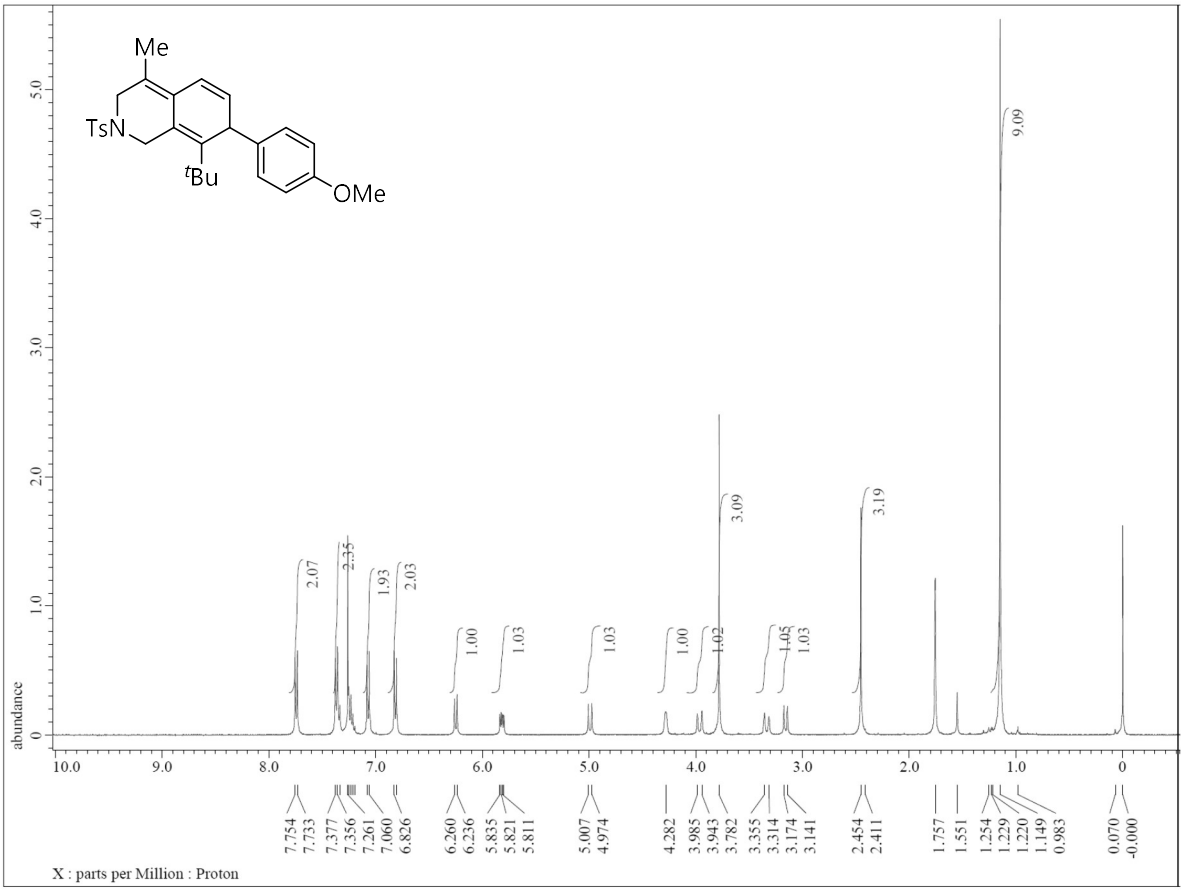


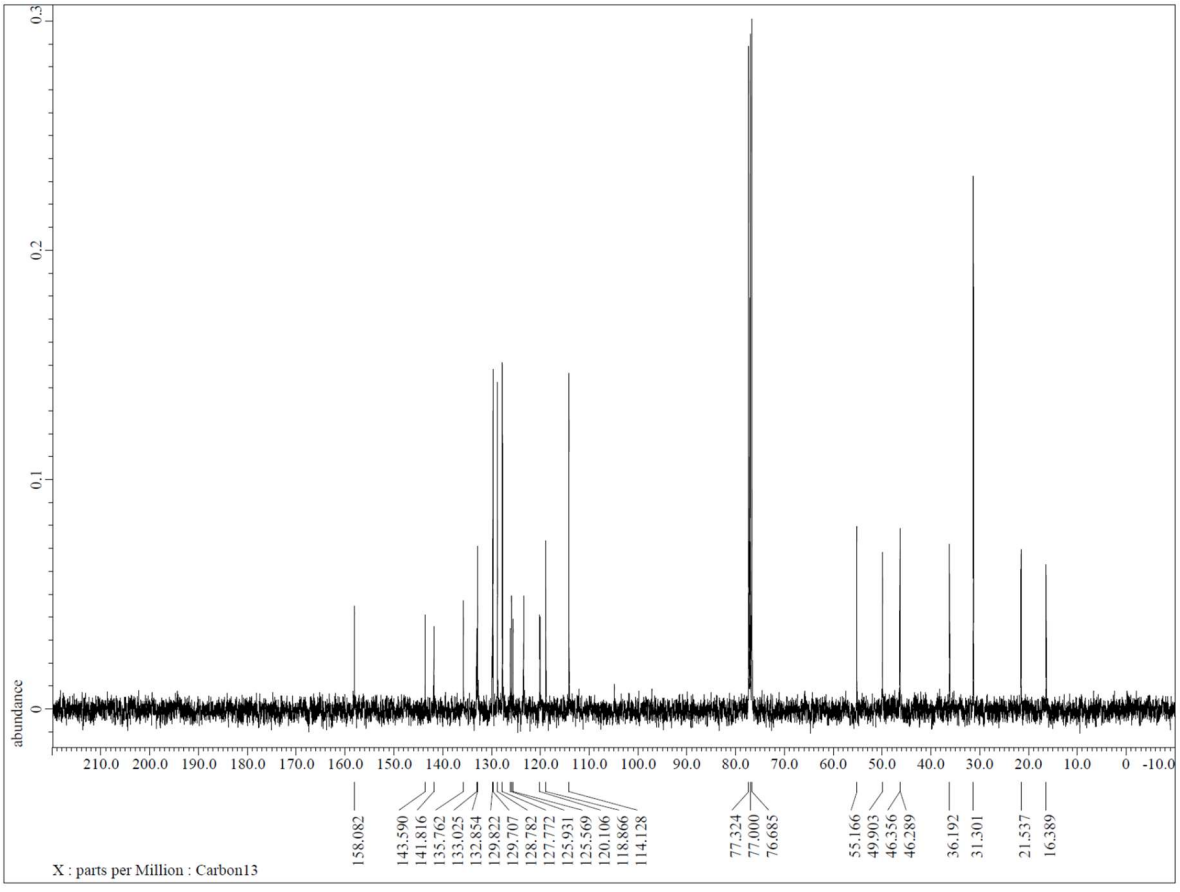

iPr
TsN
tBu
F
abundance
9.20
6.31
2.99
2.08
2.08
2.33
2.45
1.01
1.00
1.01
0.97
0.96
0.96
0.98
1.00
X : parts per Million : Proton

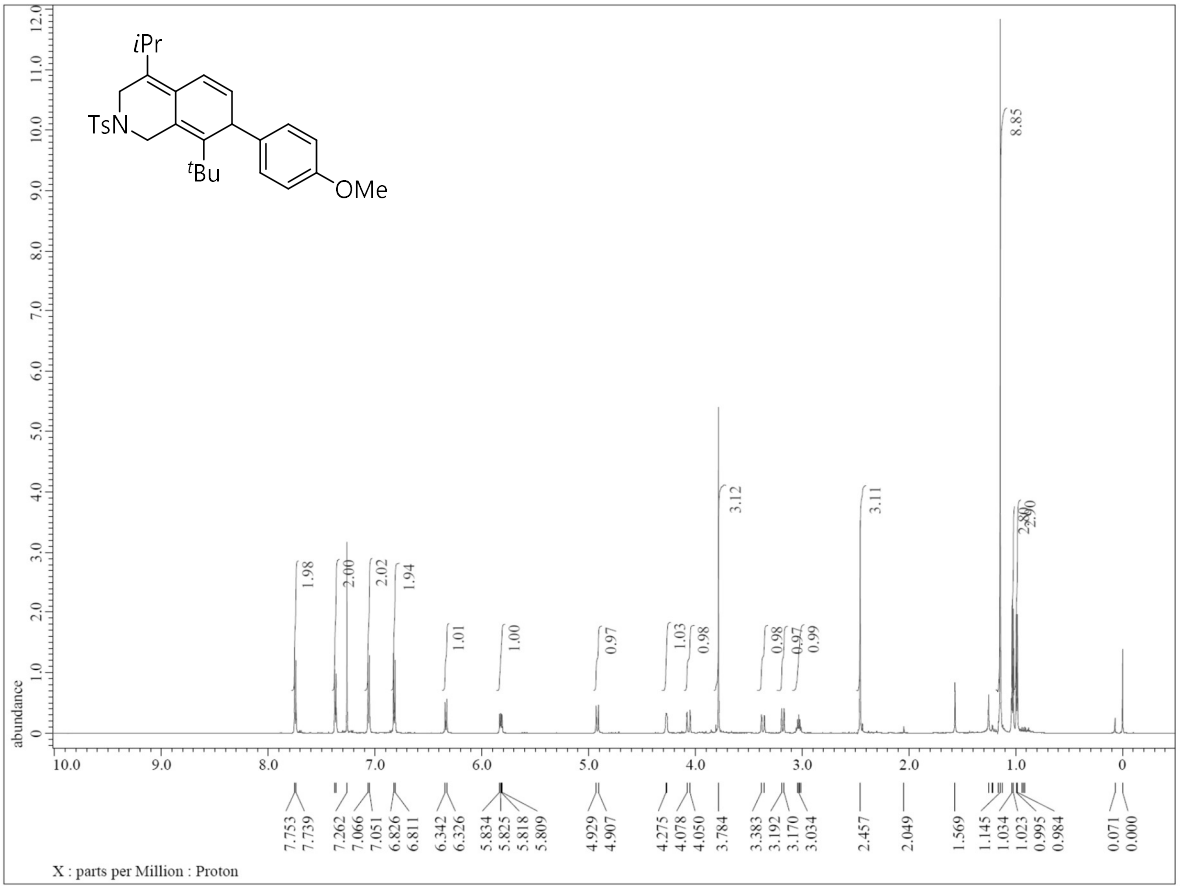

gssi-190527_8-77b-33.8mg_Carbon-1-3.jdf
abundance
X : parts per Million : Carbon13

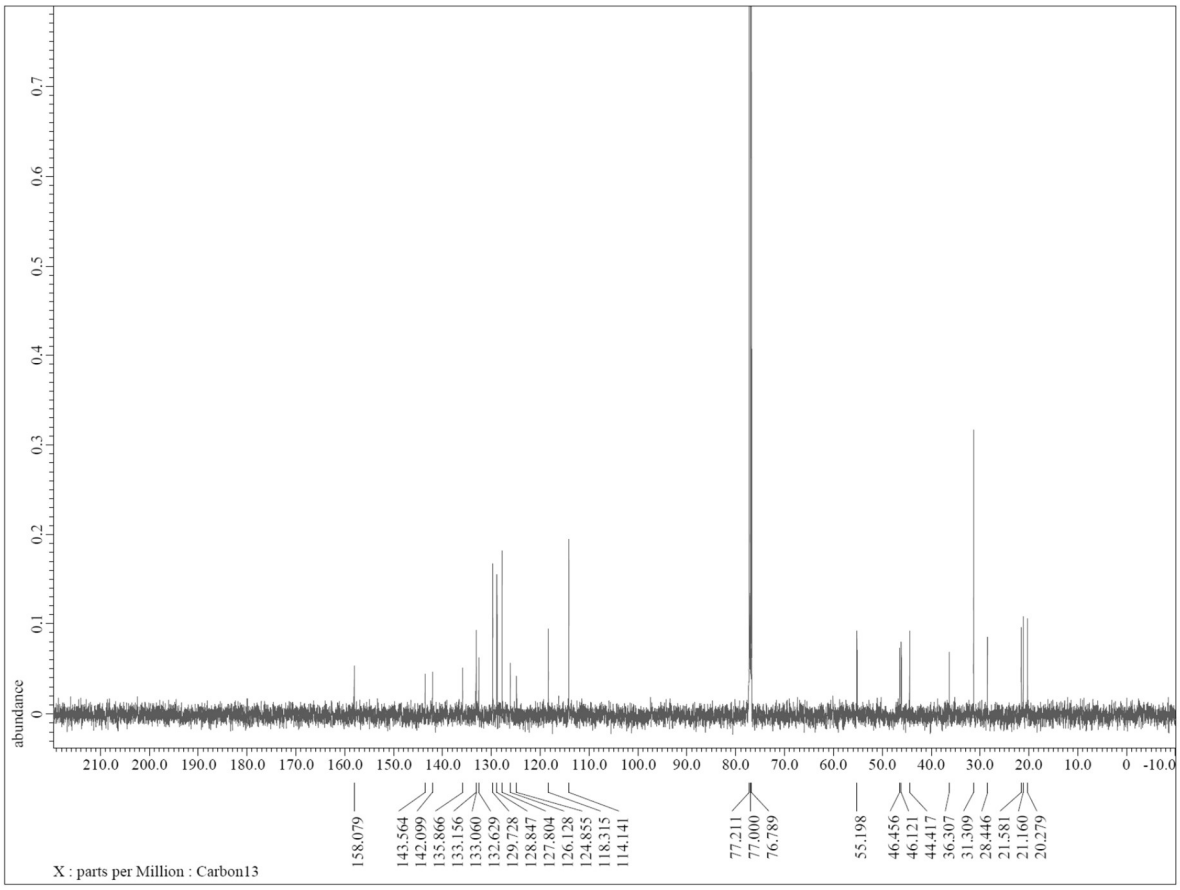
^{19}F NMR (376 MHz, $CDCl_3$)

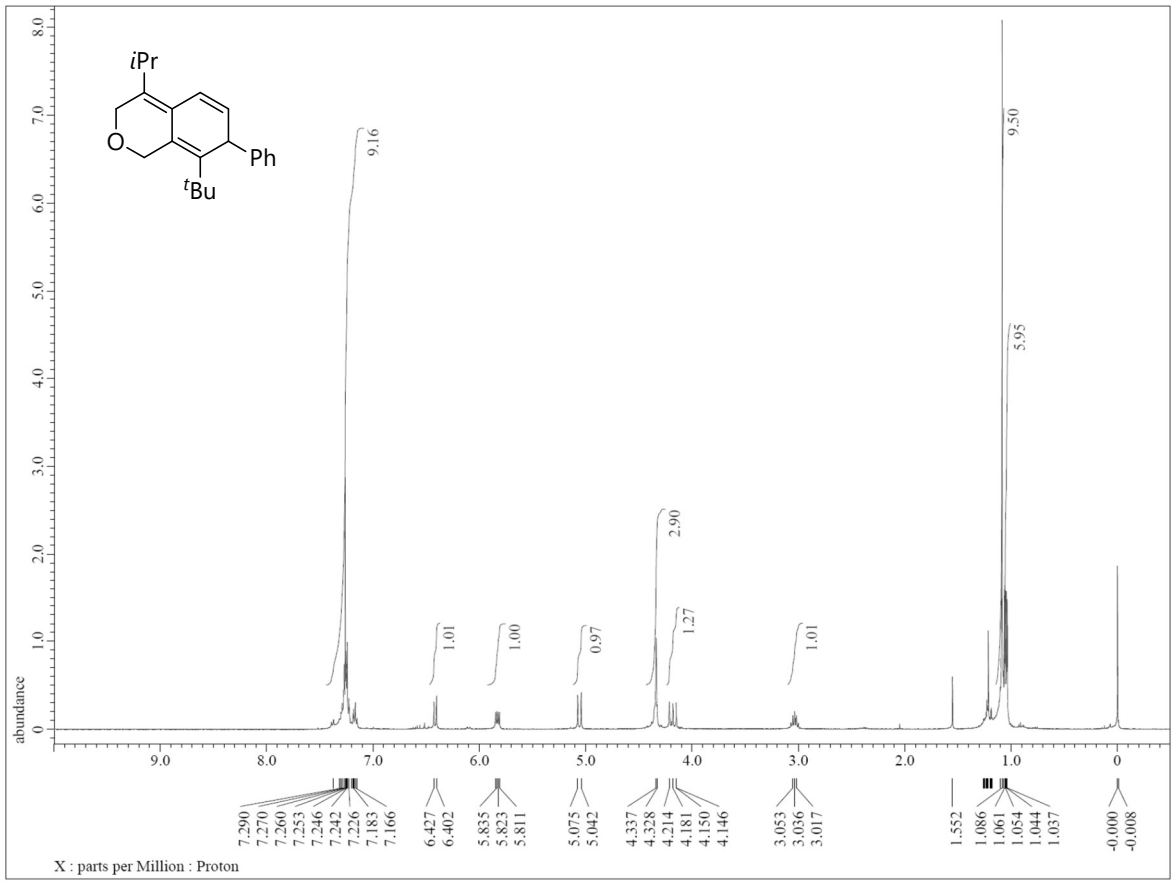


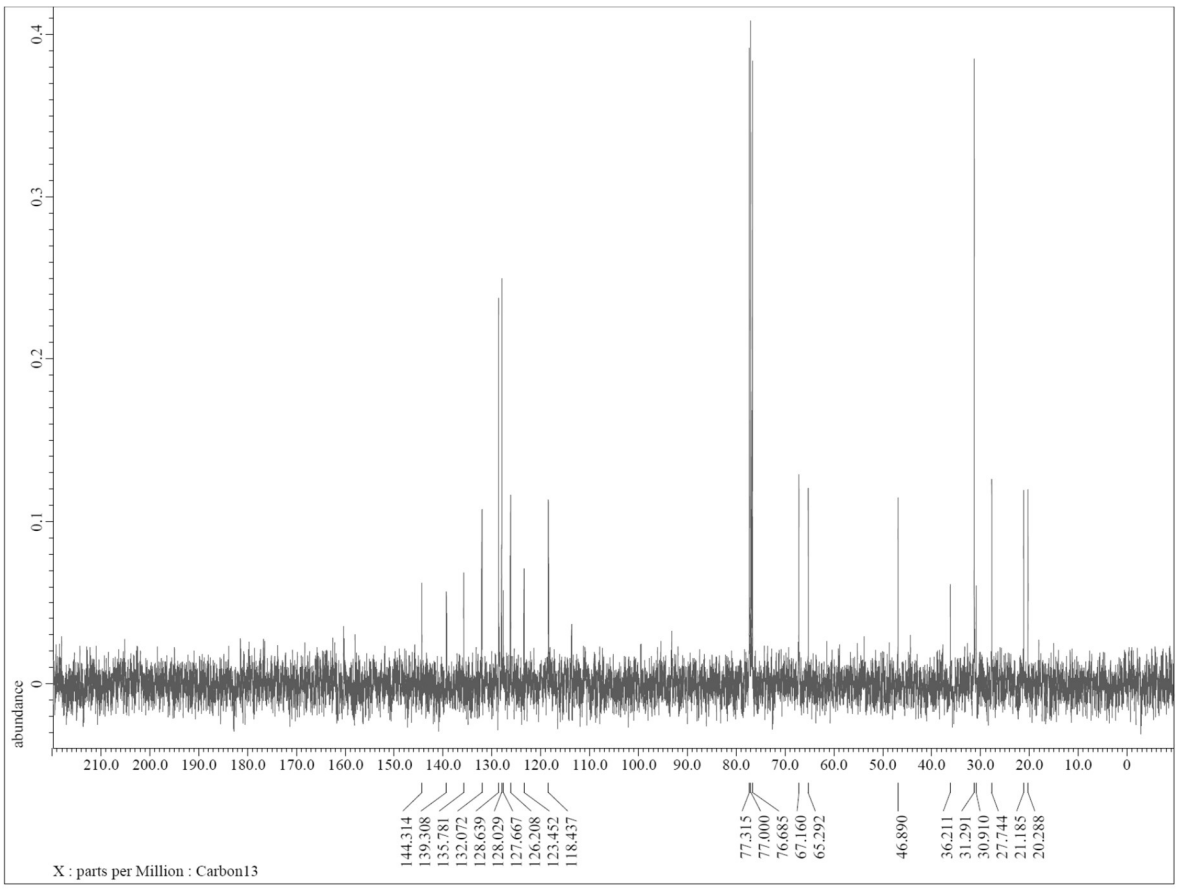

Me
TsN
tBu
OMe
abundance
9.09
3.19
3.09
2.07
2.35
1.93
2.03
1.00
1.03
1.03
1.00
1.02
1.05
1.03
7.754
7.733
7.377
7.356
7.261
7.060
6.826
6.260
6.236
5.835
5.821
5.811
5.007
4.974
4.282
3.985
3.943
3.782
3.355
3.314
3.174
3.141
2.454
2.411
1.757
1.551
1.254
1.229
1.220
1.149
0.983
0.070
-0.000
X : parts per Million : Proton

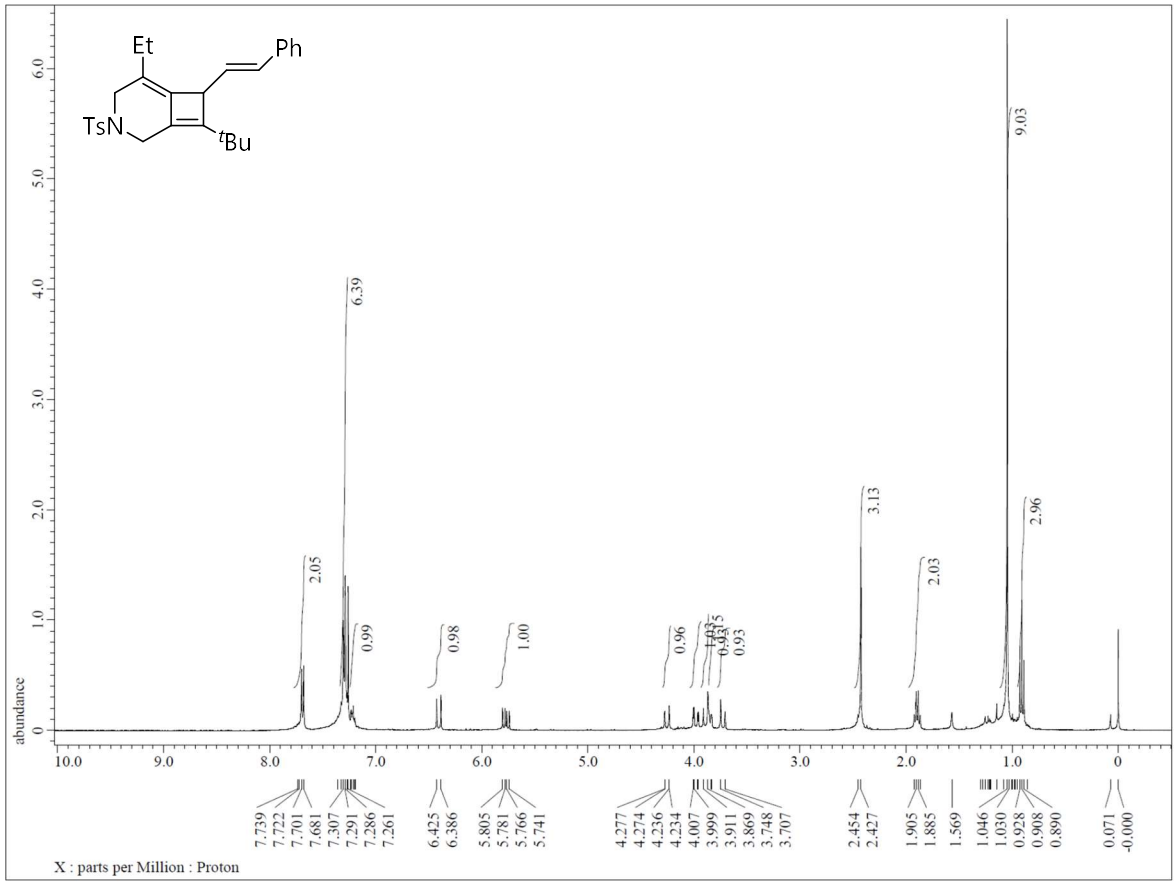

abundance
158.082
143.590
141.816
135.762
133.025
132.854
129.822
129.707
128.782
127.772
125.931
125.569
120.106
118.866
114.128
77.324
77.000
76.685
55.166
49.903
46.356
46.289
36.192
31.301
21.537
16.389
X : parts per Million : Carbon13

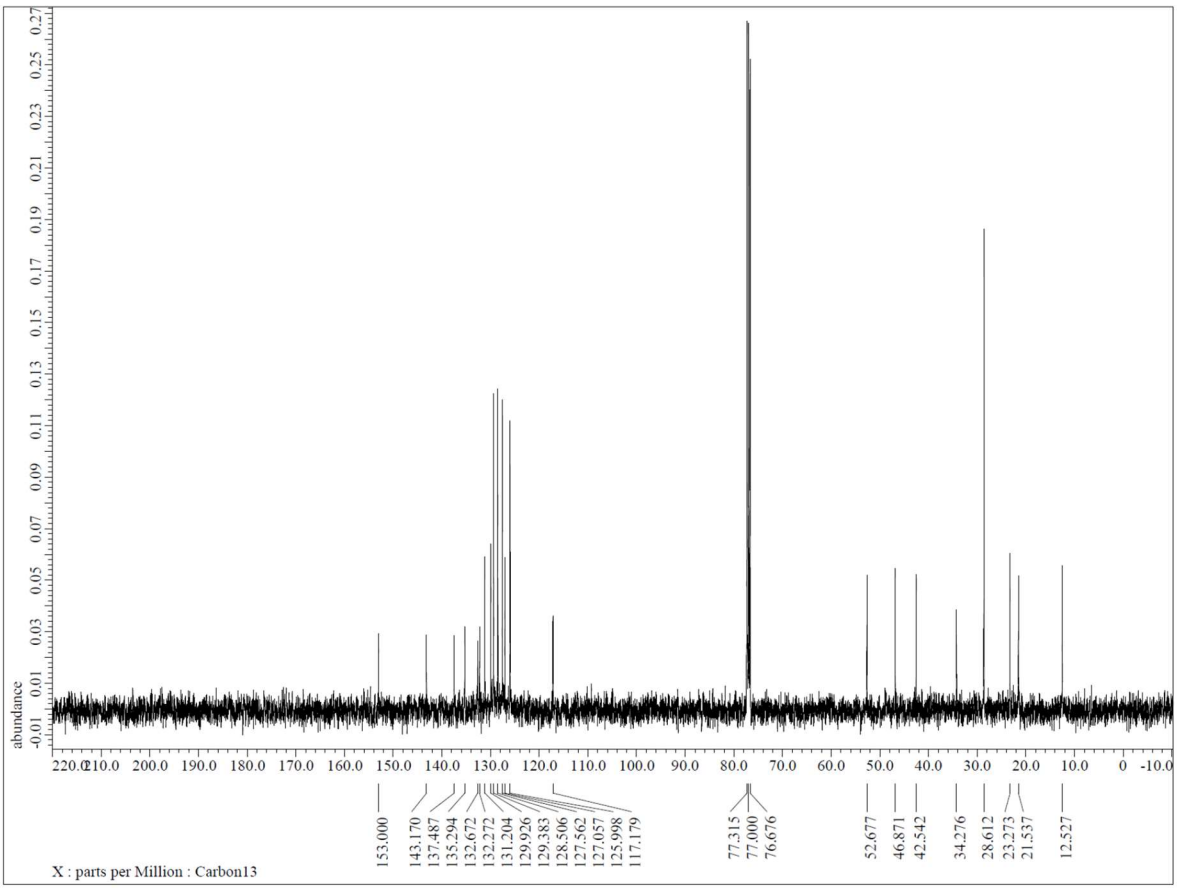

iPr
TsN
tBu
OMe
abundance
X : parts per Million : Proton

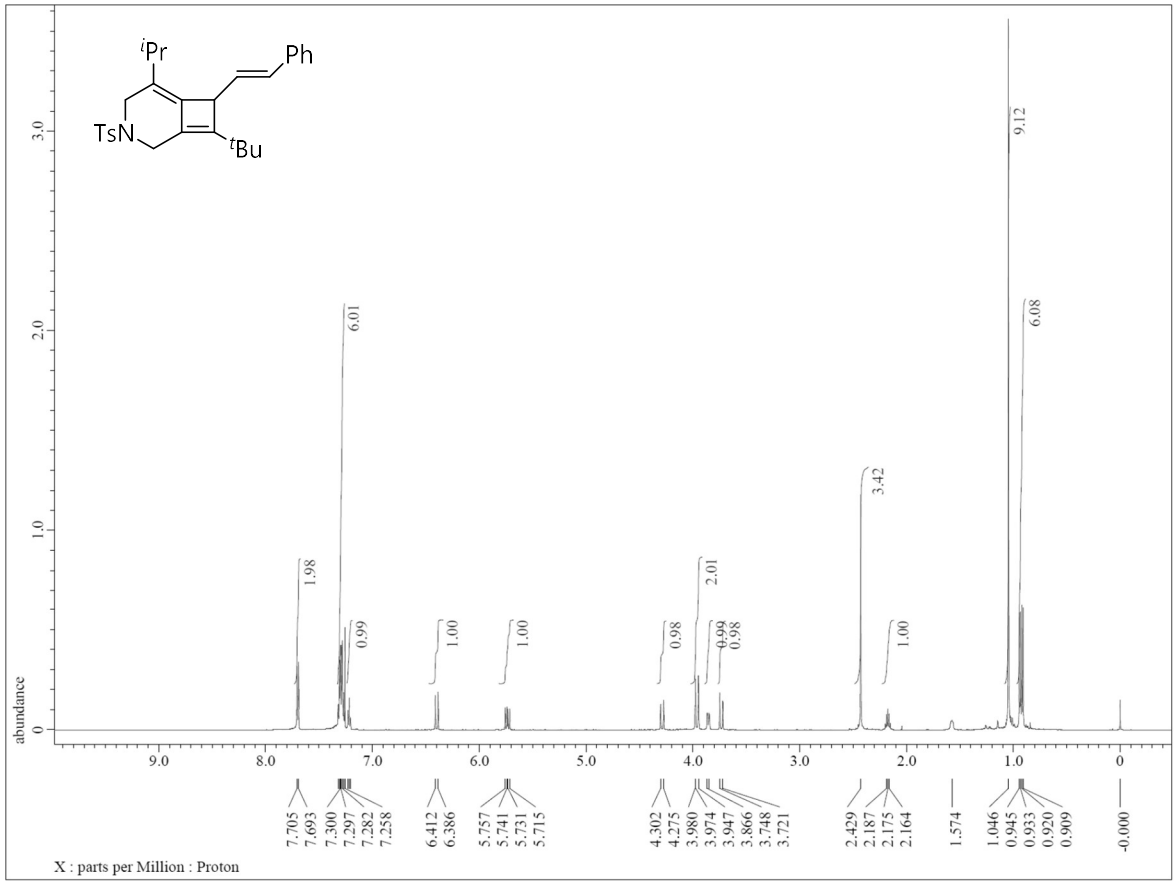

abundance
X : parts per Million : Carbon13

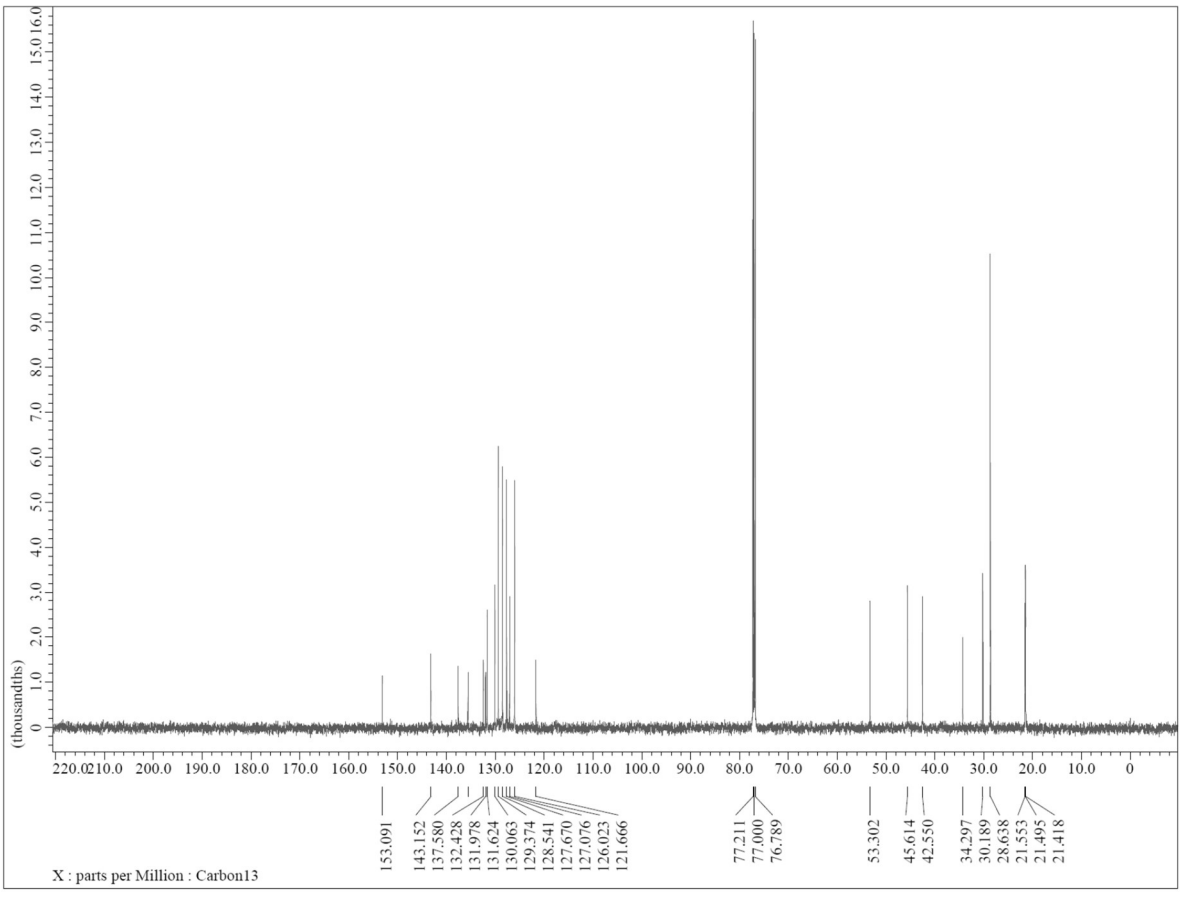

iPr
O
Ph
tBu
abundance
9.16
9.50
5.95
2.90
1.27
1.01
1.00
0.97
1.01
7.290
7.270
7.260
7.253
7.246
7.242
7.226
7.183
7.166
6.427
6.402
5.835
5.823
5.811
5.075
5.042
4.337
4.328
4.214
4.181
4.150
4.146
3.053
3.036
3.017
1.552
1.086
1.061
1.054
1.044
1.037
-0.000
-0.008
X : parts per Million : Proton

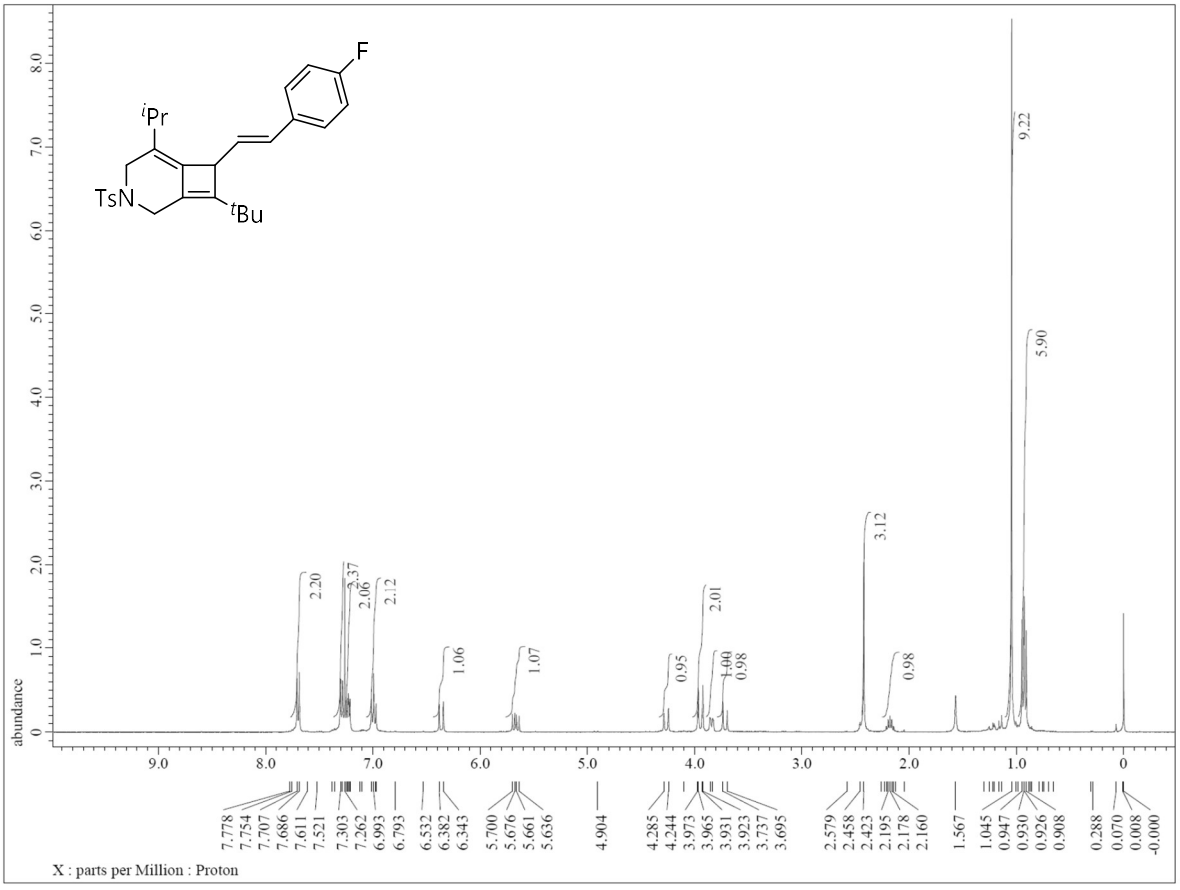

abundance
144.314
139.308
135.781
132.072
128.639
128.029
127.667
126.208
123.452
118.437
77.315
77.000
76.685
67.160
65.292
46.890
36.211
31.291
30.910
27.744
21.185
20.288
X : parts per Million : Carbon13

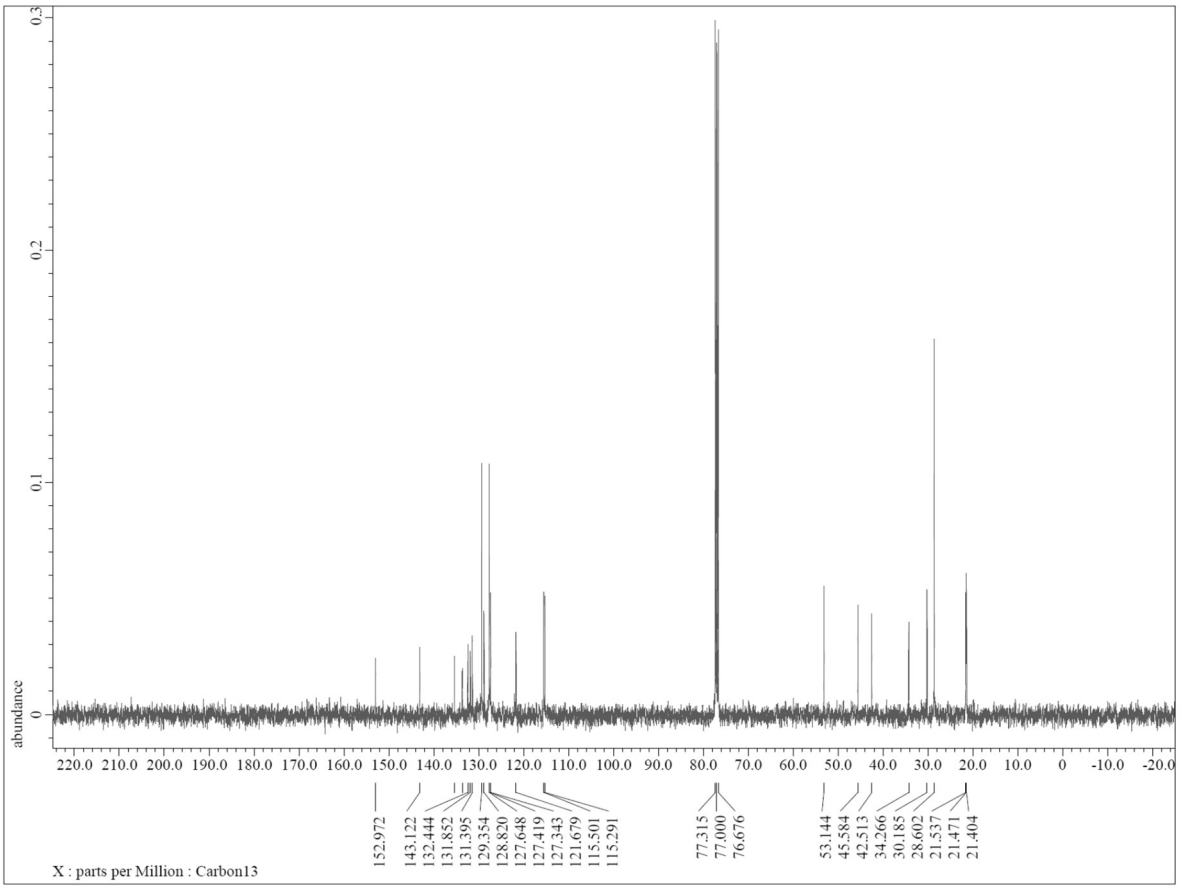

Et
Ph
TsN
tBu
abundance
6.39
2.05
0.99
0.98
1.00
0.96
0.93
3.13
2.03
9.03
2.96
7.739
7.722
7.701
7.681
7.307
7.291
7.286
7.261
6.425
6.386
5.805
5.781
5.766
5.741
4.277
4.274
4.236
4.234
4.007
3.999
3.911
3.869
3.748
3.707
2.454
2.427
1.905
1.885
1.569
1.046
1.030
0.928
0.908
0.890
0.071
-0.000
X : parts per Million : Proton


abundance
153.000
143.170
137.487
135.294
132.672
132.272
131.204
129.926
129.383
128.506
127.562
127.057
125.998
117.179
77.315
77.000
76.676
52.677
46.871
42.542
34.276
28.612
23.273
21.537
12.527
X : parts per Million : Carbon13

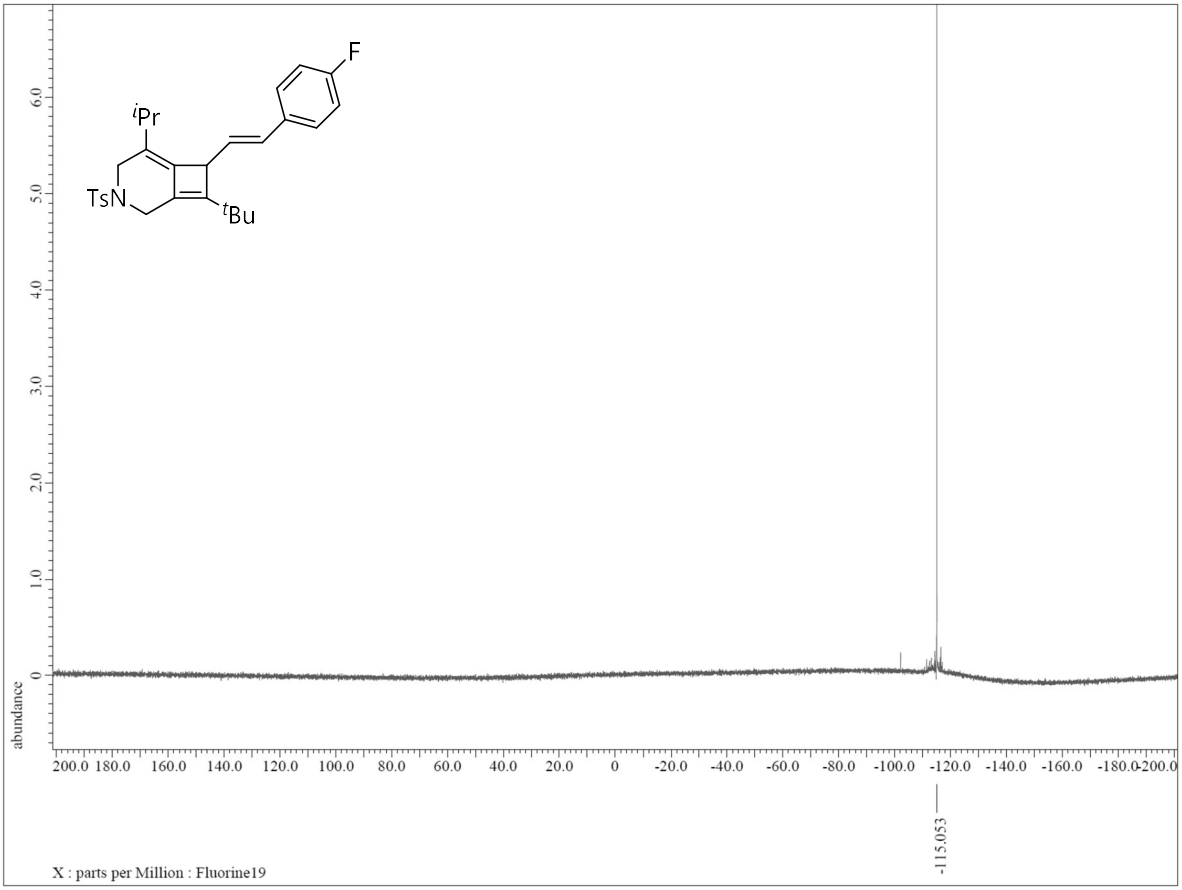

iPr
Ph
TsN
tBu
abundance
9.12
6.08
6.01
3.42
2.01
1.98
1.00
1.00
0.99
0.98
0.99
0.98
1.00
X : parts per Million : Proton

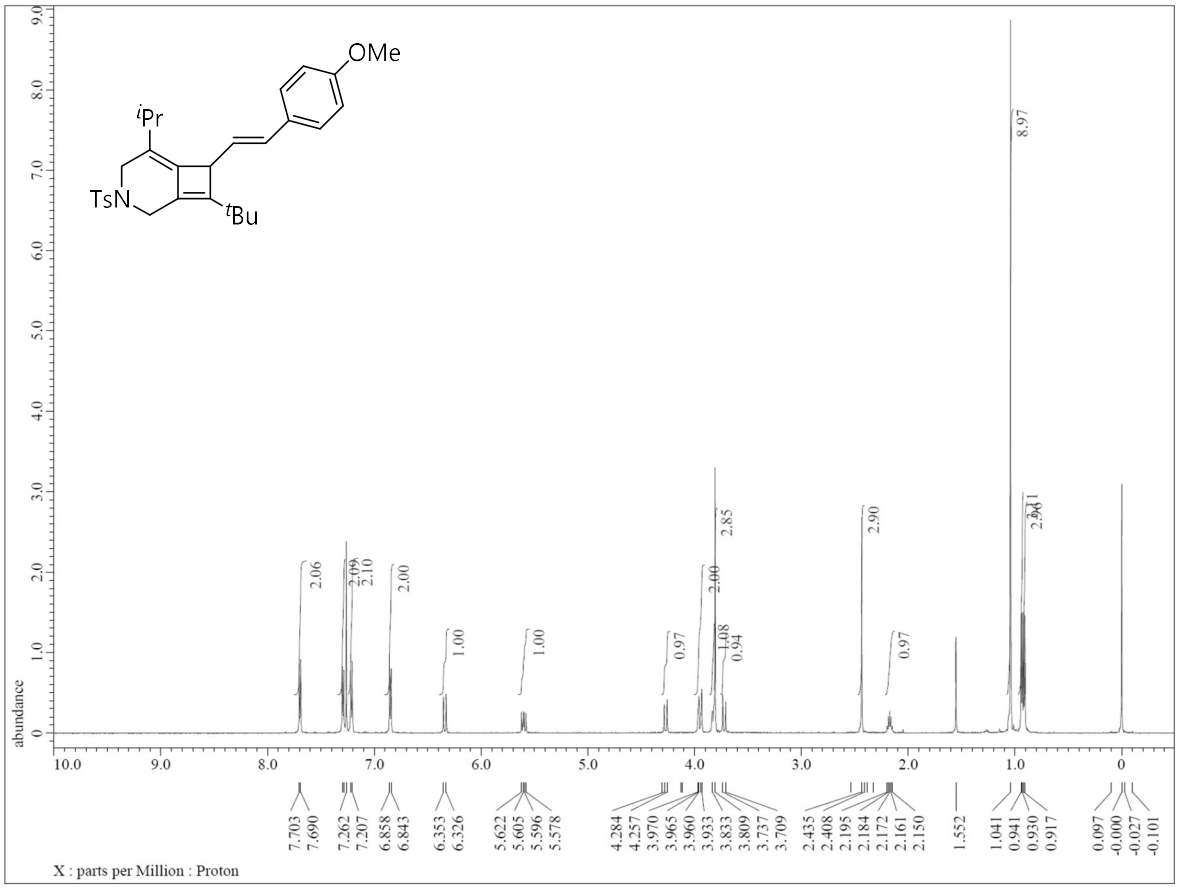

(thousandths)
153.091
143.152
137.580
132.428
131.978
131.624
130.063
129.374
128.541
127.670
127.076
126.023
121.666
77.211
77.000
76.789
53.302
45.614
42.550
34.297
30.189
28.638
21.553
21.495
21.418
X : parts per Million : Carbon13

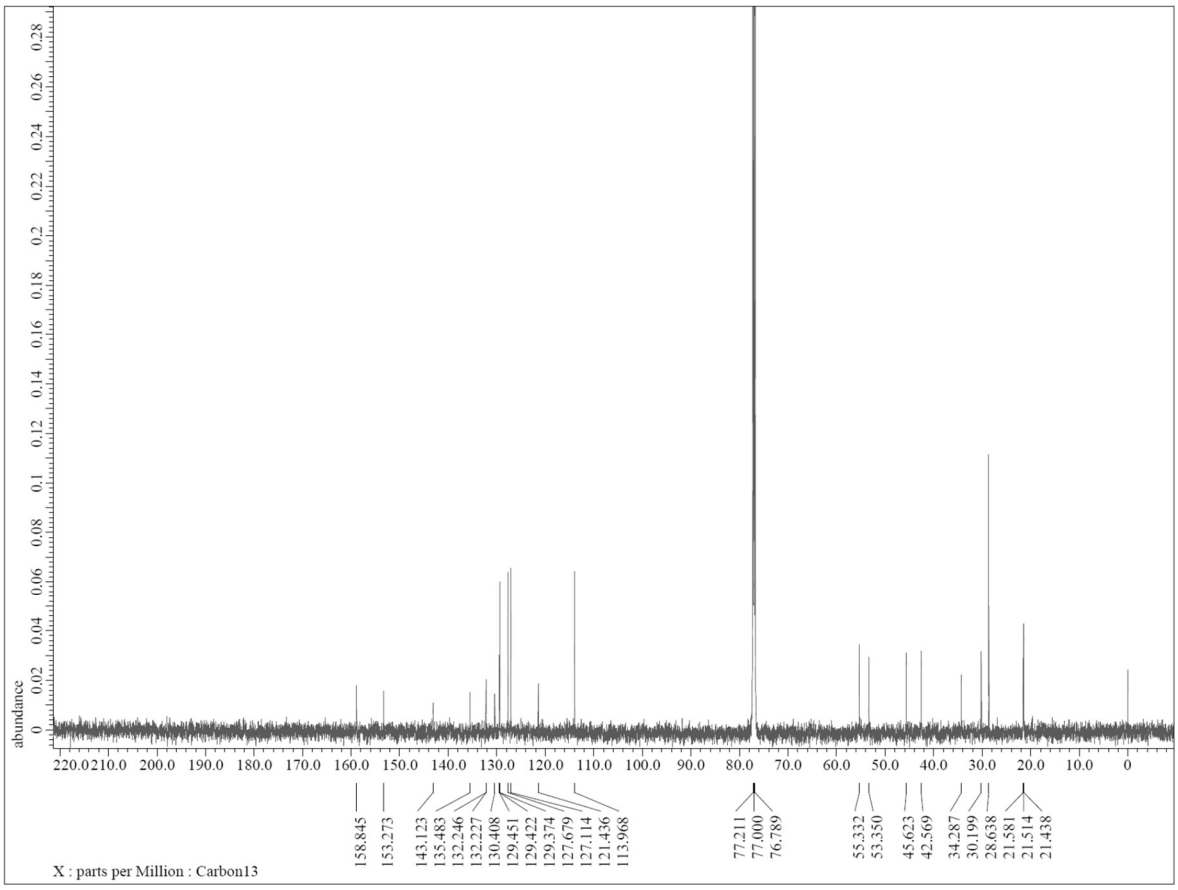

F
iPr
TsN
tBu
abundance
9.22
5.90
3.12
2.20
2.37
2.06
2.12
2.01
1.06
1.07
0.95
1.00
0.98
0.98
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.778
7.754
7.707
7.686
7.611
7.521
7.303
7.262
6.993
6.793
6.532
6.382
6.343
5.700
5.676
5.661
5.636
4.904
4.285
4.244
3.973
3.965
3.931
3.923
3.737
3.695
2.579
2.458
2.423
2.195
2.178
2.160
1.567
1.045
0.947
0.930
0.926
0.908
0.288
0.070
0.008
-0.000
X : parts per Million : Proton

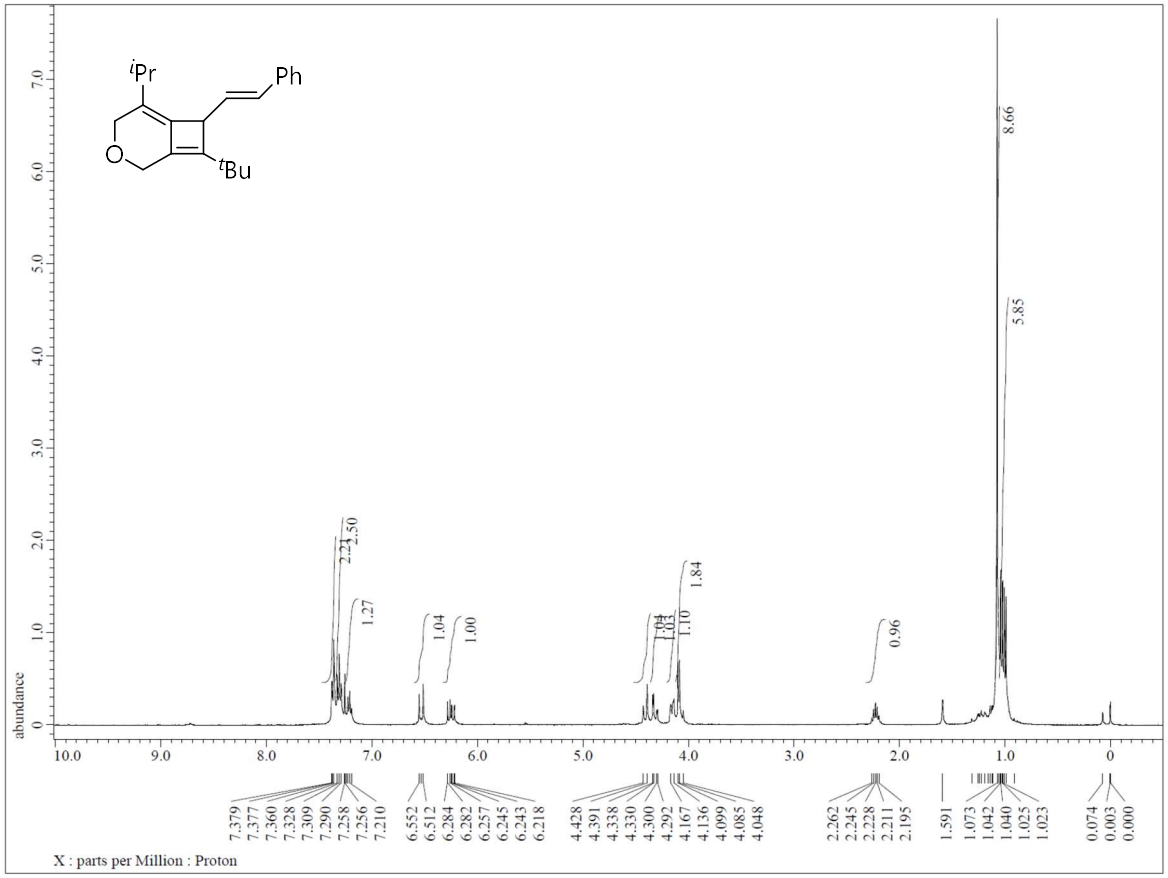

abundance
0.3
0.2
0.1
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
152.972
143.122
132.444
131.852
131.395
129.354
128.820
127.648
127.419
127.343
121.679
115.501
115.291
77.315
77.000
76.676
53.144
45.584
42.513
34.266
30.185
28.602
21.537
21.471
21.404
X : parts per Million : Carbon13

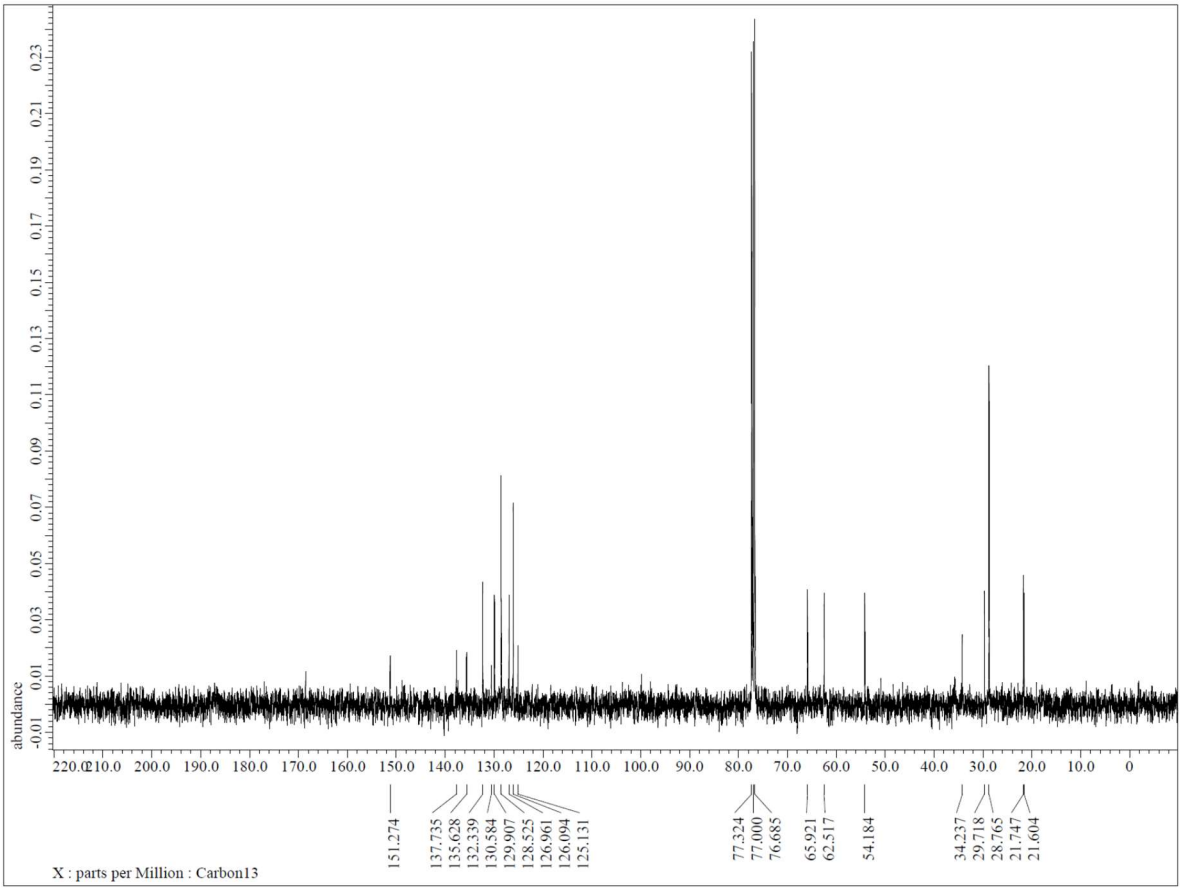
^{19}F NMR (376 MHz, $CDCl_3$)

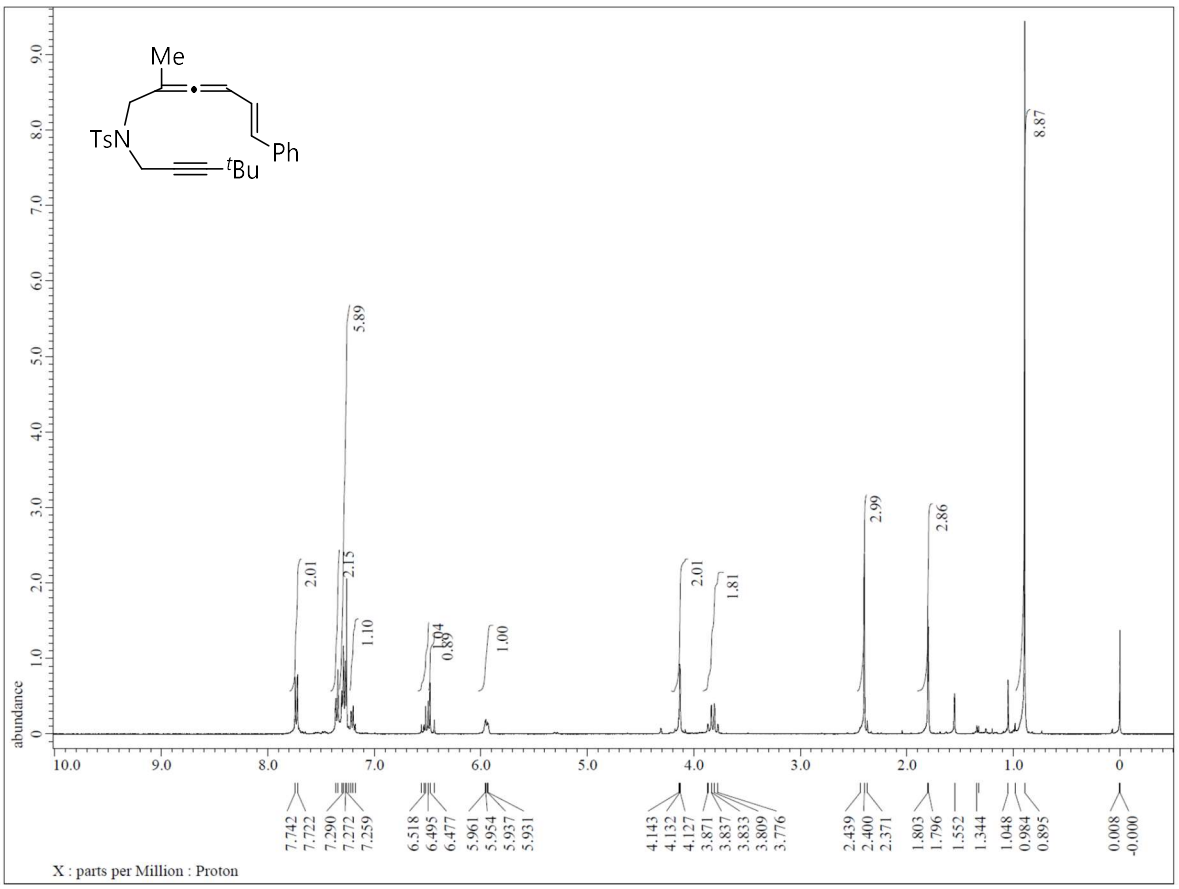


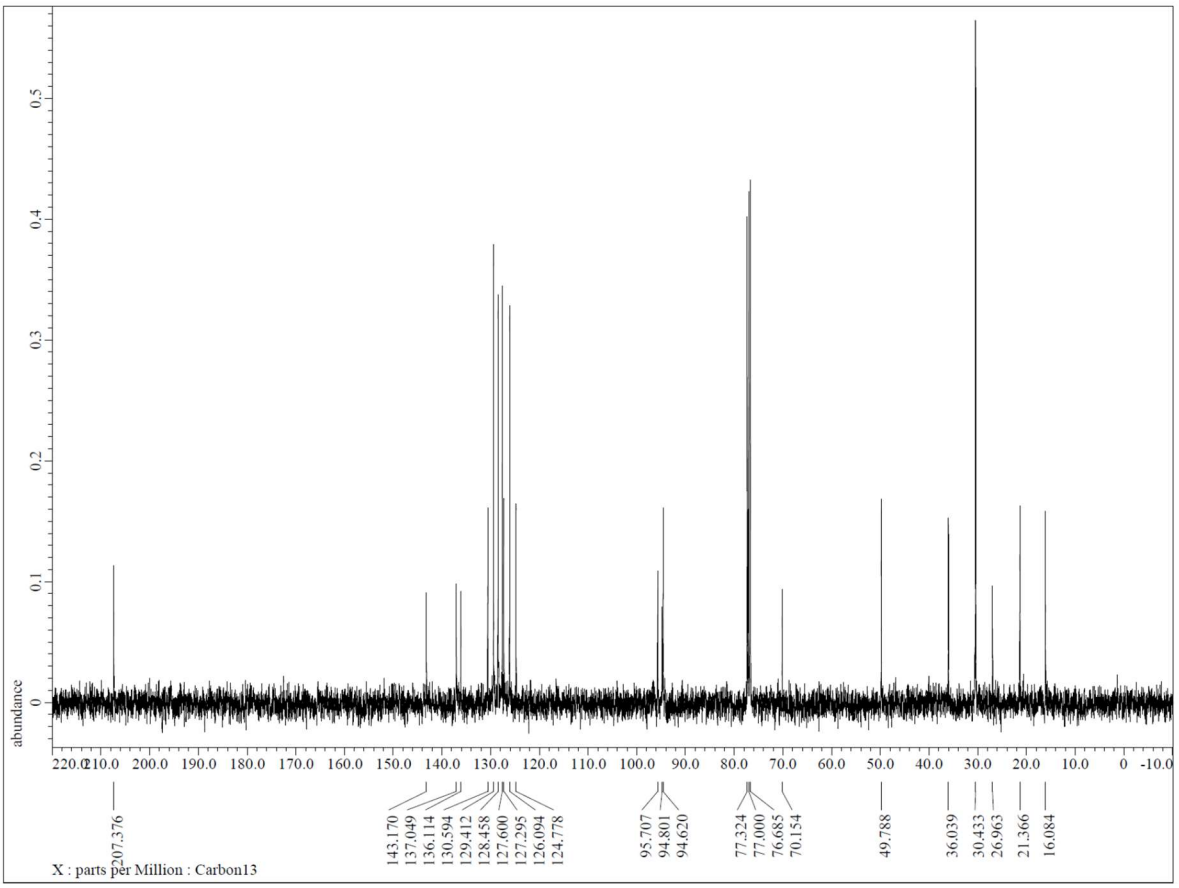

OMe
iPr
TsN
tBu
abundance
X : parts per Million : Proton

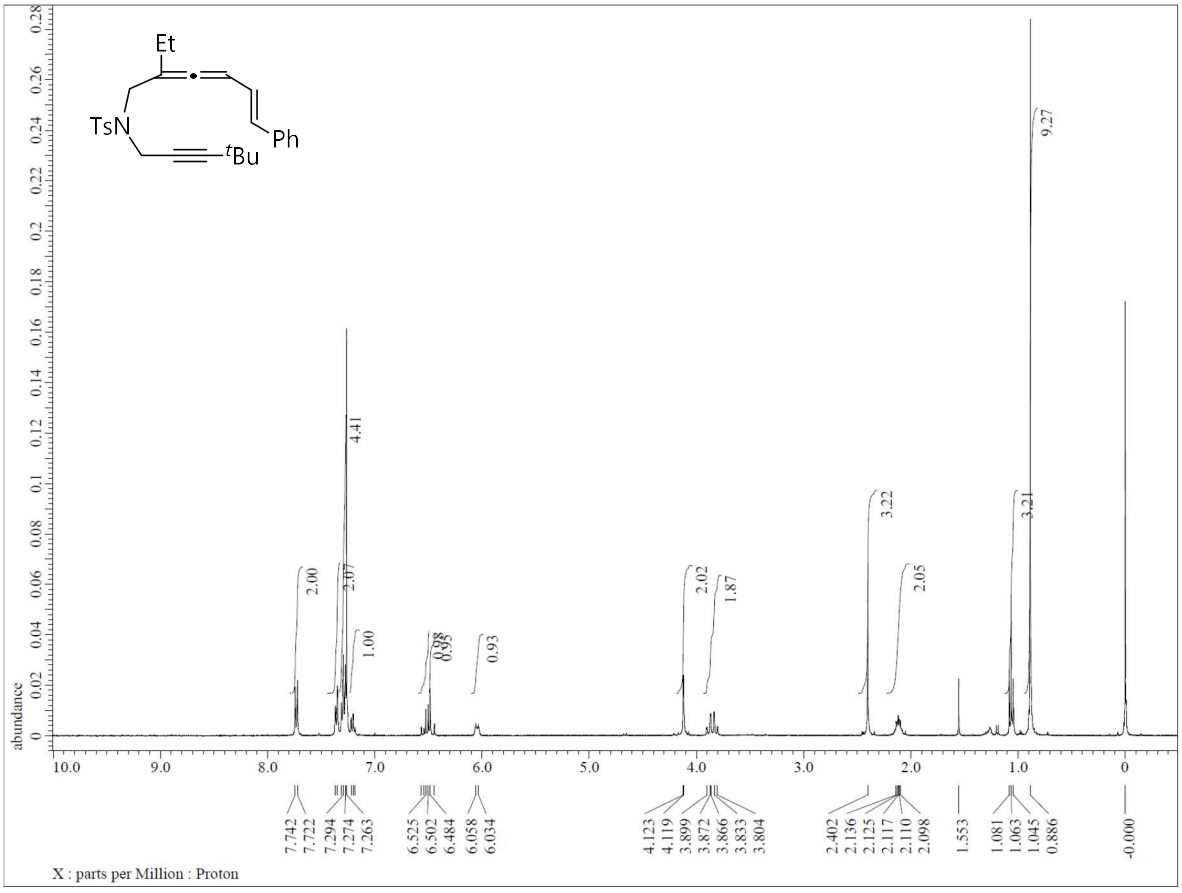

abundance
X : parts per Million : Carbon13

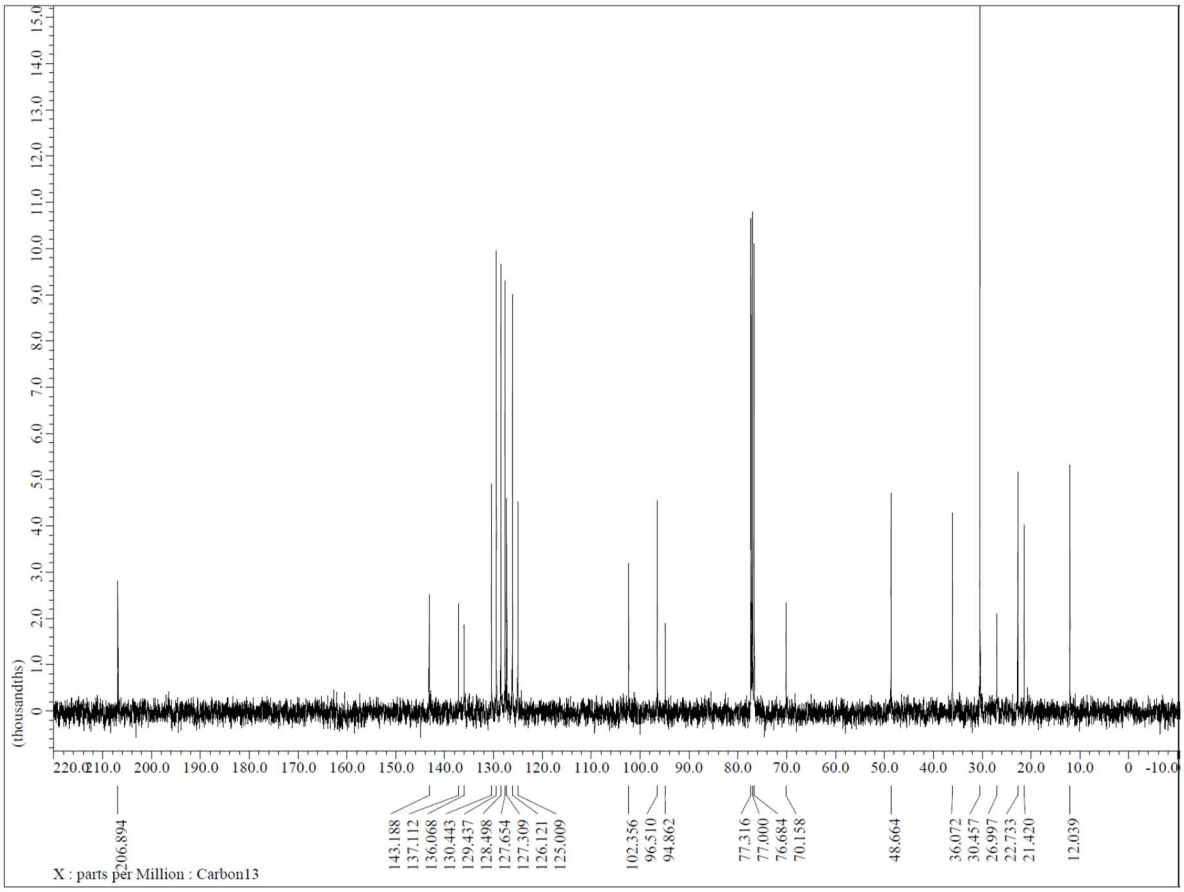

iPr
Ph
O
tBu
abundance
8.66
5.85
2.50
2.21
1.27
1.04
1.00
1.84
1.10
0.96
X : parts per Million : Proton

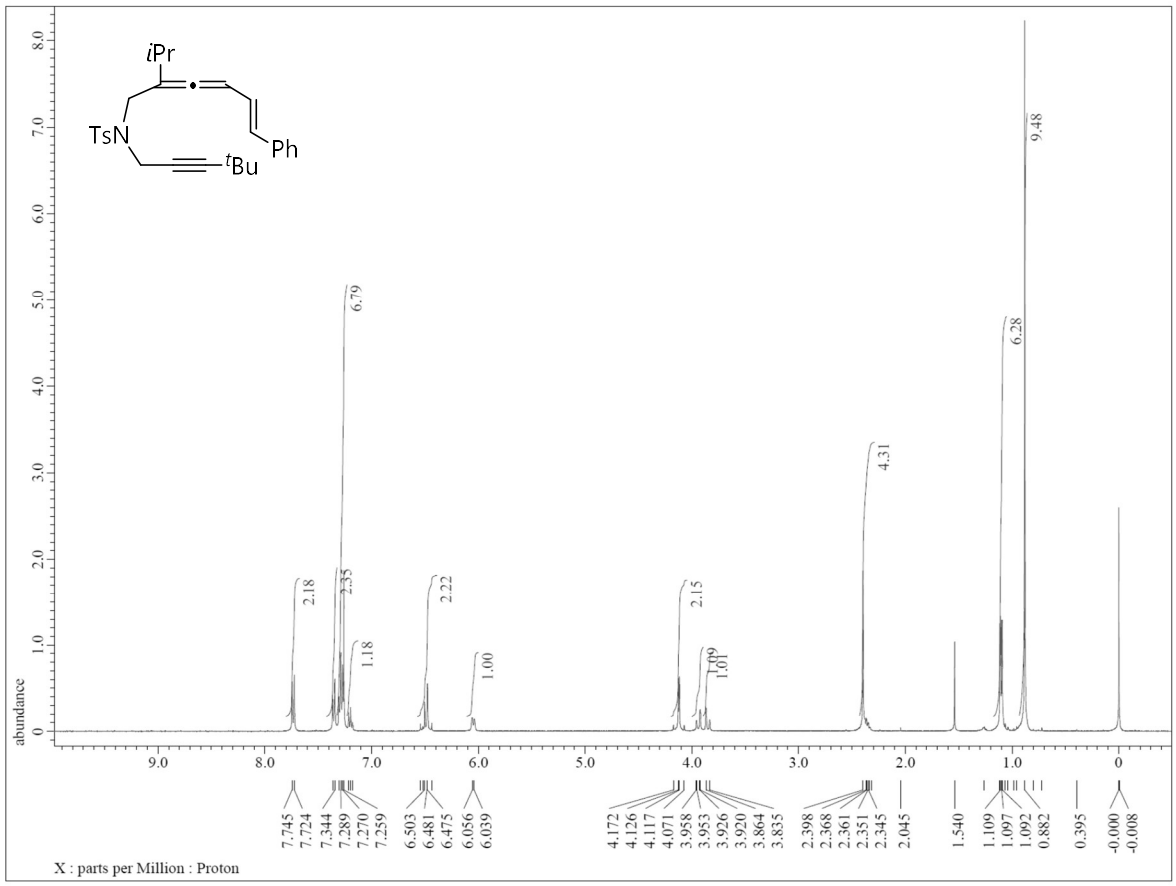

abundance
151.274
137.735
135.628
132.339
130.584
129.907
128.525
126.961
126.094
125.131
77.324
77.000
76.685
65.921
62.517
54.184
34.237
29.718
28.765
21.747
21.604
X : parts per Million : Carbon13

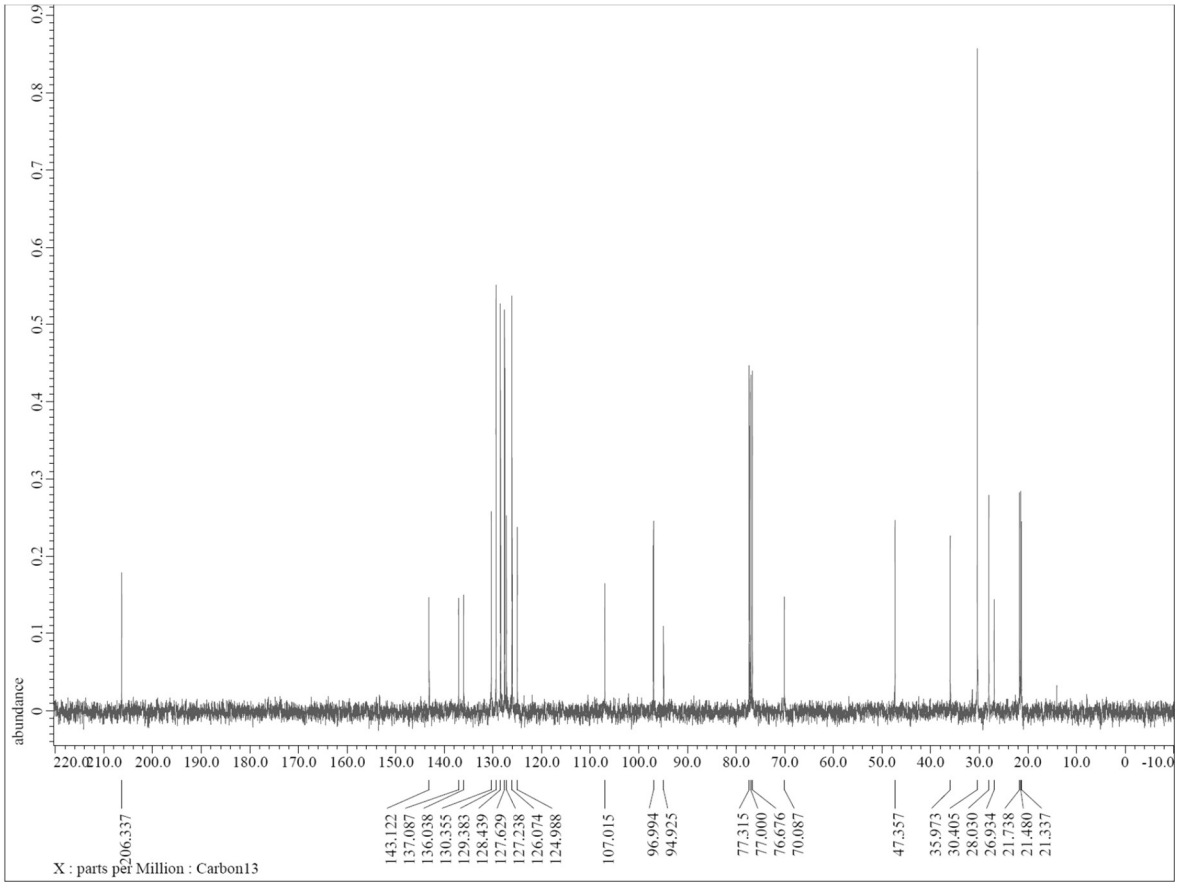

Me
TsN
Ph
tBu
abundance
8.87
5.89
2.99
2.86
2.01
2.15
2.01
1.81
1.10
1.04
0.89
1.00
7.742
7.722
7.290
7.272
7.259
6.518
6.495
6.477
5.961
5.954
5.937
5.931
4.143
4.132
4.127
3.871
3.837
3.833
3.809
3.776
2.439
2.400
2.371
1.803
1.796
1.552
1.344
1.048
0.984
0.895
0.008
-0.000
X : parts per Million : Proton

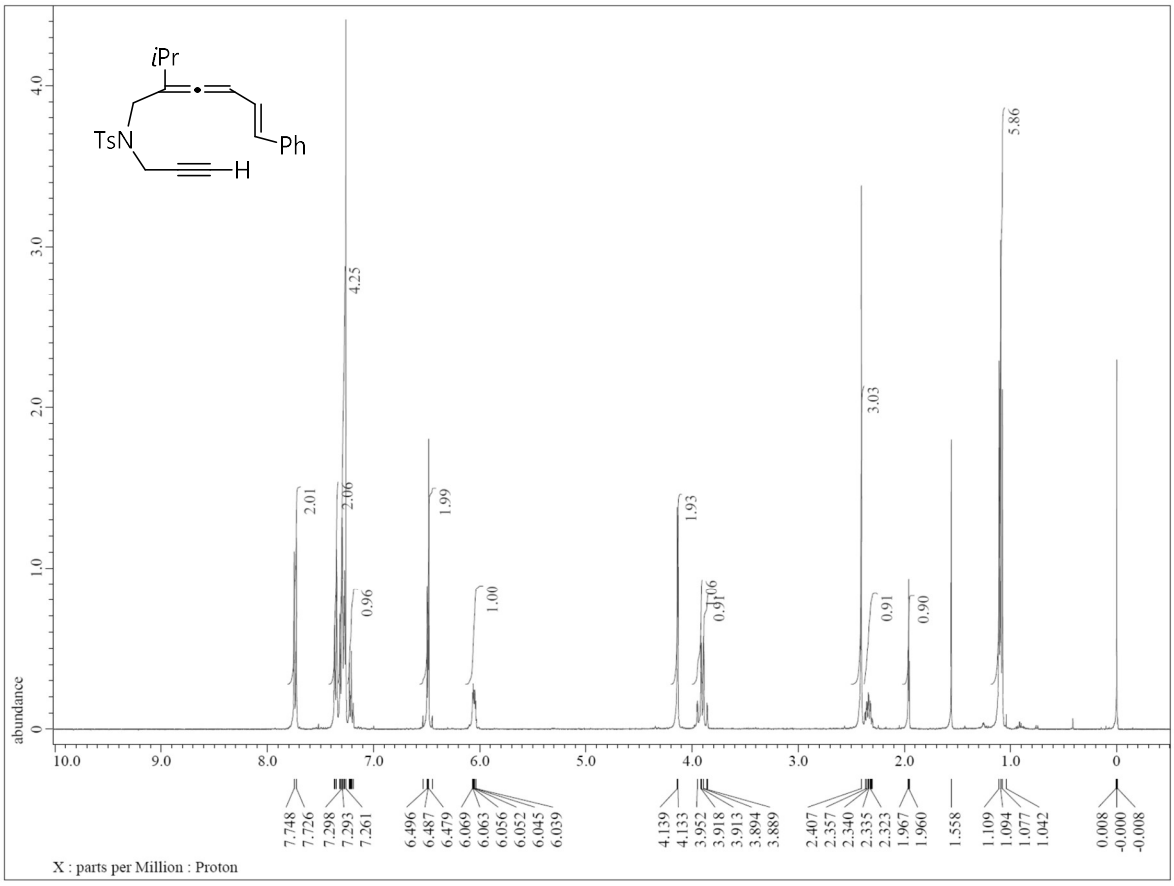

abundance
207.376
143.170
137.049
136.114
130.594
129.412
128.458
127.600
127.295
126.094
124.778
95.707
94.801
94.620
77.324
77.000
76.685
70.154
49.788
36.039
30.433
26.963
21.366
16.084
X : parts per Million : Carbon13

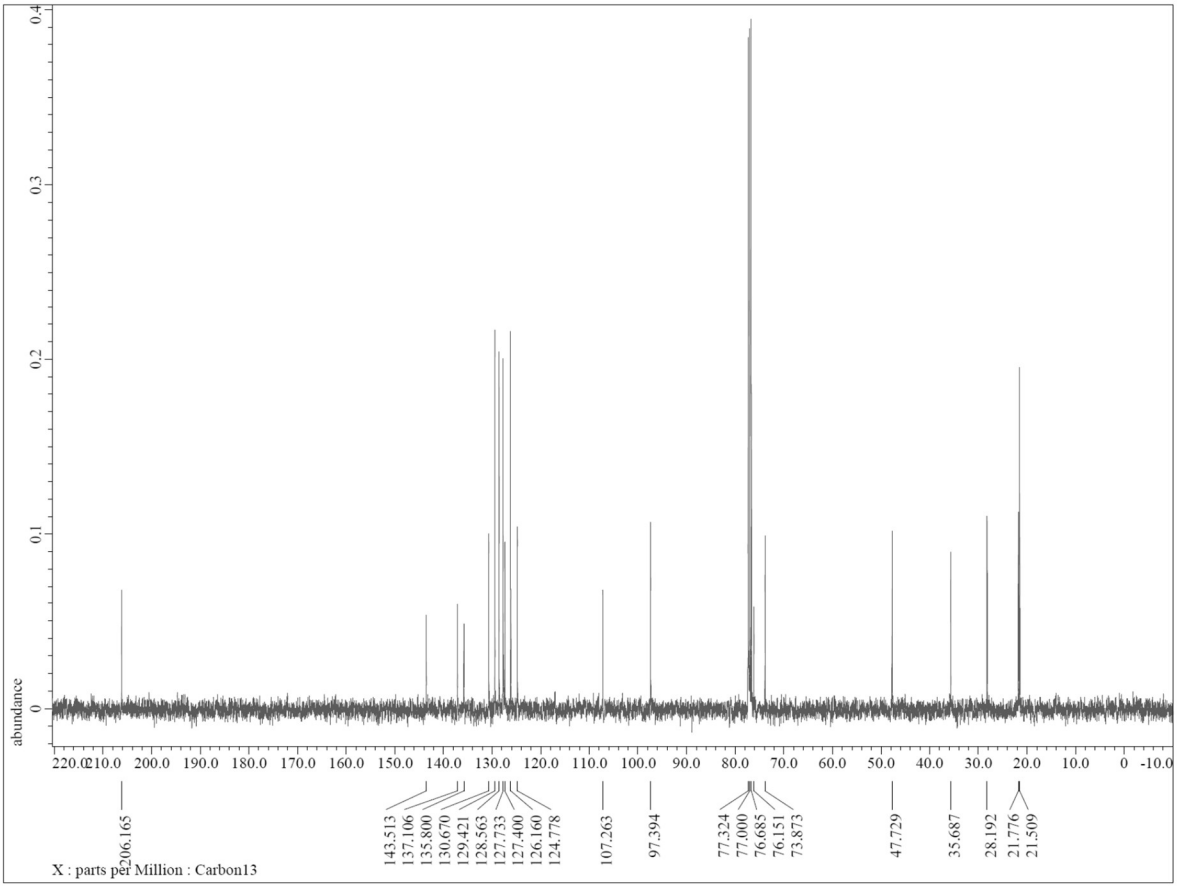

Et
TsN
Ph
tBu
abundance
X : parts per Million : Proton

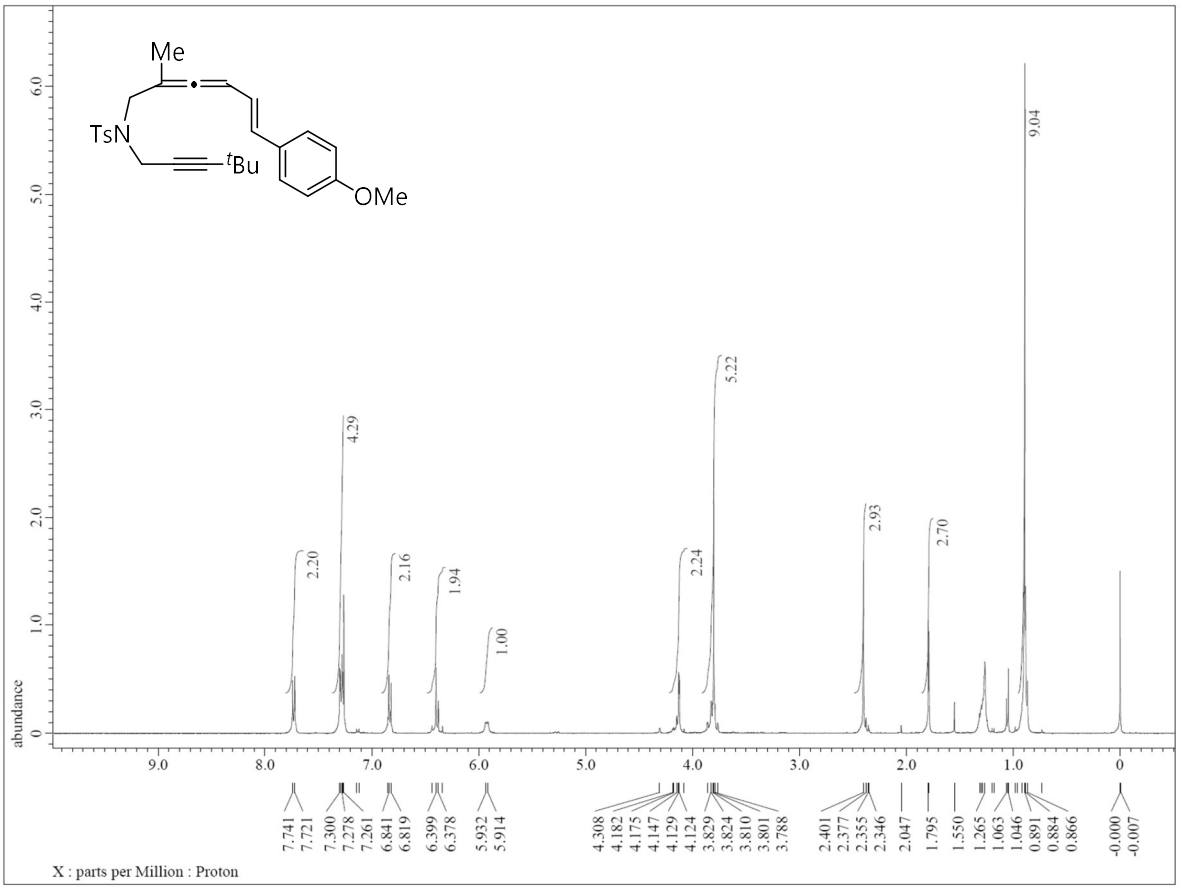

(thousandths)
X : parts per Million : Carbon13

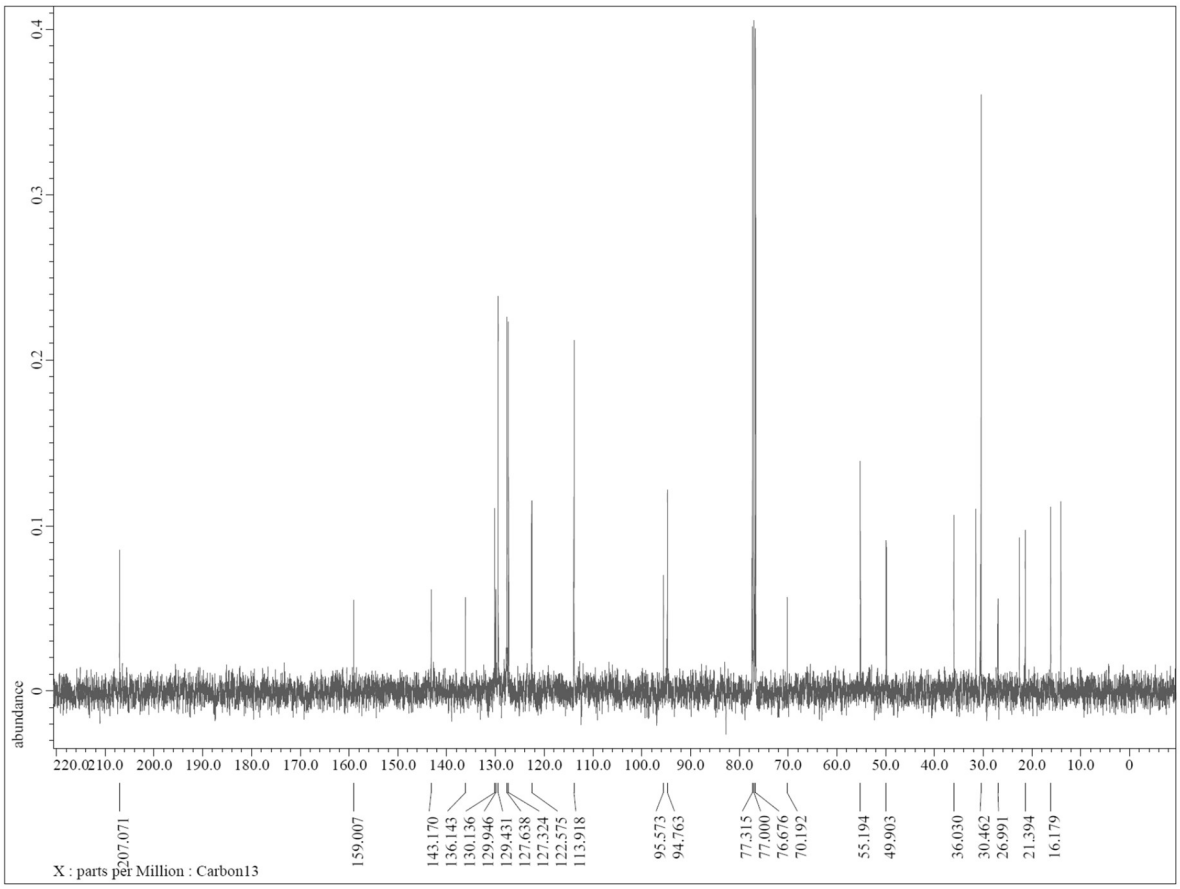

iPr
TsN
tBu
Ph
abundance
9.48
6.79
6.28
4.31
2.18
2.35
2.22
2.15
1.18
1.00
1.09
1.01
X : parts per Million : Proton

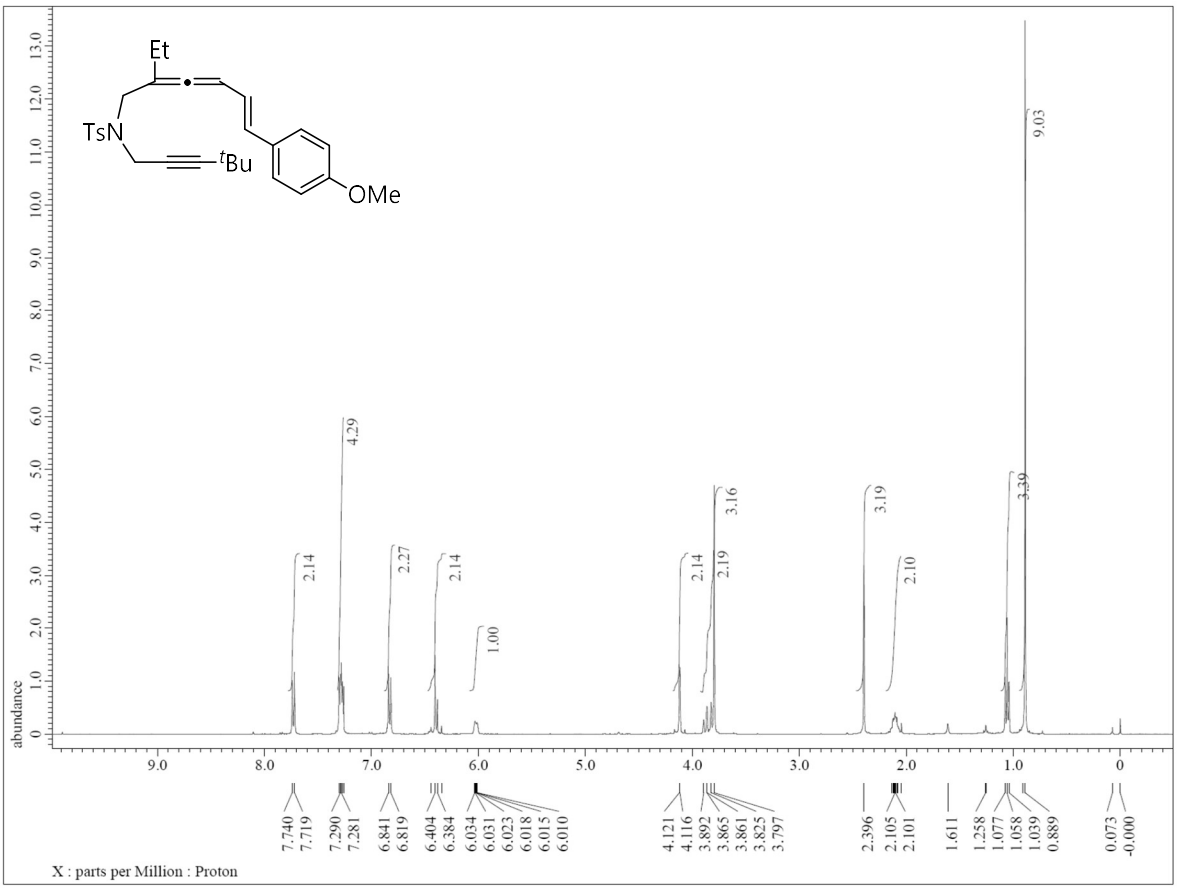

abundance
206.337
143.122
137.087
136.038
130.355
129.383
128.439
127.629
127.238
126.074
124.988
107.015
96.994
94.925
77.315
77.000
76.676
70.087
47.357
35.973
30.405
28.030
26.934
21.738
21.480
21.337
X : parts per Million : Carbon13

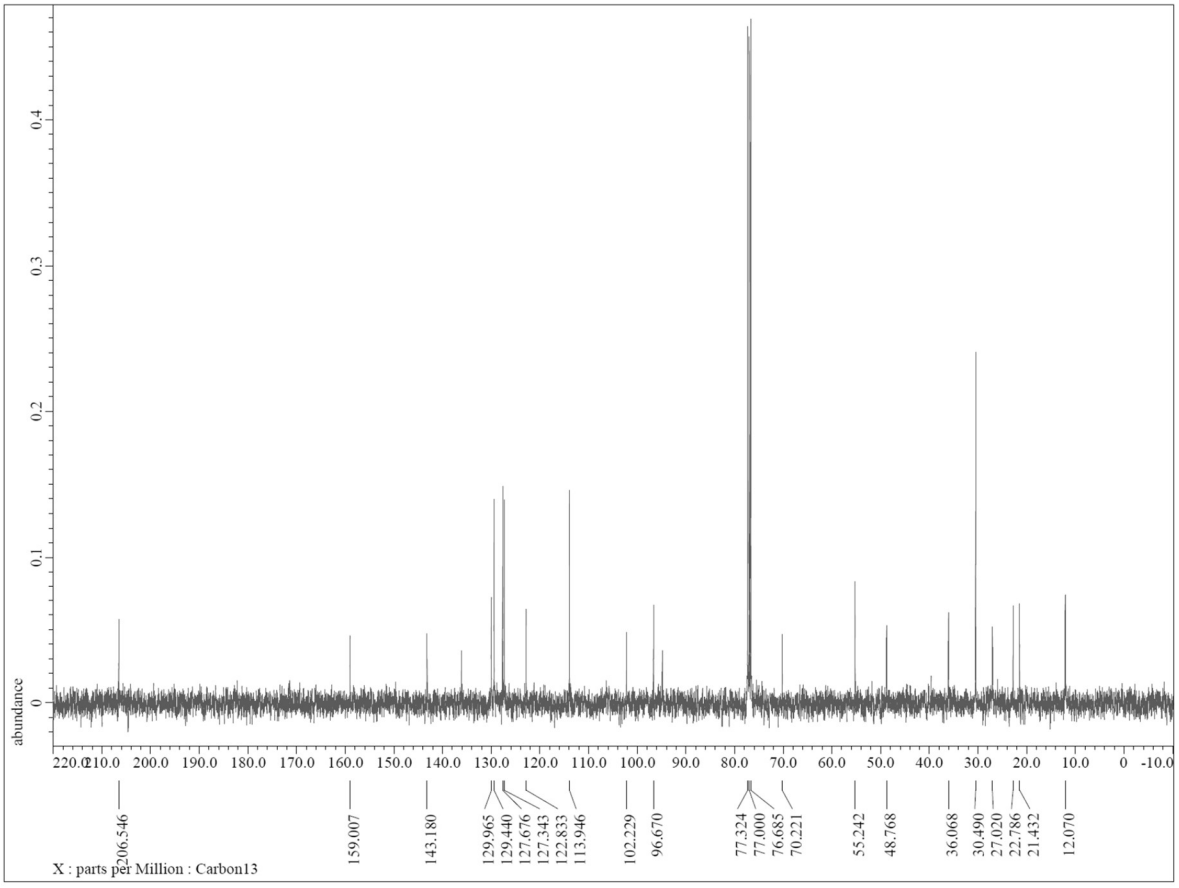

iPr
TsN
Ph
H
abundance
4.25
2.01
2.06
0.96
1.99
1.00
1.93
1.06
0.91
3.03
0.91
0.90
5.86
7.748
7.726
7.298
7.293
7.261
6.496
6.487
6.479
6.069
6.063
6.056
6.052
6.045
6.039
4.139
4.133
3.952
3.918
3.913
3.894
3.889
2.407
2.357
2.340
2.335
2.323
1.967
1.960
1.558
1.109
1.094
1.077
1.042
0.008
-0.000
-0.008
X : parts per Million : Proton

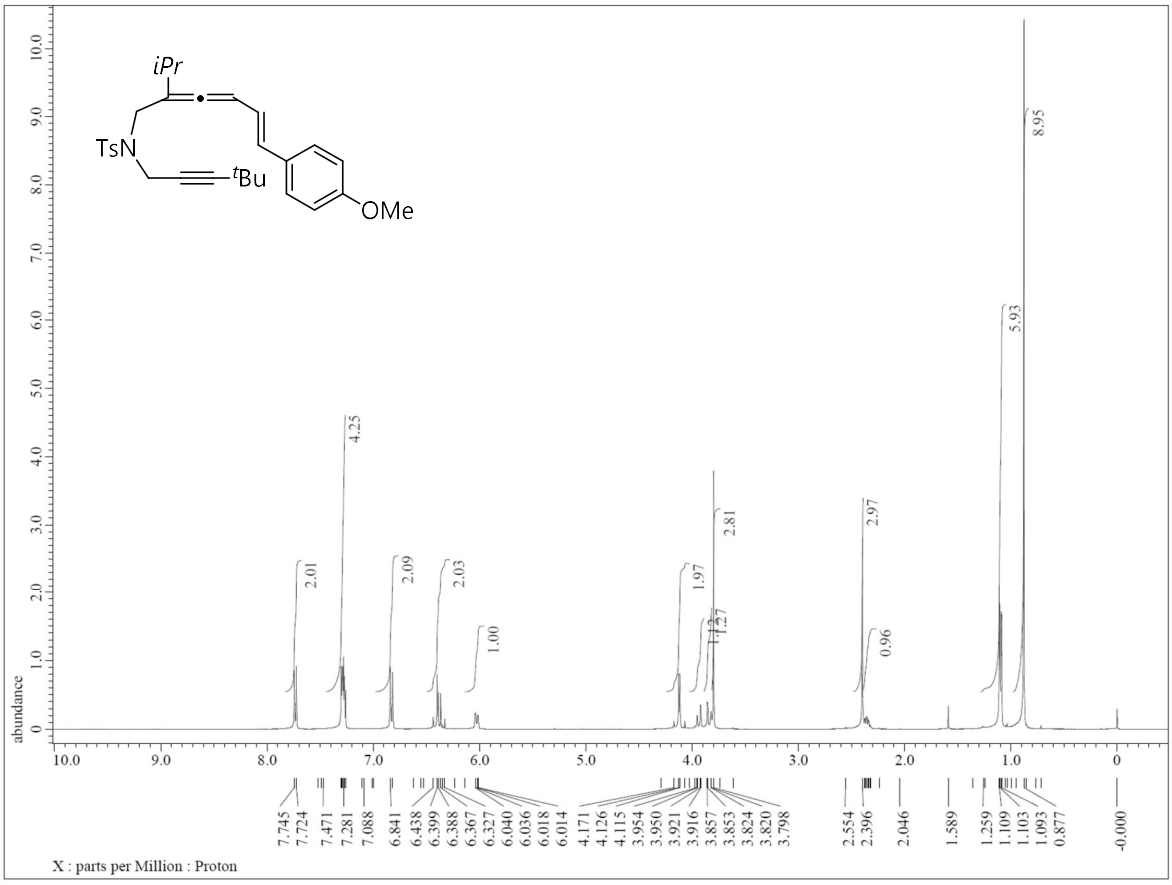

abundance
206.165
143.513
137.106
135.800
130.670
129.421
128.563
127.733
127.400
126.160
124.778
107.263
97.394
77.324
77.000
76.685
76.151
73.873
47.729
35.687
28.192
21.776
21.509
X : parts per Million : Carbon13

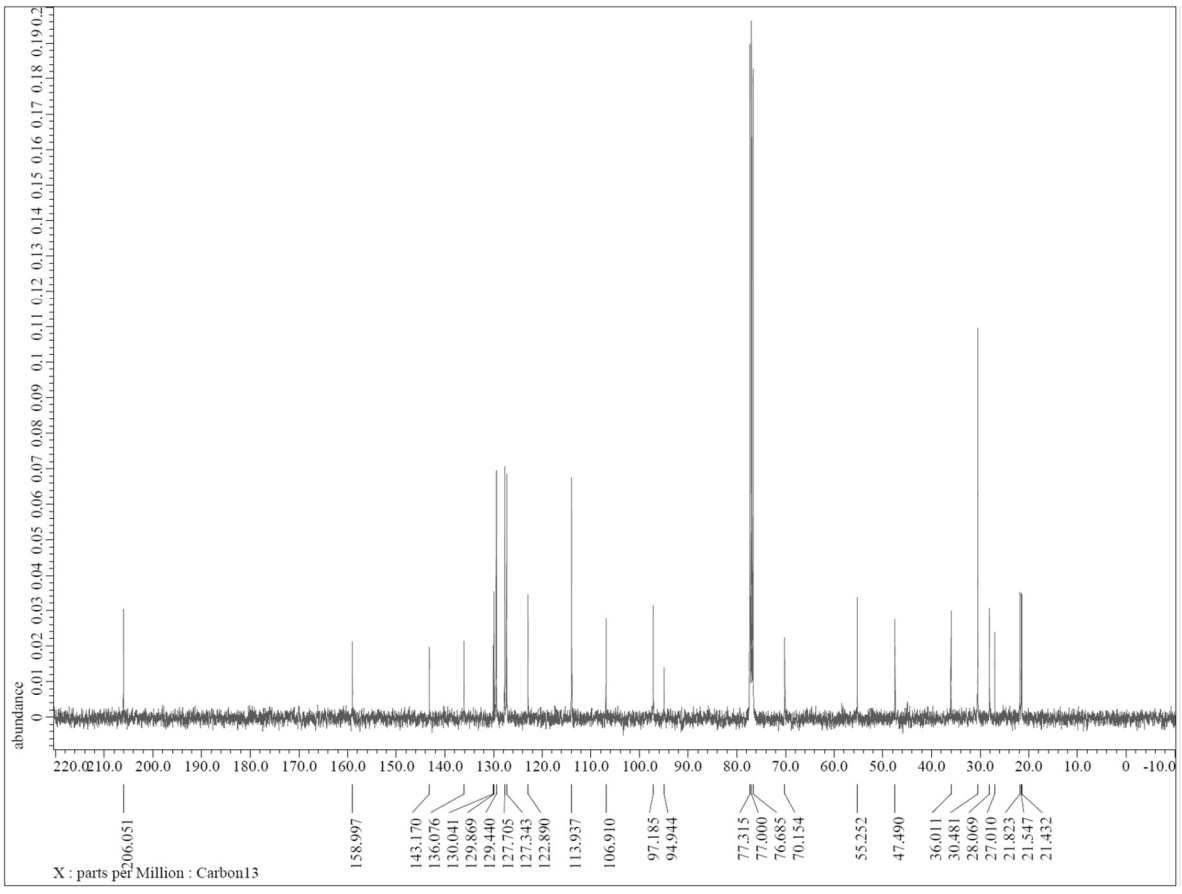

Me
TsN
tBu
OMe
abundance
9.04
5.22
4.29
2.93
2.70
2.24
2.20
2.16
1.94
1.00
7.741
7.721
7.300
7.278
7.261
6.841
6.819
6.399
6.378
5.932
5.914
4.308
4.182
4.175
4.147
4.129
4.124
3.829
3.824
3.810
3.801
3.788
2.401
2.377
2.355
2.346
2.047
1.795
1.550
1.265
1.063
1.046
0.891
0.884
0.866
-0.000
-0.007
X : parts per Million : Proton

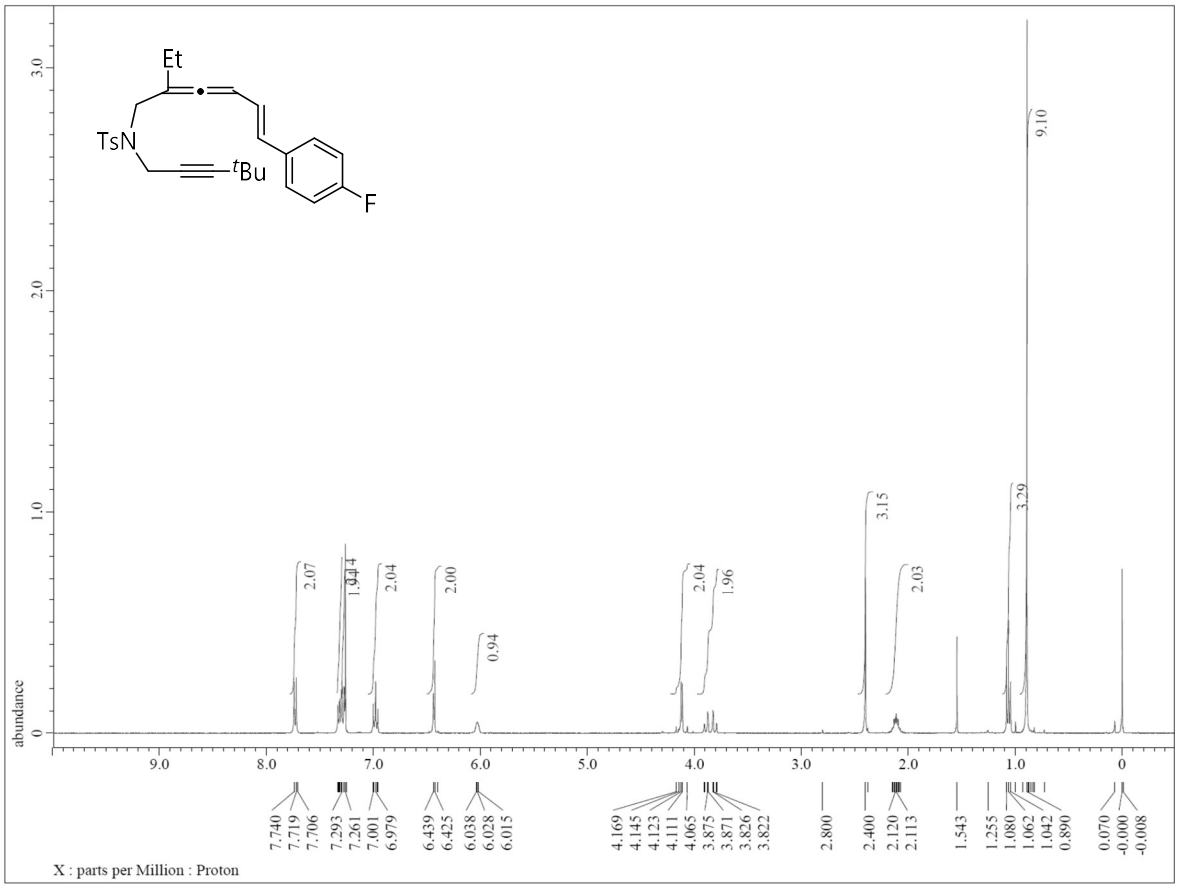

abundance
207.071
159.007
143.170
136.143
130.136
129.946
129.431
127.638
127.324
122.575
113.918
95.573
94.763
77.315
77.000
76.676
70.192
55.194
49.903
36.030
30.462
26.991
21.394
16.179
X : parts per Million : Carbon13

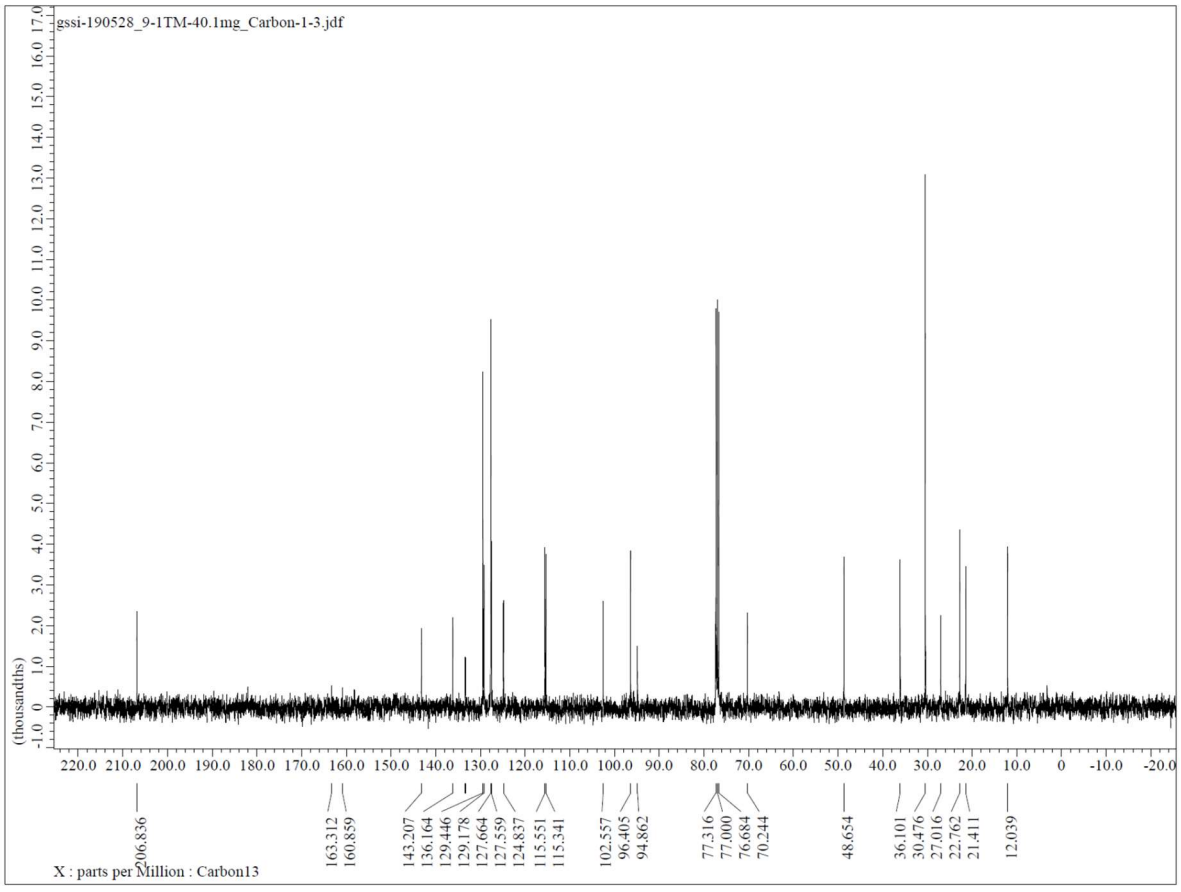

Et
TsN
tBu
OMe
abundance
9.03
4.29
2.14
2.27
2.14
1.00
2.14
2.19
3.16
3.19
2.10
3.39
7.740
7.719
7.290
7.281
6.841
6.819
6.404
6.384
6.034
6.031
6.023
6.018
6.015
6.010
4.121
4.116
3.892
3.865
3.861
3.825
3.797
2.396
2.105
2.101
1.611
1.258
1.077
1.058
1.039
0.889
0.073
-0.000
X : parts per Million : Proton


abundance
206.546
159.007
143.180
129.965
129.440
127.676
127.343
122.833
113.946
102.229
96.670
77.324
77.000
76.685
70.221
55.242
48.768
36.068
30.490
27.020
22.786
21.432
12.070
X : parts per Million : Carbon13

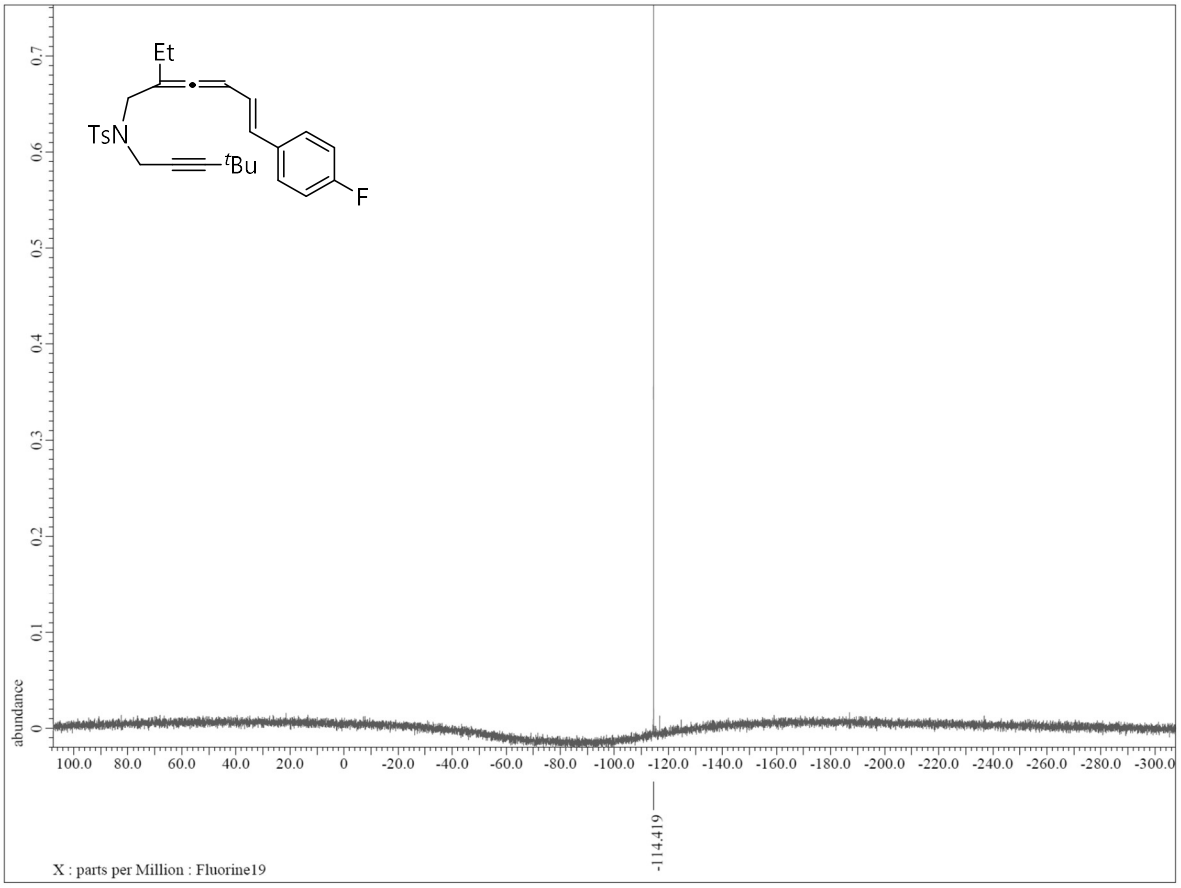

iPr
TsN
tBu
OMe
abundance
X : parts per Million : Proton

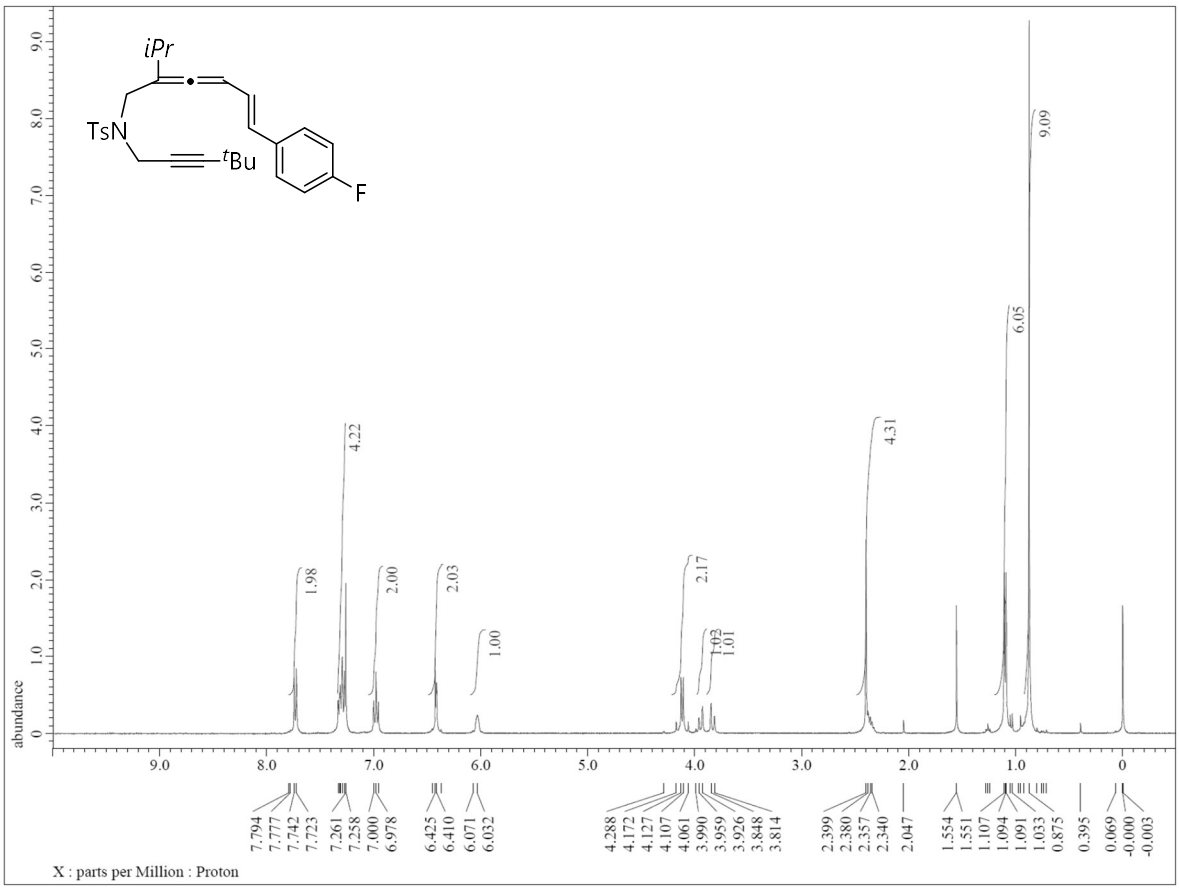

abundance
X : parts per Million : Carbon13

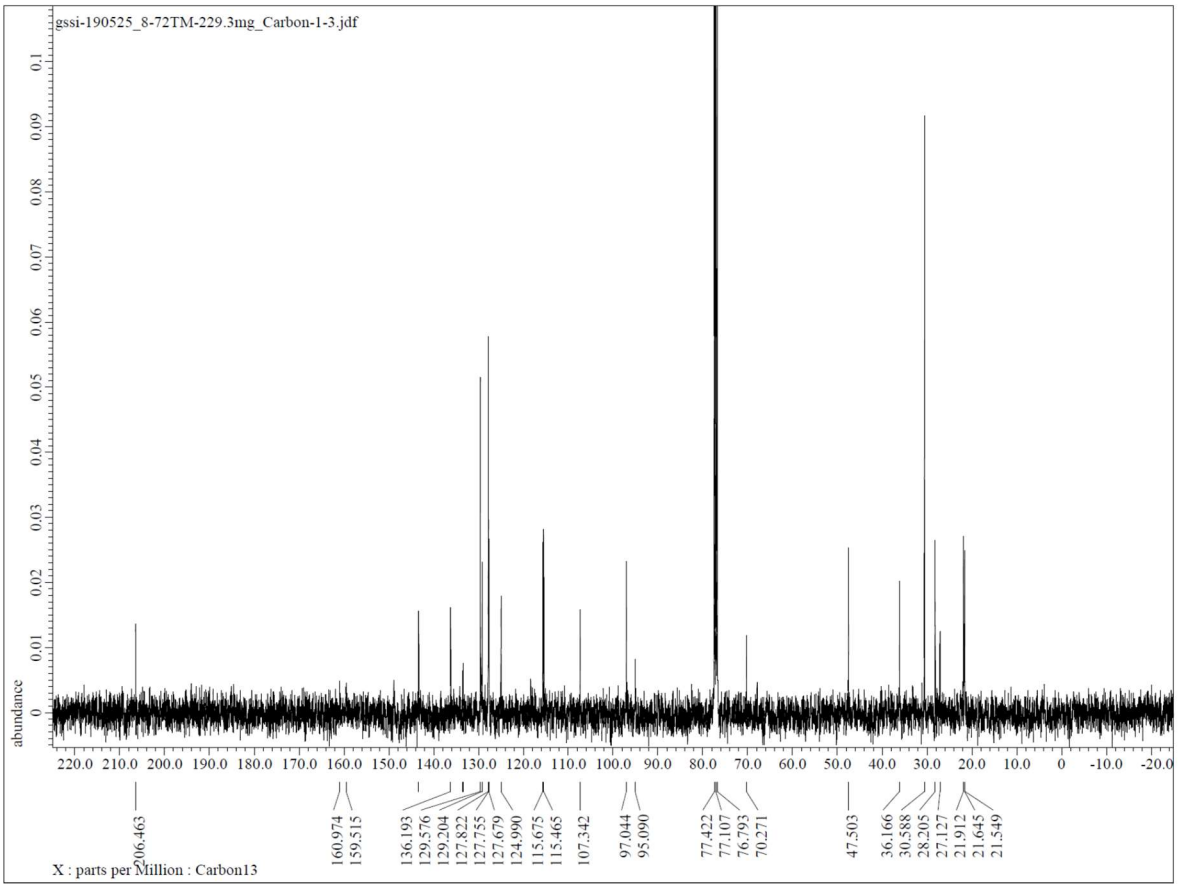

Et
TsN
tBu
F
abundance
9.10
3.15
3.79
2.07
1.94
2.04
2.00
0.94
2.04
1.96
2.03
7.740
7.719
7.706
7.293
7.261
7.001
6.979
6.439
6.425
6.038
6.028
6.015
4.169
4.145
4.123
4.111
4.065
3.875
3.871
3.826
3.822
2.800
2.400
2.120
2.113
1.543
1.255
1.080
1.062
1.042
0.890
0.070
-0.000
-0.008
X : parts per Million : Proton


gssi-190528_9-1TM-40.1mg_Carbon-1-3.jdf
(thousandths)
206.836
163.312
160.859
143.207
136.164
129.446
129.178
127.664
127.559
124.837
115.551
115.341
102.557
96.405
94.862
77.316
77.000
76.684
70.244
48.654
36.101
30.476
27.016
22.762
21.411
12.039
X : parts per Million : Carbon13

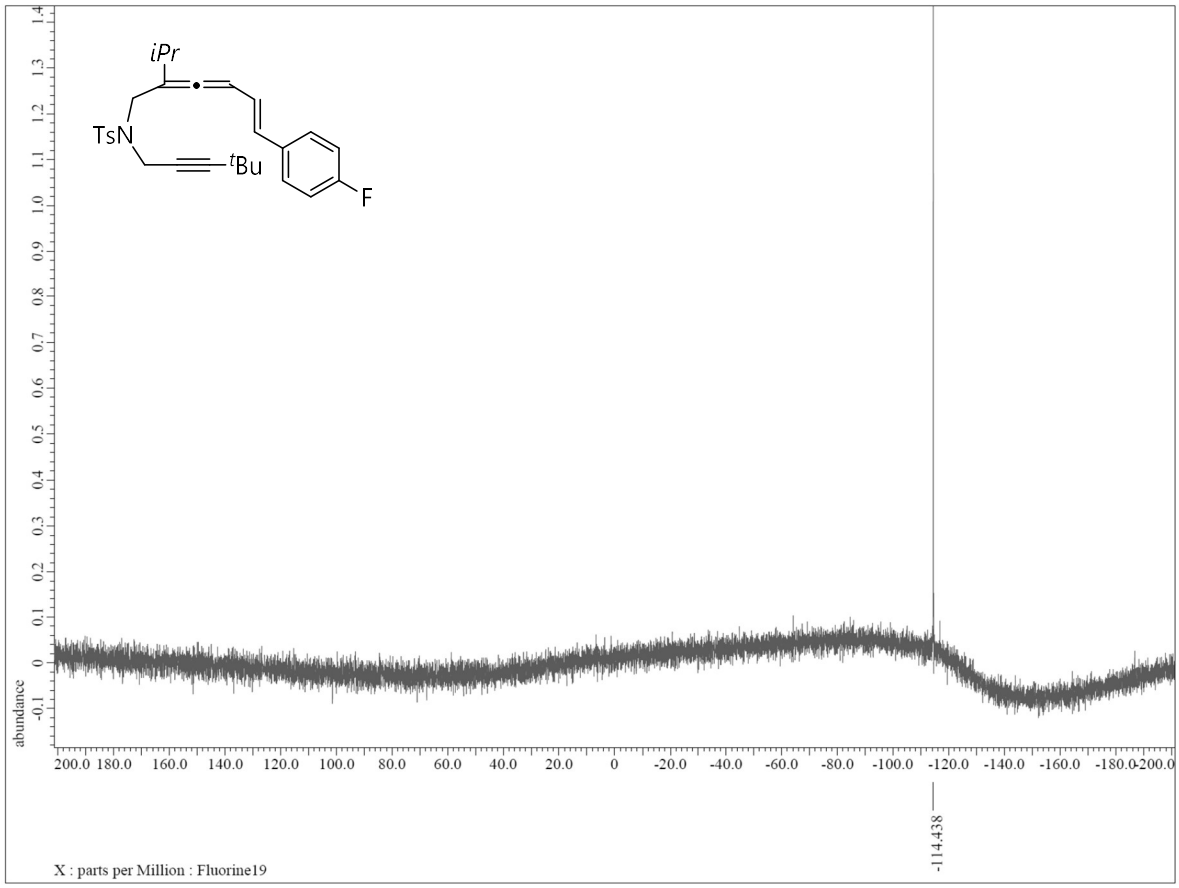
^{19}F NMR (376 MHz, $CDCl_3$)

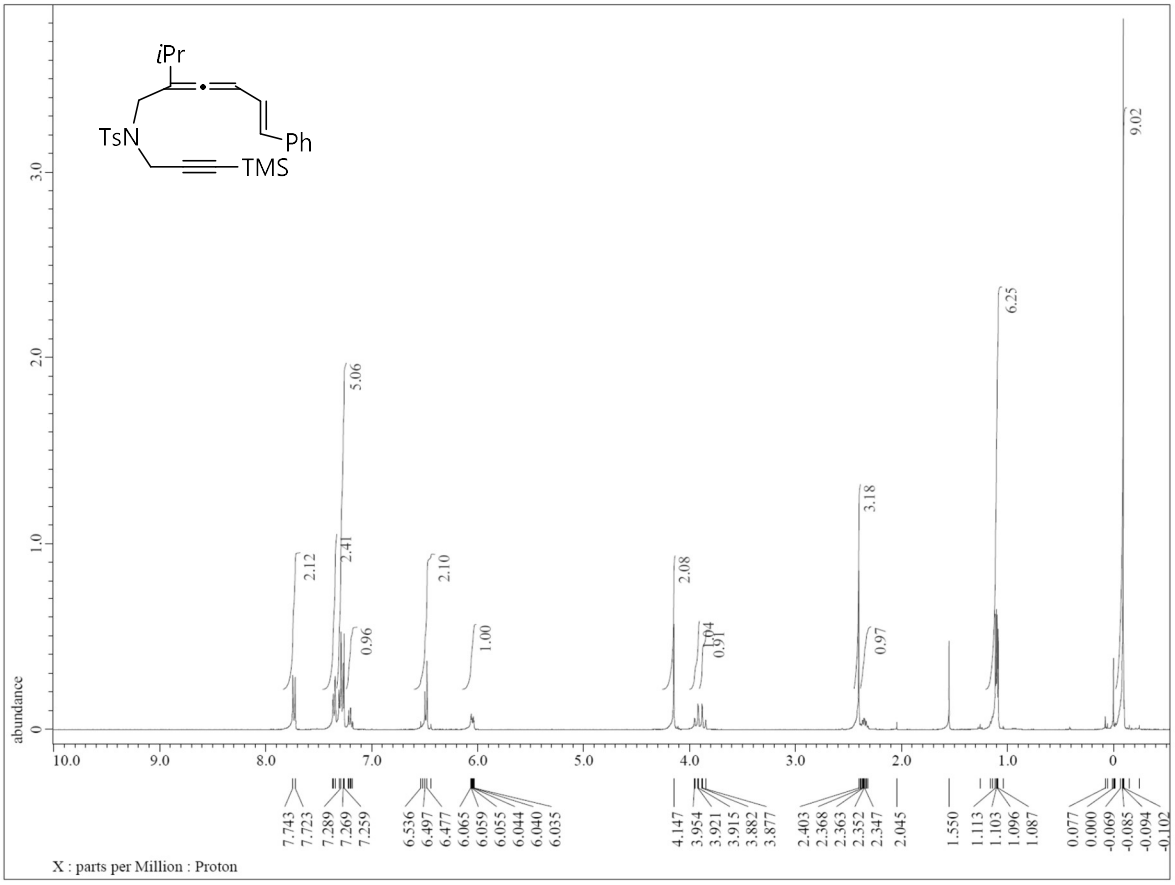


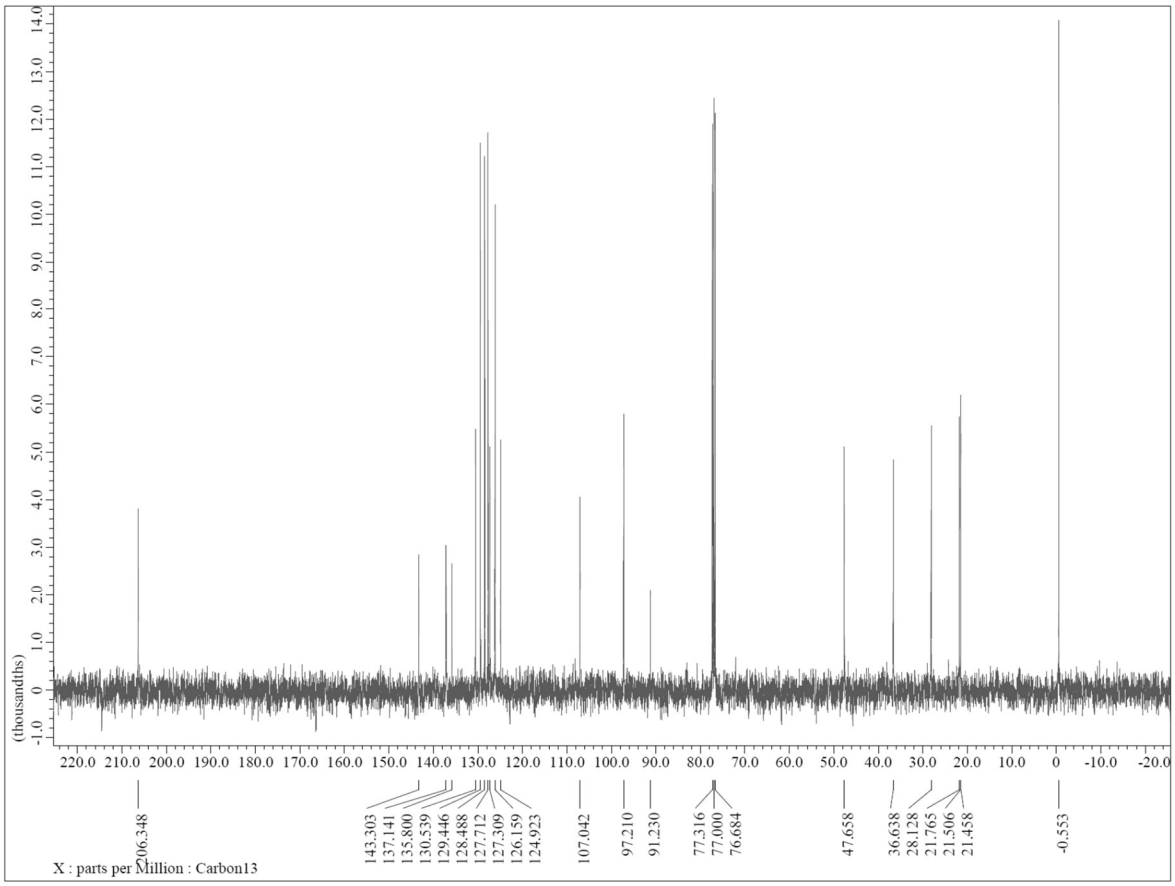

iPr
TsN
tBu
F
abundance
9.09
6.05
4.31
4.22
2.17
2.03
2.00
1.98
1.03
1.01
1.00
X : parts per Million : Proton

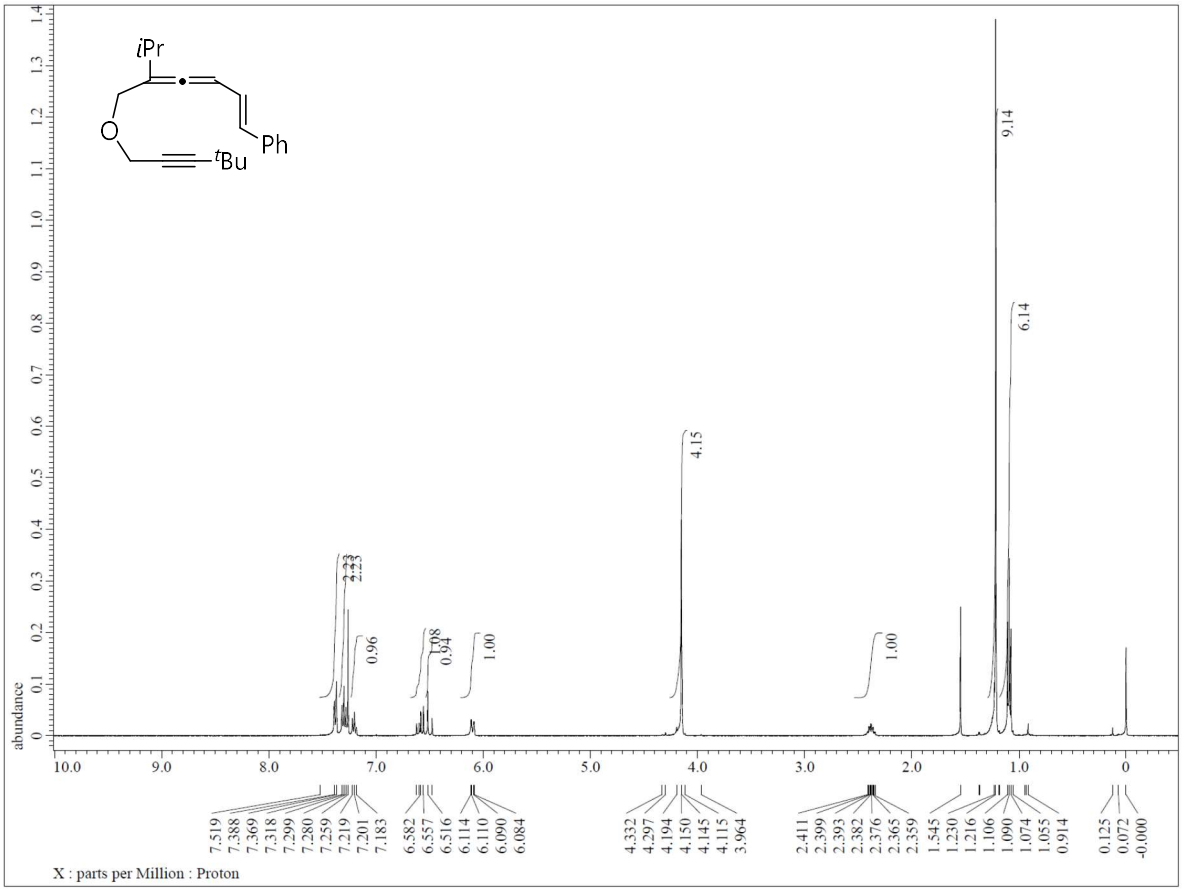

gssi-190525_8-72TM-229.3mg_Carbon-1-3.jdf
abundance
X : parts per Million : Carbon13

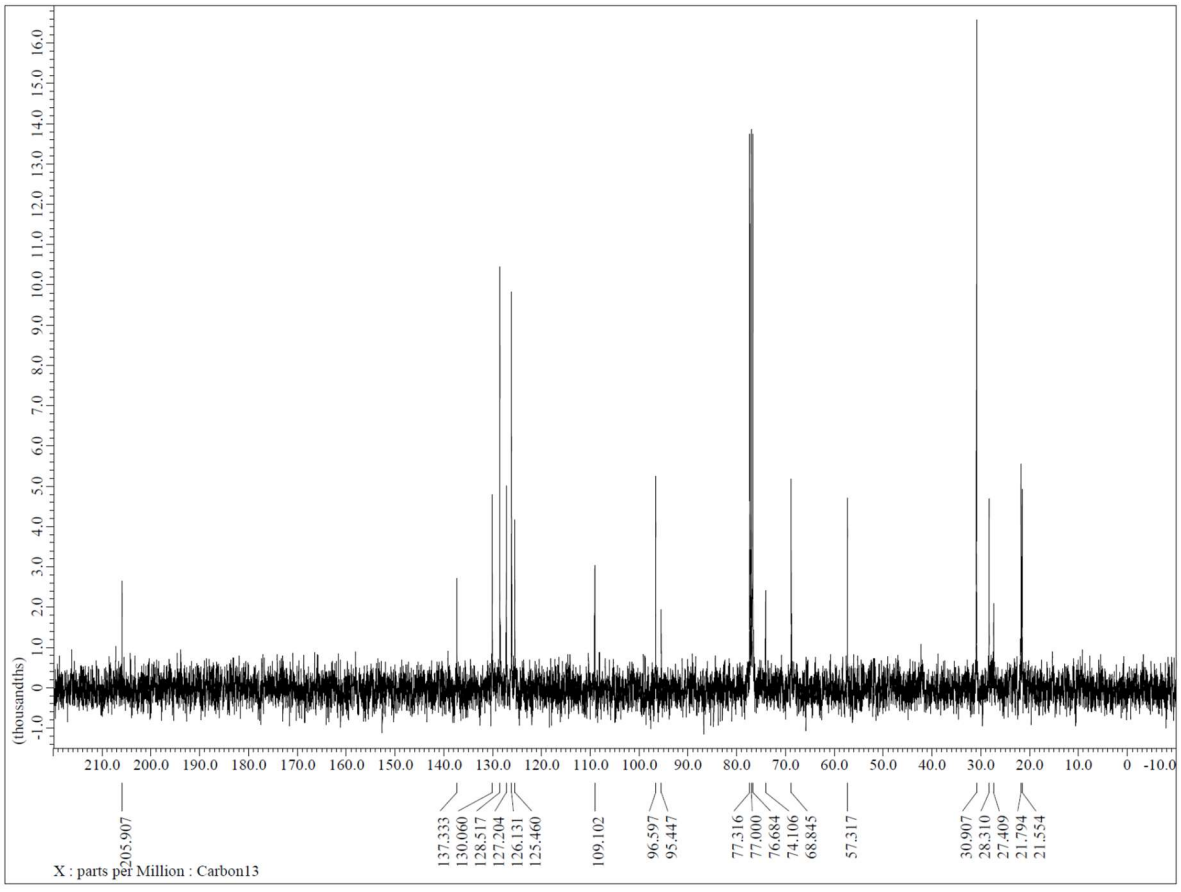
^{19}F NMR (376 MHz, $CDCl_3$)

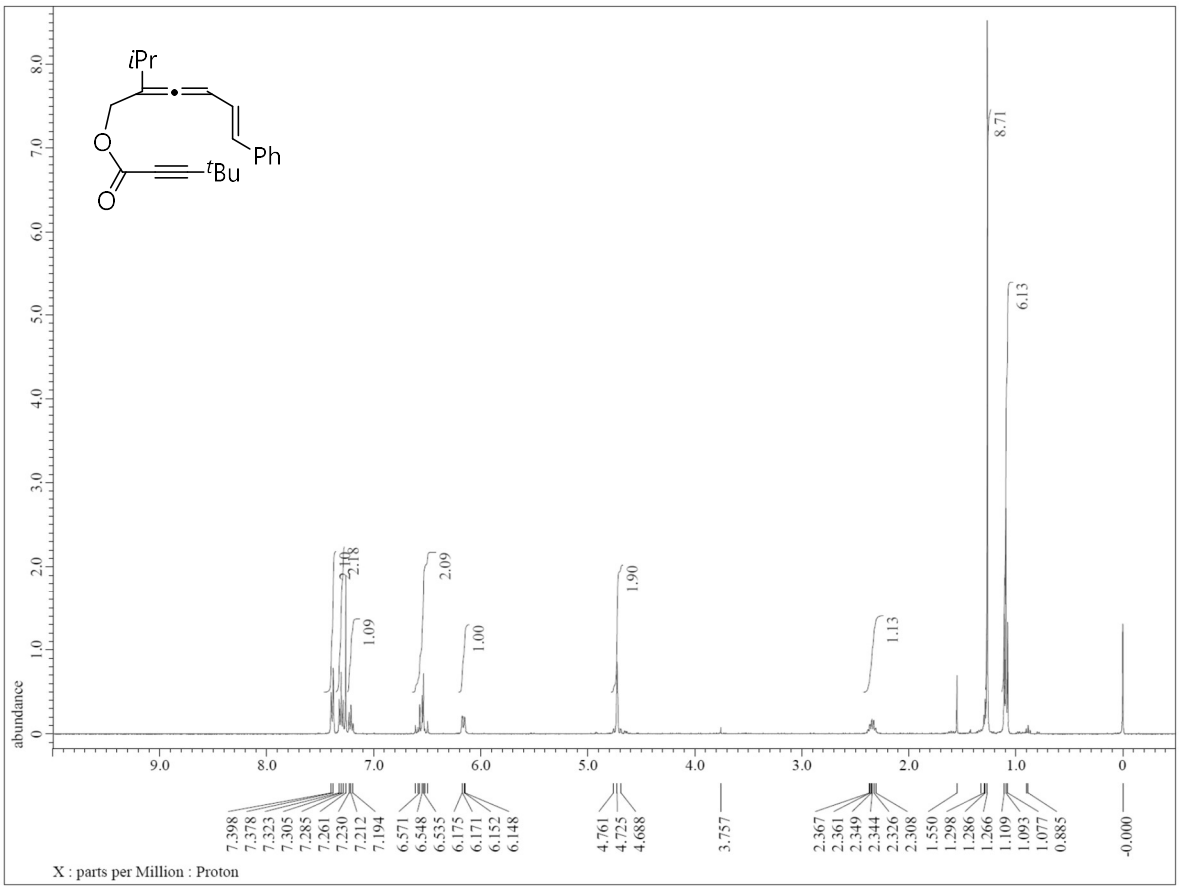



iPr
TsN
Ph
TMS
abundance
X : parts per Million : Proton


(thousandths)
X : parts per Million : Carbon13


iPr
O
tBu
Ph
abundance
9.14
6.14
4.15
1.00
1.00
0.96
1.08
0.94
1.00
X : parts per Million : Proton


(thousandths)
205.907
137.333
130.060
128.517
127.204
126.131
125.460
109.102
96.597
95.447
77.316
77.000
76.684
74.106
68.845
57.317
30.907
28.310
27.409
21.794
21.554
X : parts per Million : Carbon13


iPr
Ph
tBu
O
O
abundance
8.71
6.13
2.09
1.90
1.13
1.09
1.00
7.398
7.378
7.323
7.305
7.285
7.261
7.230
7.212
7.194
6.571
6.548
6.535
6.175
6.171
6.152
6.148
4.761
4.725
4.688
3.757
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2.361
2.349
2.344
2.326
2.308
1.550
1.298
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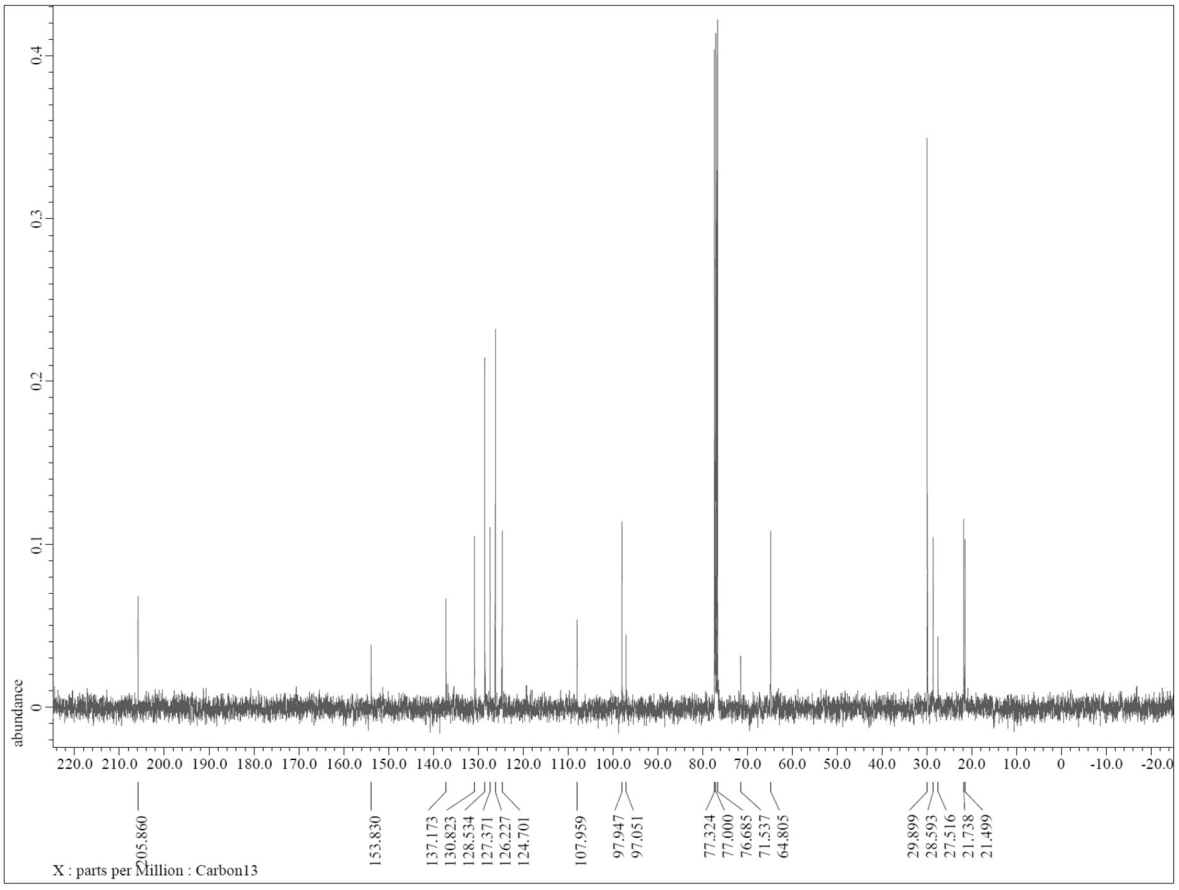
1.266
1.109
1.093
1.077
0.885
-0.000
X : parts per Million : Proton


abundance
205.860
153.830
137.173
130.823
128.534
127.371
126.227
124.701
107.959
97.947
97.051
77.324
77.000
76.685
71.537
64.805
29.899
28.593
27.516
21.738
21.499
X : parts per Million : Carbon13

Computational methods

All calculations were performed with Gaussian 16 program[1]. Structure optimizations were carried out using the M06[2] functional with an ultrafine grid and the LanL2DZ[3] (for nickel) and 6-31+G(d)[4] (for the other atoms) basis sets. Harmonic vibrational frequencies were computed at the same level of theory to confirm no imaginary vibration was observed for the optimized structure, and only one imaginary vibration was observed for the transition state. The intrinsic reaction coordinate (IRC) method was used to track minimum energy paths from transition structures to the corresponding local minima.

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Cartesian Coordinates and Energies

NiL2.log
Energy (E) = -1542.50077227 Hartree
Enthalpy (H) = -1542.216573 Hartree
Gibbs free energy (G) = -1542.299265 Hartree
Charge = 0, Spin = 1

Ni	0.093047	-0.278003	-0.660273
P	-1.967173	-0.104096	-0.286093
O	-2.342632	0.772785	1.062587
O	-2.967477	0.667972	-1.311863
O	-2.722874	-1.523290	0.011941
C	-1.668332	0.425437	2.262397
H	-0.580983	0.357629	2.101400
H	-1.882691	1.212092	2.992083
H	-2.029457	-0.539125	2.648537
C	-3.977296	1.603047	-0.961781
H	-3.545456	2.476038	-0.458978
H	-4.446040	1.913329	-1.900694
H	-4.736904	1.159738	-0.304591
C	-4.105033	-1.593740	0.320498
H	-4.710697	-1.292741	-0.545397
H	-4.327052	-2.636778	0.565122
H	-4.355098	-0.958877	1.183034
P	2.075688	-0.031946	-0.031173
O	2.330945	1.129028	1.098212
O	2.804176	-1.197286	0.858884
O	3.205916	0.318836	-1.162129
C	1.790699	2.408532	0.813046
H	0.722025	2.340163	0.552966
H	1.908539	3.013765	1.716758
H	2.327449	2.889975	-0.018486
C	2.737273	-2.511782	0.331184
H	3.354875	-2.608099	-0.574818
H	3.121971	-3.185728	1.101991
H	1.700395	-2.790743	0.088962
C	4.561819	0.550619	-0.799811

H 4.996952 -0.335234 -0.318405
H 5.103404 0.769430 -1.724623
H 4.646492 1.402852 -0.112469

SM1.log
Energy (E) = -1610.54980187 Hartree
Enthalpy (H) = -1610.032369 Hartree
Gibbs free energy (G) = -1610.128949 Hartree
Charge = 0, Spin = 1
C 1.265541 1.055987 -1.661832
C 0.645580 -1.755977 -0.344902
C 1.337869 -0.546338 0.273015
H 1.926016 1.791202 -2.136129
H 0.944026 0.351366 -2.448569
H 0.601392 0.079698 0.795146
H 2.053133 -0.889937 1.034111
C 0.099786 1.697945 -1.073903
C -0.894729 2.177603 -0.577164
C -3.241289 -1.357572 -0.187419
C -2.824740 -1.302919 -1.466208
C -1.439911 -1.437523 -1.910350
C -0.393795 -1.607866 -1.127617
H -3.547242 -1.117050 -2.263818
H -1.266609 -1.348281 -2.986865
H -2.489031 -1.559235 0.583302
N 2.059082 0.361012 -0.626675
S 3.568807 -0.164830 -1.149816
O 3.539176 -1.565296 -1.564239
O 4.049642 0.856236 -2.072416
C 1.187205 -3.111438 0.022525
H 1.208499 -3.235775 1.115746
H 0.580878 -3.917569 -0.403976
H 2.216539 -3.213265 -0.348039
C -2.113983 2.707289 0.047453
C -4.599357 -1.156383 0.306241
C -5.683218 -0.833304 -0.526479
C -4.841879 -1.267251 1.683599
C -6.952622 -0.637284 -0.001088
H -5.531226 -0.730159 -1.600735
C -6.112896 -1.070845 2.212028
H -4.010067 -1.511748 2.346406
C -7.176334 -0.755222 1.371187
H -7.777420 -0.387822 -0.667382
H -6.272759 -1.164501 3.285322
H -8.173606 -0.600307 1.779737
C -1.939555 4.196818 0.357278
H -2.850528 4.590059 0.831133
H -1.096022 4.362237 1.040706
H -1.753114 4.771518 -0.559629
C -3.296891 2.507960 -0.906366
H -3.146903 3.063824 -1.841670
H -3.422789 1.444576 -1.151144
H -4.223565 2.865091 -0.433844
C -2.366733 1.931723 1.346213
H -2.472662 0.856841 1.142017
H -1.539689 2.071641 2.056334
H -3.295566 2.281408 1.820289
C 4.512684 -0.076796 0.360043
C 4.978104 -1.248302 0.946572
C 4.789092 1.175737 0.902725
C 5.737344 -1.160624 2.111285
H 4.752511 -2.208178 0.484703
C 5.547005 1.250710 2.064535
H 4.414422 2.073517 0.413661
C 6.018815 0.084086 2.667147
H 6.111404 -2.068024 2.581824
H 5.774429 2.221676 2.500643
H 6.613968 0.148608 3.576623

TS1DA.log
Energy (E) = -1610.51457648 Hartree
Enthalpy (H) = -1609.993570 Hartree
Gibbs free energy (G) = -1610.086505 Hartree
Charge = 0, Spin = 1
Imaginary frequency: -440.0814
C 1.025033 0.771395 -1.333837
C 0.605201 -1.694082 0.153948
C 1.545468 -0.634576 0.667207
H 1.236388 1.827492 -1.545968
H 1.086318 0.221255 -2.286363
H 1.046810 -0.017328 1.430384
H 2.411087 -1.094916 1.162474
C -0.344630 0.631108 -0.777095
C -1.365773 1.255141 -0.444878
C -3.168394 -1.078635 -0.027115
C -2.732891 -1.598050 -1.215111
C -1.367339 -1.828558 -1.505819
C -0.374420 -1.383911 -0.681258
H -3.459326 -1.840813 -1.993445
H -1.097264 -2.206042 -2.495066

H -2.438673 -0.963953 0.778282
N 2.042904 0.280128 -0.369457
S 3.464846 -0.220119 -1.118774
O 3.448727 -1.653136 -1.406022
O 3.693483 0.737667 -2.193774
C 0.835499 -3.096137 0.637320
H 0.863957 -3.135452 1.737159
H 0.051921 -3.776900 0.287788
H 1.807905 -3.460005 0.271781
C -2.275578 2.371280 -0.128651
C -4.560296 -0.856377 0.341340
C -5.601469 -0.780463 -0.599467
C -4.894817 -0.721302 1.698474
C -6.916441 -0.591472 -0.196284
H -5.373304 -0.850252 -1.663262
C -6.210309 -0.530533 2.103649
H -4.100163 -0.779377 2.444413
C -7.230017 -0.465578 1.157169
H -7.705136 -0.532666 -0.945303
H -6.440933 -0.433564 3.163727
H -8.261773 -0.312907 1.469487
C -1.474362 3.666009 -0.358591
H -2.103318 4.541689 -0.138600
H -0.589936 3.702751 0.292129
H -1.137335 3.740685 -1.401747
C -3.495618 2.369827 -1.051787
H -3.188592 2.392311 -2.106383
H -4.116176 1.479725 -0.892897
H -4.113002 3.258129 -0.854211
C -2.717355 2.313791 1.335438
H -3.328857 1.424847 1.533992
H -1.849167 2.300038 2.008882
H -3.323572 3.199517 1.573761
C 4.663251 0.050534 0.173103
C 5.308086 -1.039178 0.747244
C 4.950093 1.358315 0.556681
C 6.261166 -0.810787 1.737173
H 5.065472 -2.045572 0.409738
C 5.902456 1.574038 1.544941
H 4.432502 2.188920 0.079424
C 6.555117 0.490665 2.134007
H 6.776375 -1.652772 2.195870
H 6.140475 2.589876 1.855097
H 7.301808 0.665272 2.907003

PDA.log

Energy (E) = -1610.64909229 Hartree
Enthalpy (H) = -1610.127794 Hartree
Gibbs free energy (G) = -1610.214998 Hartree
Charge = 0, Spin = 1
C 0.313768 0.289858 -0.964953
C 0.609282 -2.343485 -0.128227
C 1.748979 -1.640790 -0.799576
H 0.353165 1.374356 -1.007968
H 0.039536 -0.069283 -1.979186
H 2.696892 -1.993104 -0.358187
H 1.790482 -1.901149 -1.877324
C -0.690713 -0.248244 0.018351
C -1.720298 0.472623 0.530427
C -2.852578 -0.247487 1.239156
C -2.562039 -1.673909 1.587735
C -1.502697 -2.339916 1.121716
C -0.498315 -1.684819 0.300480
H -3.305178 -2.175851 2.209944
H -1.362478 -3.383927 1.396045
H -3.093296 0.280557 2.176318
N 1.650940 -0.199175 -0.614764
S 2.933707 0.676681 -1.265050
O 3.369435 0.110593 -2.539818
O 2.547912 2.080663 -1.180092
C 0.863085 -3.807889 0.055485
H 1.491668 -4.001212 0.939516
H -0.051419 -4.400660 0.157348
H 1.413336 -4.207229 -0.809440
C -1.833905 2.010559 0.414397
C -4.138816 -0.266786 0.409856
C -4.108366 -0.580341 -0.950145
C -5.375601 -0.059759 1.022855
C -5.287313 -0.662921 -1.684908
H -3.147818 -0.760194 -1.436462
C -6.558261 -0.147779 0.293085
H -5.409059 0.185348 2.086883
C -6.516784 -0.445792 -1.066392
H -5.245839 -0.901252 -2.747004
H -7.513894 0.022207 0.787462
H -7.438898 -0.510067 -1.641997
C -0.576329 2.674375 1.009616
H -0.681470 3.768400 0.969356
H -0.468833 2.387538 2.065777
H 0.363959 2.423976 0.507228
C -2.077059 2.462620 -1.035288

H -1.305414 2.134106 -1.739777
H -3.041034 2.080503 -1.399495
H -2.114474 3.561031 -1.081118
C -3.001300 2.588056 1.231296
H -3.980092 2.225658 0.895540
H -2.900952 2.386389 2.307201
H -3.003550 3.680142 1.112091
C 4.206119 0.350506 -0.062545
C 5.331046 -0.374399 -0.437582
C 4.052243 0.856248 1.226182
C 6.328645 -0.600964 0.508181
H 5.415854 -0.744566 -1.457810
C 5.053311 0.623166 2.160526
H 3.157631 1.421665 1.484226
C 6.188512 -0.104301 1.800891
H 7.217450 -1.165062 0.231397
H 4.950588 1.011271 3.172205
H 6.970781 -0.282890 2.536930

INT1S.log
Energy (E) = -3153.09807211 Hartree
Enthalpy (H) = -3152.294007 Hartree
Gibbs free energy (G) = -3152.435510 Hartree
Charge = 0, Spin = 1
C 2.155753 1.051035 -0.037008
C 2.293096 -1.812170 2.260831
C 2.862626 -0.523924 1.729357
H 2.779231 1.825955 0.454309
H 2.265890 1.175052 -1.118902
H 2.379475 0.315653 2.254401
H 3.933565 -0.463400 2.008386
C 0.739073 1.233974 0.360579
C -0.099522 1.768181 1.163731
C -1.397620 -2.621329 1.248267
C -0.561384 -3.537374 0.723775
C 0.893563 -3.501046 0.826256
C 1.584219 -2.633038 1.532509
H -0.967011 -4.400338 0.189092
H 1.452096 -4.270109 0.284091
H -0.957670 -1.742651 1.734192
N 2.674166 -0.282918 0.300794
S 3.852911 -0.898576 -0.714297
O 4.094756 -2.275385 -0.310492
O 3.459822 -0.567883 -2.079321
C 2.617197 -2.072891 3.706839
H 2.263516 -1.244517 4.341265
H 2.152377 -2.998159 4.062290
H 3.705066 -2.152531 3.855739
C -0.345234 2.516100 2.434413
C -2.855077 -2.656279 1.210165
C -3.590024 -3.772768 0.776168
C -3.566892 -1.512164 1.597418
C -4.975610 -3.727202 0.697447
H -3.070666 -4.690433 0.498394
C -4.954068 -1.464183 1.516872
H -3.016821 -0.635048 1.941926
C -5.666835 -2.569485 1.061129
H -5.524530 -4.604144 0.355092
H -5.475617 -0.551266 1.802377
H -6.753441 -2.535715 0.994449
Ni -1.025152 0.922270 -0.287581
P -3.069451 1.576476 -0.200510
O -3.230114 3.127285 -0.743497
O -4.316607 0.882342 -1.018560
O -3.801622 1.685864 1.243796
C -2.175068 3.723575 -1.480923
H -1.194860 3.477294 -1.044926
H -2.192430 3.389891 -2.529607
H -2.329590 4.806926 -1.444561
C -4.352706 1.024877 -2.430645
H -3.379221 0.794884 -2.891623
H -5.089510 0.307060 -2.805236
H -4.660641 2.042435 -2.706651
C -5.052505 2.348951 1.399519
H -5.801406 1.937208 0.711636
H -5.367363 2.182595 2.434394
H -4.938212 3.425385 1.218147
P -0.708683 -0.271930 -2.058456
O -1.865209 -1.136879 -2.830067
O -0.288695 0.500937 -3.443238
O 0.474603 -1.346696 -1.809279
C -2.700072 -1.987252 -2.053975
H -3.283526 -1.414714 -1.317213
H -3.384394 -2.477778 -2.753551
H -2.109126 -2.750450 -1.526981
C 0.817037 1.385265 -3.397783
H 1.756257 0.832375 -3.244646
H 0.852932 1.898470 -4.363632
H 0.696379 2.133854 -2.597281
C 0.878138 -2.284309 -2.801323
H 1.060609 -1.788829 -3.763944

H 1.809620 -2.733143 -2.443895
H 0.110702 -3.059908 -2.930290
C 5.341102 0.025341 -0.353128
C 6.265470 -0.491206 0.552758
C 5.537447 1.264351 -0.961407
C 7.400398 0.254418 0.860728
H 6.101663 -1.477934 0.983485
C 6.674793 2.000653 -0.645655
H 4.819418 1.629967 -1.693945
C 7.601771 1.498317 0.266554
H 8.133677 -0.142528 1.560832
H 6.843613 2.965353 -1.121364
H 8.492539 2.076467 0.507546
C -1.158165 3.785517 2.169818
H -0.624150 4.458519 1.482706
H -2.138183 3.552566 1.733916
H -1.324706 4.327856 3.112606
C 0.998891 2.912055 3.053366
H 1.595228 2.024377 3.311449
H 1.587502 3.531550 2.361012
H 0.844205 3.488319 3.978122
C -1.105080 1.607932 3.405284
H -0.546442 0.676754 3.587737
H -1.247743 2.117504 4.370499
H -2.091528 1.345024 3.001742

TS1S.log
Energy (E) = -3153.08081556 Hartree
Enthalpy (H) = -3152.251255 Hartree
Gibbs free energy (G) = -3152.388505 Hartree
Charge = 0, Spin = 1
Imaginary frequency: -428.7868
C 1.950593 -0.043934 1.089211
C 2.250684 -2.208341 -1.020378
C 3.213831 -1.914299 0.096139
H 2.016304 -0.263312 2.169583
H 1.936107 1.042275 0.980381
H 3.016635 -2.494040 1.013265
H 4.234900 -2.188746 -0.215477
C 0.658158 -0.652604 0.572435
C -0.285757 -1.337178 1.182501
C -1.905500 -1.379355 -1.774616
C -0.901268 -0.758062 -2.465810
C 0.489621 -0.904308 -2.261948
C 1.171227 -1.450790 -1.208260
H -1.176643 -0.087655 -3.284307
H 1.136976 -0.364124 -2.961601
H -1.632794 -2.137806 -1.041564
N 3.200986 -0.505056 0.484383
S 4.012168 0.543753 -0.548859
O 3.816117 0.241547 -1.964761
O 3.738726 1.892761 -0.055861
C 2.671507 -3.274870 -1.986639
H 2.899420 -4.224072 -1.473605
H 1.894873 -3.467214 -2.734834
H 3.591081 -2.966119 -2.514000
C -0.582742 -2.573923 1.974543
C -3.330071 -1.271471 -2.071324
C -3.856297 -0.403930 -3.046482
C -4.236408 -2.103841 -1.393218
C -5.219457 -0.350755 -3.303975
H -3.188388 0.231318 -3.627776
C -5.600516 -2.055444 -1.652316
H -3.853011 -2.795625 -0.643307
C -6.104182 -1.170249 -2.602870
H -5.596103 0.332147 -4.065086
H -6.275833 -2.716367 -1.108448
H -7.173319 -1.127070 -2.805859
Ni -1.092172 0.234154 0.546478
P -3.109701 0.334112 1.301641
O -3.258725 0.923571 2.837658
O -4.290616 1.210371 0.567133
O -3.923976 -1.057911 1.441546
C -2.154026 1.546887 3.467119
H -1.206421 1.069721 3.169150
H -2.110796 2.615704 3.209124
H -2.289623 1.439369 4.548561
C -4.294741 2.620866 0.724713
H -3.303881 3.060257 0.530961
H -5.003152 3.019824 -0.008495
H -4.623606 2.894215 1.736099
C -5.289059 -1.105130 1.843361
H -5.928651 -0.646537 1.080221
H -5.541893 -2.165363 1.950625
H -5.429919 -0.594854 2.804815
P -0.558795 2.191870 -0.225489
O -1.553594 3.156242 -1.104842
O -0.259052 3.400138 0.848002
O 0.793571 2.127649 -1.119472
C -2.321539 2.545037 -2.127003
H -2.857753 1.659119 -1.753626

H -3.048958 3.288859 -2.468376
H -1.683070 2.252849 -2.975640
C 0.744213 3.213315 1.829459
H 1.746327 3.173434 1.376214
H 0.689858 4.072828 2.504938
H 0.574700 2.291863 2.409337
C 1.361394 3.283096 -1.731559
H 1.477564 4.098336 -1.005634
H 2.345153 2.982932 -2.102101
H 0.728218 3.626220 -2.560127
C 5.707141 0.129470 -0.168891
C 6.497493 -0.477398 -1.138505
C 6.211553 0.453223 1.088513
C 7.825627 -0.773126 -0.836205
H 6.069651 -0.703378 -2.114097
C 7.537877 0.157147 1.378359
H 5.567345 0.935002 1.822764
C 8.342480 -0.456617 0.417054
H 8.456946 -1.248872 -1.584796
H 7.948095 0.407503 2.355290
H 9.381444 -0.686761 0.648605
C -1.151372 -2.162710 3.338144
H -0.443841 -1.517702 3.880898
H -2.100857 -1.623062 3.228578
H -1.334645 -3.058068 3.951752
C 0.706330 -3.371667 2.195371
H 1.134149 -3.695672 1.235843
H 1.457827 -2.774310 2.732458
H 0.501515 -4.269920 2.797189
C -1.597532 -3.470490 1.259658
H -1.212149 -3.808783 0.286279
H -1.792961 -4.365575 1.869744
H -2.545363 -2.939687 1.108773

INT2S.log
Energy (E) = -3153.08040972 Hartree
Enthalpy (H) = -3152.276467 Hartree
Gibbs free energy (G) = -3152.411669 Hartree
Charge = 0, Spin = 1
C 1.782953 -0.935568 0.355591
C 2.276256 -0.368303 -2.451959
C 3.277296 -1.068993 -1.582383
H 1.756008 -1.958580 0.771136
H 1.630777 -0.252448 1.198317
H 3.191834 -2.169255 -1.636951
H 4.302603 -0.834207 -1.906524
C 0.646190 -0.777636 -0.669294
C -0.394985 -1.691870 -0.524295
C -2.121373 -0.014222 -1.898431
C -1.213740 0.921096 -2.523407
C 0.131572 0.790970 -2.665653
C 1.023596 -0.130015 -1.984689
H -1.661516 1.828545 -2.947645
H 0.635701 1.563956 -3.249990
H -2.003132 -1.027017 -2.285386
N 3.128770 -0.707170 -0.168960
S 3.959874 0.668163 0.303453
O 3.977538 1.705584 -0.725435
O 3.497053 0.988322 1.653116
C 2.787796 0.071595 -3.786595
H 3.416198 -0.710053 -4.241654
H 1.985545 0.298851 -4.496900
H 3.424800 0.967345 -3.684262
C -0.572710 -3.168195 -0.756598
C -3.543664 0.331622 -1.747771
C -3.994272 1.647561 -1.545227
C -4.521658 -0.674805 -1.847943
C -5.350792 1.942172 -1.465302
H -3.265212 2.448141 -1.422635
C -5.876357 -0.384259 -1.753220
H -4.201048 -1.705432 -2.008193
C -6.303993 0.929820 -1.563461
H -5.666363 2.974658 -1.311630
H -6.606780 -1.189155 -1.839648
H -7.366038 1.161758 -1.494859
Ni -1.200793 -0.198692 0.037783
P -2.871676 -0.729637 1.370772
O -2.539909 -0.871754 2.989380
O -4.197948 0.188871 1.546886
O -3.599605 -2.145322 1.035480
C -1.539708 -1.780798 3.400150
H -0.667895 -1.760312 2.724141
H -1.223400 -1.491303 4.408453
H -1.934509 -2.808130 3.428508
C -4.099223 1.553333 1.932613
H -3.537729 2.136944 1.190528
H -5.123746 1.934268 1.978763
H -3.621055 1.648296 2.916497
C -4.790103 -2.545150 1.709790
H -5.645253 -1.965175 1.343754
H -4.934809 -3.606557 1.485646

H -4.694529 -2.405145 2.794855
P -0.685405 1.885190 0.656921
O -1.466015 3.214759 0.101381
O -0.888045 2.298393 2.237581
O 0.882481 2.207427 0.397197
C -1.004451 3.993556 -0.989678
H -1.833869 4.132863 -1.694640
H -0.684985 4.976309 -0.618309
H -0.168208 3.514302 -1.515309
C -0.210434 1.501098 3.194957
H 0.815453 1.867561 3.343869
H -0.769508 1.566433 4.134574
H -0.166767 0.446070 2.885324
C 1.522884 3.392450 0.877373
H 0.837555 4.001230 1.481829
H 2.383687 3.081631 1.479103
H 1.876601 3.968369 0.014421
C 5.625047 0.032708 0.418184
C 6.596969 0.488971 -0.464714
C 5.921755 -0.889741 1.419262
C 7.897287 0.000906 -0.345840
H 6.329402 1.220780 -1.225225
C 7.221679 -1.366969 1.531338
H 5.138766 -1.220742 2.100174
C 8.207242 -0.922910 0.648253
H 8.669094 0.347994 -1.030800
H 7.469922 -2.085399 2.310819
H 9.224837 -1.299934 0.739600
C -0.624316 -3.908177 0.589618
H 0.272611 -3.719218 1.196339
H -1.509750 -3.607202 1.162859
H -0.683573 -4.992138 0.406265
C 0.602283 -3.705418 -1.582192
H 0.698628 -3.159666 -2.531600
H 1.551780 -3.613519 -1.035564
H 0.451014 -4.770808 -1.811103
C -1.875914 -3.471890 -1.504678
H -1.860240 -3.062936 -2.524646
H -1.995289 -4.562451 -1.588819
H -2.741625 -3.067766 -0.966817

INT2S'.log
Energy (E) = -3153.11664303 Hartree
Enthalpy (H) = -3152.311559 Hartree
Gibbs free energy (G) = -3152.447079 Hartree

Charge = 0, Spin = 1
C 2.599269 1.348797 0.975467
C 1.823414 -0.417489 2.980849
C 3.285157 -0.234890 2.712115
H 2.662838 2.147571 1.735501
H 2.944550 1.778746 0.032363
H 3.731499 0.428901 3.478435
H 3.812872 -1.195380 2.803959
C 1.202315 0.778734 0.898844
C 0.337852 0.921883 -0.127574
C -1.881302 1.464119 1.285336
C -1.697226 0.308616 2.139905
C -0.527389 -0.345256 2.434665
C 0.858046 0.004004 2.120430
H -2.598712 -0.173348 2.527216
H -0.646625 -1.241115 3.047281
H -1.058275 2.177524 1.282006
N 3.574966 0.331778 1.401915
S 4.269155 -0.622288 0.228932
O 4.921112 -1.731759 0.921512
O 3.361435 -0.903434 -0.880783
C 1.551367 -1.132265 4.272534
H 2.431873 -1.098228 4.930659
H 0.709089 -0.705053 4.830921
H 1.328012 -2.200908 4.105828
C 0.498719 1.879399 -1.319487
C -3.189789 2.146671 1.205552
C -4.377269 1.649307 1.764948
C -3.261572 3.384845 0.547644
C -5.575468 2.348019 1.654396
H -4.380672 0.695305 2.290481
C -4.457123 4.081645 0.427239
H -2.352003 3.801701 0.111931
C -5.629035 3.565718 0.979589
H -6.477487 1.936602 2.109041
H -4.473079 5.038552 -0.094302
H -6.567848 4.112269 0.897168
Ni -1.379262 -0.059643 -0.002585
P -3.397516 -0.599932 -0.707600
O -3.607287 -1.644987 -1.959456
O -4.364109 -1.365273 0.357870
O -4.237785 0.689011 -1.224902
C -3.075143 -1.306253 -3.230468
H -1.978031 -1.283271 -3.202187
H -3.392526 -2.089744 -3.924804
H -3.456058 -0.333362 -3.574178

C -5.268045 -2.421690 0.055364
H -4.737807 -3.271304 -0.390915
H -5.717251 -2.720520 1.007725
H -6.059432 -2.096671 -0.632219
C -5.622311 0.636594 -1.526810
H -6.203426 0.455975 -0.611400
H -5.896256 1.616487 -1.929026
H -5.840631 -0.142580 -2.272199
P -0.485326 -1.998189 -0.480892
O -1.407138 -3.297699 -0.093940
O -0.232421 -2.541677 -2.000391
O 0.905179 -2.286643 0.279838
C -1.812560 -3.466457 1.253847
H -2.417309 -2.615674 1.599947
H -2.417216 -4.378431 1.284938
H -0.943789 -3.588088 1.919111
C 0.717854 -1.874605 -2.821125
H 1.659500 -1.689892 -2.285526
H 0.904882 -2.531766 -3.676074
H 0.319762 -0.915530 -3.185341
C 1.626228 -3.506529 0.149460
H 2.210832 -3.507112 -0.778366
H 2.316710 -3.549696 0.998833
H 0.951922 -4.373405 0.163047
C 5.530610 0.465177 -0.416120
C 6.570232 0.855209 0.425730
C 5.475098 0.877609 -1.742366
C 7.569096 1.681436 -0.073539
H 6.589854 0.509499 1.458714
C 6.480046 1.710101 -2.232725
H 4.654059 0.543396 -2.374389
C 7.521968 2.110030 -1.401279
H 8.388502 1.992232 0.572447
H 6.447077 2.043617 -3.268628
H 8.305942 2.759398 -1.788243
C -0.740127 1.826257 -2.224797
H -0.841358 0.842597 -2.707775
H -1.664676 2.014446 -1.661569
H -0.660713 2.581583 -3.023081
C 1.719810 1.583654 -2.213704
H 2.651369 2.004353 -1.813693
H 1.884735 0.508532 -2.344136
H 1.572037 2.040081 -3.204913
C 0.614095 3.326451 -0.812590
H 1.488888 3.472692 -0.165468
H 0.706627 4.020148 -1.663441
H -0.274316 3.621514 -0.238222

TS2.log
Energy (E) = -3153.11962804 Hartree
Enthalpy (H) = -3152.288451 Hartree
Gibbs free energy (G) = -3152.423409 Hartree
Charge = 0, Spin = 1
Imaginary frequency: -291.1606
C 2.404610 1.413382 0.622104
C 1.751885 -0.196074 2.842630
C 3.190196 -0.003764 2.468655
H 2.594621 2.318866 1.229490
H 2.648757 1.674169 -0.410183
H 3.672022 0.748578 3.124817
H 3.738532 -0.944378 2.622041
C 0.973354 0.965670 0.795306
C -0.066076 1.253053 -0.034158
C -1.644539 1.741747 1.251208
C -1.769149 0.543457 2.079876
C -0.642631 -0.202859 2.356707
C 0.734347 0.209038 2.041930
H -2.733405 0.252293 2.497943
H -0.760935 -1.080803 2.990299
H -0.878535 2.434680 1.607259
N 3.354557 0.402290 1.084170
S 4.120198 -0.563401 -0.017564
O 4.625476 -1.729273 0.701261
O 3.291298 -0.724366 -1.208785
C 1.571985 -0.965554 4.115055
H 2.420155 -0.797324 4.795569
H 0.659219 -0.696925 4.658908
H 1.541224 -2.052634 3.918468
C -0.001856 2.053075 -1.335430
C -2.877066 2.535236 0.984309
C -4.174349 2.012655 1.061491
C -2.752190 3.916748 0.775292
C -5.289449 2.828708 0.906852
H -4.329632 0.951885 1.252707
C -3.861828 4.736368 0.604857
H -1.753693 4.356555 0.747957
C -5.142840 4.192685 0.664584
H -6.285619 2.391701 0.980165
H -3.724939 5.804043 0.436861
H -6.018703 4.827687 0.537881
Ni -1.454302 -0.246760 0.223792

P -3.374571 -0.843261 -0.617949
O -3.446523 -2.067705 -1.720765
O -4.403041 -1.509861 0.475118
O -4.282906 0.294910 -1.369829
C -2.845850 -1.847412 -2.985420
H -1.959125 -1.200168 -2.905166
H -2.532153 -2.820008 -3.376519
H -3.563643 -1.376581 -3.672534
C -5.175889 -2.687176 0.283401
H -4.533191 -3.541484 0.038270
H -5.694017 -2.871804 1.230149
H -5.916985 -2.565456 -0.517548
C -5.643423 0.090329 -1.697103
H -6.245478 -0.034858 -0.784740
H -5.984776 0.984677 -2.228192
H -5.775592 -0.790084 -2.343860
P -0.373868 -2.123962 -0.237790
O -1.180032 -3.438099 0.341495
O -0.180215 -2.856244 -1.696549
O 1.102373 -2.267402 0.436621
C -1.620370 -3.442587 1.683914
H -2.315356 -2.612329 1.883772
H -2.138804 -4.394358 1.841227
H -0.771089 -3.381695 2.383995
C 0.727591 -2.314037 -2.642295
H 1.516115 -1.712409 -2.170066
H 1.190586 -3.157844 -3.167119
H 0.189694 -1.697081 -3.377816
C 1.835797 -3.487590 0.392485
H 2.352342 -3.587591 -0.571080
H 2.588152 -3.431159 1.186130
H 1.177227 -4.352360 0.548755
C 5.522150 0.424631 -0.513973
C 6.606664 0.529193 0.354639
C 5.502307 1.087256 -1.736492
C 7.689918 1.319041 -0.011403
H 6.598793 -0.013251 1.299750
C 6.592893 1.878818 -2.092241
H 4.647673 0.968120 -2.400770
C 7.681554 1.994682 -1.232545
H 8.546911 1.404795 0.654643
H 6.591667 2.401089 -3.047554
H 8.533160 2.611458 -1.515742
C -1.380386 2.221331 -1.982102
H -1.867796 1.249210 -2.129577
H -2.062476 2.837731 -1.387256
H -1.266621 2.702459 -2.965326
C 0.846197 1.304805 -2.375821
H 1.858364 1.051115 -2.042673
H 0.354745 0.360326 -2.644269
H 0.925277 1.912652 -3.290415
C 0.578768 3.457986 -1.106175
H 1.635502 3.444228 -0.811561
H 0.503718 4.051511 -2.030076
H 0.024707 3.996058 -0.324632

INT3.log
Energy (E) = -3153.16190781 Hartree
Enthalpy (H) = -3152.354793 Hartree
Gibbs free energy (G) = -3152.489921 Hartree
Charge = 0, Spin = 1
C 2.178093 1.011828 -0.066653
C 1.812744 -0.454709 2.302779
C 3.120227 -0.493784 1.571494
H 2.753298 1.830893 0.418029
H 2.168636 1.210492 -1.136562
H 3.856190 0.233726 1.981427
H 3.555444 -1.498572 1.680083
C 0.800867 0.980449 0.551683
C -0.234339 1.789070 0.168647
C -1.288138 1.973945 1.295735
C -1.701454 0.614230 1.829361
C -0.641232 -0.221085 2.197163
C 0.714599 0.125253 1.755293
H -2.652199 0.555899 2.364805
H -0.761925 -0.983251 2.968913
H -0.684030 2.422043 2.111604
N 2.883552 -0.248776 0.152423
S 4.131160 -0.593255 -0.900333
O 4.642862 -1.902049 -0.513317
O 3.612793 -0.349998 -2.241850
C 1.803901 -1.250113 3.568021
H 2.761887 -1.137087 4.098598
H 1.009353 -0.942108 4.257122
H 1.674471 -2.324964 3.357606
C -0.242429 2.530166 -1.192759
C -2.438266 2.947334 1.174605
C -3.738848 2.566674 0.838675
C -2.212335 4.288550 1.503637
C -4.762145 3.508830 0.767035
H -3.958140 1.523106 0.620781

C -3.228298 5.235989 1.432250
H -1.208338 4.594837 1.807379
C -4.511035 4.849611 1.049022
H -5.768709 3.188986 0.495859
H -3.020714 6.275688 1.683584
H -5.313639 5.583985 0.992405
Ni -1.496223 -0.942442 0.530188
P -3.240048 -0.870393 -0.682495
O -3.729912 -2.078305 -1.694038
O -4.596952 -0.836533 0.228930
O -3.370256 0.433487 -1.665772
C -2.856346 -2.441426 -2.755865
H -1.905950 -2.837927 -2.373138
H -3.363642 -3.222618 -3.329662
H -2.658384 -1.581260 -3.414110
C -5.824003 -1.485779 -0.076478
H -5.688508 -2.572649 -0.128713
H -6.511882 -1.237816 0.737937
H -6.246376 -1.139471 -1.028908
C -4.560893 0.770699 -2.356055
H -5.352255 1.051775 -1.645860
H -4.330317 1.635723 -2.987538
H -4.908456 -0.060656 -2.986201
P -0.495061 -2.823299 0.205003
O -1.445775 -4.151206 0.364287
O 0.081793 -3.294907 -1.252113
O 0.760567 -3.157789 1.198625
C -2.356740 -4.136692 1.450624
H -3.046410 -3.280239 1.381870
H -2.928441 -5.068028 1.399684
H -1.828344 -4.090601 2.415588
C 0.982879 -2.396086 -1.891503
H 1.935351 -2.341790 -1.349108
H 1.161358 -2.781172 -2.899240
H 0.555242 -1.382603 -1.956087
C 1.547864 -4.332553 1.027281
H 2.265229 -4.197201 0.207481
H 2.097758 -4.486072 1.962384
H 0.918568 -5.208289 0.822644
C 5.405275 0.613327 -0.582194
C 6.375108 0.341592 0.380980
C 5.375888 1.829090 -1.263491
C 7.331779 1.311327 0.666788
H 6.386654 -0.627528 0.877662
C 6.337156 2.790819 -0.967709
H 4.622152 2.002945 -2.030261
C 7.310513 2.532772 -0.003985
H 8.100769 1.108992 1.410386
H 6.330958 3.741527 -1.498113
H 8.062824 3.287183 0.221055
C -1.557316 3.238917 -1.557615
H -2.417241 2.564043 -1.487111
H -1.757473 4.131499 -0.955928
H -1.477470 3.569181 -2.604138
C -0.056971 1.513544 -2.340705
H 0.825792 0.870540 -2.266840
H -0.940124 0.858408 -2.389165
H 0.015592 2.050519 -3.298541
C 0.838814 3.624992 -1.229366
H 1.865060 3.248601 -1.146369
H 0.770969 4.183141 -2.175584
H 0.682375 4.343141 -0.410435

INT1c.log
Energy (E) = -3153.08844875 Hartree
Enthalpy (H) = -3152.284256 Hartree
Gibbs free energy (G) = -3152.425906 Hartree
Charge = 0, Spin = 1
C -2.151540 0.062470 0.777320
C -1.937472 3.382857 -0.426528
C -2.769317 2.496969 0.476255
H -2.636335 -0.055552 1.768485
H -2.311093 -0.873813 0.226605
H -2.360208 2.491503 1.500654
H -3.782268 2.925777 0.544910
C -0.698647 0.279317 0.988520
C 0.267076 0.748193 1.680017
C 1.792273 2.488221 -1.421917
C 0.898356 1.871350 -2.216483
C -0.509833 2.244557 -2.308322
C -1.195117 2.856557 -1.366881
H 1.212293 1.065878 -2.884692
H -1.031634 1.983771 -3.234774
H 1.433395 3.329491 -0.819408
N -2.831849 1.118612 0.028420
S -4.030030 0.663992 -1.029352
O -4.720307 1.887209 -1.419392
O -3.467370 -0.233275 -2.028450
C -2.072976 4.858365 -0.185056
H -1.822696 5.112630 0.857276
H -1.416543 5.436792 -0.843974

H -3.110479 5.182895 -0.357285
C 0.676532 1.656744 2.799975
C 3.221676 2.213697 -1.327531
C 3.835748 1.109658 -1.942110
C 4.041575 3.108862 -0.622808
C 5.210528 0.929062 -1.880148
H 3.223718 0.380988 -2.473653
C 5.420625 2.929295 -0.558009
H 3.581679 3.968286 -0.131160
C 6.014365 1.841967 -1.194757
H 5.659581 0.061352 -2.364002
H 6.034037 3.646242 -0.013012
H 7.093530 1.699893 -1.150941
Ni 0.918910 -0.536856 0.399886
P 2.780782 -1.491311 0.948888
O 3.941546 -0.964203 1.997841
O 2.392075 -2.845043 1.794809
O 3.679847 -2.179524 -0.218973
C 4.761000 0.111538 1.569241
H 4.211657 0.812247 0.920903
H 5.107518 0.645290 2.461009
H 5.627813 -0.268644 1.009439
C 1.725656 -2.692679 3.036030
H 0.884007 -1.985337 2.951764
H 1.341612 -3.678128 3.319509
H 2.421352 -2.336184 3.808179
C 4.679862 -3.147571 0.074305
H 4.217455 -4.124791 0.258224
H 5.331737 -3.204752 -0.803957
H 5.269970 -2.857812 0.953660
P 0.140825 -1.781664 -1.191085
O 0.977260 -3.010744 -1.908359
O -1.154604 -2.690728 -0.753438
O -0.476781 -0.989866 -2.453208
C 2.069272 -2.659410 -2.740929
H 2.619837 -1.794628 -2.344733
H 2.752718 -3.514690 -2.768709
H 1.718324 -2.437579 -3.759535
C -1.041269 -3.462033 0.430812
H -0.833656 -2.817743 1.300535
H -2.001919 -3.966908 0.576553
H -0.243904 -4.213220 0.340510
C -1.242318 -1.653758 -3.460184
H -2.221111 -1.936661 -3.062037
H -1.380631 -0.929671 -4.268609
H -0.713772 -2.541276 -3.832868
C -5.141794 -0.320059 -0.034419
C -5.032923 -1.708166 -0.051464
C -6.070467 0.328121 0.776878
C -5.874178 -2.459957 0.764610
H -4.302478 -2.182388 -0.707056
C -6.906826 -0.433565 1.586832
H -6.147562 1.414533 0.752099
C -6.807152 -1.824437 1.581515
H -5.804539 -3.546713 0.756821
H -7.644569 0.059182 2.218041
H -7.465954 -2.416790 2.214807
C -0.226858 1.376428 4.005819
H 0.021048 2.050290 4.840241
H -1.286623 1.523621 3.752262
H -0.104633 0.341536 4.356682
C 2.135493 1.472808 3.200573
H 2.357030 0.436850 3.489742
H 2.795906 1.734366 2.362214
H 2.381427 2.129721 4.048590
C 0.489322 3.109432 2.347162
H -0.558170 3.324090 2.097404
H 0.799854 3.796871 3.148723
H 1.095730 3.321985 1.454858

TS1c.log
Energy (E) = -3153.07352696 Hartree
Enthalpy (H) = -3152.255211 Hartree
Gibbs free energy (G) = -3152.393305 Hartree
Charge = 0, Spin = 1
Imaginary frequency: -442.4587
C -1.995977 0.584583 0.925496
C -1.732367 3.212796 -0.603418
C -2.708944 2.904379 0.500012
H -2.033139 0.491445 2.024672
H -2.217819 -0.407571 0.514599
H -2.312452 3.135956 1.504636
H -3.620064 3.503043 0.375479
C -0.590272 0.999419 0.542558
C 0.478864 1.294243 1.245429
C 2.110177 1.843788 -1.262549
C 1.162476 1.459828 -2.173882
C -0.199847 1.832670 -2.115344
C -0.863700 2.293581 -1.014164
H 1.461207 0.826077 -3.013139
H -0.838050 1.526013 -2.948099

H 1.834421 2.622467 -0.552399
N -3.080238 1.488573 0.531417
S -4.025909 0.964563 -0.762966
O -4.884107 2.093407 -1.109380
O -3.244010 0.290831 -1.796362
C -1.839866 4.573290 -1.226166
H -1.705063 5.368608 -0.473286
H -1.086973 4.714676 -2.009680
H -2.839228 4.715768 -1.667652
C 0.992954 2.239495 2.291625
C 3.536832 1.550472 -1.348266
C 4.050705 0.435991 -2.030996
C 4.452284 2.438260 -0.759572
C 5.419632 0.224014 -2.125193
H 3.360260 -0.280023 -2.477645
C 5.824309 2.227226 -0.851781
H 4.071569 3.315204 -0.231908
C 6.316392 1.116937 -1.535174
H 5.792890 -0.651661 -2.655642
H 6.512439 2.935613 -0.391439
H 7.389609 0.946505 -1.608169
Ni 0.923139 -0.234679 0.226044
P 2.463448 -1.461399 1.134231
O 3.677529 -1.038899 2.172337
O 1.737043 -2.517203 2.165538
O 3.216482 -2.530236 0.167725
C 4.766763 -0.300396 1.638625
H 4.439785 0.401683 0.858641
H 5.220019 0.264342 2.460496
H 5.513916 -0.981075 1.205404
C 1.117671 -1.995339 3.327153
H 0.417712 -1.181870 3.070495
H 0.562860 -2.815937 3.793919
H 1.868659 -1.614192 4.033208
C 3.892652 -3.668867 0.686870
H 3.167748 -4.448678 0.950727
H 4.556031 -4.031543 -0.105346
H 4.484839 -3.411718 1.575061
P -0.049841 -1.685486 -1.085458
O 0.609459 -3.149716 -1.474478
O -1.451715 -2.300489 -0.485097
O -0.570399 -1.149065 -2.513779
C 1.718435 -3.152993 -2.355619
H 2.405063 -2.320414 -2.145945
H 2.260914 -4.091541 -2.199553
H 1.376878 -3.094822 -3.399643
C -1.401566 -2.994603 0.751561
H -0.947319 -2.370583 1.536234
H -2.436291 -3.224905 1.030007
H -0.824279 -3.923824 0.656896
C -1.496009 -1.876034 -3.319273
H -2.517162 -1.601489 -3.030899
H -1.315834 -1.574685 -4.356253
H -1.348804 -2.959442 -3.218179
C -5.012269 -0.294300 0.029942
C -4.716717 -1.635887 -0.190544
C -6.073233 0.098444 0.842430
C -5.504206 -2.605975 0.426967
H -3.878299 -1.906493 -0.832842
C -6.853012 -0.878608 1.450196
H -6.282161 1.157931 0.983527
C -6.567695 -2.228767 1.242968
H -5.287527 -3.660873 0.262445
H -7.689613 -0.587678 2.083316
H -7.182780 -2.991093 1.719168
C 0.136433 2.033462 3.551041
H 0.473809 2.710258 4.350913
H -0.924638 2.244969 3.356216
H 0.218168 1.002944 3.924943
C 2.456507 1.997147 2.642531
H 2.614418 0.983569 3.034618
H 3.098932 2.114910 1.758113
H 2.788299 2.718126 3.404843
C 0.827224 3.695385 1.832630
H -0.208809 3.920476 1.548051
H 1.116175 4.372175 2.650793
H 1.463887 3.929714 0.968413

INT2c.log
Energy (E) = -3153.16576955 Hartree
Enthalpy (H) = -3152.358524 Hartree
Gibbs free energy (G) = -3152.493088 Hartree
Charge = 0, Spin = 1
C -1.782303 0.348282 0.069287
C -1.599020 1.649882 2.553625
C -2.707760 1.967799 1.606743
H -2.084781 -0.452468 -0.602716
H -1.407492 1.172142 -0.567900
H -3.618629 2.224974 2.164098
H -2.444080 2.855911 0.988223
C -0.708253 -0.116992 1.049660

C -0.001826 -1.354397 0.876696
C 0.846252 -1.844019 2.081341
C 0.920316 -0.894494 3.242622
C 0.227166 0.242323 3.340384
C -0.724843 0.641730 2.322784
H 1.593521 -1.195107 4.048315
H 0.327409 0.850724 4.238160
H 0.350606 -2.752579 2.474905
N -2.994468 0.806223 0.763868
S -4.280206 1.081351 -0.297565
O -5.333596 1.710221 0.490984
O -3.818951 1.713434 -1.533895
C -1.557991 2.567360 3.737120
H -2.198494 2.217069 4.562403
H -0.546125 2.713802 4.132934
H -1.938691 3.560115 3.450783
C -0.605509 -2.524129 0.024003
C 2.294304 -2.244565 1.806935
C 3.221729 -1.279914 1.402146
C 2.769580 -3.524413 2.098308
C 4.567640 -1.590922 1.240636
H 2.870751 -0.258981 1.220260
C 4.117324 -3.847152 1.941192
H 2.073839 -4.288784 2.448370
C 5.021709 -2.882360 1.504846
H 5.263724 -0.821444 0.905767
H 4.460380 -4.856382 2.167032
H 6.075136 -3.131427 1.382022
Ni 0.974760 0.211261 -0.020299
P 2.282361 -0.149381 -1.724082
O 2.546215 -1.524746 -2.606014
O 1.865571 0.781536 -3.007997
O 3.801171 0.399846 -1.503595
C 3.179717 -2.621291 -1.966345
H 2.889978 -2.702368 -0.908300
H 2.879448 -3.531977 -2.495873
H 4.273456 -2.512351 -2.014405
C 0.571306 0.635082 -3.570951
H -0.213206 0.769336 -2.810741
H 0.462532 1.418513 -4.327578
H 0.464620 -0.348984 -4.048260
C 4.684563 0.609338 -2.599124
H 4.459667 1.566616 -3.085949
H 5.699911 0.633066 -2.190118
H 4.602010 -0.198655 -3.337915
P 1.226816 2.376919 -0.025882
O 2.728466 3.053205 -0.089484
O 0.596609 3.099916 -1.342176
O 0.549962 3.235164 1.188019
C 3.663767 2.637630 0.894912
H 4.059353 1.642656 0.650328
H 4.482959 3.363535 0.885481
H 3.212940 2.621791 1.899610
C 1.313589 3.897850 -2.273198
H 2.128378 3.320234 -2.729933
H 0.591901 4.189781 -3.043046
H 1.726033 4.796923 -1.797412
C 0.514155 4.653937 1.153369
H -0.088109 5.004202 0.303993
H 0.047737 4.983633 2.087294
H 1.527232 5.075000 1.084561
C -4.770618 -0.584646 -0.693097
C -4.464486 -1.110550 -1.943384
C -5.468307 -1.319907 0.262489
C -4.860391 -2.413003 -2.239687
H -3.930561 -0.497508 -2.668515
C -5.860122 -2.617495 -0.045221
H -5.695468 -0.872246 1.228850
C -5.555034 -3.161910 -1.293276
H -4.627320 -2.840687 -3.213555
H -6.406968 -3.206475 0.689157
H -5.864653 -4.179132 -1.529217
C -0.674398 -2.273812 -1.493029
H -1.302651 -3.048511 -1.960289
H -1.079178 -1.304242 -1.798100
H 0.326276 -2.350591 -1.939073
C 0.188900 -3.835954 0.127415
H 1.240424 -3.716700 -0.156474
H 0.150855 -4.286569 1.127049
H -0.255724 -4.568099 -0.562308
C -1.999975 -2.849431 0.592299
H -2.725833 -2.038067 0.466749
H -2.416193 -3.745588 0.106087
H -1.933930 -3.055409 1.671314

SM2.log
Energy (E) = -1689.11735315 Hartree
Enthalpy (H) = -1688.540229 Hartree
Gibbs free energy (G) = -1688.641669 Hartree
Charge = 0, Spin = 1
C -1.046566 0.249193 -1.108299

C -1.149683 -1.137947 1.875701
C -2.015445 -0.064004 1.244830
H -1.130992 1.079396 -1.828357
H -0.000500 -0.095572 -1.132040
H -2.895021 -0.517804 0.765134
H -2.392715 0.608190 2.024381
C -1.918006 -0.843776 -1.501875
C -2.603011 -1.798457 -1.791663
C 3.198391 -2.029691 -0.217434
C 2.169103 -1.558334 0.511377
C 0.856058 -2.174735 0.536002
C -0.160458 -1.684806 1.217143
H 2.274175 -0.645425 1.101171
H 0.699887 -3.061204 -0.090528
H 3.054754 -2.961562 -0.774405
N -1.388714 0.783826 0.228518
S -0.310153 1.945700 0.780177
O -0.693108 2.236748 2.156104
O 1.066974 1.580495 0.456314
C -1.493083 -1.565787 3.294132
H -0.861429 -2.438616 3.521343
C -3.409603 -2.991770 -2.074647
C 4.519390 -1.419228 -0.333528
C 4.779972 -0.099905 0.071458
C 5.574513 -2.163792 -0.879497
C 6.054944 0.437347 -0.043393
H 3.969644 0.516736 0.460480
C 6.851379 -1.625168 -0.995493
H 5.384446 -3.186567 -1.208647
C 7.098701 -0.321728 -0.573478
H 6.235417 1.463291 0.275247
H 7.656119 -2.225888 -1.417503
H 8.096373 0.105275 -0.664012
C -2.563097 -3.994645 -2.865536
H -1.665765 -4.281724 -2.300930
H -3.149546 -4.902166 -3.069107
H -2.240994 -3.569818 -3.825356
C -3.825527 -3.613072 -0.735870
H -2.942755 -3.882782 -0.139250
H -4.434847 -2.912271 -0.147958
H -4.419326 -4.522061 -0.910082
C -4.653667 -2.610244 -2.881640
H -4.377048 -2.158037 -3.843170
H -5.259667 -3.505201 -3.083545
H -5.274688 -1.890207 -2.332493
C -2.954371 -1.997331 3.404170
H -3.164437 -2.386340 4.409713
H -3.639938 -1.153860 3.234914
H -3.198975 -2.784410 2.677510
C -1.162864 -0.468283 4.303443
H -1.762311 0.437484 4.137246
H -1.364959 -0.818834 5.325200
H -0.107941 -0.173707 4.239393
C -0.730706 3.345543 -0.242035
C 0.127768 3.736071 -1.263477
C -1.918846 4.024844 0.016416
C -0.217899 4.833606 -2.048904
H 1.054193 3.188069 -1.426656
C -2.252130 5.119218 -0.771627
H -2.563802 3.698199 0.830848
C -1.402939 5.521084 -1.803125
H 0.444135 5.152585 -2.851852
H -3.174770 5.663854 -0.579654
H -1.668109 6.379833 -2.417724

NiF2.log
Energy (E) = -368.913242634 Hartree
Enthalpy (H) = -368.905041 Hartree
Gibbs free energy (G) = -368.935754 Hartree
Charge = 0, Spin = 1
Ni -0.000000 -0.000000 0.361995
F 0.000000 1.416530 -0.563103
F -0.000000 -1.416530 -0.563103

INT4.log
Energy (E) = -2058.07998550 Hartree
Enthalpy (H) = -2057.492504 Hartree
Gibbs free energy (G) = -2057.607412 Hartree
Charge = 0, Spin = 1
C 2.751106 -0.050416 -1.247381
C 1.428780 1.443697 1.580012
C 2.594517 0.547451 1.215526
H 3.830721 -0.253741 -1.355424
H 2.232770 -0.738611 -1.929994
H 3.457571 1.158506 0.907055
H 2.908289 -0.019127 2.104889
C 2.464206 1.328013 -1.625910
C 2.254350 2.487430 -1.906292
C -2.753600 0.123323 -0.612171
C -1.775090 0.439798 0.345299

C -0.750778 1.445469 0.122618
C 0.349597 1.446759 0.846265
H -1.617388 -0.233609 1.190312
H -0.893267 2.148336 -0.701620
H -2.781639 0.756448 -1.503375
N 2.334522 -0.375938 0.120813
S 1.371581 -1.710859 0.362587
O 1.123142 -1.765229 1.798123
O 0.263405 -1.713741 -0.587513
C 1.513850 2.239538 2.870516
C 1.968678 3.895781 -2.210967
Ni -3.510066 1.426284 0.768317
F -3.361288 2.763566 -0.372230
F -3.872183 0.318951 2.078174
H 0.710892 2.992284 2.834959
C 0.694131 3.993565 -3.056582
H -0.176132 3.593180 -2.520162
H 0.487295 5.045727 -3.299128
H 0.801666 3.437665 -3.997531
C 3.145897 4.498193 -2.985307
H 3.303857 3.972111 -3.936317
H 2.945217 5.556339 -3.206817
H 4.075067 4.438139 -2.402879
C 1.777550 4.653171 -0.891179
H 0.961938 4.220180 -0.294857
H 2.695777 4.622365 -0.288015
H 1.534809 5.705766 -1.096144
C 2.847828 2.968688 3.004075
H 2.836934 3.622434 3.886204
H 3.683463 2.265170 3.134396
H 3.061171 3.591855 2.124446
C 1.255257 1.326613 4.069000
H 2.024825 0.546024 4.157053
H 1.264873 1.906821 5.002085
H 0.283159 0.824722 3.982100
C -3.535954 -1.104712 -0.688308
C -4.438060 -1.236871 -1.754436
C -3.404321 -2.161044 0.225429
C -5.196184 -2.390832 -1.906478
H -4.542099 -0.415202 -2.464205
C -4.160212 -3.313500 0.070433
H -2.713265 -2.077526 1.061731
C -5.057666 -3.432428 -0.992035
H -5.894586 -2.478076 -2.737222
H -4.051303 -4.127673 0.784972
H -5.648633 -4.340283 -1.105701
C 2.436587 -3.068568 -0.091371
C 3.513066 -3.381160 0.736906
C 2.176825 -3.786020 -1.253989
C 4.348561 -4.434471 0.384894
H 3.681125 -2.810912 1.650349
C 3.021831 -4.839331 -1.597311
H 1.316396 -3.523147 -1.867073
C 4.103310 -5.160516 -0.781578
H 5.190209 -4.695068 1.024296
H 2.829860 -5.412279 -2.502794
H 4.759815 -5.986078 -1.051977

TS3.log
Energy (E) = -2058.04270415 Hartree
Enthalpy (H) = -2057.456438 Hartree
Gibbs free energy (G) = -2057.566125 Hartree
Charge = 0, Spin = 1
Imaginary frequency: -292.7518
C 2.737379 1.161564 -0.601838
C 0.597190 1.103494 1.517849
C 2.076560 0.972562 1.762175
H 3.602446 1.840479 -0.599224
H 2.849175 0.496466 -1.468853
H 2.549200 1.959208 1.918183
H 2.281877 0.375893 2.658788
C 1.499555 1.990553 -0.772009
C 1.079275 3.049969 -1.280141
C -2.844059 -0.663218 -0.949270
C -1.664447 -0.318734 -0.249997
C -0.881268 0.831039 -0.544216
C 0.162024 1.181994 0.255734
H -1.267431 -1.002832 0.502691
H -1.151898 1.439722 -1.407611
H -3.109082 -0.016769 -1.791096
N 2.775338 0.365204 0.624603
S 2.546938 -1.302130 0.437968
O 2.412551 -1.825269 1.791500
O 1.541537 -1.606072 -0.576645
C -0.344523 1.262423 2.693005
C 0.288029 4.229482 -1.631979
Ni -3.409373 0.522395 0.579954
F -3.601272 1.920546 -0.498815
F -3.388805 -0.637308 1.909366
H -1.345779 1.473669 2.279058
C -0.545102 3.977594 -2.893048

H -1.292786 3.189794 -2.731887
H -1.085832 4.895237 -3.163778
H 0.091464 3.690368 -3.740507
C 1.244570 5.408324 -1.875998
H 1.918259 5.206257 -2.719255
H 0.660929 6.310050 -2.110034
H 1.854959 5.614682 -0.986911
C -0.636646 4.561845 -0.446891
H -1.365514 3.760914 -0.262329
H -0.053935 4.723794 0.470511
H -1.192570 5.483712 -0.670879
C 0.066742 2.440540 3.575103
H -0.665436 2.592183 4.379586
H 1.041600 2.260582 4.053411
H 0.137137 3.373379 2.998157
C -0.434714 -0.027340 3.507549
H 0.534131 -0.293072 3.955039
H -1.163396 0.092368 4.320574
H -0.768332 -0.871214 2.891327
C -3.513216 -1.961669 -0.923130
C -4.472748 -2.221632 -1.913028
C -3.223366 -2.963334 0.016667
C -5.117417 -3.451061 -1.976418
H -4.709063 -1.442804 -2.639126
C -3.867239 -4.190082 -0.049286
H -2.516790 -2.767669 0.820231
C -4.813709 -4.440229 -1.044225
H -5.858072 -3.636595 -2.752799
H -3.636436 -4.957480 0.687789
H -5.316927 -5.405159 -1.087754
C 4.126047 -1.787683 -0.230751
C 5.256415 -1.698724 0.579201
C 4.192868 -2.275677 -1.531309
C 6.482757 -2.101715 0.065457
H 5.167159 -1.322298 1.597317
C 5.428734 -2.675623 -2.035877
H 3.283992 -2.347118 -2.126442
C 6.567660 -2.587513 -1.240463
H 7.375556 -2.041921 0.685426
H 5.498163 -3.061253 -3.051471
H 7.531190 -2.903285 -1.637541

INT5.log
Energy (E) = -2058.14273276 Hartree
Enthalpy (H) = -2057.553813 Hartree
Gibbs free energy (G) = -2057.659501 Hartree
Charge = 0, Spin = 1
C -2.195733 0.213215 -1.252790
C -0.329323 -1.750513 0.018053
C -1.612861 -2.148881 -0.692171
H -2.022586 0.066172 -2.330782
H -3.010015 0.943393 -1.162190
H -1.417391 -2.403463 -1.747568
H -2.069089 -3.035255 -0.236305
C -0.937330 0.594851 -0.555688
C -0.146457 1.605818 -0.118609
C 3.281377 -0.123820 0.526371
C 2.184472 0.446226 -0.137179
C 0.864766 0.637492 0.530363
C -0.105614 -0.434780 0.022754
H 2.158582 0.431991 -1.232081
H 0.966293 0.716349 1.622161
H 3.187780 -0.198439 1.614765
N -2.646578 -1.090981 -0.717264
S -3.564893 -0.947847 0.698384
O -3.696902 -2.300204 1.228543
O -3.083889 0.136863 1.550482
C 0.561736 -2.787595 0.639596
C -0.232273 3.097083 -0.093356
Ni 3.477254 1.920891 0.295346
F 2.987521 2.204917 1.960345
F 4.084924 1.963395 -1.351849
H 1.424017 -2.249546 1.073494
C -0.225437 3.551752 1.371990
H 0.708449 3.262413 1.874157
H -0.315609 4.646898 1.426649
H -1.068596 3.107734 1.921094
C -1.534278 3.532739 -0.762392
H -2.404545 3.114731 -0.233489
H -1.626524 4.627959 -0.745550
H -1.575947 3.208753 -1.813608
C 0.957414 3.725789 -0.825008
H 1.902985 3.530961 -0.293756
H 1.062875 3.343456 -1.850280
H 0.841344 4.818501 -0.871084
C 1.097784 -3.761802 -0.409223
H 1.797338 -4.477535 0.044202
H 0.282519 -4.344155 -0.865062
H 1.627626 -3.231981 -1.213868
C -0.144576 -3.530216 1.774246

H -0.992532 -4.124004 1.403705
H 0.548927 -4.222637 2.271091
H -0.537689 -2.832698 2.525162
C 4.374378 -0.895548 -0.055778
C 5.167833 -1.650283 0.821362
C 4.623446 -0.971869 -1.435671
C 6.175978 -2.475523 0.337419
H 4.980781 -1.587936 1.894083
C 5.633963 -1.791743 -1.914856
H 4.048849 -0.357254 -2.124908
C 6.409568 -2.547643 -1.033347
H 6.780515 -3.058867 1.029768
H 5.826276 -1.838614 -2.985387
H 7.200657 -3.189427 -1.418447
C -5.133065 -0.428076 0.027283
C -5.879622 -1.338458 -0.717406
C -5.591874 0.859665 0.283036
C -7.112118 -0.942136 -1.221834
H -5.494898 -2.342463 -0.890642
C -6.828816 1.246437 -0.229260
H -4.986344 1.536539 0.884187
C -7.584065 0.348734 -0.978849
H -7.709926 -1.642079 -1.803052
H -7.202949 2.250519 -0.037074
H -8.551278 0.653880 -1.375363

I.log
Energy (E) = -2058.04746784 Hartree
Enthalpy (H) = -2057.460677 Hartree
Gibbs free energy (G) = -2057.575006 Hartree
Charge = 0, Spin = 1
C -3.339909 0.064508 -1.415403
C -1.565043 -0.729880 1.567147
C -2.503544 0.272820 0.936755
H -4.245087 0.683275 -1.265950
H -2.979691 0.242908 -2.435919
H -3.546900 -0.058424 1.058493
H -2.428207 1.230408 1.480002
C -3.657278 -1.343563 -1.217101
C -3.881317 -2.506823 -0.966008
C 2.344393 -1.793807 -1.008255
C 1.342270 -1.332918 -0.227336
C 0.119486 -2.046607 0.059332
C -0.792206 -1.471746 0.821719
H 1.434301 -0.357813 0.254332
H -0.042083 -3.032975 -0.385179
H 2.304731 -2.809714 -1.408868
N -2.274291 0.474263 -0.491470
S -1.253516 1.711791 -0.943534
O -0.108061 1.660844 -0.044764
O -1.098076 1.614543 -2.388176
C -1.486977 -0.775863 3.083013
C -4.109714 -3.918636 -0.633805
Ni 4.912043 -0.023691 0.544233
F 6.311521 0.081878 1.610108
F 3.699789 -0.384905 1.775774
H -0.932849 -1.689323 3.347111
C -3.284866 -4.804461 -1.573319
H -2.213083 -4.581899 -1.485269
H -3.439865 -5.863814 -1.322728
H -3.578770 -4.650869 -2.620108
C -5.597583 -4.251096 -0.783329
H -5.937702 -4.086788 -1.814478
H -5.772652 -5.305930 -0.527067
H -6.210657 -3.628735 -0.117925
C -3.669954 -4.149790 0.817406
H -2.610060 -3.893732 0.958172
H -4.260952 -3.531676 1.507958
H -3.813671 -5.205465 1.089806
C -2.868062 -0.848079 3.728221
H -2.775126 -0.980488 4.814260
H -3.441953 0.076278 3.564110
H -3.456977 -1.688581 3.334254
C -0.685805 0.421186 3.595875
H -1.189664 1.372997 3.367550
H -0.571123 0.366584 4.687066
H 0.315323 0.451582 3.146183
C 3.548047 -1.035936 -1.257526
C 4.747857 -1.714040 -1.603518
C 3.575795 0.380395 -1.133868
C 5.945390 -1.031715 -1.606101
H 4.721277 -2.791844 -1.755156
C 4.783442 1.089957 -1.258850
H 2.646908 0.919922 -0.957796
C 5.983116 0.365824 -1.354645
H 6.881472 -1.569104 -1.743880
H 4.793603 2.173575 -1.169688
H 6.938006 0.882398 -1.307455
C -2.136543 3.219677 -0.583390
C -1.892126 3.888350 0.614268
C -3.085805 3.679667 -1.495291

C -2.624451 5.036306 0.905951
H -1.119470 3.521978 1.288972
C -3.811196 4.826892 -1.191228
H -3.230799 3.158824 -2.440945
C -3.583169 5.500691 0.008196
H -2.437824 5.573748 1.834056
H -4.548998 5.203010 -1.897852
H -4.150527 6.400814 0.239369

II.log
Energy (E) = -2058.07383488 Hartree
Enthalpy (H) = -2057.486975 Hartree
Gibbs free energy (G) = -2057.600134 Hartree
Charge = 0, Spin = 1
C -1.760424 0.687328 -1.096273
C 0.020832 -0.430008 1.792246
C -0.764833 0.707962 1.180684
H -2.540498 1.427342 -0.842520
H -1.476841 0.838110 -2.146311
H -1.842172 0.571400 1.364377
H -0.489409 1.646364 1.689526
C -2.305238 -0.669307 -0.947058
C -2.496025 -1.882972 -0.774212
C 4.282881 -1.817532 -0.201590
C 3.281760 -1.175376 0.429687
C 1.919430 -1.673990 0.471749
C 0.944078 -1.072784 1.123593
H 3.455473 -0.223536 0.935304
H 1.710233 -2.593167 -0.087441
H 4.059082 -2.780077 -0.673535
N -0.572657 0.850064 -0.266487
S 0.546024 1.984789 -0.798013
O 1.686588 1.884600 0.096886
O 0.659343 1.795664 -2.236883
C -0.316579 -0.790051 3.231916
C -2.466652 -3.356125 -0.711332
Ni -4.250382 -0.876742 -0.415199
F -4.960617 -1.583119 -1.840193
F -3.908541 -0.068386 1.106425
H 0.513365 -1.408505 3.607491
C -2.864753 -3.936489 -2.072398
H -2.169380 -3.610115 -2.856704
H -2.830440 -5.033574 -2.015169
H -3.875693 -3.620621 -2.353553
C -3.409662 -3.863776 0.383230
H -4.457933 -3.659706 0.124400
H -3.294121 -4.951482 0.485593
H -3.188698 -3.399313 1.354034
C -1.016526 -3.738217 -0.377378
H -0.326482 -3.372953 -1.150021
H -0.702386 -3.322949 0.590246
H -0.939725 -4.833484 -0.334461
C -1.596301 -1.625259 3.287490
H -1.865600 -1.853051 4.328720
H -2.447265 -1.100296 2.827235
H -1.459012 -2.580109 2.759750
C -0.434041 0.442362 4.126047
H -1.320933 1.042409 3.875004
H -0.539257 0.138461 5.176072
H 0.452604 1.086929 4.049125
C 5.667175 -1.368691 -0.316091
C 6.642330 -2.266657 -0.774153
C 6.071414 -0.062741 0.005202
C 7.975612 -1.886742 -0.887856
H 6.342638 -3.282114 -1.038349
C 7.402103 0.317359 -0.107642
H 5.330559 0.668787 0.326970
C 8.362915 -0.592248 -0.551412
H 8.714527 -2.604411 -1.242503
H 7.692824 1.337059 0.142581
H 9.404977 -0.289013 -0.642251
C -0.216339 3.574820 -0.520612
C 0.044148 4.260611 0.664339
C -1.083729 4.090002 -1.483256
C -0.591224 5.477775 0.892791
H 0.757276 3.853021 1.378974
C -1.713154 5.307111 -1.242391
H -1.237198 3.556636 -2.420252
C -1.471101 5.996070 -0.055080
H -0.390978 6.026866 1.811178
H -2.386459 5.723923 -1.989371
H -1.963761 6.949713 0.127494

III.log
Energy (E) = -2058.09031404 Hartree
Enthalpy (H) = -2057.502951 Hartree
Gibbs free energy (G) = -2057.613697 Hartree
Charge = 0, Spin = 1
C -0.075685 -1.376892 -2.002629
C 1.321083 -0.935584 1.215758

C	0.497176	-1.896964	0.386564
H	-0.251173	-2.415669	-2.342884
H	-0.767876	-0.725951	-2.551557
H	1.166593	-2.566004	-0.177664
H	-0.080816	-2.547684	1.062133
C	1.308142	-1.001498	-2.255306
C	2.480073	-0.719285	-2.378885
C	-0.780171	2.991099	-0.500931
C	-0.327283	2.027697	0.337413
C	0.943400	1.408492	0.112879
C	1.395687	0.323045	0.844164
H	-0.920298	1.649695	1.171200
H	1.553315	1.754799	-0.729467
H	-0.103108	3.338057	-1.288354
N	-0.390277	-1.241131	-0.570408
S	-1.994677	-1.081124	-0.135199
O	-2.002271	-0.664844	1.260876
O	-2.627371	-0.281907	-1.175277
C	1.990768	-1.482256	2.455869
C	3.909225	-0.405587	-2.508568
Ni	2.348974	1.745709	1.706667
F	3.666386	1.864200	0.540801
F	1.242749	1.806735	3.067568
H	2.726458	-0.730842	2.782780
C	4.099854	1.103828	-2.692703
H	3.773276	1.651404	-1.798661
H	5.166712	1.323124	-2.844442
H	3.546503	1.468017	-3.569584
C	4.473492	-1.156340	-3.719727
H	3.975258	-0.843967	-4.647678
H	5.547952	-0.945202	-3.818518
H	4.344369	-2.241759	-3.609897
C	4.622788	-0.859821	-1.228672
H	4.236251	-0.318594	-0.353562
H	4.496102	-1.941493	-1.074302
H	5.698588	-0.646950	-1.311204
C	2.731532	-2.790112	2.190411
H	3.283758	-3.099479	3.087464
H	2.039293	-3.608285	1.940990
H	3.453074	-2.689580	1.367676
C	0.955117	-1.632651	3.570621
H	0.181358	-2.370418	3.307069
H	1.437985	-1.980046	4.494363
H	0.462622	-0.672943	3.769335
C	-2.086987	3.617633	-0.473458
C	-2.323827	4.725478	-1.302627
C	-3.129151	3.154441	0.348187
C	-3.555696	5.367342	-1.300795
H	-1.522045	5.084280	-1.949374
C	-4.359105	3.795107	0.346841
H	-2.978964	2.276907	0.975679
C	-4.576150	4.904057	-0.473094
H	-3.721329	6.228941	-1.945600
H	-5.159968	3.424216	0.984380
H	-5.544733	5.401904	-0.470431
C	-2.685493	-2.723879	-0.203485
C	-2.748139	-3.487616	0.960430
C	-3.120427	-3.225231	-1.429609
C	-3.245572	-4.785831	0.887680
H	-2.436569	-3.053098	1.909429
C	-3.614596	-4.524480	-1.488415
H	-3.096061	-2.592699	-2.316014
C	-3.672883	-5.303155	-0.333417
H	-3.308370	-5.391038	1.790381
H	-3.965982	-4.926454	-2.437117
H	-4.064803	-6.317737	-0.384298