

Supporting Information

Primary phosphines and phosphine oxides with a stereogenic carbon center adjacent to the phosphorus atom: synthesis and anti-Markovnikov-radical addition to alkenes

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X-ray structure analysis: The single crystals of **7a** suitable for X-ray diffraction were obtained by slow diffusion of hexane into toluene solution of **7a**. Single-crystal X-ray diffraction experiment for **7a** was carried out at the BL02B1 of SPring-8 synchrotron. A wavelength of $\lambda = 0.41180 \text{ \AA}$ and a single crystal of $0.005 \times 0.01 \times 0.01 \text{ mm}^3$ were used. The crystal was selected from the grown fine tiny needles and was attached to the tip of a MiTeGen MicroMountTM. All frame images (Dectris) were collected at $-173 \text{ }^\circ\text{C}$ and converted to SFRM format by the *Henkankun-R*¹⁾. Data reduction was performed using Bruker SAINT. Structure was solved by direct methods (*SHELXT*)²⁾ and refined against F^2 by weighted full-matrix least-squares (*SHELXL*)³⁾. Crystal data and measurement descriptions are summarized Table S1.

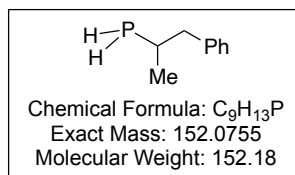
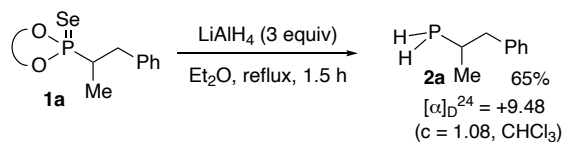
Table S1. Crystal data and structure refinement for (*S*_{ax}, *S*_p)-**7a**

Crystal data	
Chemical formula	C ₁₈ H ₃₁ OPSi
<i>M</i> _r	322.49
Crystal system, space group	Orthorhombic, <i>P</i> 2 ₁ 2 ₁ 2 ₁
Temperature (K)	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	6.4316 (6), 13.8703 (14), 20.916 (2)
<i>V</i> (Å ³)	1865.9 (3)
<i>Z</i>	4
Radiation type	Synchrotron, $\lambda = 0.4119 \text{ \AA}$
μ (mm ⁻¹)	0.06
Crystal size (mm)	0.01 × 0.01 × 0.01
Data collection	
Diffractometer	Dectris PILATUS-CdTe
Absorption correction	Empirical (using intensity measurements) <i>SADABS</i>
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	43417, 4209, 4145
<i>R</i> _{int}	0.046
($\sin \theta/\lambda$) _{max} (Å ⁻¹)	0.647
Refinement	

$R[F^2 > 2\sigma(F^2)],$ $wR(F^2), S$	0.022, 0.062, 1.03
No. of reflections	4209
No. of parameters	199
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\max}, \Delta\rho_{\min}$ (e Å ⁻³)	0.25, -0.20
Absolute structure	Flack x determined using 1756 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
Absolute structure parameter	0.05 (6)

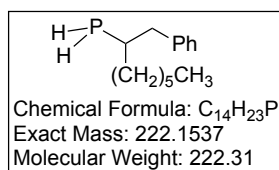
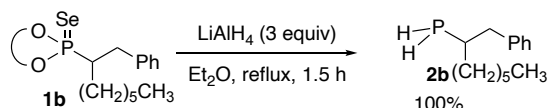
Experimental procedures and spectroscopic data

(1-Phenylprop-2-yl)phosphane (2a)



Et_2O (5 mL) and (*S*_{ax}, *S*)-phosphonoselenoate **1a** (858 mg, 1.7 mmol, dr = 5:95) was placed in a side-arm flask, degassed by *freeze-pump-thaw* cycle. The solution was cooled in ice bath. LiAlH_4 (228 mg, 6 mmol) was added, and the mixture was stirred at reflux temperature for 1.5 h. The resulting mixture was quenched with water (0.23 mL), sodium hydroxide 15% aqueous solution (0.23 mL) and water (0.7 mL). The solution was filtered through diatomite and washed with sodium hydroxide (5% aqueous solution) five times and hydrochloric acid (1M aqueous solution) two times. The washed solution was dried over Na_2SO_4 , filtered, and concentrated to give the primary phosphine **2a** (166 mg, 65%) as a colorless liquid; $[\alpha]_{\text{D}}^{24} = +9.48$ ($C = 0.108$, CHCl_3); IR (neat): 2338 cm^{-1} ; ^1H NMR (CDCl_3): δ 1.17 (dd, $^3J_{\text{P-H}} = 6.9 \text{ Hz}$, $J = 13.1 \text{ Hz}$, 3H, CH_3), 2.14-2.22 (m, 1H, PCH), 2.66-2.72 (m, 1H, CH_2Ph), 2.70 (ddd, $J = 6.4, 12.0 \text{ Hz}$, $^1J_{\text{P-H}} = 194.4 \text{ Hz}$, 1H, PH_2), 2.72 (ddd, $J = 5.6, 12.0 \text{ Hz}$, $^1J_{\text{P-H}} = 194.5 \text{ Hz}$, 1H, PH_2), 2.75-2.81 (m, 1H, CH_2Ph), 7.14-7.23 (m, 3H), 7.28-7.31 (m, 2H); ^{13}C NMR (CDCl_3): δ 22.3 (d, $^2J_{\text{C-P}} = 9.6 \text{ Hz}$), 24.4 (d, $^2J_{\text{C-P}} = 6.0 \text{ Hz}$), 45.6 (d, $^1J_{\text{C-P}} = 7.2 \text{ Hz}$), 126.2, 128.3, 129.0, 140.7 (d, $^3J_{\text{C-P}} = 6.0 \text{ Hz}$); ^{31}P NMR (CDCl_3): δ -111.8 (t, $^1J_{\text{P-H}} = 196.2 \text{ Hz}$); MS (EI) m/z 152 (M^+); HRMS Calcd for $\text{C}_9\text{H}_{13}\text{P}$: 152.0755, Found: 152.0741.

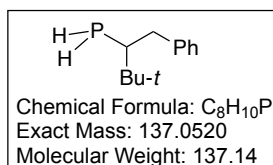
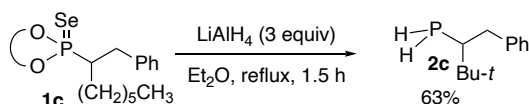
(1-Phenyloct-2-yl)phosphane (2b)



Et_2O (3 mL) and (*S*_{ax}, *S*)-phosphonoselenoate **1b** (189 mg, 0.33 mmol, dr = 5:95) was placed in a side-arm flask. LAH (57 mg, 1 mmol) was added, and the mixture was stirred at reflux temperature for 1.5 h. The resulting mixture was quenched with water (0.06 mL), sodium hydroxide 15% aqueous solution (0.06 mL) and water (0.18

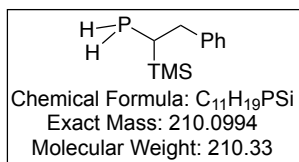
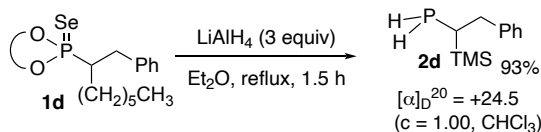
mL). The solution was filtered through diatomite and washed with sodium hydroxide (5% aqueous solution) five times and hydrochloric acid (1M aqueous solution) two times. The washed solution was dried over Na₂SO₄, filtered, and concentrated to give the primary phosphine **2b** (83 mg, 100%) as colorless liquid; IR (neat): 2342 cm⁻¹; ¹H NMR (CDCl₃): δ 0.88 (t, *J* = 7.1 Hz, 3H), 1.22-1.49 (m, 9H), 1.50-1.60 (m, 1H), 2.07-2.12 (m, 1H), 2.59 (ddd, *J* = 6.6, 12.1 Hz, ¹*J*_{P-H} = 195.3 Hz, 1H, PH₂), 2.66 (ddd, *J* = 5.3, 12.0 Hz, ¹*J*_{P-H} = 196.1 Hz, 1H, PH₂), 2.63-2.70 (m, 1H), 2.85-2.92 (m, 1H), 7.14-7.23 (m, 3H), 7.26-7.31 (m, 2H); ¹³C NMR (CDCl₃): δ 14.1, 22.6, 27.8 (d, *J*_{C-P} = 6.7 Hz), 29.2, 30.0 (d, *J*_{C-P} = 6.7 Hz), 31.7, 36.1 (d, *J*_{C-P} = 8.6 Hz), 43.9 (d, *J*_{C-P} = 6.7 Hz), 126.1, 128.2, 129.1, 140.6 (d, ³*J*_{C-P} = 4.8 Hz); ³¹P NMR (CDCl₃): δ -123.4 (t, ¹*J*_{P-H} = 185.3 Hz)

(3,3-Dimethyl-1-phenylbut-2-yl)phosphane (2c)



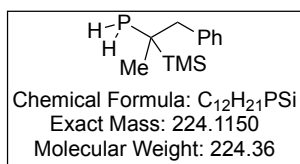
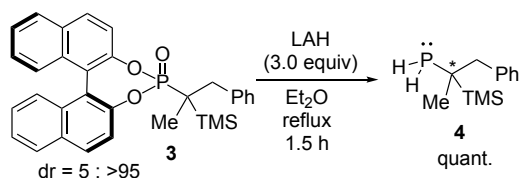
Et₂O (3 mL) and (*S*_{ax}, *S*)- phosphonoselenoate **1d** (135 mg, 0.25 mmol, dr = 72:28) was placed in a side-arm flask. LAH (30 mg, 0.75 mmol) was added, and the mixture was stirred at reflux temperature for 1.5 h. The resulting mixture was quenched with water (0.03 mL), sodium hydroxide 15% aqueous solution (0.03 mL) and water (0.09 mL). The solution was filtered through diatomite and washed with sodium hydroxide (5% aqueous solution) five times and hydrochloric acid (1M aqueous solution) two times. The washed solution was dried over Na₂SO₄, filtered, and concentrated to give the primary phosphine **2c** (30 mg, 63%) as colorless liquid; IR (neat): 2344 cm⁻¹; ¹H NMR (CDCl₃): δ 1.10 (s, 9H, C(CH₃)₃), 2.02-2.06 (m, 1H, PCH), 2.24-2.33 (m, 1H, CH₂Ph), 2.26 (ddd, *J* = 6.3, 12.3 Hz, ¹*J*_{P-H} = 198.8 Hz, 1H, PH₂), 2.46 (ddd, *J* = 5.1, 12.2 Hz, ¹*J*_{P-H} = 199.1 Hz, 1H, PH₂), 3.21-3.29 (m, 1H, CH₂Ph), 7.16-7.23 (m, 3H), 7.27-7.32 (m, 2H); ¹³C NMR (CDCl₃): δ 28.2 (d, ³*J*_{C-P} = 7.5 Hz), 33.6 (d, ²*J*_{C-P} = 9.4 Hz), 38.9 (d, ²*J*_{C-P} = 5.6 Hz), 42.3 (d, ¹*J*_{C-P} = 10.3 Hz), 126.0, 128.3, 129.1, 141.8; ³¹P NMR (CDCl₃): δ -145.9 (t, ¹*J*_{P-H} = 196.2 Hz)

(2-Phenyl-1-(trimethylsilyl)ethyl)phosphane (2d)



Et₂O (3 mL) and (*S*_{ax}, *S*)- phosphonoselenoate **1e** (284 mg, 0.50 mmol, dr = 90:10) was placed in a side-arm flask. LAH (57 mg, 1.5 mmol) was added, and the mixture was stirred at reflux temperature for 1.5 h. The resulting mixture was quenched with water (0.06 mL), sodium hydroxide 15% aqueous solution (0.06 mL) and water (0.18 mL). The solution was filtered through diatomite and washed with sodium hydroxide (5% aqueous solution) five times and hydrochloric acid (1M aqueous solution) two times. The washed solution was dried over Na₂SO₄, filtered, and concentrated to give the primary phosphine **2d** (98 mg, 93%) as colorless liquid; IR (neat): 2342 cm⁻¹; ¹H NMR (CDCl₃): δ 0.10 (s, 9H, Si(CH₃)₃), 1.13-1.21 (m, 1H, PCH), 2.47 (ddd, *J* = 7.2, 11.1, 14.0 Hz, 1H, CH₂Ph), 2.48 (ddd, *J* = 9.8, 11.7 Hz, ¹*J*_{P-H} = 195.5 Hz, 1H, PH₂), 2.61 (ddd, *J* = 5.1, 11.9 Hz, ¹*J*_{P-H} = 196.1 Hz, 1H, PH₂), 3.11-3.20 (m, 1H, CH₂Ph), 7.16-7.23 (m, 3H), 7.27-7.32 (m, 2H); ¹³C NMR (CDCl₃): δ -2.6 (d, ³*J*_{C-P} = 4.7 Hz), 14.9 (d, ¹*J*_{C-P} = 20.7 Hz), 38.7 (d, ²*J*_{C-P} = 4.7 Hz), 126.0, 128.2, 128.8, 141.6 (d, ³*J*_{C-P} = 2.8 Hz); ³¹P NMR (CDCl₃): δ -138.3 (t, ¹*J*_{P-H} = 196.2 Hz)

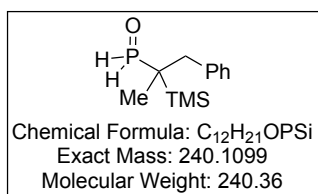
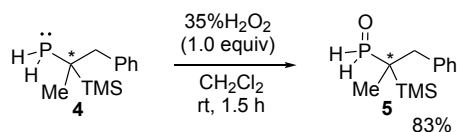
(1-Phenyl-2-(trimethylsilyl)prop-2-yl)phosphane (**4**)



Et₂O (3 mL) and phosphonate **3** (104 mg, 0.20 mmol) were placed in a 20 mL two-necked flask. LiAlH₄ (23 mg, 0.60 mmol, 3.0 equiv) was added, and the mixture was stirred at reflux temperature for 1.5 h. The resulting mixture was quenched at 0 °C with water (23 μL), sodium hydroxide 15% aqueous solution (23 μL), and water (69 μL). The solution was filtered through diatomite, and washed with sodium hydroxide (5% aqueous solution) five times. The washed solution was dried over MgSO₄, filtered, and concentrated to give the primary phosphane **4** (44 mg, quant) as a colorless liquid; IR (neat): 2961, 1603, 1494, 1453, 1409, 1261, 1099, 1022 cm⁻¹; ¹H NMR(CDCl₃):

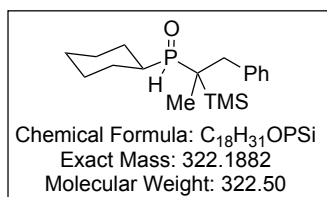
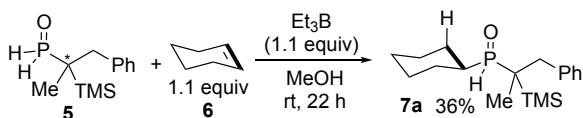
δ 0.11 (s, 9H), 1.16 (d, $J = 11.2$ Hz, 3H), 2.14-2.38 (m, 1H), 2.64-2.77 (m, 1H), 2.78-2.87 (m, 2H), 7.16-7.25 (m, 3H), 7.29-7.30 (m, 2H); ^{13}C NMR (CDCl_3): δ -3.6, -3.5, 1.4, 17.8 (d, $J_{\text{P-C1}} = 18.8$ Hz), 24.2 (d, $J_{\text{P-C2}} = 6.6$ Hz), 43.4 (d, $J_{\text{P-C3}} = 8.5$ Hz), 126.4, 127.7, 130.8, 137.7 (d, $J = 3.8$ Hz); ^{31}P NMR (CDCl_3): δ -110.8; MS (EI) m/z 224 (M^+); HRMS Calcd for $\text{C}_{12}\text{H}_{21}\text{PSi}$: 224.1150, Found: 224.1159.

(1-Phenyl-2-(trimethylsilyl)prop-2-yl)phosphine oxide (5)



To a 30 mL round-bottom flask were added (1-phenyl-2-(trimethylsilyl)propan-2-yl)phosphane (**4**) (224 mg, 1.0 mmol), CH_2Cl_2 (2.0 mL) and hydrogen peroxide (35% aqueous solution, 70 μL , 1.0 mmol, 1.0 equiv), and the mixture was stirred at room temperature for 1.5 h. After that, the mixture was filtered, washed with CH_2Cl_2 , and the filtrate was concentrated to give the (1-phenyl-2-(trimethylsilyl)propan-2-yl)phosphine oxide (**5**) (198 mg, 83%) as a colorless solid; mp : 81-83 $^{\circ}\text{C}$; IR (KBr): 2922, 2312, 1255, 1179, 1010, 915 cm^{-1} ; ^1H NMR(CDCl_3): δ 0.20 (s, 9H), 0.84 (d, $J = 25.1$ Hz, 3H), 2.71 (dd, $J = 13.5, 29.6$ Hz, 1H), 3.27 (dd, $J = 8.1, 13.9$ Hz, 1H), 6.39 (d, $J_{\text{P-H1}} = 458.7$ Hz, 1H), 6.49 (d, $J_{\text{P-H2}} = 453.7$ Hz, 1H), 7.18-7.21 (m, 3H), 7.24-7.26 (m, 2H); ^{13}C NMR (CDCl_3): δ -3.3, 1.1, 11.3 (d, $J_{\text{C-P1}} = 4.7$ Hz), 24.9 (d, $J_{\text{C-P2}} = 56.4$ Hz), 29.8, 35.8 (d, $J_{\text{C-P3}} = 2.8\text{Hz}$), 127.0, 128.4, 130.7, 134.9 (d, $J = 5.6$ Hz); ^{31}P NMR (CDCl_3): δ 20.0; MS (EI) m/z 240 (M^+); HRMS Calcd for $\text{C}_{12}\text{H}_{21}\text{OPSi}$: 240.1099, Found: 240.1080.

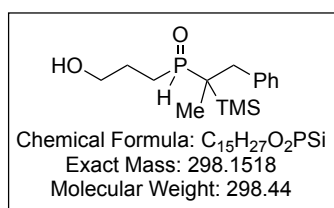
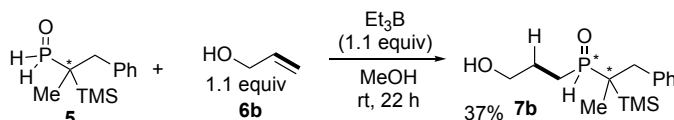
Cyclohexyl(1-phenyl-2-(trimethylsilyl)prop-2-yl)phosphine oxide (7a)



To a solution of (1-phenyl-2-(tmethylsilyl)propan-2-yl)phosphine oxide (**5**) (120 mg, 0.50 mmol) and cyclohexene (56 μL , 0.55 mmol) in methanol (2.5 mL) was added Et_3B (1.0 M, 0.55 mL, 0.55 mmol), at room

temperature in an open reaction vessel. The solution was stirred at room temperature for 22 h. The reaction mixture was concentrated on a rotary evaporator, and the solution was extracted with CH₂Cl₂ three times, and the combined organic layers were dried and concentrated to afford the crude phosphine oxide. The crude product was purified by column chromatography on Al₂O₃ (CH₂Cl₂:MeOH = 50:1, R_f = 0.20) to give the mixture (96 mg). The resulting oil was passed through GPC to give **7a** (58 mg, 36%, dr = 95 : 5) as a colorless solid; mp: 85-88 °C; IR (KBr): 2924, 2301, 1453, 1250, 1165, 956, 844, 757 cm⁻¹; ¹H NMR(CDCl₃): δ 0.11 (s, 8.4H), 0.16 (s, 0.6H), 0.98-1.05 (m, 2H), 1.12 (d, *J* = 19.8 Hz, 3H), 1.23-1.28 (m, 4H), 1.48-1.57 (m, 2H), 1.66-1.73 (m, 2H), 1.80-1.81 (m, 1H), 2.72 (dd, *J* = 13.5, 28.7 Hz, 0.06H), 2.90 (dd, *J* = 13.9, 21.3 Hz, 0.94H), 3.17 (dd, *J* = 7.2, 13.5 Hz, 1H), 6.32 (d, *J*_{P-H} = 436.2 Hz, 1H), 7.22-7.25 (m, 3H), 7.26-7.27 (m, 2H); ¹³C NMR (CDCl₃): δ -2.6, -2.3, 14.3, 25.8, 26.1, 26.3 (d, *J*_{C-P1} = 3.8 Hz), 26.4 (d, *J*_{C-P2} = 3.8 Hz), 29.1 (d, *J*_{C-P3} = 48.9 Hz), 29.8, 33.6 (d, *J*_{C-P4} = 59.4 Hz), 35.9 (d, *J*_{C-P5} = 2.9 Hz), 38.1, 126.8, 128.2, 130.8, 137.7 (d, *J* = 7.7 Hz); ³¹P NMR (CDCl₃): δ 54.0 (major), 55.8 (minor); MS (EI) *m/z* 322 (M⁺); HRMS Calcd for C₁₈H₃₁OPSi: 322.1882, Found: 322.1860.

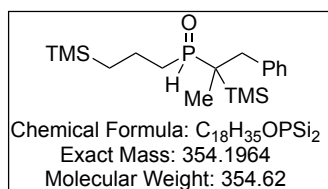
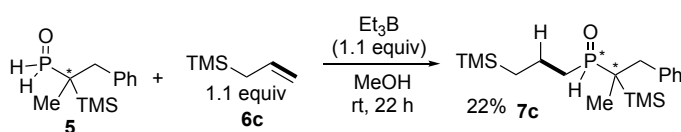
(2- Hydroxypropyl)(1-phenyl-2-(trimethylsilyl)prop-2-yl)phosphine oxide (**7b**)



To a solution of (1-phenyl-2-(trimethylsilyl)propan-2-yl)phosphine oxide (**5**) (120 mg, 0.50 mmol) and allyl alcohol (37 μl, 0.55 mmol) in methanol (2.5 mL) was added Et₃B (1.0 M, 0.55 mL, 0.55 mmol) at room temperature in an open reaction vessel. The solution was stirred at room temperature for 22 h. The reaction mixture was concentrated on a rotary evaporator, and the solution was extracted with CH₂Cl₂ three times, and the combined organic layers were dried and concentrated to afford the crude phosphine oxide. The crude product was purified by column chromatography on Al₂O₃ (CH₂Cl₂:MeOH = 50:1, R_f = 0.20) to give the mixture (98 mg). The resulting oil was passed through GPC to give **7b** (55 mg, 37%, dr = 81:19) as a colorless oil; IR (neat): 3343, 2925, 1454, 1252, 1164, 962, 843, 761 cm⁻¹; ¹H NMR(CDCl₃): δ 0.13 (s, 6.9H), 0.20 (s, 2.1H), 1.09 (d, *J* = 20.6 Hz, 3H), 1.21-1.43

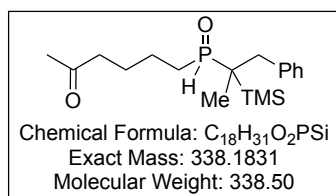
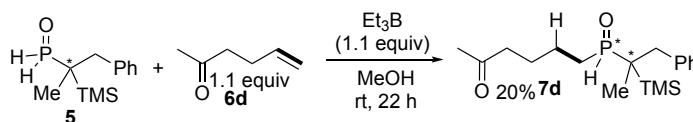
(m, 2H), 1.79-1.81 (m, 2H), 2.83 (dd, $J = 13.5, 22.9$ Hz, 1H), 3.13-3.18 (m, 1H), 3.55 (br, 2H), 4.64 (br, 1H), 6.50 (d, $J_{\text{P-H}} = 383.3$ Hz, 1H), 7.17-7.22 (m, 2H), 7.24-7.25 (m, 3H); ^{13}C NMR (CDCl_3): δ -2.6, -2.2, 14.1, 14.5, 21.9 (d, $J_{\text{P-C1}} = 60.4$ Hz), 27.0 (d, $J_{\text{P-C2}} = 14.4$ Hz), 35.7, 37.7, 62.7, 127.0, 128.3, 131.1, 137.2 (d, $J = 6.7$ Hz); ^{31}P NMR (CDCl_3): δ 48.7 (major), 50.8 (minor); MS (EI) m/z 298 (M^+); HRMS Calcd for $\text{C}_{15}\text{H}_{27}\text{O}_2\text{PSi}$: 298.1518, Found: 298.1505.

(1-Phenyl-2-(trimethylsilyl)prop-2-yl)(3-(trimethylsilyl)propyl)phosphine oxide (7c)



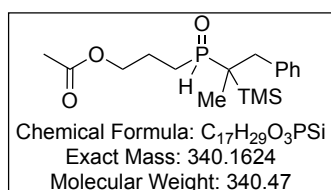
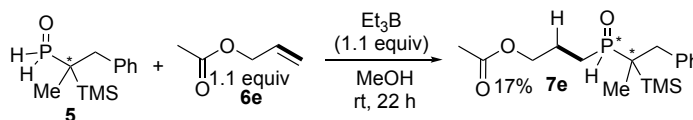
To a solution of (1-phenyl-2-(trimethylsilyl)prop-2-yl)phosphine oxide (**5**) (120 mg, 0.50 mmol) and allyltrimethylsilane (85 μL , 0.55 mmol) in methanol (2.5 mL) was added Et_3B in hexane (0.6 M, 1.1 mL, 0.65 mmol) at room temperature in an open reaction vessel. The solution was stirred at room temperature for 22 h. The reaction mixture was concentrated on a rotary evaporator, and the solution was extracted with CH_2Cl_2 three times, and the combined organic layers were dried and concentrated to afford the crude phosphine oxide. The crude product was purified by column chromatography on Al_2O_3 (CH_2Cl_2 : $\text{MeOH} = 50 : 1$, $R_f = 0.20$) to give the mixture (111 mg). The resulting solid was passed through GPC to give **7c** (39 mg, 22%, dr = 7:22) as a colorless oil; IR (neat): 3369, 3029, 2953, 2309, 1603, 1455, 1174, 840 cm^{-1} ; ^1H NMR(CDCl_3): δ -0.07 (s, 9H), 0.14 (s, 9H), 0.44-0.52 (m, 1H), 0.55-0.88 (m, 1H), 1.08 (d, $J = 20.6$ Hz, 3H), 1.15-1.47 (m, 3H), 1.62-1.75 (m, 1H), 2.71 (dd, $J = 13.9, 29.2$ Hz, 0.27H), 2.87 (dd, $J = 13.9, 22.4$ Hz, 0.73H), 3.15 (dd, $J = 7.6, 13.9$ Hz, 0.73H), 3.27 (dd, $J = 7.6, 13.9$ Hz, 0.27H), 6.57 (d, $J_{\text{P-H}} = 453.3$ Hz, 1H), 7.21-7.23 (m, 2H), 7.27-7.37 (m, 3H); ^{13}C NMR (CDCl_3): δ -2.7, -2.6, -2.2, -1.7, -0.7, -0.5, 14.1, 14.5, 18.4, 28.2 (d, $J_{\text{P-C1}} = 58.2$ Hz), 35.7 (d, $J_{\text{P-C2}} = 16.0$ Hz), 37.7, 126.9, 128.2, 131.0, 137.5 (d, $J = 7.5$ Hz); ^{31}P NMR (CDCl_3): δ 46.2 (major), 47.8 (minor); MS (EI) m/z 354 (M^+); HRMS Calcd for $\text{C}_{18}\text{H}_{35}\text{OPSi}_2$: 354.1964, Found: 354.1964.

6-((1-Phenyl-2-(trimethylsilyl)prop-2-yl)hydrophosphoryl)hexan-2-one (7d)



To a solution of (1-phenyl-2-(trimethylsilyl)propan-2-yl)phosphine oxide (**5**) (120 mg, 0.50 mmol) and 5-hexen-2-one (64 μ L, 0.55 mmol) in methanol (2.5 mL) was added Et₃B in hexane (1.0 M, 0.55 mL, 0.55 mmol) at room temperature in an open reaction vessel. The solution was stirred at room temperature for 22 h. The reaction mixture was concentrated on a rotary evaporator, and the solution was extracted with CH₂Cl₂ three times, and the combined organic layers were dried and concentrated to afford the crude phosphine oxide. The crude product was purified by column chromatography on Al₂O₃ (CH₂Cl₂:MeOH = 50:1, R_f = 0.20) to give the mixture (120 mg). The resulting oil was passed through GPC to give **7d** (34 mg, 20%, dr = 81:19) as a colorless oil; IR (neat): 2953, 2309, 1714, 1455, 1360, 1252, 1171 cm⁻¹; ¹H NMR(CDCl₃): δ 0.14 (s, 7.4H), 0.21 (s, 1.6H), 1.07 (d, J = 20.6 Hz, 2.3H), 1.08 (d, J = 18.9 Hz, 0.7H), 1.12-1.27 (m, 2H), 1.40-1.64 (m, 4H), 2.08 (s, 3H), 2.35 (t, J = 7.0 Hz, 2H), 2.71 (dd, J = 13.5, 30.0 Hz, 0.29H), 2.83 (dd, J = 13.5, 23.1 Hz, 0.71H), 3.17 (dd, J = 7.6, 13.7 Hz, 0.75H), 3.24 (dd, J = 7.6, 13.9 Hz, 0.25H), 6.45 (d, J_{P-H} = 441.6 Hz, 0.22H), 6.56 (d, J_{P-H} = 438.0 Hz, 0.78H), 7.19-7.23 (m, 2H), 7.25-7.30 (m, 3H); ¹³C NMR (CDCl₃): δ -2.7, -2.3, 14.3, 23.0 (d, J_{P-C1} = 3.8 Hz), 24.3 (d, J_{P-C2} = 53.6 Hz), 24.6 (d, J_{P-C3} = 6.6 Hz), 25.7 (d, J_{P-C4} = 62.0 Hz), 27.7 (d, J_{P-C5} = 52.6 Hz), 30.0, 35.7, 43.2, 126.9, 128.2, 131.1, 137.4 (d, J = 7.5 Hz), 208.5; ³¹P NMR (CDCl₃): δ 45.6 (major), 47.6 (minor); MS (EI) m/z 338 (M⁺); HRMS Calcd for C₁₈H₃₁O₂PSi: 338.1831, Found: 338.1803.

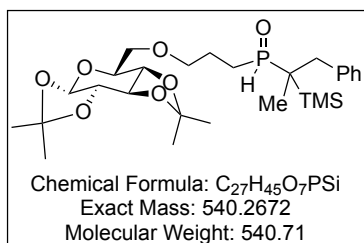
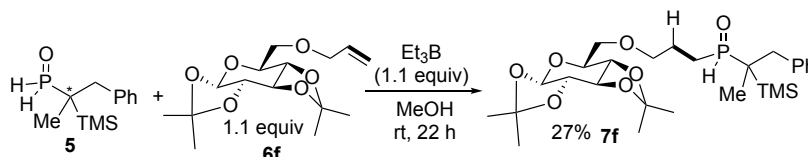
3-((1-Phenyl-2-(trimethylsilyl)prop-2-yl)hydrophosphoryl)propyl acetate (**7e**)



To a solution of (1-phenyl-2-(trimethylsilyl)propan-2-yl)phosphine oxide (**5**) (120 mg, 0.50 mmol) and allyl acetate (60 μ L, 0.55 mmol) in methanol (2.5 mL) was added Et₃B in hexane (1.0 M, 0.55 mL, 0.55 mmol) at room

temperature in an open reaction vessel. The solution was stirred at room temperature for 22 h. The reaction mixture was concentrated on a rotary evaporator, and the solution was extracted with CH₂Cl₂ three times, and the combined organic layers were dried and concentrated to afford the crude phosphine oxide. The crude product was purified by column chromatography on Al₂O₃ (CH₂Cl₂ : MeOH = 50 : 1, R_f = 0.20) to give the mixture (105 mg). The resulting oil was passed through GPC to give **7e** (29 mg, 17%, dr = 79 : 21) as a colorless oil; IR (neat): 2956, 2310, 1739, 1455, 1365, 1241, 1178, 1036 cm⁻¹; ¹H NMR(CDCl₃): δ 0.15 (s, 7.2H), 0.22 (s, 1.8H), 1.08 (d, *J* = 20.6 Hz, 2.4H), 1.10 (d, *J* = 18.9 Hz, 0.6H), 1.15-1.41 (m, 2H), 1.68-1.78 (m, 1H), 1.97 (s, 0.7H), 1.98 (s, 2.3H), 2.01-2.06 (m, 1H), 2.82 (dd, *J* = 13.9, 24.2 Hz, 1H), 3.20 (dd, *J* = 7.2, 13.7 Hz, 1H), 3.91-4.02 (m, 2H), 6.51 (d, *J*_{P-H} = 443.4 Hz, 0.2H), 6.60 (d, *J*_{P-H} = 439.4 Hz, 0.8H), 7.18-7.23 (m, 2H), 7.26-7.29 (m, 3H); ¹³C NMR (CDCl₃): δ -2.7, -2.3, 14.2, 21.0, 21.5, 22.7 (d, *J*_{P-C1} = 2.8 Hz), 22.9 (d, *J*_{P-C2} = 5.6 Hz), 27.7 (d, *J*_{P-C3} = 53.4 Hz), 35.7, 64.3 (d, *J*_{P-C4} = 14.1 Hz), 126.9, 128.3, 131.1, 137.3 (d, *J* = 6.6 Hz), 171.0; ³¹P NMR (CDCl₃): δ 44.8 (major), 47.1 (minor); MS (EI) *m/z* 340 (M⁺); HRMS Calcd for C₁₇H₂₉O₃PSi: 340.1624, Found: 340.1616.

(1)-Phenyl-2-(trimethylsilyl)prop-2-yl(3-(((3*aR*,5*R*,5*aS*,8*aS*,8*bR*)-2,2,7,7-tetramethyltetrahydro-5H-bis([1,3]dioxolo)[4,5-*b*:4',5'-*d*]pyran-5-yl)methoxy)propyl)phosphine oxide (7f**)**

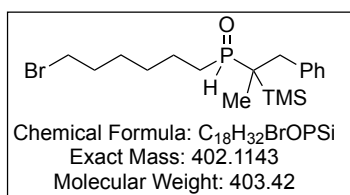
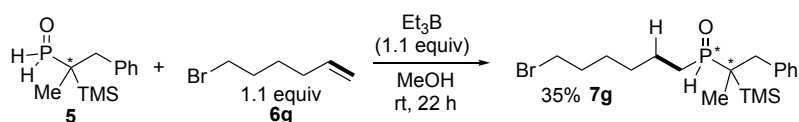


To a solution of (1-phenyl-2-(trimethylsilyl)propan-2-yl)phosphine oxide (**5**) (120 mg, 0.50 mmol) and (3*aR*,5*R*,5*aS*,8*aS*,8*bR*)-5-((allyloxy)methyl)-2,2,7,7-tetramethyltetrahydro-5H-bis([1,3]dioxolo)[4,5-*b*:4',5'-*d*]pyran (165 mg, 0.55 mmol) in methanol (2.5 mL) was added Et₃B in THF (1.0 M, 0.55 mL, 0.55 mmol) at room

temperature in an open reaction vessel. After 22 h, To the reaction mixture was added Et₃B in THF (1.0 M, 0.55 mL, 0.55 mmol). The solution was stirred at room temperature for 48 h. The reaction mixture was concentrated on a rotary evaporator, and the solution was extracted with CH₂Cl₂ three times, and the combined organic layers were dried and

concentrated to afford the crude phosphine oxide. The resulting oil was passed through column chromatography on Al₂O₃ (CH₂Cl₂:MeOH = 50:1) to give the mixture (201 mg). The resulting oil was passed through GPC to give **7f** (72 mg, 27%, dr = 85 : 15) as a colorless oil; IR (neat): 2934, 1719, 1456, 1380, 1254, 1212, 1169, 1070 cm⁻¹; ¹H NMR(CDCl₃): δ 0.11 (s, 7.4H), 0.19 (s, 1.6H), 1.05 (d, *J* = 19.3 Hz, 0.6H), 1.07 (d, *J* = 20.6 Hz, 2.4H), 1.18-1.32 (m, 8H), 1.39 (br, 4H), 1.47 (s, 3H), 1.63-1.95 (m, 1H), 2.87 (dd, *J* = 13.5, 21.8 Hz, 1H), 3.12 (dd, *J* = 8.1, 13.7 Hz, 1H), 3.32-3.45 (m, 1H), 3.49-3.60 (m, 3H), 3.85-3.91 (m, 1H), 4.15-4.17 (m, 1H), 4.25-4.27 (m, 1H), 4.43-4.56 (m, 1H), 5.47 (d, *J* = 4.9 Hz, 1H), 6.44 (d, *J*_{P-H} = 444.8 Hz, 0.2H), 6.58 (d, *J*_{P-H} = 440.7 Hz, 0.8H), 7.20-7.21 (m, 2H), 7.23-7.29 (m, 3H); ¹³C NMR (CDCl₃): δ -2.6, -2.2, 14.1, 14.4, 21.1 (d, *J*_{P-C1} = 61.1 Hz), 23.5, 23.6, 24.5, 25.0, 26.1 (d, *J*_{P-C2} = 12.2 Hz), 27.7 (d, *J*_{P-C3} = 51.7 Hz), 35.7, 37.6, 66.8, 69.5, 70.6 (d, *J*_{P-C4} = 11.3 Hz), 71.0 (d, *J*_{P-C5} = 13.2 Hz), 71.2, 96.4, 108.6, 109.3, 126.9, 127.9, 128.2, 130.8, 131.0, 137.4 (d, *J* = 8.5 Hz); ³¹P NMR (CDCl₃): δ 46.5 (major), 48.1 (minor); MS (EI) *m/z* 540 (M⁺); HRMS Calcd for C₂₇H₄₅O₇PSi: 540.2672, Found: 540.2655.

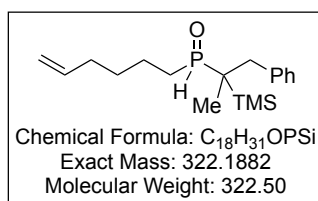
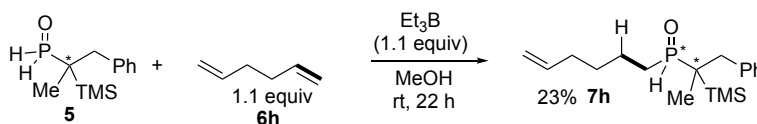
(6-Bromohexyl)(1-phenyl-2-(trimethylsilyl)prop-2-yl)phosphine oxide (**7g**)



To a solution of (1-phenyl-2-(trimethylsilyl)propan-2-yl)phosphine oxide (**5**) (120 mg, 0.50 mmol) and 6-bromo-1-hexene (80 μL, 0.55 mmol) in methanol (2.5 mL) was added Et₃B in THF (1.0 M, 0.55 mL, 0.55 mmol) at room temperature in an open reaction vessel. After 10 h, the solution was added Et₃B in THF (1.0 M, 0.55 mL, 0.55 mmol). The solution was stirred at room temperature for 22 h. The reaction mixture was concentrated on a rotary evaporator, and the solution was extracted with CH₂Cl₂ three times, and the combined organic layers were dried and concentrated to afford the crude phosphine oxide. The crude product was purified by column chromatography on Al₂O₃ (CH₂Cl₂:MeOH = 50:1, R_f = 0.20) to give the mixture (100 mg). The resulting solid was passed through GPC to give **7g** (71 mg, 35%, dr = 83:17) as a colorless oil; IR (neat): 2934, 2309, 1495, 1455, 1251, 1173 cm⁻¹; ¹H NMR(CDCl₃): δ 0.12 (s, 7.5H), 0.20 (s, 1.5H), 1.06 (d, *J* = 20.2 Hz, 3H), 1.11-1.22 (m, 2H), 1.26-1.43 (m,

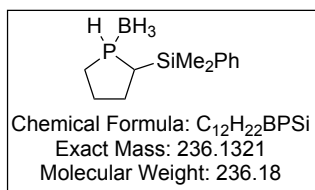
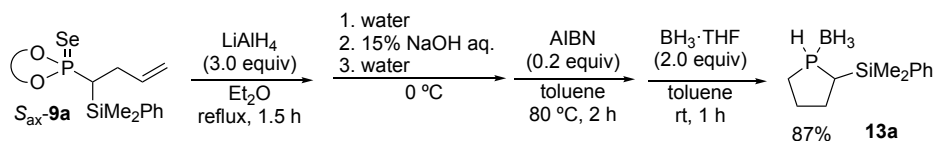
5H), 1.63-1.80 (m, 3H), 2.82 (dd, $J = 13.5, 23.1$ Hz, 1H), 3.15 (dd, $J = 7.2, 13.7$ Hz, 1H), 3.32 (t, $J = 6.7$ Hz, 2H), 6.44 (d, $J_{\text{P-H}} = 441.2$ Hz, 0.25H), 6.54 (d, $J_{\text{P-H}} = 437.1$ Hz, 0.75H), 7.18-7.20 (m, 2H), 7.24-7.28 (m, 3H); ^{13}C NMR (CDCl_3): δ -2.7, -2.2, 14.0, 14.4, 23.2 (d, $J_{\text{P-C1}} = 3.8$ Hz), 24.2 (d, $J_{\text{P-C2}} = 60.1$ Hz), 27.6, 27.7 (d, $J_{\text{P-C3}} = 52.6$ Hz), 29.7 (d, $J_{\text{P-C4}} = 12.2$ Hz), 33.1 (d, $J_{\text{P-C5}} = 139.1$ Hz), 35.7, 37.7, 126.9, 127.9, 128.2, 130.7, 131.0, 137.4 (d, $J = 7.5$ Hz); ^{31}P NMR (CDCl_3): δ 46.2 (major), 48.1 (minor); MS (EI) m/z 402 (M^+); HRMS Calcd for $\text{C}_{18}\text{H}_{32}\text{BrOPSi}$: 402.1143, Found: 402.1136.

Hex-5-en-1-yl(1-phenyl-2-(trimethylsilyl)prop-2-yl)phosphine oxide (7h)



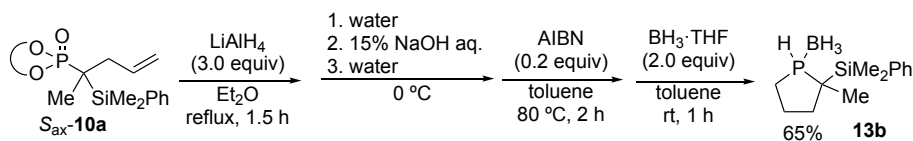
To a solution of (1-phenyl-2-(trimethylsilyl)propan-2-yl)phosphine oxide (**5**) (120 mg, 0.50 mmol) and 1,5-hexadiene (66 μL , 0.55 mmol) in methanol (2.5 mL) was added Et_3B in hexane (0.6 M, 0.92 mL, 0.55 mmol) at room temperature in an open reaction vessel. The solution was stirred at room temperature for 22 h. The reaction mixture was concentrated on a rotary evaporator, and the solution was extracted with CH_2Cl_2 three times, and the combined organic layers were dried and concentrated to afford the crude phosphine oxide. The crude product was purified by column chromatography on Al_2O_3 (CH_2Cl_2 :MeOH = 50:1, R_f = 0.20) to give the mixture (120 mg). The resulting oil was passed through GPC to give **7h** (37 mg, 23%, dr = 81 : 19) as a colorless oil; IR (neat): 2927, 2305, 1639, 1454, 1252, 1177 cm^{-1} ; ^1H NMR(CDCl_3): δ 0.14 (s, 7.2H), 0.22 (s, 1.8H), 0.75-0.85 (m, 1H), 1.08 (d, $J = 20.6$ Hz, 3H), 1.16-1.24 (m, 2H), 1.36-1.40 (m, 2H), 1.65-1.70 (m, 1H), 1.96-1.98 (m, 2H), 2.85 (dd, $J = 13.5, 22.9$ Hz, 1H), 3.18 (dd, $J = 7.6, 13.9$ Hz, 1H), 4.90-4.97 (m, 2H), 5.67-5.77 (m, 1H), 6.46 (d, $J_{\text{P-H}} = 441.6$ Hz, 0.24H), 6.57 (d, $J_{\text{P-H}} = 438.0$ Hz, 0.76H), 7.23-7.25 (m, 2H), 7.26-7.29 (m, 3H); ^{13}C NMR (CDCl_3): δ -2.7, -2.2, 14.4, 22.9 (d, $J_{\text{P-C1}} = 3.8$ Hz), 24.3 (d, $J_{\text{P-C2}} = 59.2$ Hz), 27.7 (d, $J_{\text{P-C3}} = 52.6$ Hz), 29.9 (d, $J_{\text{P-C4}} = 13.2$ Hz), 33.3, 35.8, 37.7, 114.9, 126.9, 128.2, 131.1, 137.5 (d, $J = 7.5$ Hz), 138.3; ^{31}P NMR (CDCl_3): δ 46.5 (major), 48.1 (minor); MS (EI) m/z 322 (M^+); HRMS Calcd for $\text{C}_{18}\text{H}_{31}\text{OPSi}$: 322.1882, Found: 322.1879.

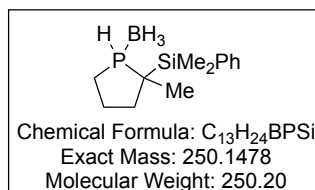
2-(Dimethyl(phenyl)silyl)phospholane-Borane (**13a**)



Et₂O (5 mL) and phosphonoselenoate **9a** (292 mg, 0.5 mmol) was placed in a 20 mL two-necked flask. LAH (57 mg, 1.5 mmol, 3.0 equiv) was added, and the mixture was stirred at reflux temperature for 1.5 h. The resulting mixture was quenched with water (60 μ L), sodium hydroxide 15% aqueous solution (60 μ L), and water (180 μ L). The solution was filtered through diatomite, and concentrated to give the primary phosphine as a colorless oil. This oil and toluene (5 mL) were placed in a 20 mL two-necked flask. To this AIBN (16 mg, 0.1 mmol, 0.2 equiv) was added, and the mixture was stirred at 80 °C for 2 h. The reaction mixture was cooled to room temperature. BH₃·THF (1.0 M THF solution, 1 mL, 1.0 mmol, 2.0 equiv) was then added to the solution, and it was stirred for 1 h. To the resulting solution were added water and ether. The aqueous phase was extracted with ether three times. The combined organic layer was dried over MgSO₄, filtered, and concentrated. The crude product was purified by column chromatography on silica gel (CH₂Cl₂:hexane = 1:3, R_f = 0.3) to give the product **13a** (103 mg, 87%, dr = 88:12) as a colorless oil; IR (neat): 3069, 2952, 2380, 2245, 1487, 1427, 1305, 1253, 1059, 924, 834, 771, 735, 620, 472 cm⁻¹; ¹H NMR (CDCl₃): δ 0.46 (s, 2.7H), 0.46 (s, 2.7H), 0.50 (s, 0.3H), 0.53 (s, 0.3H), 0.65 (br, 3H), 1.25-1.35 (m, 1H), 1.50-1.59 (m, 1H), 1.61-1.70 (m, 1H), 1.78-1.84 (m, 1H), 1.88-1.99 (m, 2H), 2.07-2.19 (m, 1H), 4.50 (ddt, J = 348.5 Hz, 17.2 Hz, 6.3 Hz, 0.45H), 4.48-4.52 (m, 0.05H), 5.39-5.42 (m, 0.05H), 7.36-7.42 (m, 3H), 7.52-7.55 (m, 2H); ¹³C NMR (CDCl₃): δ -4.3, -3.0, 21.2 (d, J = 35.7 Hz), 22.1 (d, J = 23.5 Hz), 27.8, 31.2, 128.0, 129.7, 133.9, 135.7; ³¹P NMR (CDCl₃): δ 1.6 (minor), 3.7 (major) (J = 55.1 Hz); ¹¹B NMR (CDCl₃): δ -42.3; MS (EI) m/z 236 (M⁺); HRMS Calcd for C₁₂H₂₂BPSi: 236.1321, Found: 236.1316.

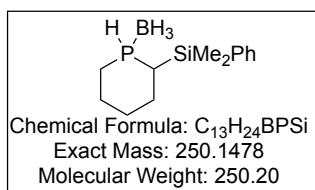
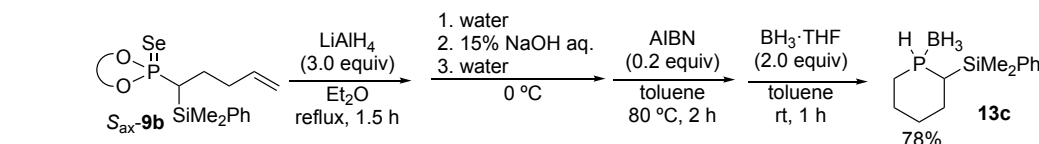
2-(Dimethyl(phenyl)silyl)-2-methylphospholane-Borane (**13b**)





Et₂O (3 mL) and phosphonoselenoate **10a** (80 mg, 0.15 mmol) was placed in a 20 mL two-necked flask. LAH (17 mg, 0.45 mmol, 3.0 equiv) was added, and the mixture was stirred at reflux temperature for 1.5 h. The resulting mixture was quenched with water (20 μL), sodium hydroxide 15% aqueous solution (20 μL), and water (60 μL). The solution was filtered through diatomite, and concentrated to give the primary phosphine as a colorless oil. This oil and toluene (5 mL) were placed in a 20 mL two-necked flask. To this AIBN (5 mg, 0.03 mmol, 0.2 equiv) was added, and the mixture was stirred at 80 °C for 2 h. The reaction mixture was cooled to room temperature. BH₃·THF (1.0 M THF solution, 0.3 mL, 0.3 mmol, 2.0 equiv) was then added to the solution, and it was stirred for 1 h. To the resulting solution were added water and ether. The aqueous phase was extracted with ether three times. The combined organic layer was dried over MgSO₄, filtered, and concentrated. The crude product was purified by column chromatography on silica gel (CH₂Cl₂:hexane = 1:3, R_f = 0.3) to give the product **13b** (24 mg, 65%, dr = 87:13) as a colorless oil; IR (neat): 3069, 2951, 2385, 2248, 1888, 1455, 1377, 1254, 1061, 970, 939, 702, 609, 492, 410 cm⁻¹; ¹H NMR (CDCl₃): δ 0.45 (s, 2.4H), 0.48 (s, 2.4H), 0.53 (s, 0.6H), 0.55 (s, 0.6H), 0.61 (br, 3H), 1.17 (d, *J* = 18.4 Hz, 2.4H), 1.22 (d, *J* = 16.2 Hz, 0.6H) 1.51-2.06 (m, 6H), 4.48-4.52 (m, 0.05H), 4.53 (ddt, *J* = 350.1 Hz, 6.8 Hz, 6.3 Hz, 0.9H), 5.39-5.42 (m, 0.05H), 7.35-7.44 (m, 3H), 7.52-7.55 (m, 1.6H), 7.57-7.60 (m, 0.4H); ¹³C NMR (CDCl₃): δ -5.3, -5.2, 16.7, 20.1 (d, *J* = 32.9 Hz), 21.5 (d, *J* = 34.8 Hz), 23.6, 38.9, 127.9, 129.7, 134.5, 134.8; ³¹P NMR (CDCl₃): δ 14.4 (major) (*J* = 50.9 Hz), 34.5 (minor); ¹¹B NMR (CDCl₃): δ -44.8(major), -42.3(minor); MS (EI) *m/z* 250 (M⁺); HRMS Calcd for C₁₃H₂₄BPSi: 250.1478, Found: 250.1469.

2-(Dimethyl(phenyl)silyl)phosphinane-Borane (**13c**)



Et₂O (10 mL) and phosphonoselenoate **9b** (598 mg, 1.0 mmol) was placed in a 20 mL two-necked flask. LAH (110 mg, 3.0 mmol, 3.0 equiv) was added, and the mixture was stirred at reflux temperature for 1.5 h. The resulting mixture was quenched with water (110 μL), sodium hydroxide 15% aqueous solution (110 μL)

and water (330 μ L). The solution was filtered through diatomite, and concentrated to give the primary phosphine as a colorless oil. This oil and toluene (10 mL) were placed in a 20 mL two-necked flask. To this AIBN (33 mg, 0.2 mmol, 0.2 equiv) added, and the mixture was stirred at 80 $^{\circ}$ C for 2 h. The reaction mixture was cooled to room temperature. $\text{BH}_3 \cdot \text{THF}$ (1.0 M THF solution, 2 mL, 2.0 mmol, 2.0 equiv) was then added to the solution, and it was stirred for 1 h. To the resulting solution were added water and ether. The aqueous phase was extracted with ether three times. The combined organic layer was dried over MgSO_4 , filtered, and concentrated. The crude product was purified by column chromatography on silica gel (CH_2Cl_2 : hexane = 1 : 3, R_f = 0.3) to give the product **13c** (195 mg, 78%, dr = 87:13) as a colorless oil; IR (neat): 3068, 2856, 2378, 2256, 1957, 1715, 1589, 1427, 1251, 1028, 917, 831, 701, 553, 470 cm^{-1} ; ^1H NMR (CDCl_3): δ 0.46 (s, 0.4H), 0.46 (s, 0.4H), 0.48 (s, 2.6H), 0.51 (s, 2.6H), 0.61 (br, 3H), 1.03-1.14 (m, 1H), 1.16-1.34 (m, 2H), 1.41-1.63 (m, 2H), 1.78-1.81 (m, 1H), 1.86-1.95 (m, 2H), 1.98-2.11 (m, 1H), 4.25-4.26 (m, 0.05H), 4.32 (ddt, J = 352.3 Hz, 16.6 Hz, 6.1 Hz, 0.9H), 5.16-5.19 (m, 0.05H), 7.36-7.43 (m, 3H), 7.52-7.56 (m, 2H); ^{13}C NMR (CDCl_3): δ -4.0, -2.5, 19.2 (d, J = 18.8 Hz), 20.8 (d, J = 34.8 Hz), 25.1 (d, J = 7.5 Hz), 27.3 (d, J = 8.5 Hz), 27.4 (d, J = 5.6 Hz), 127.9, 129.6, 134.1, 135.5; ^{31}P NMR (CDCl_3): δ -19.7 (minor), -8.6 (major) (J = 57.2 Hz); ^{11}B NMR (CDCl_3): δ -44.9 (minor), -42.3 (major); MS (EI) m/z 250 (M^+); HRMS Calcd for $\text{C}_{13}\text{H}_{24}\text{BPSi}$: 250.1478, Found: 250.1494.

Cartesian Coordinates

Radical 8b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	15	0	-2.394628	-1.583971	-0.203126
2	6	0	-0.871100	-0.698832	0.342933
3	6	0	-0.650032	-1.098304	1.819725
4	1	0	0.231749	-0.618375	2.222566
5	1	0	-1.488071	-0.809901	2.446759
6	1	0	-0.515796	-2.172958	1.928776
7	8	0	-2.959785	-1.184880	-1.515413
8	14	0	-1.196329	1.223068	0.216175
9	6	0	-1.210389	1.812298	-1.575998
10	1	0	-1.619835	2.819357	-1.616475
11	1	0	-0.219880	1.851613	-2.015128
12	1	0	-1.836017	1.174773	-2.191641
13	6	0	0.091459	2.175580	1.222870
14	1	0	-0.092540	3.242426	1.113459
15	1	0	0.025853	1.946943	2.283059
16	1	0	1.107832	1.981671	0.899882
17	6	0	-2.893601	1.605659	0.968662
18	1	0	-3.006222	1.226747	1.981043
19	1	0	-3.018872	2.685073	1.017528
20	1	0	-3.709165	1.214388	0.368423
21	6	0	0.270369	-1.243133	-0.579992
22	1	0	-0.014107	-1.070924	-1.612096
23	1	0	0.307723	-2.323906	-0.455277
24	6	0	1.675870	-0.706062	-0.371040
25	6	0	2.230290	0.200333	-1.267988
26	6	0	2.474449	-1.154424	0.678920
27	6	0	3.521290	0.677692	-1.101470

28	1	0	1.655074	0.527823	-2.115175
29	6	0	3.763405	-0.680229	0.850269
30	1	0	2.094002	-1.893020	1.361812
31	6	0	4.290648	0.245438	-0.035979
32	1	0	3.925063	1.379446	-1.809968
33	1	0	4.359176	-1.041109	1.670305
34	1	0	5.293102	0.612520	0.095016
35	1	0	-3.288712	-1.433043	0.865409

Radical, **8a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
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3	6	0	-0.873581	-0.658681	0.361484
4	6	0	-0.615551	-1.019178	1.842909
5	1	0	0.286269	-0.545427	2.206627
6	1	0	-1.432555	-0.702058	2.483409
7	1	0	-0.495104	-2.093011	1.977978
8	8	0	-2.897033	-1.333121	-1.498455
9	14	0	-1.232168	1.251311	0.199887
10	6	0	-1.282177	1.800601	-1.604781
11	1	0	-1.699197	2.803618	-1.662957
12	1	0	-0.300744	1.835120	-2.064635
13	1	0	-1.913834	1.143244	-2.193083
14	6	0	0.051784	2.245710	1.168756
15	1	0	-0.151338	3.306975	1.041224
16	1	0	0.003950	2.036512	2.233897
17	1	0	1.067131	2.062282	0.836379
18	6	0	-2.927952	1.609684	0.966766

19	1	0	-3.021443	1.234954	1.982546
20	1	0	-3.077777	2.686318	1.008654
21	1	0	-3.741188	1.193785	0.379769
22	6	0	0.259236	-1.211234	-0.571382
23	1	0	-0.031467	-1.035126	-1.600366
24	1	0	0.292139	-2.292717	-0.448670
25	6	0	1.670222	-0.685872	-0.366055
26	6	0	2.216491	0.244553	-1.243345
27	6	0	2.480560	-1.168109	0.659392
28	6	0	3.512223	0.710151	-1.081143
29	1	0	1.631363	0.600099	-2.072178
30	6	0	3.774441	-0.705705	0.826439
31	1	0	2.104707	-1.923619	1.326369
32	6	0	4.294257	0.242512	-0.039940
33	1	0	3.909918	1.430427	-1.774333
34	1	0	4.379470	-1.093187	1.627328
35	1	0	5.300521	0.600370	0.087310

Product 7a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
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2	6	0	-0.355598	0.262854	-1.948531
3	1	0	-1.355604	-0.013850	-2.291040
4	1	0	-0.051132	1.149550	-2.514869
5	1	0	0.319365	-0.554950	-2.234304
6	8	0	1.467767	1.690302	1.437367
7	14	0	-1.531431	2.029964	-0.018300
8	6	0	-1.802054	2.230902	1.838938
9	1	0	-2.302341	3.186541	2.034776

10	1	0	-2.426220	1.442743	2.268446
11	1	0	-0.835934	2.236782	2.351164
12	6	0	-3.184116	1.803660	-0.918422
13	1	0	-3.838154	2.650791	-0.679493
14	1	0	-3.060985	1.787578	-2.006339
15	1	0	-3.702597	0.888371	-0.622068
16	6	0	-0.741581	3.624523	-0.677613
17	1	0	-0.474817	3.565276	-1.738221
18	1	0	-1.459775	4.445923	-0.571378
19	1	0	0.154016	3.896323	-0.111277
20	6	0	-0.664338	-0.782717	0.386614
21	1	0	-0.510696	-0.574316	1.450662
22	1	0	0.080091	-1.541927	0.109470
23	6	0	-2.035447	-1.413078	0.208442
24	6	0	-3.017094	-1.291721	1.202182
25	6	0	-2.340922	-2.185945	-0.922975
26	6	0	-4.271994	-1.885535	1.057077
27	1	0	-2.790879	-0.735654	2.107164
28	6	0	-3.593965	-2.779794	-1.074668
29	1	0	-1.584740	-2.338531	-1.687669
30	6	0	-4.568565	-2.625956	-0.087361
31	1	0	-5.013546	-1.775399	1.843177
32	1	0	-3.805148	-3.371932	-1.960645
33	1	0	-5.543399	-3.090396	-0.202743
34	15	0	1.363129	1.070459	0.066480
35	1	0	1.678824	1.953260	-1.003831
36	6	0	2.599912	-0.291436	-0.222327
37	6	0	3.891729	0.298593	-0.833877
38	6	0	2.909194	-1.045906	1.089148
39	1	0	2.168870	-0.995502	-0.949206
40	6	0	4.971695	-0.776305	-1.029924
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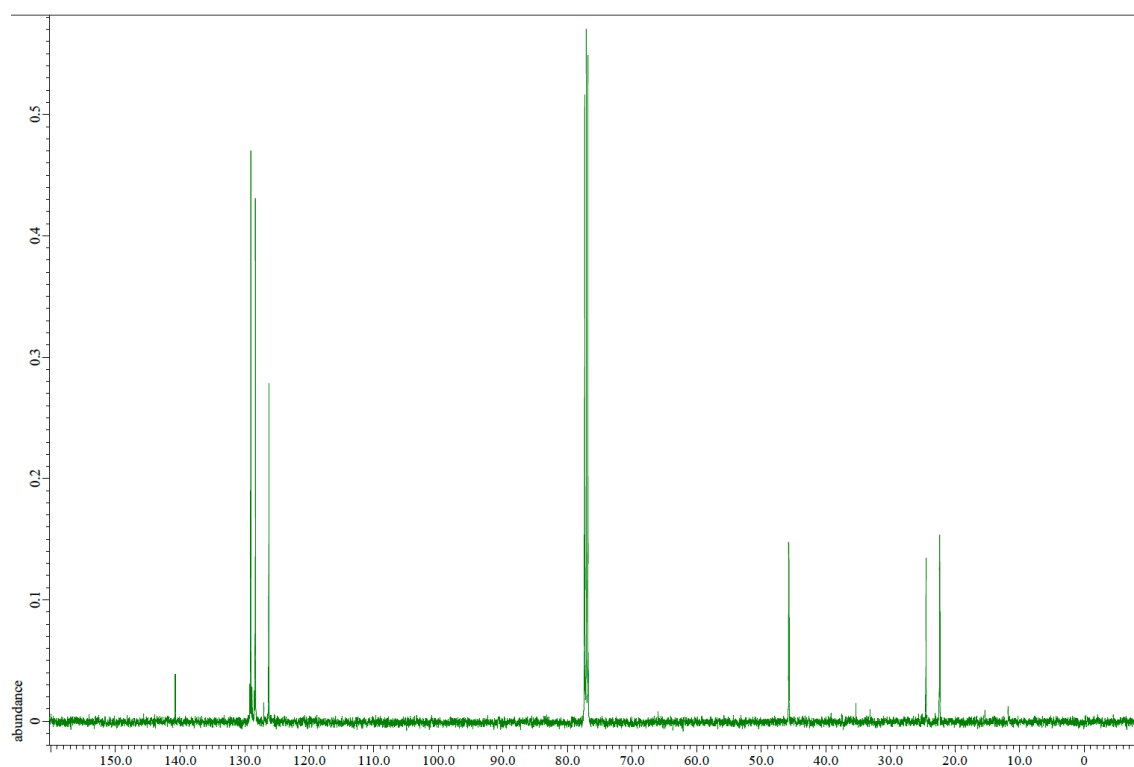
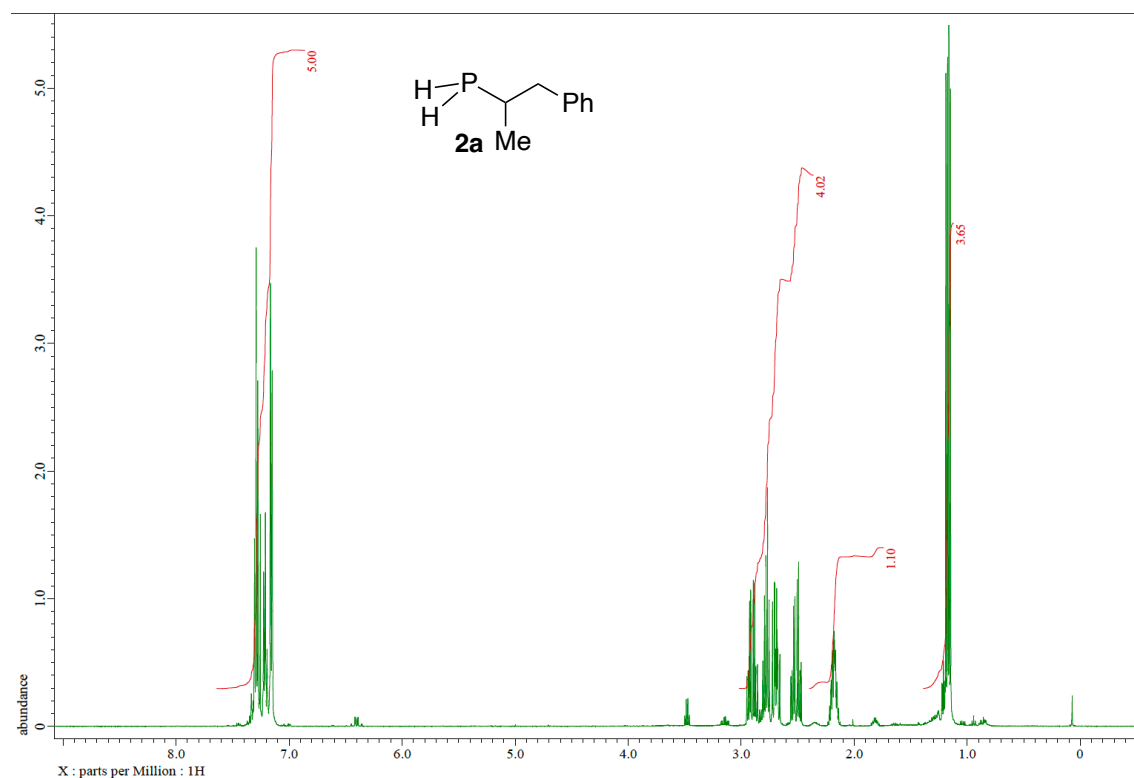
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49	1	0	4.219385	-2.597003	1.844151
50	1	0	3.613933	-2.901699	0.221472
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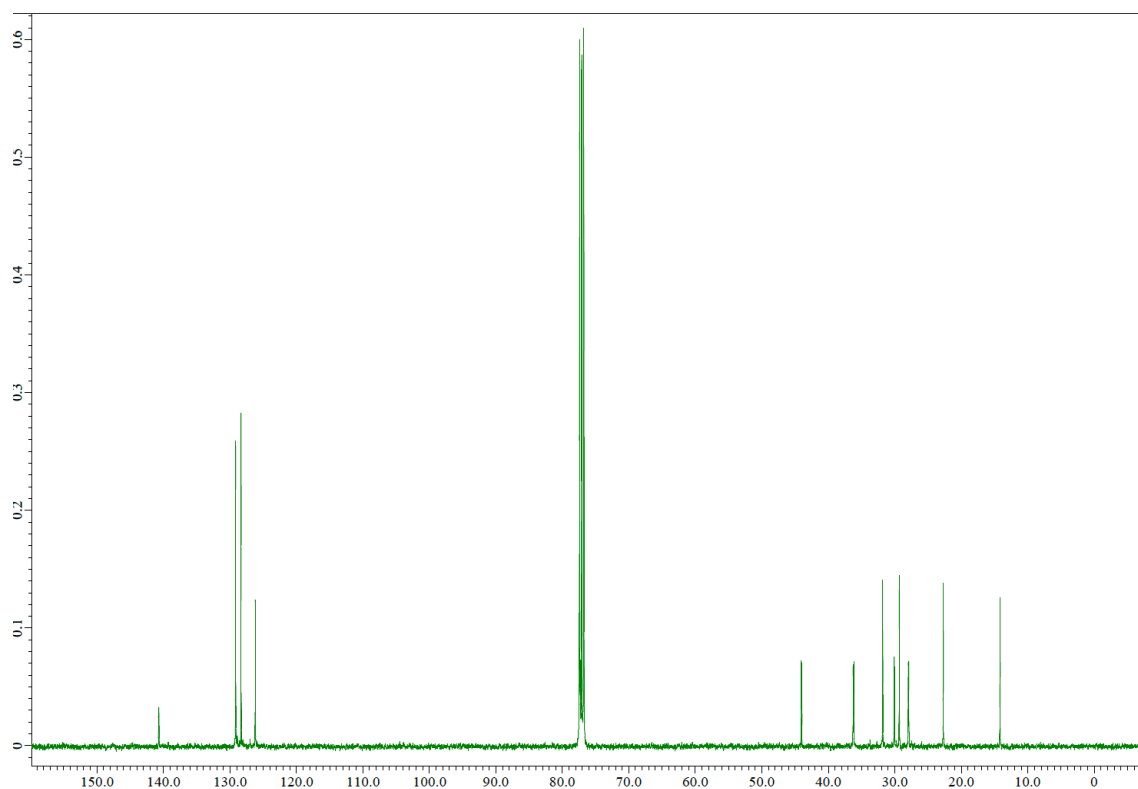
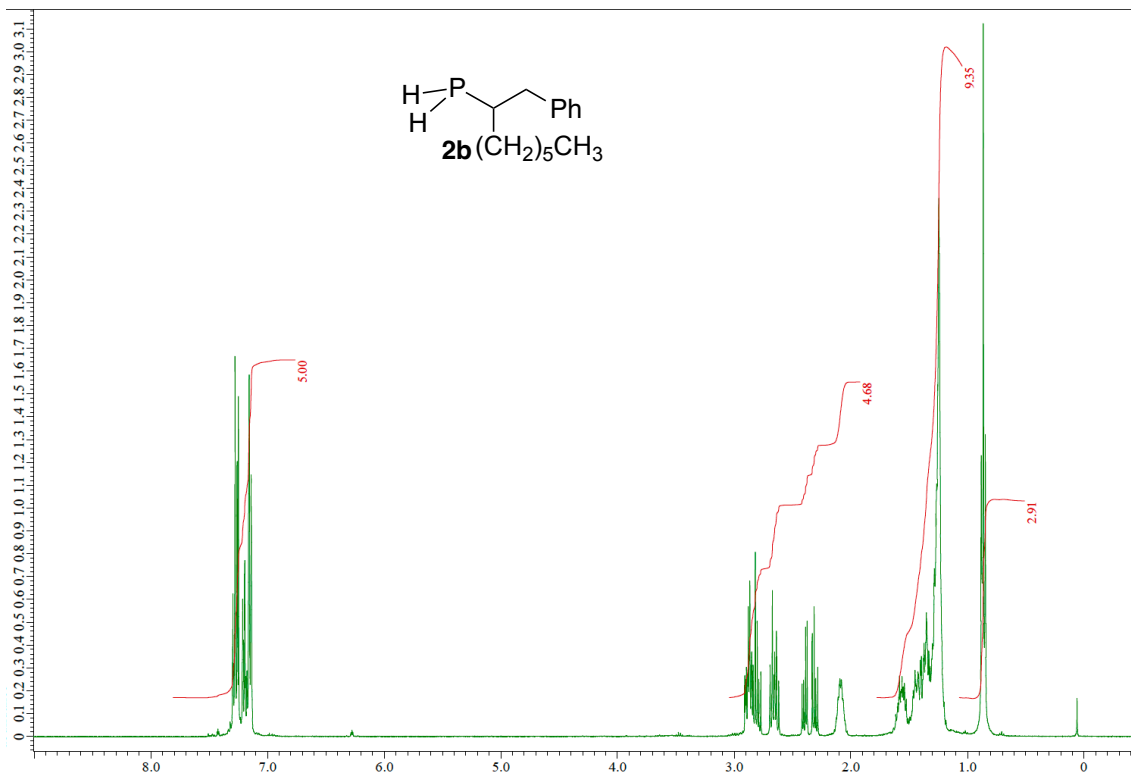
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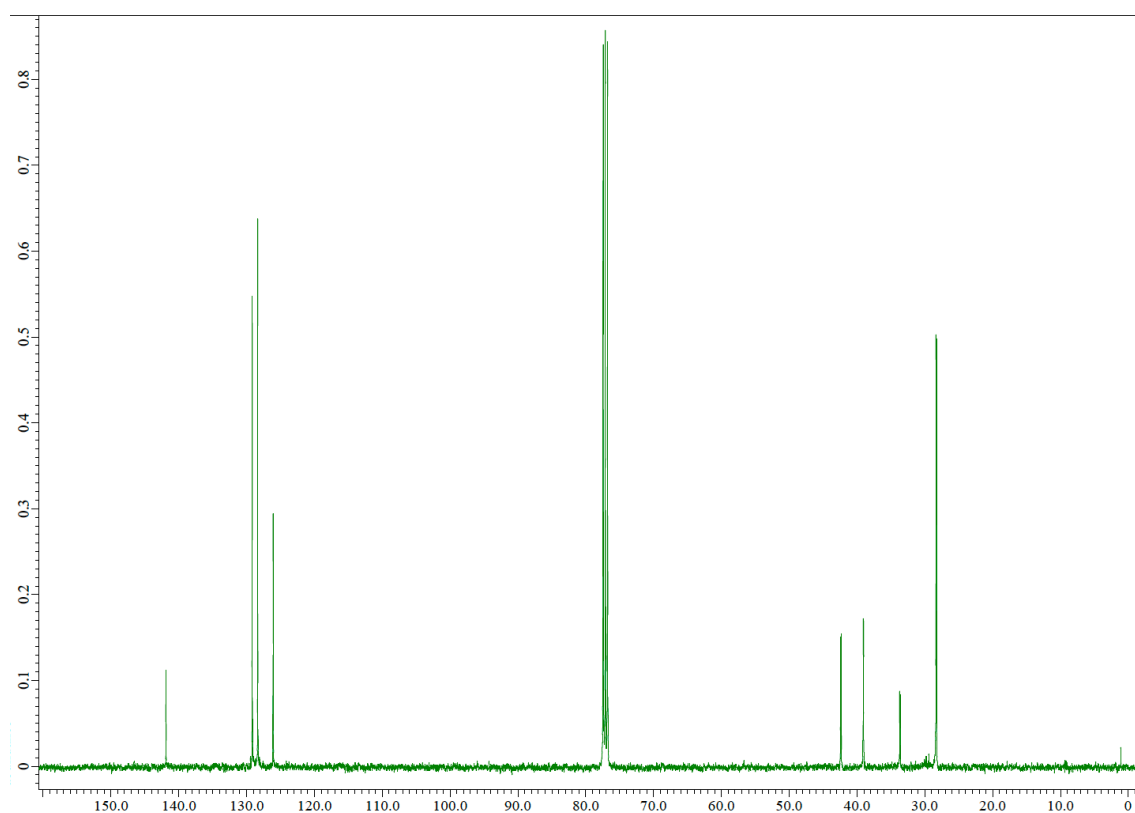
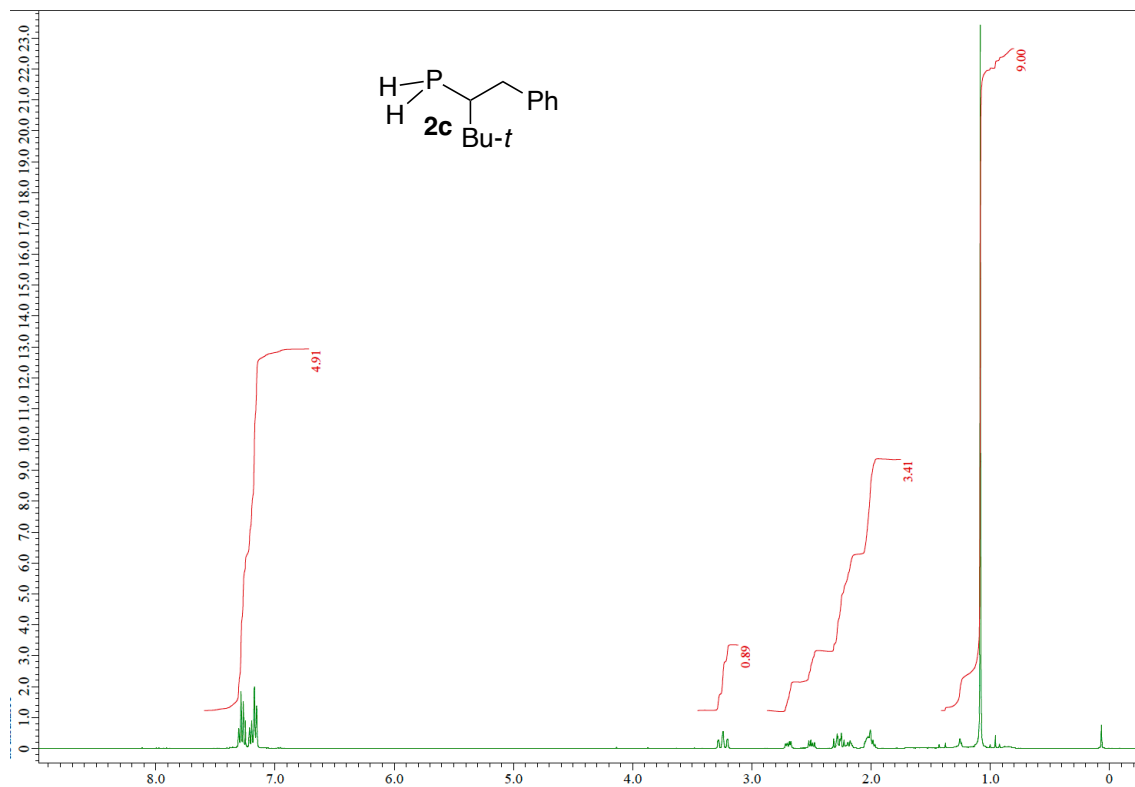
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
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4	1	0	-0.551825	-0.901183	1.778256
5	1	0	-0.000230	-2.186750	0.694783
6	8	0	-1.204462	1.051610	-2.079083
7	14	0	0.716555	1.628259	0.648215
8	6	0	1.225603	2.846474	-0.700863
9	1	0	1.213145	3.866374	-0.299101
10	1	0	2.231404	2.661613	-1.087427
11	1	0	0.516361	2.790463	-1.531334
12	6	0	2.036010	1.526581	2.005203
13	1	0	2.211855	2.531153	2.408102
14	1	0	1.716583	0.894544	2.840610
15	1	0	2.990745	1.143220	1.636962
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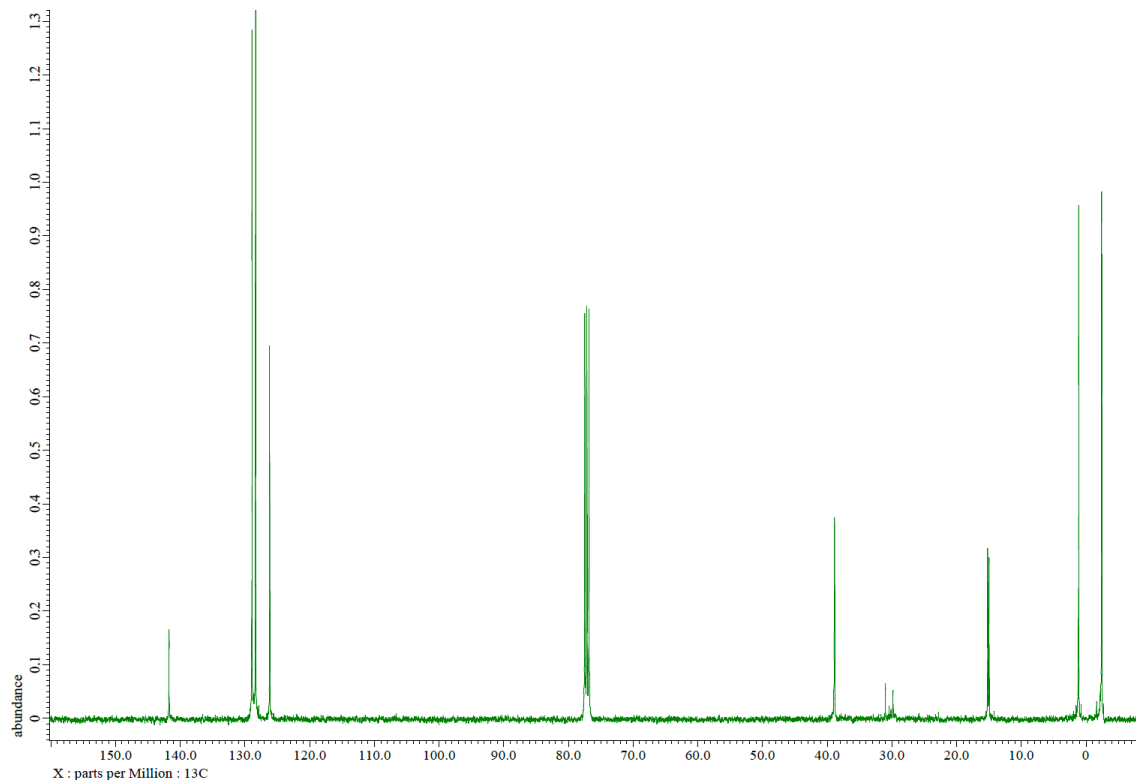
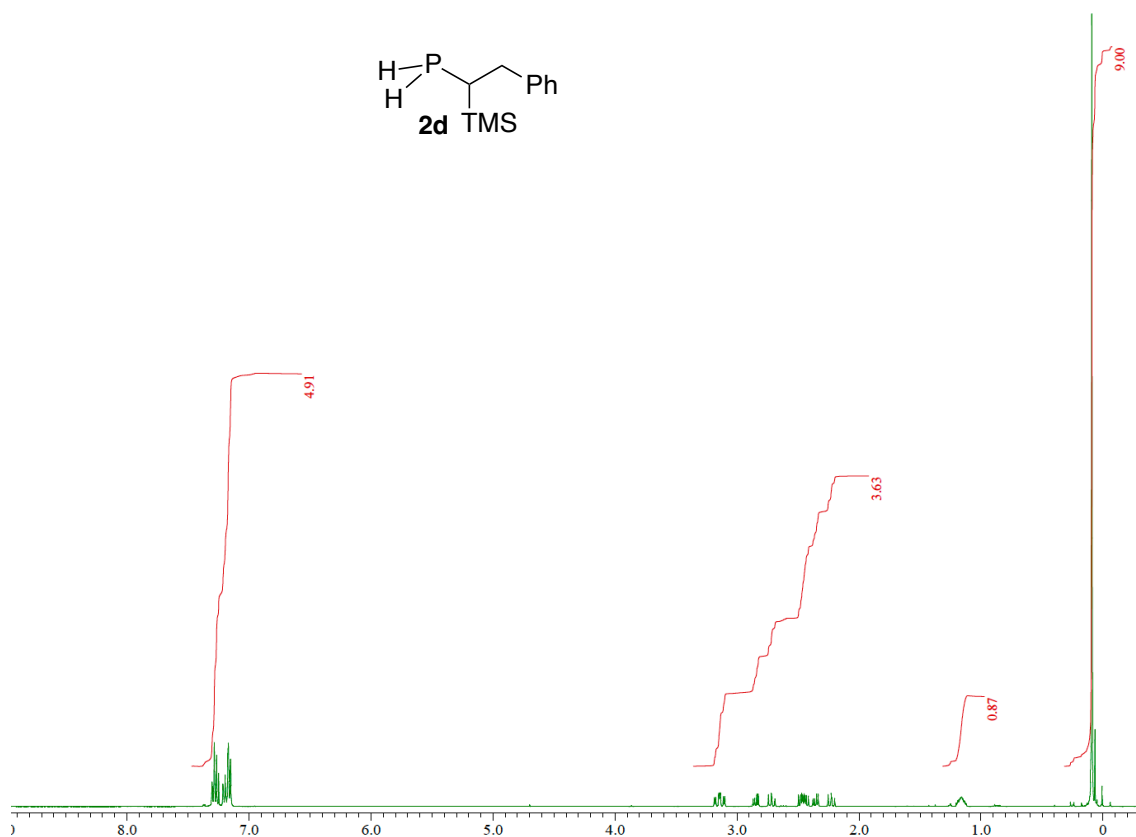
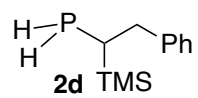
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22	1	0	1.166497	-1.596387	-1.509063
23	6	0	2.912247	-0.799596	-0.597882
24	6	0	3.900623	0.149643	-0.895583
25	6	0	3.298489	-1.943049	0.119431
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29	1	0	2.567200	-2.720239	0.321990
30	6	0	5.576411	-1.142824	0.275658
31	1	0	5.962178	0.736785	-0.707652
32	1	0	4.883919	-3.005410	1.111978
33	1	0	6.600169	-1.274124	0.613335
34	15	0	-1.160794	-0.109208	-1.118430
35	1	0	-1.107527	-1.385129	-1.759500
36	6	0	-2.696167	-0.292857	-0.075751
37	6	0	-3.837342	0.558330	-0.675110
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44	1	0	-3.322409	-2.183852	-0.928293
45	1	0	-2.345062	-2.370830	0.520318
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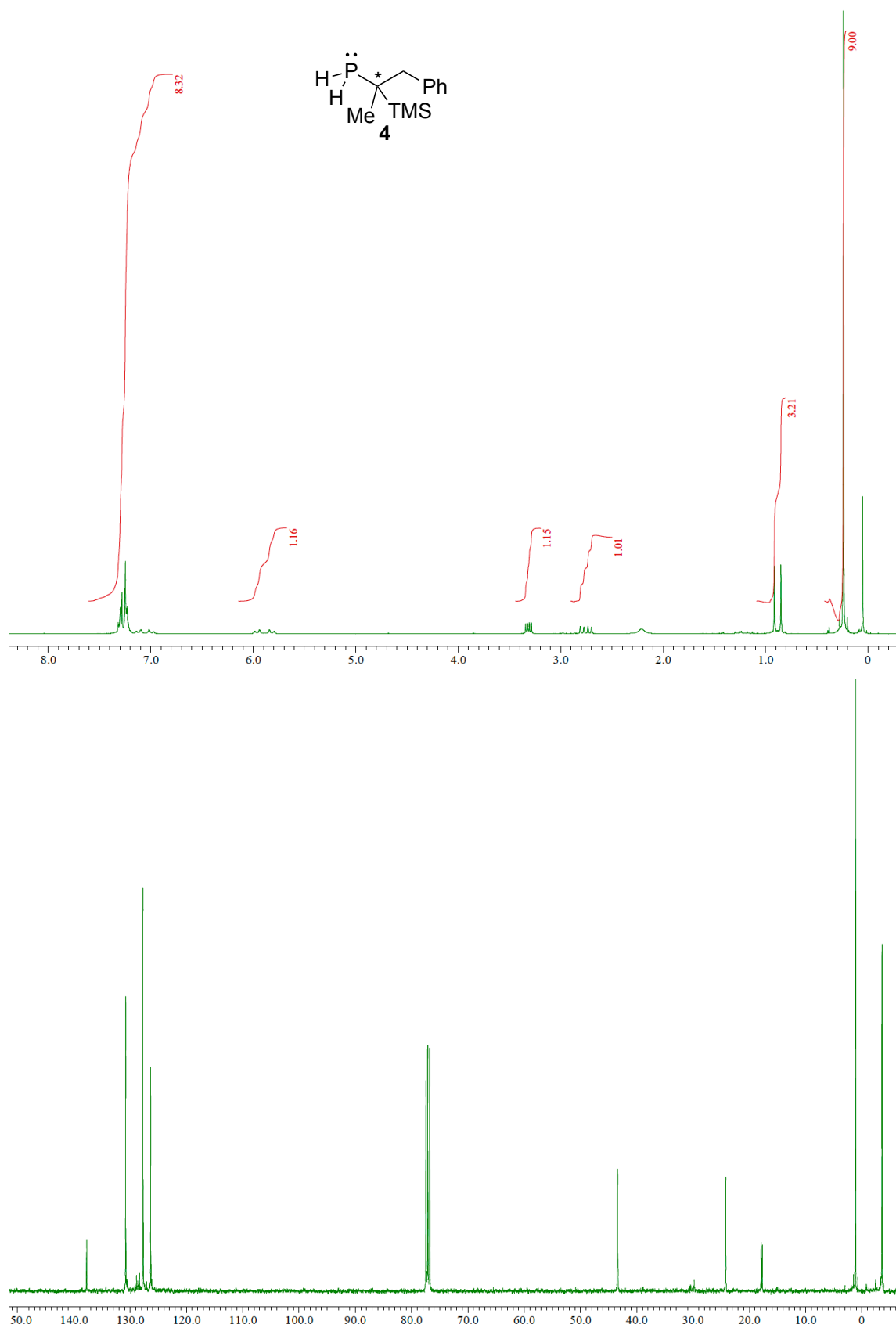
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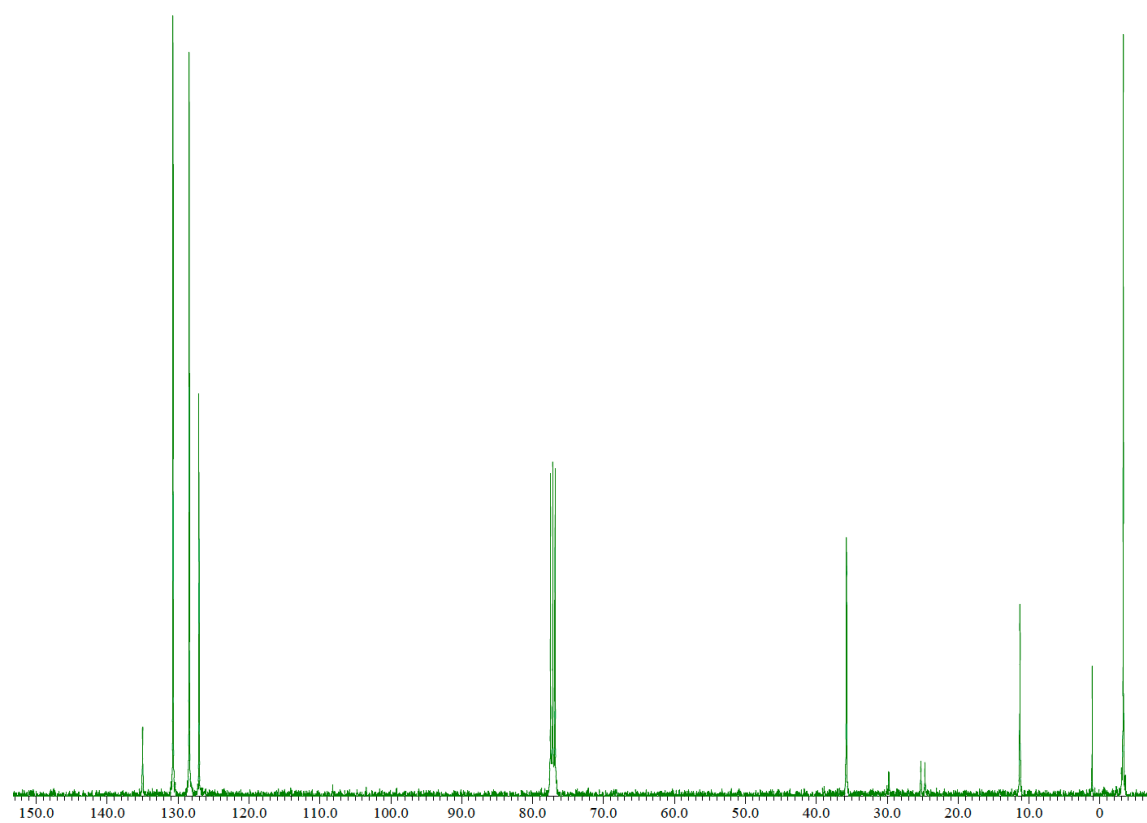
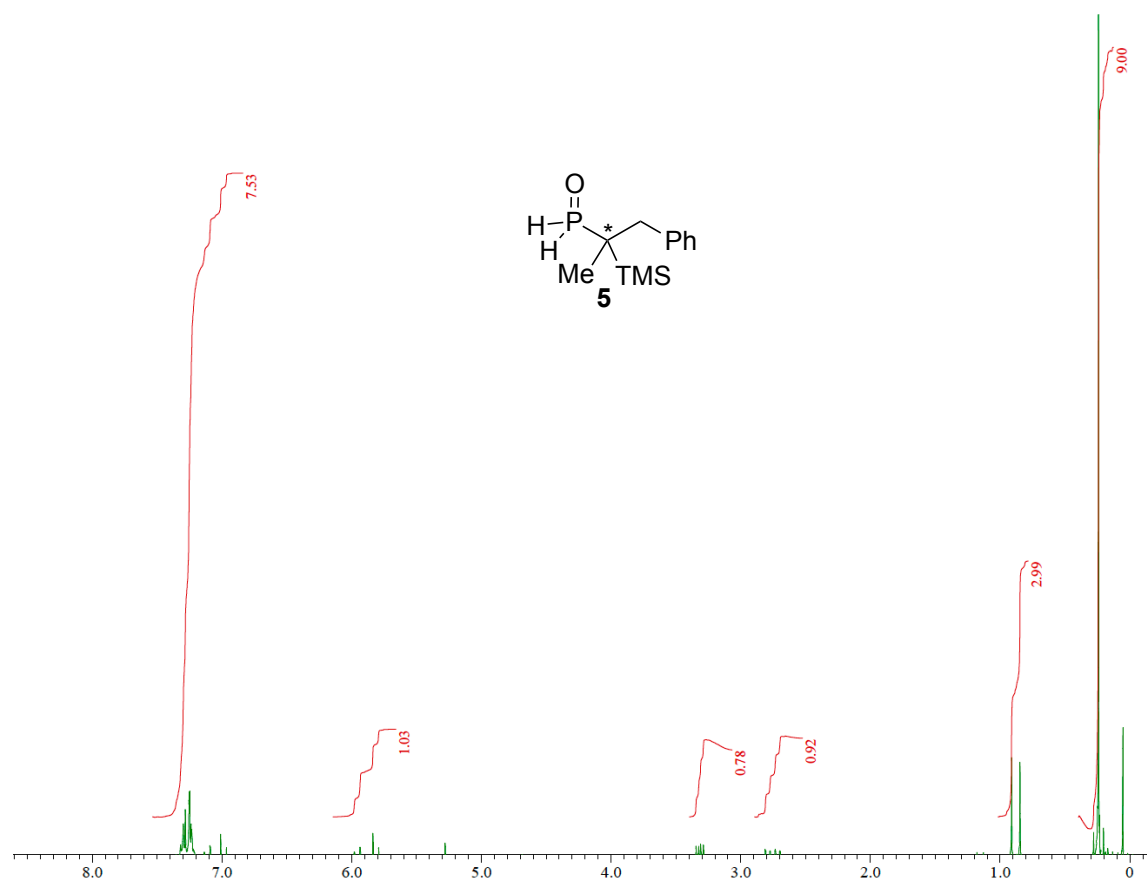


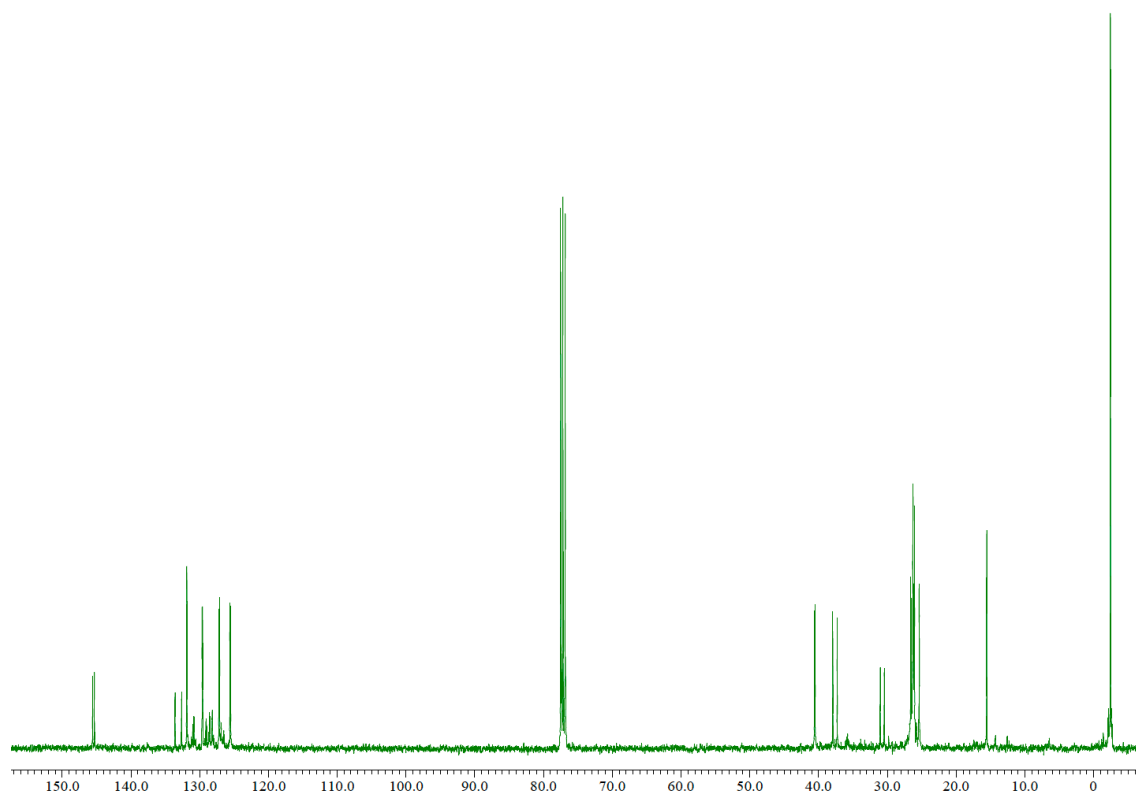
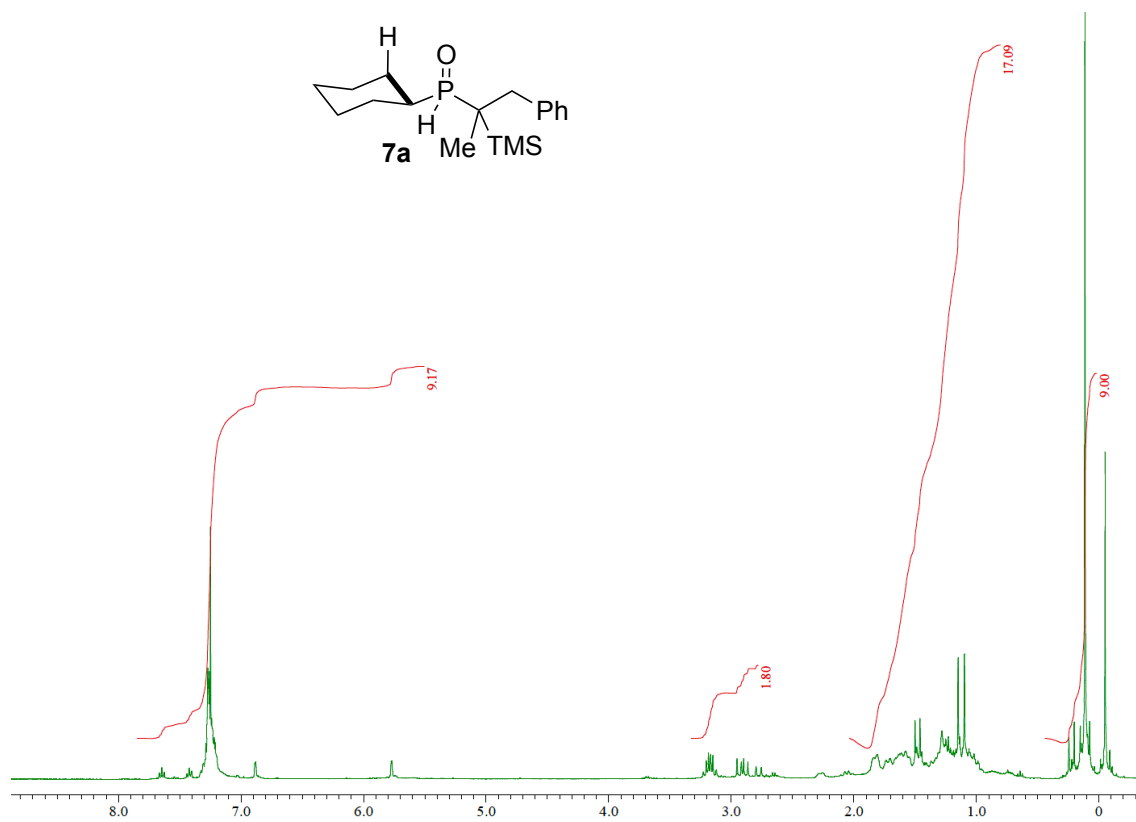
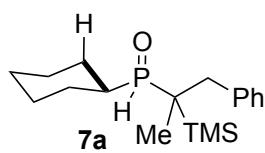


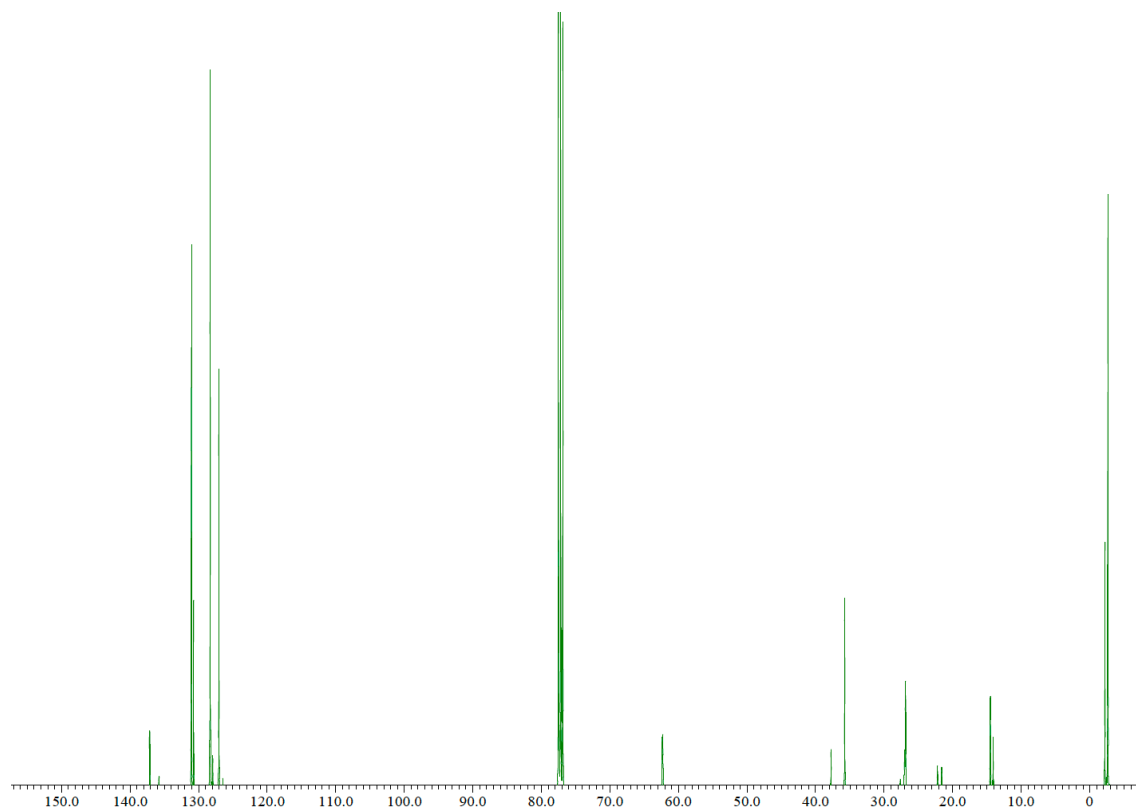
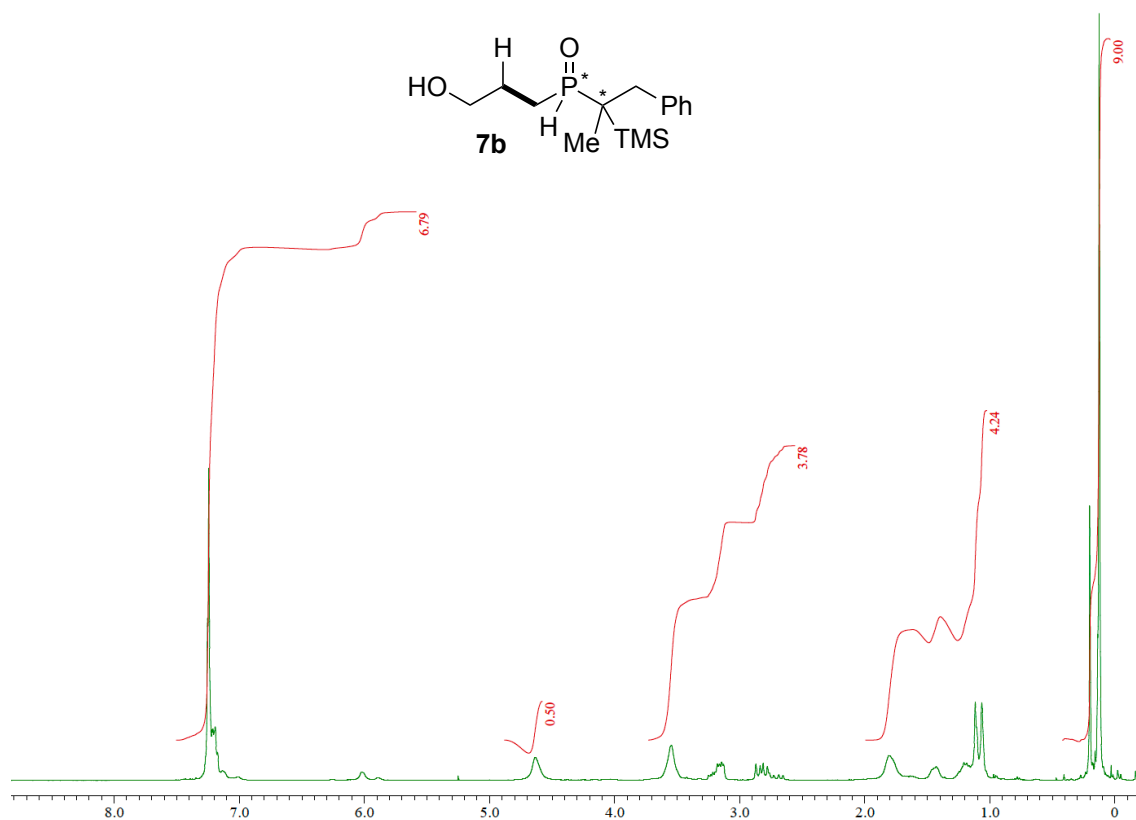
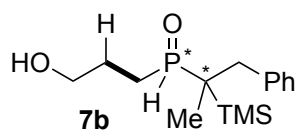


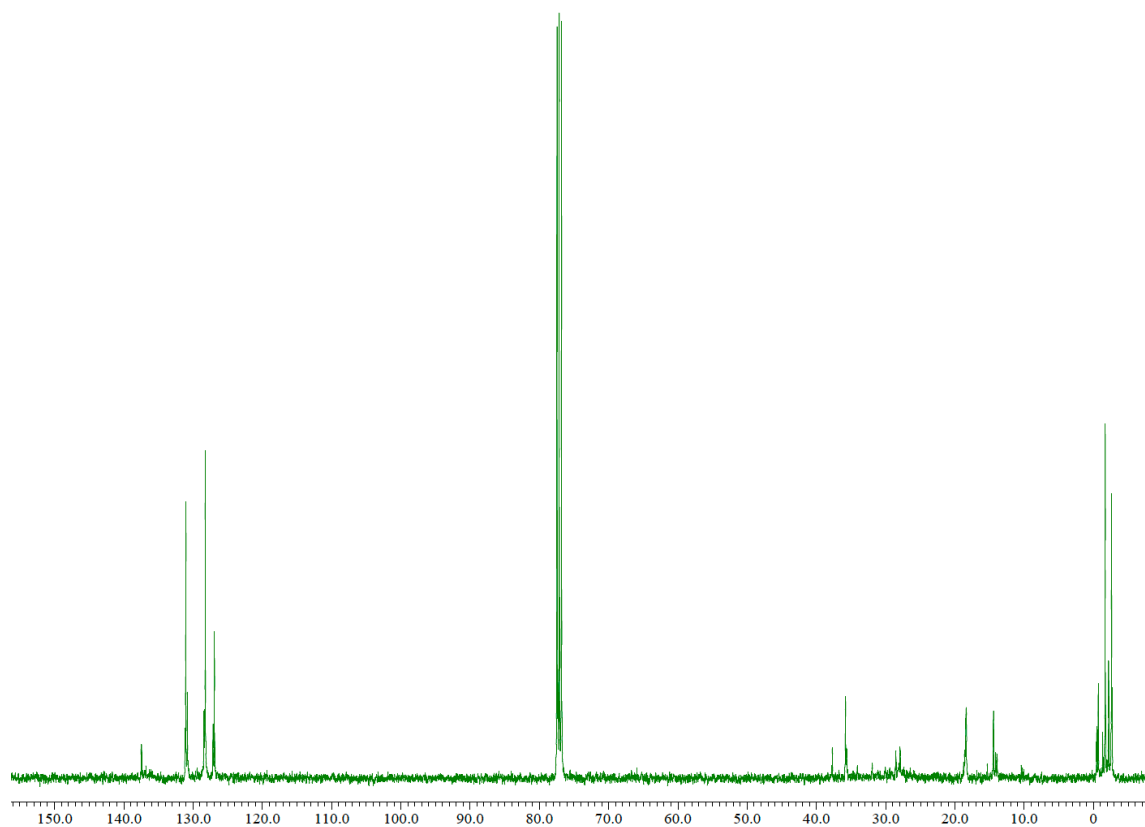
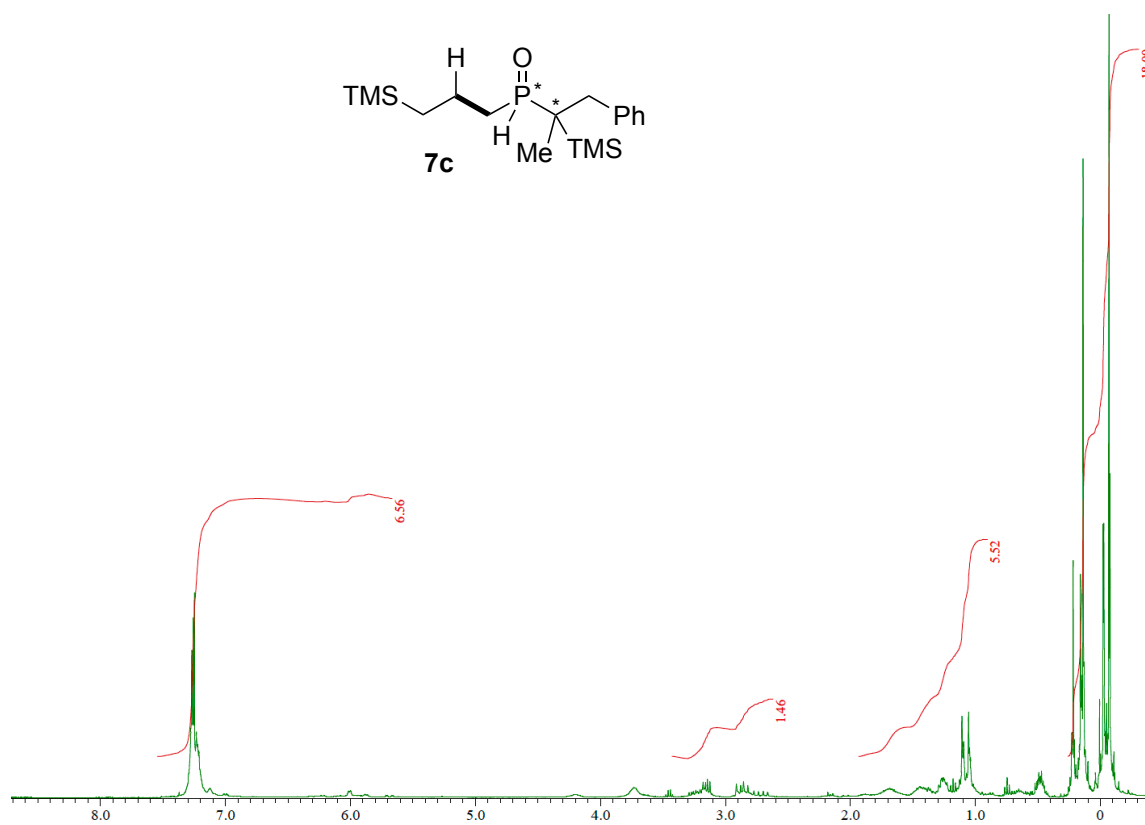
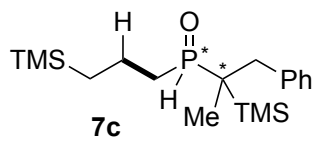


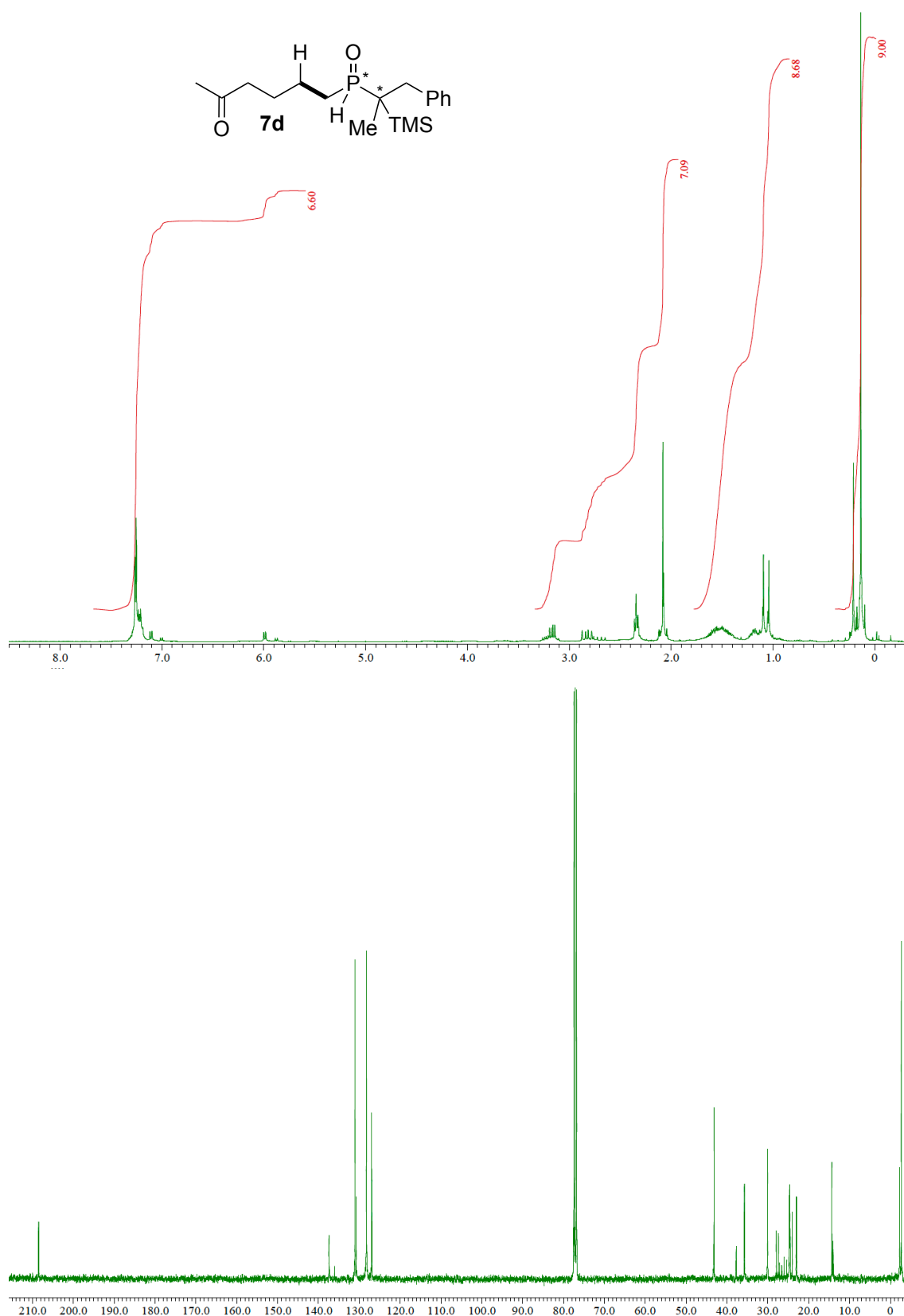


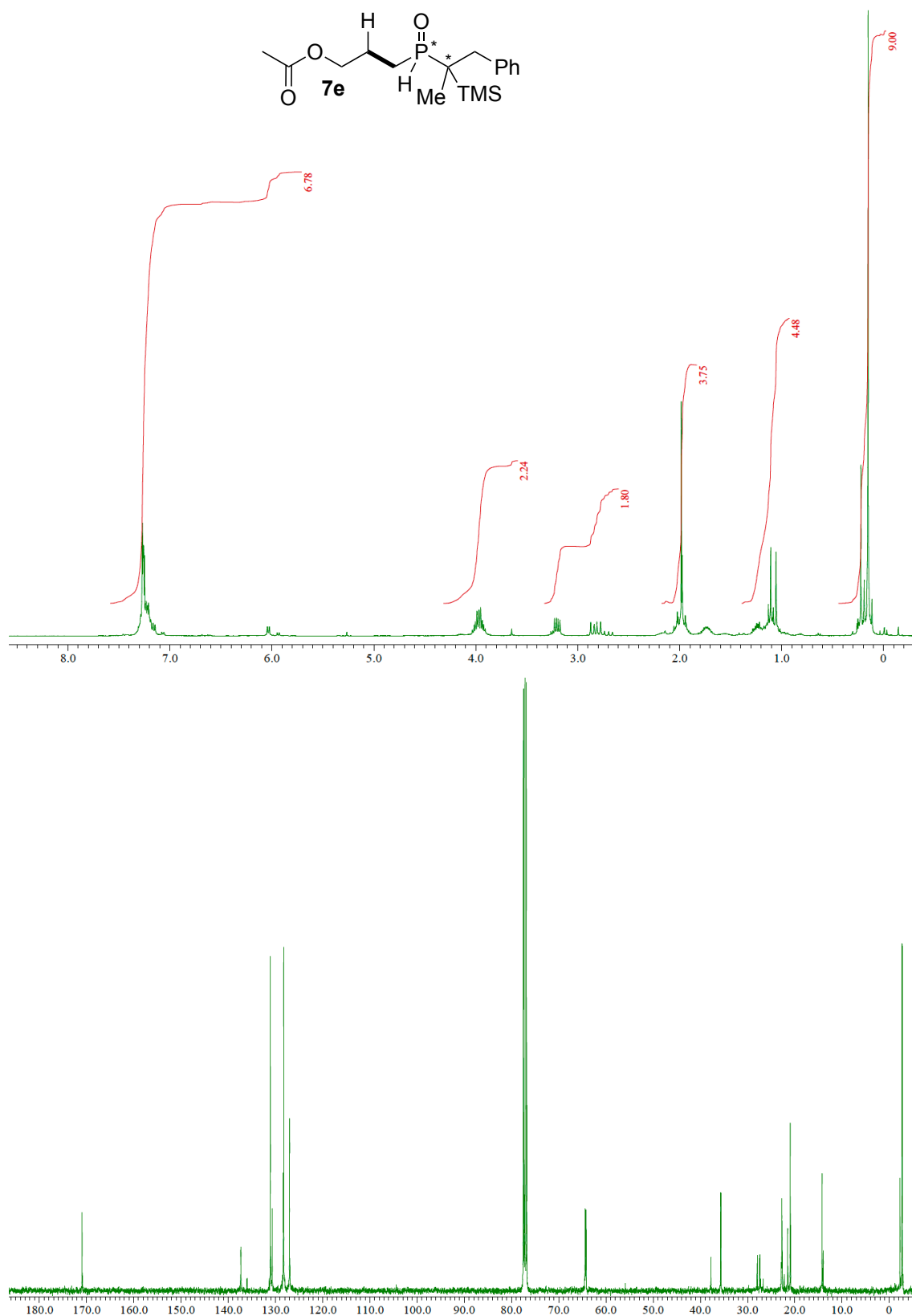
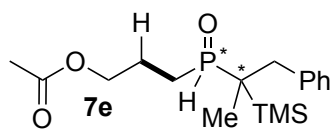


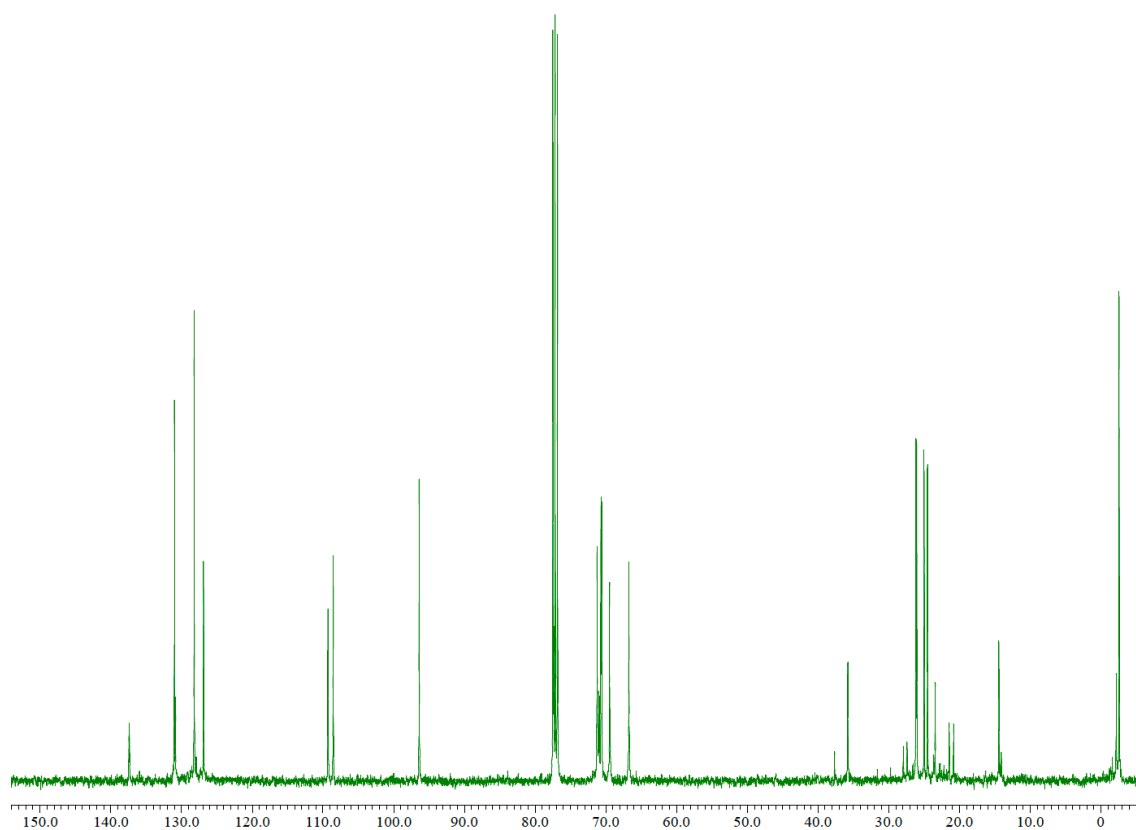
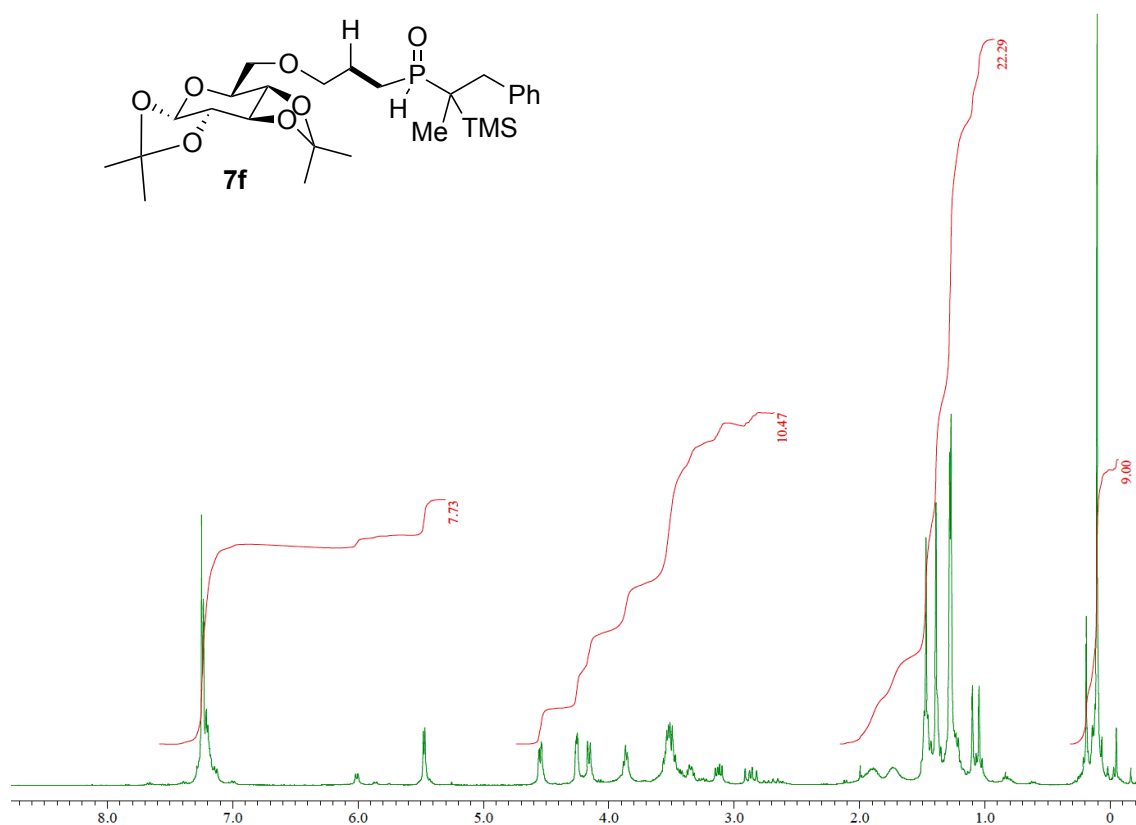
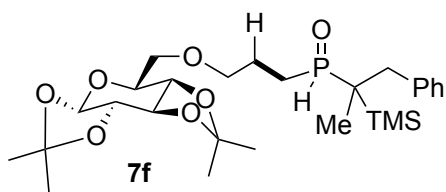


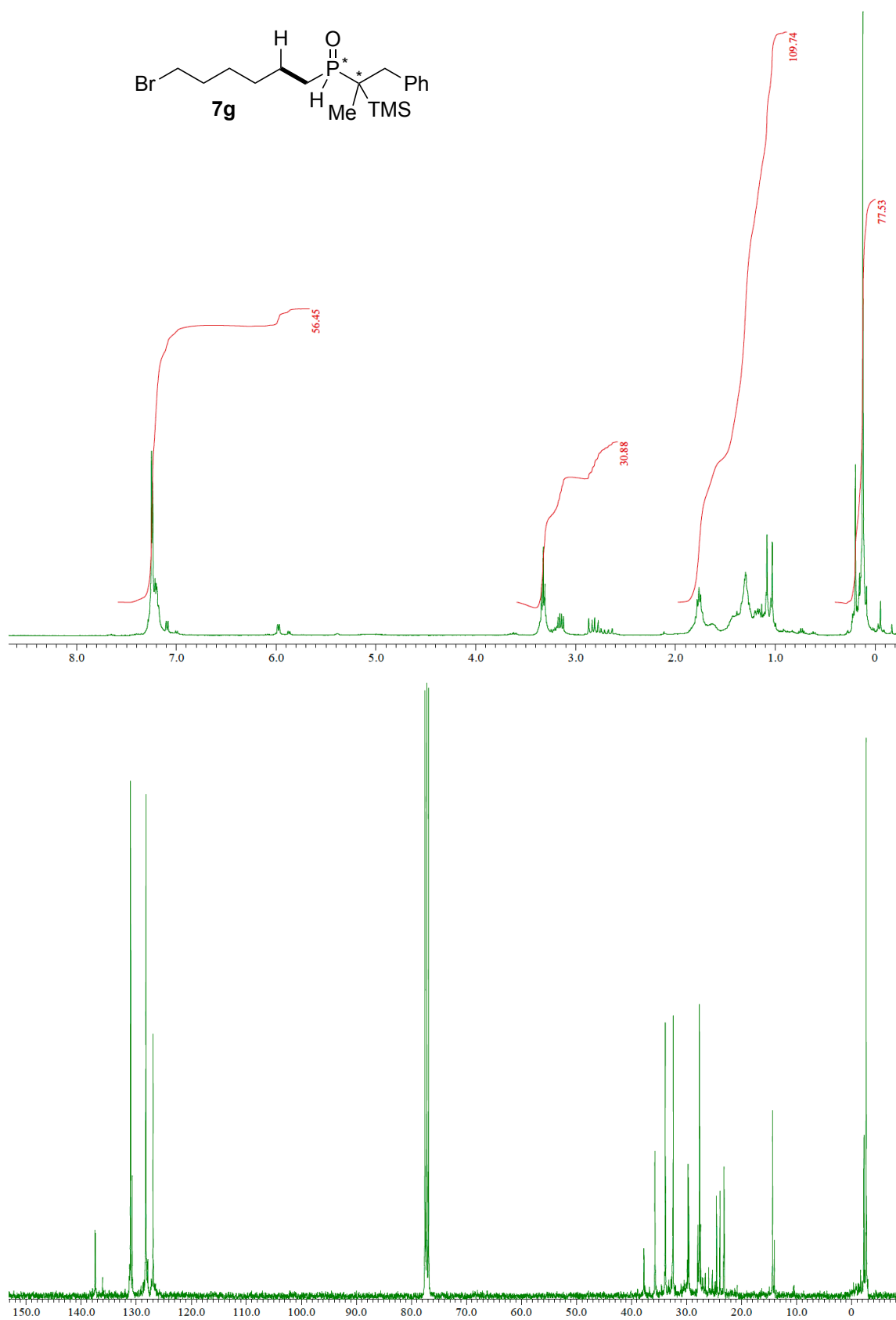
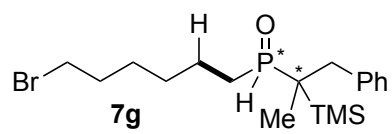


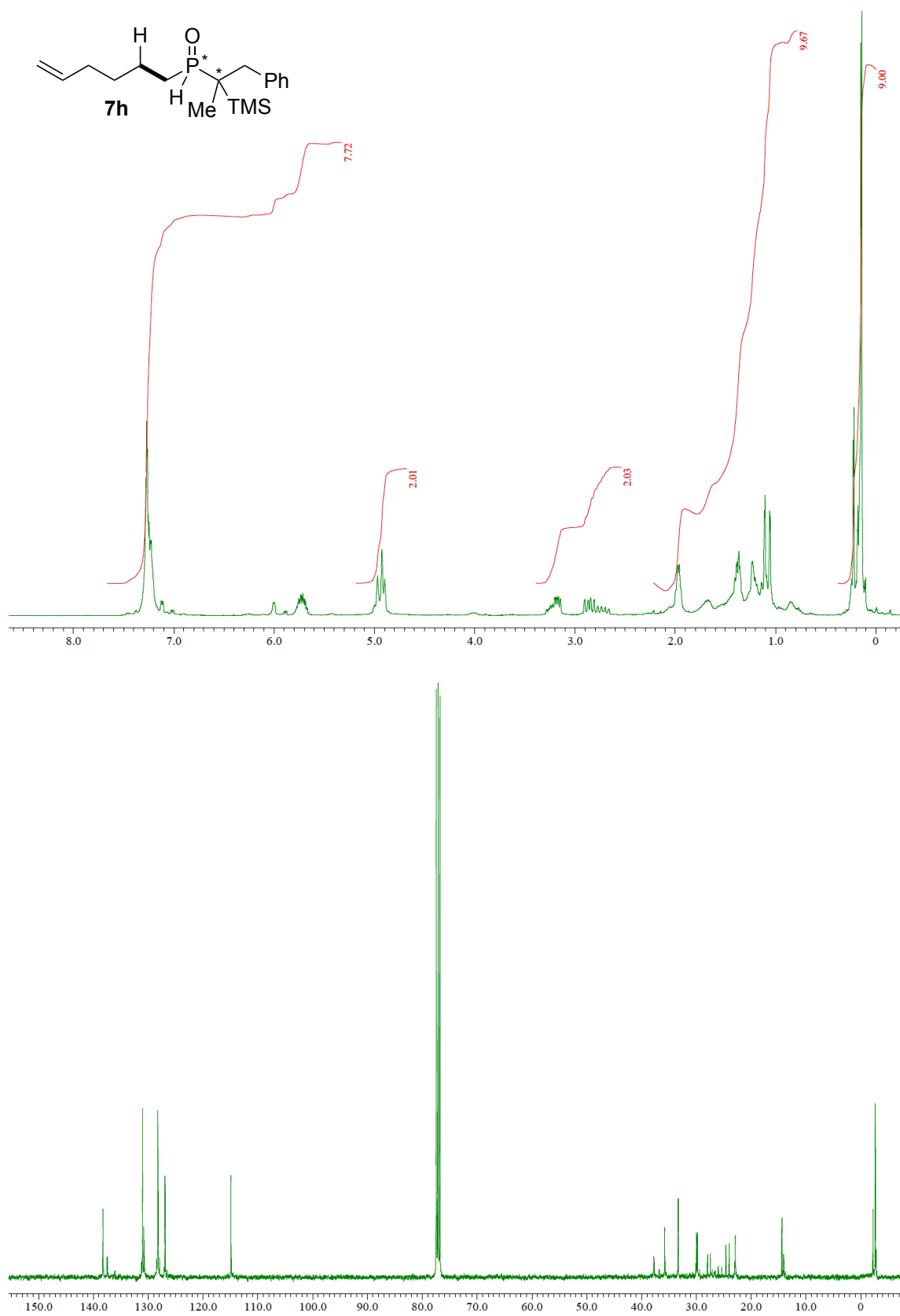


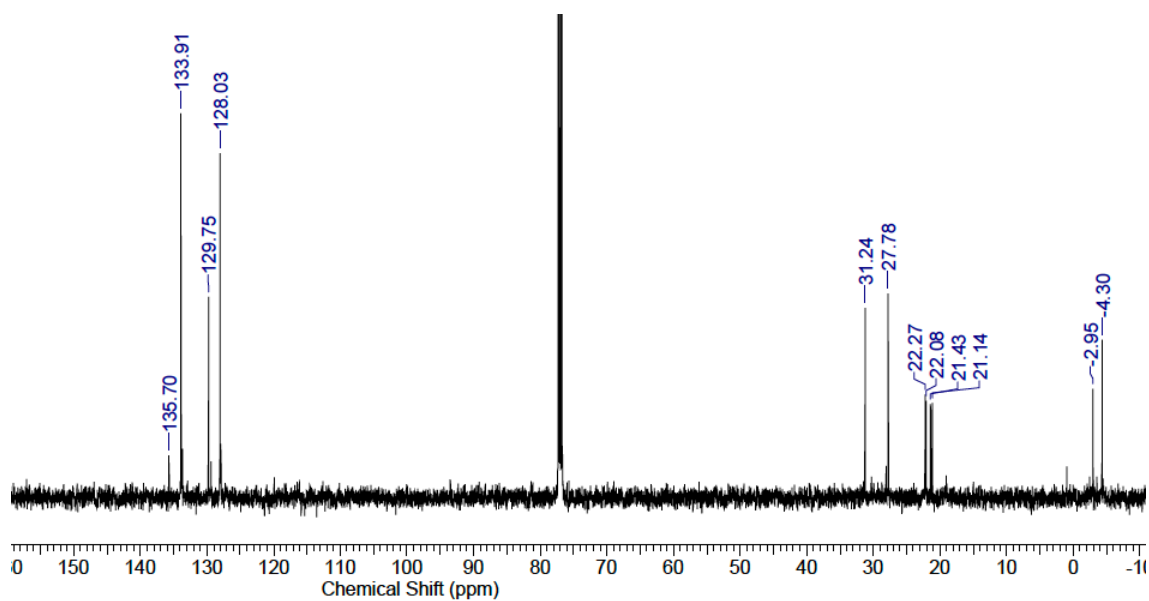
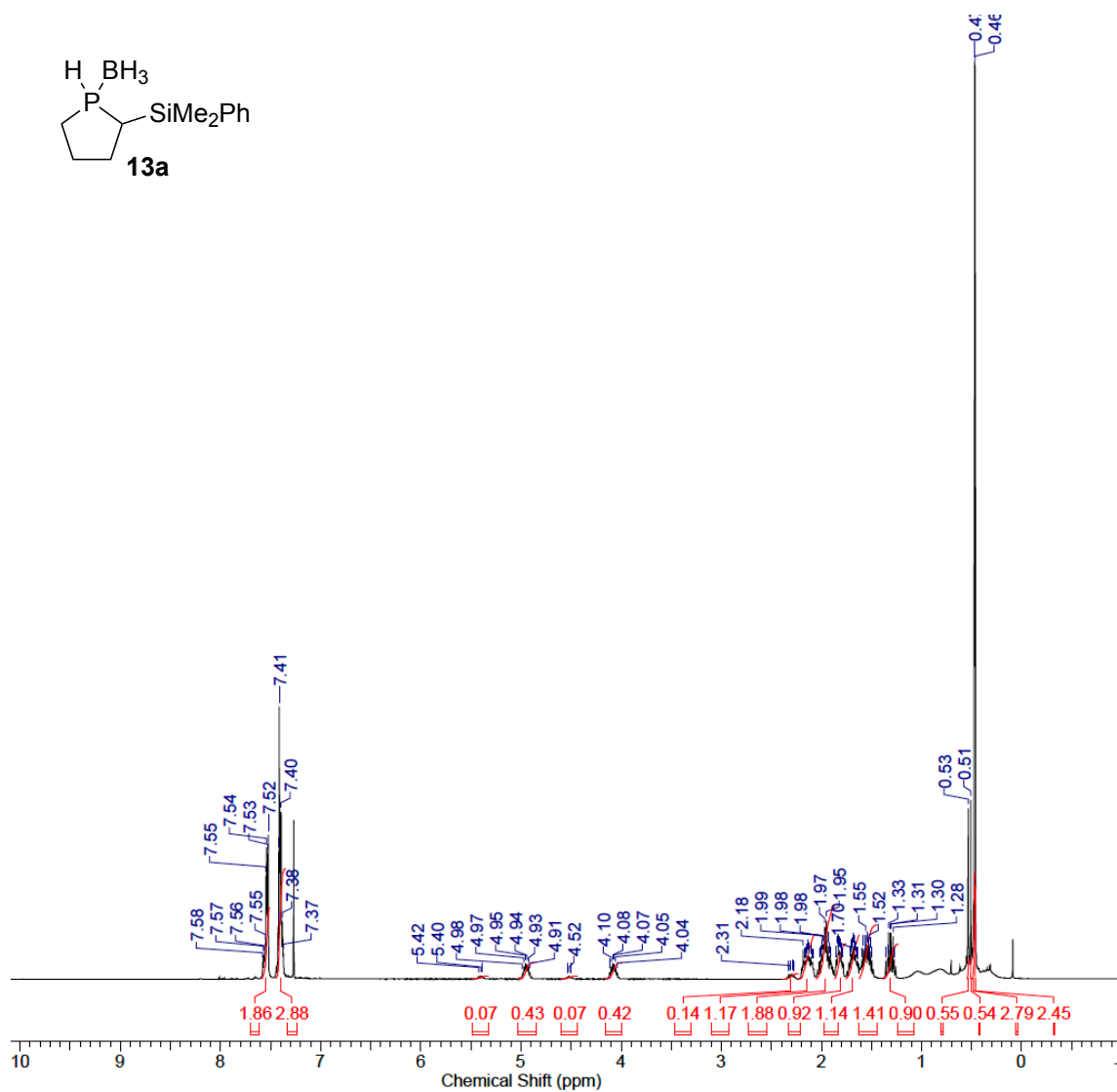
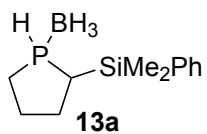


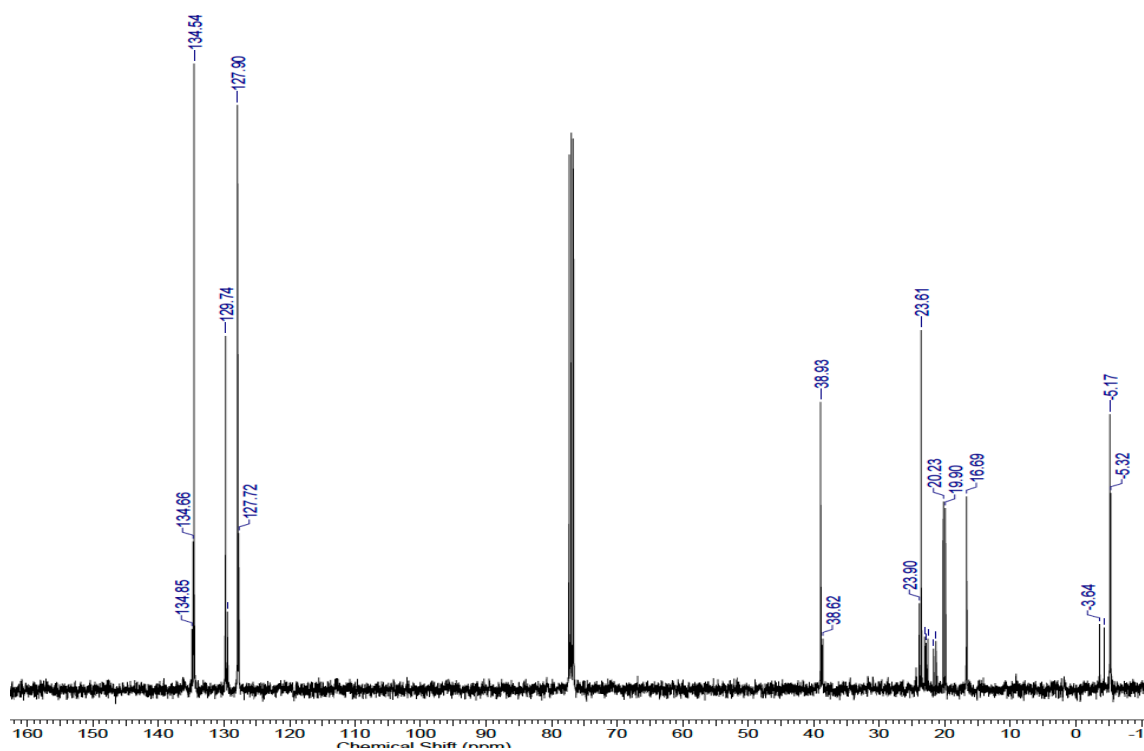
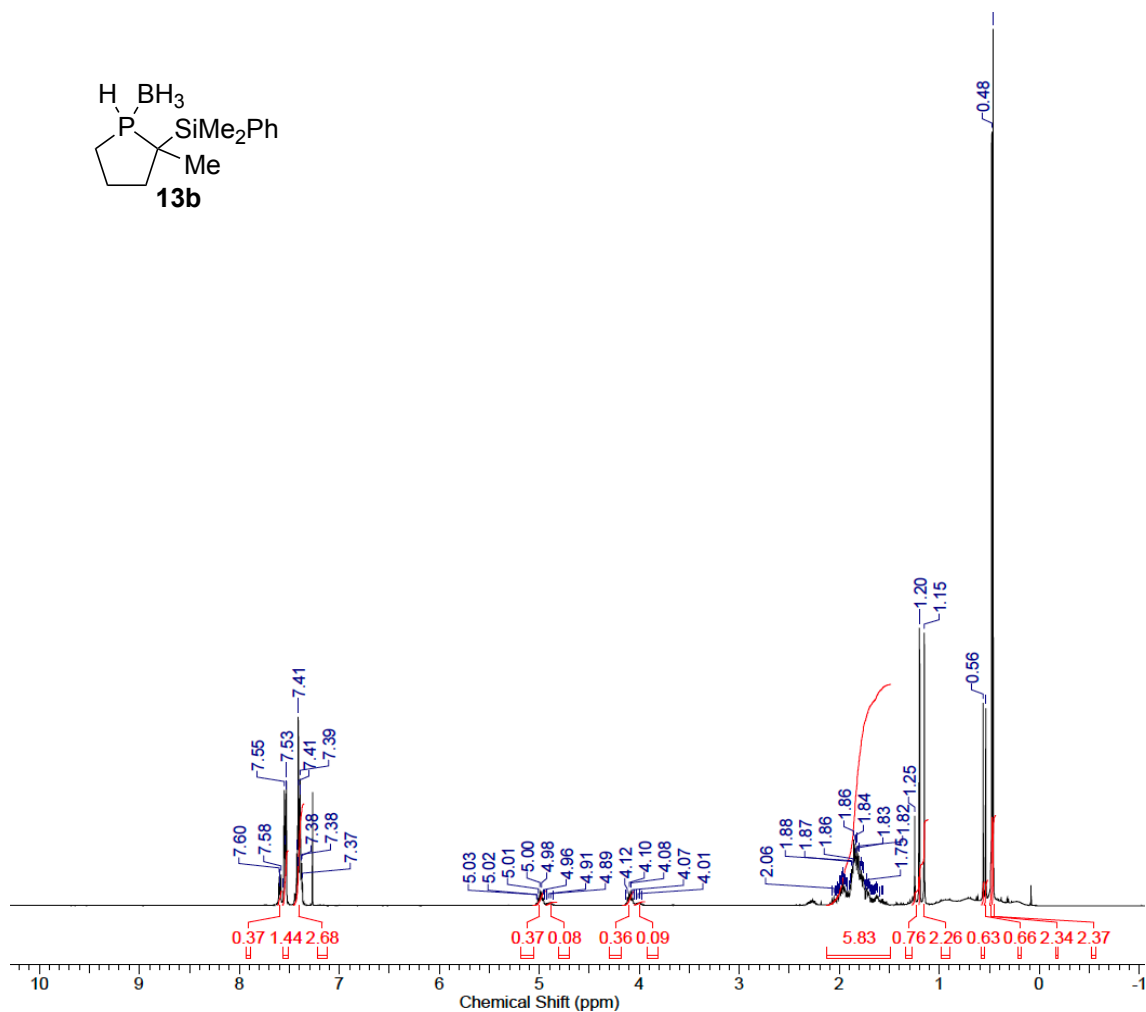
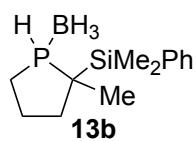


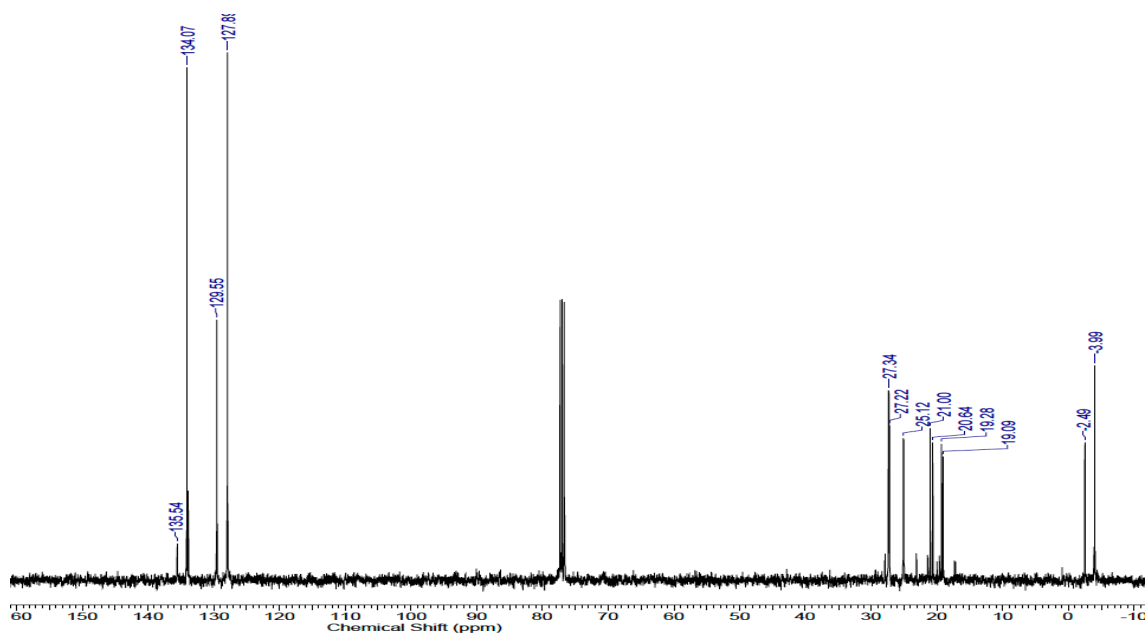
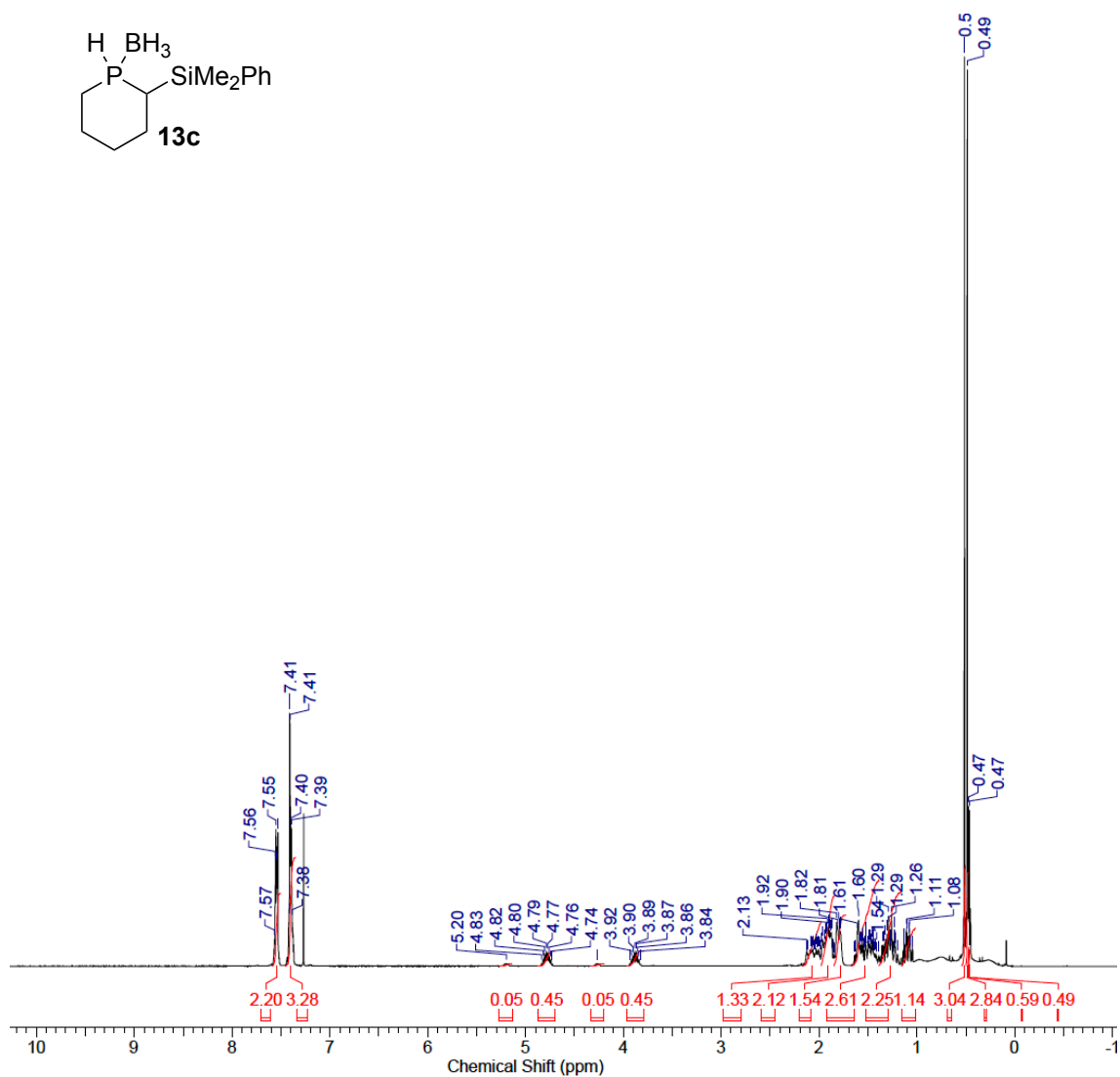
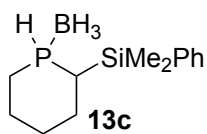












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