Supporting Information

Distinct reactivities of *Ortho*-chalcone-substituted Organophosphines with Activated Alkynes: Skeletal Editing or Periphery Modification

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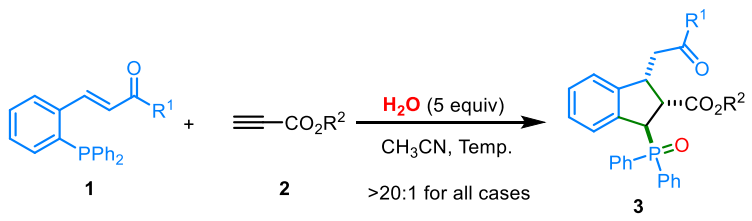
Table of Contents

1. General methods

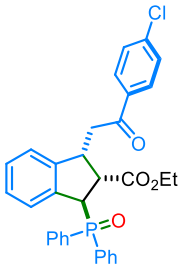
NMR spectra were recorded with tetramethylsilane as the internal standard. For compounds **3e-j** and **3n-r**, ^{1}H NMR spectra were recorded at 500 MHz (Bruker Avance). For other compounds, ^{1}H NMR spectra were recorded at 400 MHz (Bruker Avance). For compounds **3b**, **3e-j**, **3n-r**, **5a**, **7** and **10**, ^{13}C NMR spectra were recorded at 125 MHz (Bruker Avance). For other compounds, ^{13}C NMR spectra were recorded at 100 MHz (Bruker Avance). For compounds **3a**, **3c**, ^{31}P NMR spectra were recorded at 162 MHz (JNM-ECZ 400S/L1). For compound **15**, ^{31}P NMR spectra were recorded at 162 MHz (Bruker Avance). For other compounds, ^{31}P NMR spectra were recorded at 202 MHz (Bruker Avance). For compounds **3b**, ^{19}F NMR spectra were recorded at 471 MHz (Bruker Avance). For compound **5b**, ^{19}F NMR spectra were recorded at 376 MHz (Bruker Avance). ^{1}H NMR chemical shifts (δ) are reported in ppm relative to tetramethylsilane (TMS) with the solvent signal as the internal standard ($CDCl_3$ at 7.26 ppm, $(CD_3)_2SO$ at 2.50 ppm). ^{13}C NMR chemical shifts are reported in ppm from tetramethylsilane (TMS) with the solvent resonance as the internal standard ($CDCl_3$ at 77.00 ppm, $(CD_3)_2SO$ at 39.52 ppm). Data are given as: s (singlet), d (doublet), t (triplet), q (quartet), dd (double of doublet), br (broad) or m (multiplets), coupling constants (Hz) and integration. Flash column chromatography was carried out using silica gel eluting with ethyl acetate and petroleum ether. High resolution mass spectra were obtained with the Q-TOF-Premier mass spectrometer. Reactions were monitored by TLC and visualized with ultraviolet light. IR spectra were recorded on a Thermo Fisher Nicolet Avatar 360 FTIR spectrometer on a KBr beam splitter. All the solvents were used directly without any purification. (NOTE: *Ortho*-chalcone-substituted organophosphines could undergo biomolecular [2+2] cycloaddition slowly. For details, please see the sixth section on this ESI)

2. Experimental data for the formation of 3



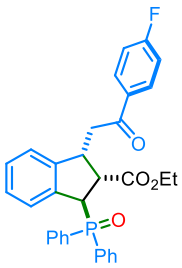
General procedure： To a 5.0 mL vial were successively added functionalized organic phosphine **1** (0.20 mmol), propiolic acid ester **2** (0.40 mmol, 2.0 equiv), H_2O (18 μL, 1.0 mmol) and 1.0 mL of CH_3CN. The resulting mixture was stirred at specified temperature until the

complete consumption of **1** as monitored by thin layer chromatography. And then, the reaction mixture was directly subjected to flash column chromatography on silica gel (petroleum ether/ethyl acetate) to afford the corresponding products **3**. For the formation of **3a**, **3c**, **3e**, **3f**, **3h**, **3i** and **3n**, the reactions were performed at 0 ^{o}C. For the formation of **3b**, **3d**, **3g**, **3j-m**, **3o**, **3p** and **3r-t**, the reactions were performed at 25 ^{o}C. For the formation of **3q**, the reaction was performed at 60 ^{o}C.



Ethyl 1-(2-(4-chlorophenyl)-2-oxoethyl)-3-(diphenylphosphoryl)-2,3-dihydro-1*H*-indene-2-carboxylate (**3a**)

White solid obtained by column chromatography (petroleum ether/ethyl acetate = 8:1 to 2:1); 54.2 mg, 50% yield, >20:1 dr; reaction time = 48 h; mp 138.2-139.1 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83-7.72 (m, 6H), 7.56-7.37 (m, 8H), 7.15 (t, *J* = 8.0 Hz, 1H), 7.06 (d, *J* = 8.0 Hz, 1H), 7.00 (t, *J* = 8.0 Hz, 1H), 6.65 (d, *J* = 8.0 Hz, 1H), 4.64 (q, *J* = 4.0 Hz, 1H), 4.08-4.06 (m, 1H), 3.99-3.92 (m, 1H), 3.73-3.58 (m, 2H), 3.33 (dd, J_1 = 20.0 Hz, J_2 = 12.0 Hz, 1H), 3.13 (dd, J_1 = 20.0 Hz, J_2 = 4.0 Hz, 1H), 0.92 (t, *J* = 8.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.3, 173.1 (d, *J* = 8.0 Hz, 1C), 145.1 (d, *J* = 6.0 Hz, 1C), 139.5, 136.7 (d, *J* = 4.0 Hz, 1C), 135.0, 132.2, 131.9 (dd, J_1 = 20.0 Hz, J_2 = 3.0 Hz, 1C), 131.8 (d, *J* = 5.0 Hz, 1C), 131.6 (q, *J* = 9.0 Hz, 1C), 130.9 (d, *J* = 68.0 Hz, 1C), 129.0 (d, *J* = 37.0 Hz, 1C), 128.5 (q, *J* = 2.0 Hz, 1C), 127.5 (dd, J_1 = 69.0 Hz, J_2 = 13.0 Hz, 1C), 125.3 (d, *J* = 3.0 Hz, 1C), 123.5 (d, *J* = 1.0 Hz, 1C), 60.9, 48.2, 47.8 (d, *J* = 70.0 Hz, 1C), 41.8 (d, *J* = 3.0 Hz, 1C), 40.6, 13.7; ^{31}P NMR (162 MHz, $CDCl_3$) δ 31.62; IR (KBr) ν 3054, 2949, 1736, 1186, 754 cm^{-1}. HRMS (ESI) calcd for $C_{32}H_{29}ClO_4P$ $[M+H]^+$: 543.1487, found: 543.1485.

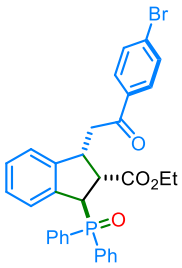


Ethyl

1-(diphenylphosphoryl)-3-(2-(4-fluorophenyl)-2-oxoethyl)-2,3-dihydro-1*H*-indene-2-carboxylate

(**3b**)

Yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 5:1 to 2:1); 43.1 mg, 41% yield, >20:1 dr; reaction time = 6 h; mp 66.8-67.6 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.71 (s, 1H), 8.65 (d, *J* = 8.0 Hz, 1H), 8.44 (d, *J* = 8.0 Hz, 1H), 8.10 (d, *J* = 12.0 Hz, 1H), 7.75-7.71 (m, 2H), 7.66-7.61 (m, 4H), 7.55 (d, *J* = 8.0 Hz, 1H), 7.45-7.34 (m, 4H), 7.32-7.28 (m, 1H), 7.25-7.11 (m, 5H), 6.52 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 195.8, 173.1 (d, *J* = 7.5 Hz, 1C), 165.6 (d, *J* = 252.5 Hz, 1C), 145.2 (d, *J* = 6.0 Hz, 1C), 136.6 (d, *J* = 5.0 Hz, 1C), 133.1 (d, *J* = 4.0 Hz, 1C), 132.0 (dd, J_1 = 25.0 Hz, J_2 = 1.0 Hz, 1C), 131.5 (q, *J* = 9.0 Hz, 1C), 131.2 (d, *J* = 11.0 Hz, 1C), 130.4 (d, *J* = 10.0 Hz, 1C), 128.6-128.4 (m, 1C), 127.8 (d, *J* = 1.0 Hz, 1C), 127.1 (d, *J* = 2.5 Hz, 1C), 125.2 (d, *J* = 2.5 Hz, 1C), 123.4 (d, *J* = 1.0 Hz, 1C), 115.5 (d, *J* = 22.5 Hz, 1C), 60.8, 48.2, 47.8 (d, *J* = 70.0 Hz, 1C), 41.8 (d, *J* = 2.5 Hz, 1C), 40.5, 13.6; ^{19}F NMR (471 MHz, $CDCl_3$) δ -105.07; ^{31}P NMR (202 MHz, $CDCl_3$) δ 30.99; IR (KBr) ν 3062, 2990, 1726, 1684, 1193, 729 cm^{-1}. HRMS (ESI) calcd for $C_{32}H_{29}FO_4P$ $[M+H]^+$: 527.1782, found: 527.1785.



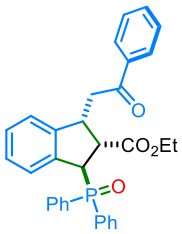
Ethyl

1-(2-(4-bromophenyl)-2-oxoethyl)-3-(diphenylphosphoryl)-2,3-dihydro-1*H*-indene-2-carboxylate

(**3c**)

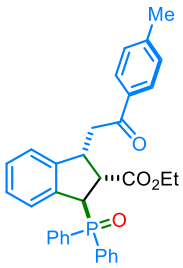
White solid obtained by column chromatography (petroleum ether/ethyl acetate = 8:1 to 2:1); 59.1 mg, 50% yield, >20:1 dr; reaction time = 48 h; mp 156.4-157.2 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ

7.81-7.73 (m, 6H), 7.55 (d, J = 8.0 Hz, 3H), 7.47 (dd, J_1 = 16.0 Hz, J_2 = 4.0 Hz, 5H), 7.15 (t, J = 8.0 Hz, 1H), 7.06 (d, J = 8.0 Hz, 1H), 7.00 (t, J = 8.0 Hz, 1H), 6.65 (d, J = 8.0 Hz, 1H), 4.65 (q, J = 4.0 Hz, 1H), 4.07-4.06 (m, 1H), 3.99-3.92 (m, 1H), 3.70-3.59 (m, 2H), 3.33 (dd, J_1 = 16.0 Hz, J_2 = 8.0 Hz, 1H), 3.13 (dd, J_1 = 16.0 Hz, J_2 = 4.0 Hz, 1H), 0.91 (t, J = 8.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.5, 173.1 (d, J = 9.0 Hz, 1C), 145.1 (d, J = 6.0 Hz, 1C), 136.7 (d, J = 5.0 Hz, 1C), 135.3, 132.1, 132.1 (d, J = 2.0 Hz, 1C), 131.8 (d, J = 5.0 Hz, 1C), 131.6 (q, J = 9.0 Hz, 1C), 131.2, 130.5, 129.3, 128.5 (q, J = 8.0 Hz, 1C), 128.2, 127.9 (d, J = 2.0 Hz, 1C), 127.2 (d, J = 2.0 Hz, 1C), 60.9, 48.2, 47.8 (d, J = 70.0 Hz, 1C), 41.8 (d, J = 3.0 Hz, 1C), 40.6, 13.7; ^{31}P NMR (162 MHz, $CDCl_3$) δ 31.62; IR (KBr) ν 3053, 2950, 1734, 1186, 753 cm^{-1}. HRMS (ESI) calcd for $C_{32}H_{29}BrO_4P$ $[M+H]^+$: 587.0981, found: 587.0984.



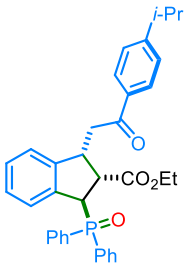
Ethyl 1-(diphenylphosphoryl)-3-(2-oxo-2-phenylethyl)-2,3-dihydro-1*H*-indene-2-carboxylate (**3d**)

Light yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 5:1 to 2:1); 67.1 mg, 66% yield, >20:1 dr; reaction time = 54 h; mp 66.7-67.4 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, J = 4.0 Hz, 2H), 7.79-7.72 (m, 4H), 7.55-7.40 (m, 9H), 7.16 (t, J = 8.0 Hz, 1H), 7.07 (d, J = 8.0 Hz, 1H), 7.01 (t, J = 4.0 Hz, 1H), 6.67 (d, J = 8.0 Hz, 1H), 4.66 (q, J = 4.0 Hz, 1H), 4.10-4.04 (m, 1H), 4.00-3.93 (m, 1H), 3.74-3.57 (m, 2H), 3.36 (dd, J_1 = 20.0 Hz, J_2 = 12.0 Hz, 1H), 3.18 (dd, J_1 = 16.0 Hz, J_2 = 4.0 Hz, 1H), 0.90 (t, J = 4.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.4, 173.2 (d, J = 8.0 Hz, 1C), 145.3 (d, J = 6.0 Hz, 1C), 138.2, 136.7 (d, J = 5.0 Hz, 1C), 136.6, 133.1, 132.0 (dd, J_1 = 20.0 Hz, J_2 = 2.0 Hz, 1C), 131.6 (dd, J_1 = 15.0 Hz, J_2 = 9.0 Hz, 1C), 131.2 (d, J = 23.0 Hz, 1C), 130.4, 128.5 (q, J = 6.0 Hz, 1C), 127.8, 127.5 (dd, J_1 = 72.0 Hz, J_2 = 3.0 Hz, 1C), 125.3 (d, J = 4.0 Hz, 1C), 123.5 (d, J = 1.0 Hz, 1C), 60.9, 48.2, 47.8 (d, J = 69.0 Hz, 1C), 41.9 (d, J = 3.0 Hz, 1C), 40.6, 13.6; ^{31}P NMR (202 MHz, $CDCl_3$) δ 31.01; IR (KBr) ν 3060, 2949, 1726, 1193, 754 cm^{-1}. HRMS (ESI) calcd for $C_{32}H_{30}O_4P$ $[M+H]^+$: 509.1876, found: 509.1882.



Ethyl 1-(diphenylphosphoryl)-3-(2-oxo-2-(*p*-tolyl)ethyl)-2,3-dihydro-1*H*-indene-2-carboxylate (**3e**)

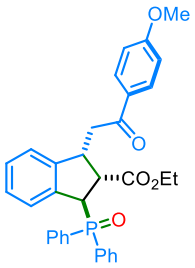
Yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 8:1 to 2:1); 49.8 mg, 48% yield, >20:1 dr; reaction time = 72 h; mp 59.2-60.3 ℃; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.79-7.71 (m, 6H), 7.54-7.41 (m, 6H), 7.18 (d, *J* = 10.0 Hz, 2H), 7.12 (t, *J* = 5.0 Hz, 1H), 7.05 (d, *J* = 10.0 Hz, 1H), 6.97 (t, *J* = 5.0 Hz, 1H), 6.65 (d, *J* = 5.0 Hz, 1H), 4.66 (q, *J* = 5.0 Hz, 1H), 4.10-4.06 (m, 1H), 3.98-3.93 (m, 1H), 3.72-3.66 (m, 1H), 3.63-3.57 (m, 1H), 3.31 (dd, J_1 = 20.0 Hz, J_2 = 10.0 Hz, 1H), 3.13 (dd, J_1 = 15.0 Hz, J_2 = 5.0 Hz, 1H), 2.34 (s, 3H), 0.87 (t, *J* = 10.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 196.9, 173.0 (d, *J* = 9.0 Hz, 1C), 145.3 (d, *J* = 9.0 Hz, 1C), 143.7, 136.6 (d, *J* = 5.0 Hz, 1C), 134.1, 131.9 (dd, J_1 = 25.0 Hz, J_2 = 1.0 Hz, 1C), 131.9, 131.4 (dd, J_1 = 19.0 Hz, J_2 = 9.0 Hz, 1C), 131.1 (d, *J* = 9.0 Hz, 1C), 129.1, 128.4 (q, *J* = 9.0 Hz, 1C), 127.7 (d, *J* = 4.0 Hz, 1C), 127.0 (d, *J* = 1.0 Hz, 1C), 125.2 (d, *J* = 2.5 Hz, 1C), 123.5 (d, *J* = 1.0 Hz, 1C), 60.7, 48.2, 47.8 (d, *J* = 69.0 Hz, 1C), 41.8 (d, *J* = 2.5 Hz, 1C), 40.4, 21.4, 13.5; ^{31}P NMR (202 MHz, $CDCl_3$) δ 31.22; IR (KBr) ν 3058, 2925, 1725, 1680, 1190, 754 cm^{-1}. HRMS (ESI) calcd for $C_{33}H_{32}O_4P$ $[M+H]^+$: 523.2033, found: 523.2037.



Ethyl 1-(diphenylphosphoryl)-3-(2-(4-isopropylphenyl)-2-oxoethyl)-2,3-dihydro-1*H*-indene-2-carboxylate (**3f**)

White solid obtained by column chromatography (petroleum ether/ethyl acetate = 8:1 to 2:1); 67.6 mg, 61% yield, >20:1 dr; reaction time = 72 h; mp 74.4-75.6 ℃; ^{1}H NMR (500 MHz, $CDCl_3$) δ

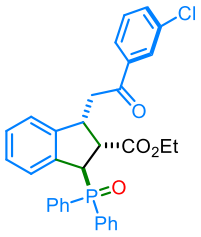
7.82-7.74 (m, 6H), 7.57-7.54 (m, 1H), 7.50-7.42 (m, 5H), 7.26 (d, *J* = 8.0 Hz, 2H), 7.15 (t, *J* = 8.0 Hz, 1H), 7.07 (d, *J* = 8.0 Hz, 1H), 6.99 (t, *J* = 8.0 Hz, 1H), 6.67 (d, *J* = 8.0 Hz, 1H), 4.65 (q, *J* = 4.0 Hz, 1H), 4.10-4.06 (m, 1H), 3.99-3.93 (m, 1H), 3.73-3.59 (m, 2H), 3.34 (dd, J_1 = 12.0 Hz, J_2 = 4.0 Hz, 1H), 3.15 (dd, J_1 = 16.0 Hz, J_2 = 4.0 Hz, 1H), 2.95-2.90 (m, 1H), 1.24 (s, 3H), 1.22 (s, 3H), 0.90 (t, *J* = 8.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 197.1, 173.1 (d, *J* = 8.0 Hz, 1C), 154.5, 145.4 (d, *J* = 5.0 Hz, 1C), 136.7 (d, *J* = 5.0 Hz, 1C), 134.5, 131.9 (dd, J_1 = 25.0 Hz, J_2 = 1.0 Hz, 1C), 131.6 (dd, J_1 = 16.0 Hz, J_2 = 7.5 Hz, 1C), 131.3 (d, *J* = 10.0 Hz, 1C), 128.5 (q, *J* = 11.0 Hz, 1C), 128.0, 127.8 (d, *J* = 2.5 Hz, 1C), 127.1 (d, *J* = 2.5 Hz, 1C), 126.6, 125.3 (d, *J* = 2.5 Hz, 1C), 123.6 (d, *J* = 1.0 Hz, 1C), 60.8, 48.3, 47.8 (d, *J* = 70.0 Hz, 1C), 41.9 (d, *J* = 4.0 Hz, 1C), 40.5, 34.1, 23.5, 13.6; ^{31}P NMR (202 MHz, $CDCl_3$) δ 31.08; IR (KBr) ν 3058, 2961, 1725, 1681, 1191, 753 cm^{-1}. HRMS (ESI) calcd for $C_{35}H_{36}O_4P$ $[M+H]^+$: 551.2346, found: 551.2351.



Ethyl 1-(diphenylphosphoryl)-3-(2-(4-methoxyphenyl)-2-oxoethyl)-2,3-dihydro-1*H*-indene-2-carboxylate (**3g**)

Yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 5:1 to 2:1); 48.7 mg, 45% yield, >20:1 dr; reaction time = 14 h; mp 177.8-178.9 ℃; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.86 (d, *J* = 10.0 Hz, 2H), 7.80-7.72 (m, 4H), 7.58-7.54 (m, 1H), 7.52-7.42 (m, 5H), 7.15 (t, *J* = 10.0 Hz, 1H), 7.06 (d, *J* = 5.0 Hz, 1H), 7.00 (t, *J* = 10.0 Hz, 1H), 6.88 (d, *J* = 10.0 Hz, 2H), 6.66 (d, *J* = 5.0 Hz, 1H), 4.65 (q, *J* = 5.0 Hz, 1H), 4.09-4.05 (m, 1H), 3.98-3.92 (m, 1H), 3.83 (s, 3H), 3.74-3.68 (m, 1H), 3.65-3.60 (m, 1H), 3.29 (dd, J_1 = 20.0 Hz, J_2 = 10.0 Hz, 1H), 3.12 (dd, J_1 = 15.0 Hz, J_2 = 5.0 Hz, 1H), 0.91 (t, *J* = 10.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 196.0, 173.2 (d, *J* = 9.0 Hz, 1C), 163.4, 145.5 (d, *J* = 6.0 Hz, 1C), 136.7 (d, *J* = 5.0 Hz, 1C), 132.0 (dd, J_1 = 25.0 Hz, J_2 = 2.5 Hz, 1C), 131.6 (dd, J_1 = 19.0 Hz, J_2 = 9.0 Hz, 1C), 131.2 (d, *J* = 10.0 Hz, 1C), 130.1, 129.8, 128.5 (dd, J_1 = 11.0 Hz, J_2 = 9.0 Hz, 1C), 127.8 (d, *J* = 2.5 Hz, 1C), 127.1 (d, *J* = 2.5 Hz, 1C), 125.3 (d, *J* = 2.5 Hz, 1C), 123.6, 113.7, 60.8, 55.4, 48.3, 47.9 (d, *J* = 69.0 Hz, 1C), 42.0

(d, J = 4.0 Hz, 1C), 40.3, 13.7; ^{31}P NMR (202 MHz, $CDCl_3$) δ 31.24; IR (KBr) ν 3063, 2995, 1725, 1674, 1186, 754 cm^{-1}. HRMS (ESI) calcd for $C_{33}H_{32}O_5P$ $[M+H]^+$: 539.1982, found: 539.1985.

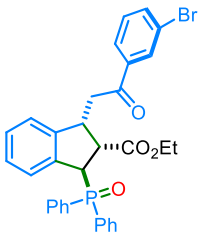


Ethyl

1-(2-(3-chlorophenyl)-2-oxoethyl)-3-(diphenylphosphoryl)-2,3-dihydro-1*H*-indene-2-carboxylate

(**3h**)

White solid obtained by column chromatography (petroleum ether/ethyl acetate = 8:1 to 2:1); 36.5 mg, 34% yield, >20:1 dr; reaction time = 72 h; mp 133.9-134.8 ℃; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.86 (t, J = 5.0 Hz, 1H), 7.81-7.73 (m, 5H), 7.59-7.56 (m, 1H), 7.53-7.43 (m, 6H), 7.36 (t, J = 10.0 Hz, 1H), 7.17 (t, J = 10.0 Hz, 1H), 7.07 (d, J = 5.0 Hz, 1H), 7.01 (t, J = 10.0 Hz, 1H), 6.65 (d, J = 10.0 Hz, 1H), 4.65 (q, J = 5.0 Hz, 1H), 4.10-4.05 (m, 1H), 3.99-3.93 (m, 1H), 3.72-3.60 (m, 2H), 3.35 (dd, J_1 = 20.0 Hz, J_2 = 10.0 Hz, 1H), 3.15 (dd, J_1 = 20.0 Hz, J_2 = 5.0 Hz, 1H), 0.93 (t, J = 10.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 196.3, 173.1 (d, J = 9.0 Hz, 1C), 145.1 (d, J = 5.0 Hz, 1C), 138.2, 136.7 (d, J = 5.0 Hz, 1C), 134.9, 133.0, 132.1, 132.0 (dd, J_1 = 25.0 Hz, J_2 = 3.0 Hz, 1C), 131.6 (dd, J_1 = 15.0 Hz, J_2 = 7.5 Hz, 1C), 131.3 (d, J = 14.0 Hz, 1C), 129.9, 128.6 (t, J = 11.0 Hz, 1C), 128.0, 127.3 (d, J = 2.5 Hz, 1C), 125.9, 125.4 (d, J = 4.0 Hz, 1C), 123.5 (d, J = 1.0 Hz, 1C), 60.9, 48.2, 47.8 (d, J = 70.0 Hz, 1C), 41.8 (d, J = 4.0 Hz, 1C), 40.8, 13.7; ^{31}P NMR (202 MHz, $CDCl_3$) δ 30.90; IR (KBr) ν 3058, 1727, 1688, 1182, 756 cm^{-1}. HRMS (ESI) calcd for $C_{32}H_{29}ClO_4P$ $[M+H]^+$: 543.1487, found: 543.1490.



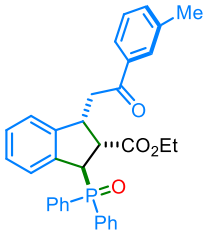
Ethyl

1-(2-(3-bromophenyl)-2-oxoethyl)-3-(diphenylphosphoryl)-2,3-dihydro-1*H*-indene-2-carboxylate

(**3i**)

White solid obtained by column chromatography (petroleum ether/ethyl acetate = 5:1 to 2:1); 41.8

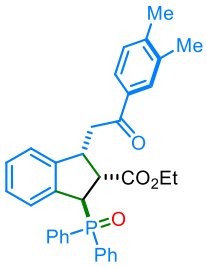
mg, 36% yield, >20:1 dr; reaction time = 72 h; mp 130.4-131.2 ℃; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.81-7.73 (m, 5H), 7.65 (d, *J* = 10.0 Hz, 1H), 7.57 (t, *J* = 10.0 Hz, 1H), 7.53-7.44 (m, 5H), 7.30 (t, *J* = 10.0 Hz, 1H), 7.17 (t, *J* = 10.0 Hz, 1H), 7.07 (d, *J* = 10.0 Hz, 1H), 7.01 (t, *J* = 10.0 Hz, 1H), 6.65 (d, *J* = 10.0 Hz, 1H), 4.64 (q, *J* = 5.0 Hz, 1H), 4.09-4.05 (m, 1H), 3.98-3.93 (m, 1H), 3.72-3.60 (m, 2H), 3.34 (dd, J_1 = 20.0 Hz, J_2 = 10.0 Hz, 1H), 3.14 (dd, J_1 = 20.0 Hz, J_2 = 5.0 Hz, 1H), 0.93 (t, *J* = 5.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 196.2, 173.2 (d, *J* = 7.5 Hz, 1C), 145.2 (d, *J* = 6.0 Hz, 1C), 138.4, 136.8 (d, *J* = 5.0 Hz, 1C), 136.0, 132.1 (dd, J_1 = 25.0 Hz, J_2 = 1.0 Hz, 1C), 131.7 (q, *J* = 9.0 Hz, 1C), 131.4 (d, *J* = 14.0 Hz, 1C), 131.0, 130.3, 128.6 (t, *J* = 11.0 Hz, 1C), 128.0 (d, *J* = 2.5 Hz, 1C), 127.3 (d, *J* = 1.0 Hz, 1C), 126.4, 125.4 (d, *J* = 2.5 Hz, 1C), 123.6 (d, *J* = 1.0 Hz, 1C), 123.0, 61.0, 48.3, 47.9 (d, *J* = 70.0 Hz, 1C), 41.9 (d, *J* = 4.0 Hz, 1C), 40.9, 13.8; ^{31}P NMR (202 MHz, $CDCl_3$) δ 30.79; IR (KBr) ν 3057, 2909, 1727, 1688, 1183, 756 cm^{-1}. HRMS (ESI) calcd for $C_{32}H_{29}BrO_4P$ $[M+H]^+$: 587.0981, found: 587.0983.



Ethyl 1-(diphenylphosphoryl)-3-(2-oxo-2-(*m*-tolyl)ethyl)-2,3-dihydro-1*H*-indene-2-carboxylate (**3j**)

Yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 5:1 to 2:1); 44.7 mg, 43% yield, >20:1 dr; reaction time = 8 h; mp 87.4-88.5 ℃; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.81-7.72 (m, 4H), 7.70 (s, 1H), 7.67 (d, *J* = 5.0 Hz, 1H), 7.58-7.55 (m, 1H), 7.53-7.43 (m, 5H), 7.34 (d, *J* = 10.0 Hz, 1H), 7.29 (t, *J* = 10.0 Hz, 1H), 7.16 (t, *J* = 10.0 Hz, 1H), 7.07 (d, *J* = 5.0 Hz, 1H), 7.00 (t, *J* = 10.0 Hz, 1H), 6.66 (d, *J* = 10.0 Hz, 1H), 4.65 (q, *J* = 5.0 Hz, 1H), 4.10-4.06 (m, 1H), 3.99-3.93 (m, 1H), 3.74-3.68 (m, 1H), 3.66-3.59 (m, 1H), 3.34 (dd, J_1 = 20.0 Hz, J_2 = 10.0 Hz, 1H), 3.16 (dd, J_1 = 20.0 Hz, J_2 = 5.0 Hz, 1H), 2.36 (s, 3H), 0.91 (t, *J* = 10.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 197.7, 173.2 (d, *J* = 7.5 Hz, 1C), 145.4 (d, *J* = 5.0 Hz, 1C), 138.3, 136.7 (d, *J* = 5.0 Hz, 1C), 136.7, 133.8, 132.0 (dd, J_1 = 25.0 Hz, J_2 = 2.5 Hz, 1C), 132.0, 131.6 (dd, J_1 = 19.0 Hz, J_2 = 9.0 Hz, 1C), 131.3 (d, *J* = 9.0 Hz, 1C), 130.6, 128.6-128.4 (m, 1C), 127.9 (d, *J* = 2.5 Hz, 1C), 127.1 (d, *J* = 2.5 Hz, 1C), 125.3 (d, *J* = 2.5 Hz, 1C), 125.0, 123.6 (d, *J* = 1.0 Hz, 1C), 60.9, 48.3, 47.8 (d, *J* = 69.0 Hz, 1C), 41.9 (d, *J* = 4.0 Hz, 1C), 40.7, 21.3, 13.7; ^{31}P NMR (202 MHz,

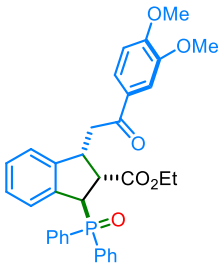
$CDCl_3$) δ 31.17; IR (KBr) ν 3055, 2991, 1727, 1685, 1189, 755 cm^{-1}. HRMS (ESI) calcd for $C_{33}H_{32}O_4P$ $[M+H]^+$: 523.2033, found: 523.2038.



Ethyl

1-(2-(3,4-dimethylphenyl)-2-oxoethyl)-3-(diphenylphosphoryl)-2,3-dihydro-1*H*-indene-2-carboxylate (**3k**)

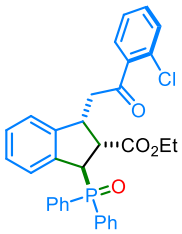
White solid obtained by column chromatography (petroleum ether/ethyl acetate = 5:1 to 2:1); 43.6 mg, 41% yield, >20:1 dr; reaction time = 11 h; mp 151.2-152.0 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80-7.72 (m, 4H), 7.66 (s, 1H), 7.61 (d, *J* = 8.0 Hz, 1H), 7.58-7.54 (m, 1H), 7.51-7.41 (m, 5H), 7.16-7.13 (m, 2H), 7.07 (d, *J* = 8.0 Hz, 1H), 7.00 (t, *J* = 8.0 Hz, 1H), 6.67 (d, *J* = 4.0 Hz, 1H), 4.66 (q, *J* = 4.0 Hz, 1H), 4.09-4.03 (m, 1H), 3.99-3.92 (m, 1H), 3.73-3.67 (m, 1H), 3.66-3.60 (m, 1H), 3.32 (dd, J_1 = 16.0 Hz, J_2 = 8.0 Hz, 1H), 3.13 (dd, J_1 = 20.0 Hz, J_2 = 8.0 Hz, 1H), 2.28 (s, 3H), 2.26 (s, 3H), 0.91 (t, *J* = 8.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.4, 173.2 (d, *J* = 8.0 Hz, 1C), 145.5 (d, *J* = 6.0 Hz, 1C), 142.7, 136.9, 136.8 (d, *J* = 4.0 Hz, 1C), 134.7, 132.0 (dd, J_1 = 20.0 Hz, J_2 = 2.0 Hz, 1C), 131.7 (dd, J_1 = 14.0 Hz, J_2 = 9.0 Hz, 1C), 131.3 (d, *J* = 27.0 Hz, 1C), 129.8, 129.1, 128.6 (dd, J_1 = 12.0 Hz, J_2 = 10.0 Hz, 1C), 127.9 (d, *J* = 2.0 Hz, 1C), 127.2 (d, *J* = 2.0 Hz, 1C), 125.6, 125.4 (d, *J* = 3.0 Hz, 1C), 123.7 (d, *J* = 2.0 Hz, 1C), 60.9, 48.4, 47.9 (d, *J* = 69.0 Hz, 1C), 42.0 (d, *J* = 4.0 Hz, 1C), 40.6, 20.1, 19.8, 13.8; ^{31}P NMR (202 MHz, $CDCl_3$) δ 31.10; IR (KBr) ν 3057, 2947, 1729, 1680, 1185, 754 cm^{-1}. HRMS (ESI) calcd for $C_{34}H_{34}O_4P$ $[M+H]^+$: 537.2189, found: 537.2196.



Ethyl

1-(2-(3,4-dimethoxyphenyl)-2-oxoethyl)-3-(diphenylphosphoryl)-2,3-dihydro-1*H*-indene-2-carbox ylate (**3l**)

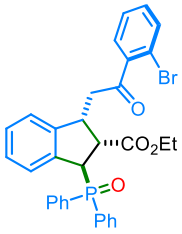
Light yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 5:1 to 1:1); 58.1 mg, 51% yield, >20:1 dr; reaction time = 8 h; mp 93.4-94.6 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79-7.69 (m, 4H), 7.56-7.43 (m, 8H), 7.15 (t, *J* = 8.0 Hz, 1H), 7.06 (d, *J* = 8.0 Hz, 1H), 6.99 (t, *J* = 8.0 Hz, 1H), 6.82 (d, *J* = 8.0 Hz, 1H), 6.65 (d, *J* = 8.0 Hz, 1H), 4.65 (q, *J* = 4.0 Hz, 1H), 4.06-4.03 (m, 1H), 3.98-3.94 (m, 1H), 3.90 (s, 3H), 3.88 (s, 3H), 3.76-3.68 (m, 1H), 3.65-3.57 (m, 1H), 3.29 (dd, J_1 = 20.0 Hz, J_2 = 8.0 Hz, 1H), 3.14 (dd, J_1 = 20.0 Hz, J_2 = 4.0 Hz, 1H), 0.90 (t, *J* = 8.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.0, 173.1 (d, *J* = 8.0 Hz, 1C), 153.2, 148.9, 145.3 (d, *J* = 6.0 Hz, 1C), 136.7 (d, *J* = 4.0 Hz, 1C), 132.0 (dd, J_1 = 20.0 Hz, J_2 = 2.0 Hz, 1C), 131.5 (dd, J_1 = 21.0 Hz, J_2 = 8.0 Hz, 1C), 131.3, 130.5, 129.9, 128.4 (dd, J_1 = 11.0 Hz, J_2 = 4.0 Hz, 1C), 127.8 (d, *J* = 2.0 Hz, 1C), 127.0 (d, *J* = 2.0 Hz, 1C), 125.2 (d, *J* = 2.0 Hz, 1C), 123.5, 122.4, 109.9 (d, *J* = 4.0 Hz, 1C), 60.8, 55.9, 55.9, 48.3, 47.9 (d, *J* = 69.0 Hz, 1C), 42.0 (d, *J* = 2.0 Hz, 1C), 40.0, 13.7; ^{31}P NMR (202 MHz, $CDCl_3$) δ 31.16; IR (KBr) ν 3064, 2948, 1726, 1267, 1195, 1162, 730 cm^{-1}. HRMS (ESI) calcd for $C_{34}H_{34}O_6P$ $[M+H]^+$: 569.2088, found: 569.2091.



Ethyl 1-(2-(2-chlorophenyl)-2-oxoethyl)-3-(diphenylphosphoryl)-2,3-dihydro-1*H*-indene-2-carboxylate (**3m**)

White solid obtained by column chromatography (petroleum ether/ethyl acetate = 5:1 to 2:1); 41.7 mg, 38% yield, >20:1 dr; reaction time = 5 h; mp 119.4-120.5 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (t, *J* = 8.0 Hz, 2H), 7.72 (t, *J* = 8.0 Hz, 2H), 7.56-7.46 (m, 7H), 7.36 (s, 2H), 7.28 (s, 1H), 7.16-7.09 (m, 2H), 6.99 (t, *J* = 8.0 Hz, 1H), 6.61 (d, *J* = 8.0 Hz, 1H), 4.61 (q, *J* = 4.0 Hz, 1H), 4.02-3.91 (m, 2H), 3.78 (q, *J* = 8.0 Hz, 2H), 3.27 (d, *J* = 4.0 Hz, 2H), 1.04 (t, *J* = 4.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.2, 173.0 (d, *J* = 8.0 Hz, 1C), 145.1 (d, *J* = 6.0 Hz, 1C), 138.5, 136.6 (d, *J* = 5.0 Hz, 1C), 132.0 (dd, J_1 = 19.0 Hz, J_2 = 3.0 Hz, 1C), 131.9, 131.6 (dd, J_1 = 13.0 Hz, J_2 = 9.0 Hz, 1C), 131.2 (d, *J* = 15.0 Hz, 1C), 131.0, 130.6, 129.5, 128.5 (dd, J_1 = 11.0 Hz, J_2 = 5.0

Hz, 1C), 127.9 (d, *J* = 3.0 Hz, 1C), 127.2 (d, *J* = 2.0 Hz, 1C), 126.9, 125.2 (d, *J* = 4.0 Hz, 1C), 123.7 (d, *J* = 2.0 Hz, 1C), 60.9, 48.2, 47.5. 45.0, 42.0 (d, *J* = 3.0 Hz, 1C), 13.8; ^{31}P NMR (202 MHz, $CDCl_3$) δ 30.91; IR (KBr) ν 3057, 2914, 1722, 1186, 757 cm^{-1}. HRMS (ESI) calcd for $C_{32}H_{29}ClO_4P$ $[M+H]^+$: 543.1487, found: 543.1489.

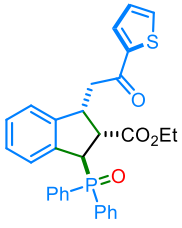


Ethyl

1-(2-(2-bromophenyl)-2-oxoethyl)-3-(diphenylphosphoryl)-2,3-dihydro-1*H*-indene-2-carboxylate

(**3n**)

White solid obtained by column chromatography (petroleum ether/ethyl acetate = 8:1 to 2:1); 57.4 mg, 49% yield, >20:1 dr; reaction time = 72 h; mp 141.3-142.1 ℃; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.82-7.78 (m, 2H), 7.75-7.72 (m, 2H), 7.58-7.54 (m, 2H), 7.52 (d, *J* = 10.0 Hz, 1H), 7.49-7.44 (m, 4H), 7.40 (dd, J_1 = 10.0 Hz, J_2 = 5.0 Hz, 1H), 7.33 (t, *J* = 10.0 Hz, 1H), 7.27 (dd, J_1 = 15.0 Hz, J_2 = 5.0 Hz, 1H), 7.17 (t, *J* = 10.0 Hz, 1H), 7.12 (d, *J* = 5.0 Hz, 1H), 6.99 (t, *J* = 10.0 Hz, 1H), 6.61 (d, *J* = 5.0 Hz, 1H), 4.61 (q, *J* = 5.0 Hz, 1H), 4.01 (q, *J* = 10.0 Hz, 1H), 3.96-3.91 (m, 1H), 3.83-3.74 (m, 2H), 3.25 (d, *J* = 5.0 Hz, 2H), 1.06 (t, *J* = 5.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 201.2, 173.0 (d, *J* = 7.5 Hz, 1C), 145.2 (d, *J* = 5.0 Hz, 1C), 140.8, 136.5 (d, *J* = 5.0 Hz, 1C), 133.8, 132.0 (dd, J_1 = 24.0 Hz, J_2 = 2.5 Hz, 1C), 131.7-131.6 (m, 1C), 131.3 (d, *J* = 6.0 Hz, 1C), 130.6, 129.0, 128.5 (t, *J* = 11.0 Hz, 1C), 128.0 (d, *J* = 2.5 Hz, 1C), 127.4, 127.2 (d, *J* = 1.0 Hz, 1C), 125.3 (d, *J* = 4.0 Hz, 1C), 123.8, 118.7, 61.0, 48.2, 47.9 (d, *J* = 69.0 Hz, 1C), 44.8, 41.8 (d, *J* = 4.0 Hz, 1C), 13.9; ^{31}P NMR (202 MHz, $CDCl_3$) δ 31.07; IR (KBr) ν 3056, 2950, 1721, 1185, 756 cm^{-1}. HRMS (ESI) calcd for $C_{32}H_{29}BrO_4P$ $[M+H]^+$: 587.0981, found: 587.0981.

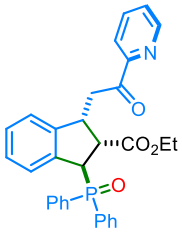


Ethyl

1-(diphenylphosphoryl)-3-(2-oxo-2-(thiophen-2-yl)ethyl)-2,3-dihydro-1*H*-indene-2-carboxylate

(**3o**)

Light yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 5:1 to 1:1); 50.1 mg, 49% yield, >20:1 dr; reaction time = 3 h; mp 81.7-83.1 ℃; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.79-7.71 (m, 4H), 7.60-7.54 (m, 3H), 7.51-7.42 (m, 5H), 7.14 (t, *J* = 10.0 Hz, 1H), 7.06 (t, *J* = 5.0 Hz, 2H), 6.99 (t, *J* = 10.0 Hz, 1H), 6.66 (d, *J* = 10.0 Hz, 1H), 4.65 (q, *J* = 5.0 Hz, 1H), 4.07-4.03 (m, 1H), 3.96-3.90 (m, 1H), 3.77-3.70 (m, 1H), 3.67-3.60 (m, 1H), 3.25 (dd, J_1 = 20.0 Hz, J_2 = 10.0 Hz, 1H), 3.13 (dd, J_1 = 15.0 Hz, J_2 = 5.0 Hz, 1H), 0.93 (t, *J* = 4.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 190.3, 173.0 (d, *J* = 9.0 Hz, 1C), 145.0 (d, *J* = 6.0 Hz, 1C), 143.9, 136.7 (d, *J* = 4.0 Hz, 1C), 133.5, 132.0 (d, *J* = 2.5 Hz, 1C), 131.8 (dd, J_1 = 5.0 Hz, J_2 = 2.5 Hz, 1C), 131.7-131.5 (m, 1C), 131.2 (d, *J* = 7.5 Hz, 1C), 130.5, 128.6, 128.4 (t, *J* = 9.0 Hz, 1C), 128.0, 127.9 (d, *J* = 2.5 Hz, 1C), 127.2 (d, *J* = 2.5 Hz, 1C), 125.3 (d, *J* = 2.5 Hz, 1C), 123.6, 60.9, 48.2, 47.8 (d, *J* = 69.0 Hz, 1C), 41.8 (d, *J* = 2.5 Hz, 1C), 41.2, 13.6; ^{31}P NMR (202 MHz, $CDCl_3$) δ 31.02; IR (KBr) ν 3062, 2911, 1727, 1190, 710 cm^{-1}. HRMS (ESI) calcd for $C_{30}H_{28}O_4P$ $[M+H]^+$: 515.1440, found: 515.1446.



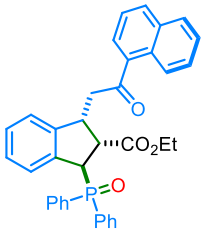
Ethyl

1-(diphenylphosphoryl)-3-(2-oxo-2-(pyridin-2-yl)ethyl)-2,3-dihydro-1*H*-indene-2-carboxylate

(**3p**)

White solid obtained by column chromatography (petroleum ether/ethyl acetate = 3:1 to 2:1); 50.3 mg, 49% yield, >20:1 dr; reaction time = 5 h; mp 132.4-133.6 ℃; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.60 (d, *J* = 5.0 Hz, 1H), 8.01 (d, *J* = 10.0 Hz, 1H), 7.80 (t, *J* = 10.0 Hz, 2H), 7.71 (t, *J* = 10.0 Hz, 2H), 7.56-7.45 (m, 8H), 7.15 (t, *J* = 10.0 Hz, 1H), 7.09 (d, *J* = 5.0 Hz, 1H), 6.98 (t, *J* = 10.0 Hz, 1H), 6.61 (d, *J* = 10.0 Hz, 1H), 4.66 (d, *J* = 10.0 Hz, 1H), 4.03-3.95 (m, 2H), 3.74-3.64 (m, 3H), 3.40 (dd, J_1 = 30.0 Hz, J_2 = 5.0 Hz, 1H), 0.86 (t, *J* = 10.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 199.3, 173.1 (d, *J* = 11.0 Hz, 1C), 153.1, 148.9, 145.4 (d, *J* = 6.0 Hz, 1C), 136.8 (d, *J* = 6.0 Hz, 1C), 132.0 (dd, J_1 = 21.0 Hz, J_2 = 4.0 Hz, 1C), 131.7 (dd, J_1 = 27.5 Hz, J_2 = 11.0 Hz, 1C), 131.4, 130.4, 128.5 (d, *J* = 15.0 Hz, 1C), 127.8 (d, *J* = 2.5 Hz, 1C), 127.1, 127.0 (d, *J* = 2.5 Hz, 1C),

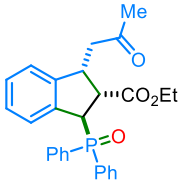
125.2 (d, J = 5.0 Hz, 1C), 123.6 (d, J = 1.0 Hz, 1C), 121.6, 60.8, 48.5, 47.8 (d, J = 87.5 Hz, 1C), 42.0, 39.7, 13.6; ^{31}P NMR (202 MHz, $CDCl_3$) δ 31.23; IR (KBr) ν 3056, 1726, 1186, 1113, 757 cm^{-1}. HRMS (ESI) calcd for $C_{31}H_{29}NO_4P$ $[M+H]^+$: 510.1829, found: 510.1836.



Ethyl

1-(diphenylphosphoryl)-3-(2-(naphthalen-1-yl)-2-oxoethyl)-2,3-dihydro-1*H*-indene-2-carboxylate (**3q**)

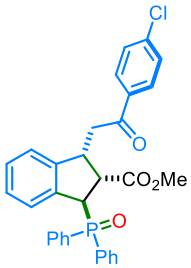
Light yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 5:1 to 1:1); 46.3 mg, 42% yield, >20:1 dr; reaction time = 1 h; mp 132.9-134.0 ℃; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.65 (d, J = 10.0 Hz, 1H), 7.95 (d, J = 5.0 Hz, 1H), 7.86-7.80 (m, 4H), 7.77-7.74 (m, 2H), 7.59-7.42 (m, 9H), 7.17 (t, J = 10.0 Hz, 1H), 7.13 (d, J = 10.0 Hz, 1H), 7.01 (t, J = 5.0 Hz, 1H), 6.66 (d, J = 5.0 Hz, 1H), 4.68 (q, J = 5.0 Hz, 1H), 4.17-4.13 (m, 1H), 4.08-4.02 (m, 1H), 3.75-3.68 (m, 1H), 3.66-3.60 (m, 1H), 3.43 (dd, J_1 = 20.0 Hz, J_2 = 10.0 Hz, 1H), 3.33 (dd, J_1 = 20.0 Hz, J_2 = 5.0 Hz, 1H), 0.90 (t, J = 5.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 201.3, 173.2 (d, J = 9.0 Hz, 1C), 145.4 (d, J = 5.0 Hz, 1C), 136.7 (d, J = 5.0 Hz, 1C), 135.3, 133.9, 132.8, 132.0 (dd, J_1 = 24.0 Hz, J_2 = 2.5 Hz, 1C), 131.6 (dd, J_1 = 19.0 Hz, J_2 = 9.0 Hz, 1C), 131.3 (d, J = 6.0 Hz, 1C), 130.6, 130.1, 128.4 (dd, J_1 = 11.0 Hz, J_2 = 5.0 Hz, 1C), 128.3, 127.9 (d, J = 2.5 Hz, 1C), 127.8 (d, J = 20.0 Hz, 1C), 127.1 (d, J = 2.5 Hz, 1C), 126.4, 125.8, 125.3 (d, J = 4.0 Hz, 1C), 124.2, 123.6, 60.9, 48.3, 48.0 (d, J = 70.0 Hz, 1C), 43.9, 42.2 (d, J = 2.5 Hz, 1C), 13.7; ^{31}P NMR (202 MHz, $CDCl_3$) δ 30.99; IR (KBr) ν 3055, 1727, 1186, 707 cm^{-1}. HRMS (ESI) calcd for $C_{36}H_{32}O_4P$ $[M+H]^+$: 559.2033, found: 559.2038.



Ethyl 1-(diphenylphosphoryl)-3-(2-oxopropyl)-2,3-dihydro-1*H*-indene-2-carboxylate (**3r**)

White solid obtained by column chromatography (petroleum ether/ethyl acetate = 4:1 to 1:1); 48.4

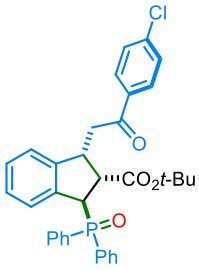
mg, 54% yield, >20:1 dr; reaction time = 1 h; mp 144.0-145.1 ℃; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.77-7.73 (m, 4H), 7.55 (t, *J* = 10.0 Hz, 1H), 7.51-7.42 (m, 5H), 7.13 (t, *J* = 10.0 Hz, 1H), 7.00 (d, *J* = 10.0 Hz, 1H), 6.96 (t, *J* = 10.0 Hz, 1H), 6.60 (d, *J* = 10.0 Hz, 1H), 4.58 (q, *J* = 5.0 Hz, 1H), 3.91-3.73 (m, 4H), 2.76 (dd, J_1 = 20.0 Hz, J_2 = 10.0 Hz, 1H), 2.64 (dd, J_1 = 20.0 Hz, J_2 = 5.0 Hz, 1H), 2.06 (s, 3H), 1.09 (t, *J* = 5.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 206.0, 172.9 (d, *J* = 7.5 Hz, 1C), 145.2 (d, *J* = 6.0 Hz, 1C), 136.5 (d, *J* = 5.0 Hz, 1C), 131.9 (dd, J_1 = 26.0 Hz, J_2 = 2.5 Hz, 1C), 131.5 (dd, J_1 = 14.0 Hz, J_2 = 9.0 Hz, 1C), 131.0 (d, *J* = 72.5 Hz, 1C), 128.4 (dd, J_1 = 14.0 Hz, J_2 = 12.5 Hz, 1C), 127.8 (d, *J* = 2.5 Hz, 1C), 127.1 (d, *J* = 2.5 Hz, 1C), 125.2 (d, *J* = 4.0 Hz, 1C), 123.4 (d, *J* = 1.0 Hz, 1C), 60.8, 48.1, 47.6 (d, *J* = 70.0 Hz, 1C), 45.5, 41.6 (d, *J* = 4.0 Hz, 1C), 29.9, 13.8; ^{31}P NMR (202 MHz, $CDCl_3$) δ 30.80; IR (KBr) ν 3055, 2906, 1726, 1182, 757 cm^{-1}. HRMS (ESI) calcd for $C_{27}H_{28}O_4P$ $[M+H]^+$: 447.1720, found: 447.1725.



Methyl 1-(2-(4-chlorophenyl)-2-oxoethyl)-3-(diphenylphosphoryl)-2,3-dihydro-1*H*-indene-2-carboxylate (**3s**)

White solid obtained by column chromatography (petroleum ether/ethyl acetate = 5:1 to 3:1); 40.5 mg, 38% yield, >20:1 dr; reaction time = 2 h; mp 72.6-73.7 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82-7.72 (m, 6H), 7.57 (t, *J* = 8.0 Hz, 1H), 7.51-7.45 (m, 5H), 7.39 (d, *J* = 8.0 Hz, 2H), 7.16 (t, *J* = 8.0 Hz, 1H), 7.07 (d, *J* = 8.0 Hz, 1H), 7.00 (t, *J* = 8.0 Hz, 1H), 6.65 (d, *J* = 4.0 Hz, 1H), 4.64 (q, *J* = 8.0 Hz, 1H), 4.11-4.08 (m, 1H), 4.00-3.92 (m, 1H), 3.31 (dd, J_1 = 20.0 Hz, J_2 = 8.0 Hz, 1H), 3.21 (s, 3H), 3.11 (dd, J_1 = 16.0 Hz, J_2 = 4.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.4, 173.5 (d, *J* = 8.0 Hz, 1C), 145.1 (d, *J* = 6.0 Hz, 1C), 139.5, 136.6 (d, *J* = 5.0 Hz, 1C), 135.1, 132.1, 132.0 (dd, J_1 = 20.0 Hz, J_2 = 2.0 Hz, 1C), 131.6 (dd, J_1 = 14.0 Hz, J_2 = 8.0 Hz, 1C), 129.2, 128.9, 128.5 (dd, J_1 = 12.0 Hz, J_2 = 7.0 Hz, 1C), 127.9 (d, *J* = 2.0 Hz, 1C), 127.3 (d, *J* = 2.0 Hz, 1C), 125.3 (d, *J* = 4.0 Hz, 1C), 123.6 (d, *J* = 2.0 Hz, 1C), 51.7, 48.1, 47.4, 42.0 (d, *J* = 4.0 Hz, 1C), 40.7; ^{31}P NMR (202 MHz, $CDCl_3$) δ 30.94; IR (KBr) ν 3059, 2946, 1732, 1187, 758 cm^{-1}. HRMS (ESI) calcd for

$C_{31}H_{27}ClO_4P$ $[M+H]^+$: 529.1330, found: 529.1341.



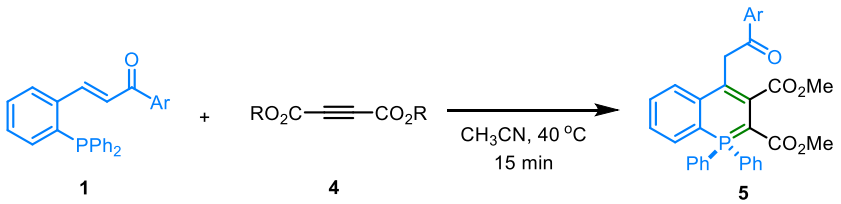
tert-Butyl

1-(2-(4-chlorophenyl)-2-oxoethyl)-3-(diphenylphosphoryl)-2,3-dihydro-1*H*-indene-2-carboxylate

(**3t**)

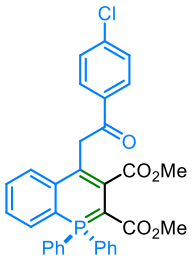
White solid obtained by column chromatography (petroleum ether/ethyl acetate = 5:1 to 4:1); 52.9 mg, 46% yield, >20:1 dr; reaction time = 7 h; mp 153.4-154.2 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.0 Hz, 2H), 7.81-7.77 (m, 2H), 7.71-7.66 (m, 2H), 7.53 (t, *J* = 8.0 Hz, 2H), 7.47-7.42 (m, 4H), 7.41 (d, *J* = 8.0 Hz, 2H), 7.14 (t, *J* = 8.0 Hz, 1H), 7.00 (q, *J* = 8.0 Hz, 2H), 6.64 (d, *J* = 8.0 Hz, 1H), 4.58 (d, *J* = 8.0 Hz, 1H), 3.96-3.86 (m, 2H), 3.30 (d, *J* = 8.0 Hz, 2H), 1.18 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.3, 172.4 (d, *J* = 11.0 Hz, 1C), 145.2 (d, *J* = 5.0 Hz, 1C), 139.6, 137.0 (d, *J* = 5.0 Hz, 1C), 135.1, 132.0 (dd, J_1 = 9.0 Hz, J_2 = 2.0 Hz, 1C), 131.7 (dd, J_1 = 26.0 Hz, J_2 = 9.0 Hz, 1C), 130.3, 129.4, 129.0, 128.8-128.5 (m, 1C), 127.8 (d, *J* = 3.0 Hz, 1C), 127.1 (d, *J* = 2.0 Hz, 1C), 125.5 (d, *J* = 3.0 Hz, 1C), 123.3 (d, *J* = 3.0 Hz, 1C), 81.5, 49.5, 48.4 (d, *J* = 68.0 Hz, 1C), 41.7, 40.2, 27.8; ^{31}P NMR (202 MHz, $CDCl_3$) δ 31.61; IR (KBr) ν 3061, 1723, 1369, 1188, 1148, 757 cm^{-1}. HRMS (ESI) calcd for $C_{34}H_{33}ClO_4P$ $[M+H]^+$: 571.1800, found: 571.1812.

3. Experimental data for the formation of 5



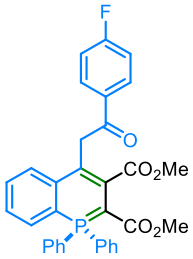
General procedure： To a 5.0 mL vial were successively added functionalized organic phosphine **1** (0.20 mmol), but-2-ynedioate **4** (0.22 mmol, 1.1 equiv) and 1.0 mL of extra dry CH_3CN. The resulting mixture was stirred at 40 ^{o}C for 15 min until the complete consumption of **1** as monitored by thin layer chromatography. And then, the reaction mixture was directly subjected to flash column chromatography on silica gel (petroleum ether/ethyl acetate) to afford the

corresponding products **5**.



Dimethyl 4-(2-(4-chlorophenyl)-2-oxoethyl)-1,1-diphenyl-1λ^5-phosphinoline-2,3-dicarboxylate (**5a**)

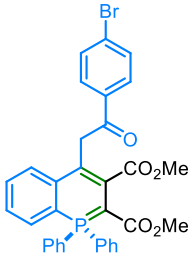
Yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 5:1); 89.0 mg, 78% yield; reaction time = 15 min; mp 202.3-202.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8.0 Hz, 2H), 7.63 (dd, J_1 = 12.0 Hz, J_2 = 8.0 Hz, 4H), 7.59-7.55 (m, 2H), 7.50-7.46 (m, 4H), 7.41 (t, *J* = 8.0 Hz, 1H), 7.33-7.28 (m, 4H), 7.09 (t, *J* = 8.0 Hz, 1H), 4.18 (s, 2H), 3.85 (s, 3H), 3.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.0, 171.4 (d, *J* = 15.0 Hz, 1C), 166.7, 140.8 (d, *J* = 6.0 Hz, 1C), 138.9, 135.1, 133.0 (d, *J* = 11.0 Hz, 1C), 132.5 (d, *J* = 8.0 Hz, 1C), 131.9, 131.9, 131.8, 129.6, 128.6, 128.5, 128.5, 124.5 (d, *J* = 12.0 Hz, 1C), 124.3 (d, *J* = 9.0 Hz, 1C), 111.4, 110.5, 105.2 (d, *J* = 9.0 Hz, 1C), 52.2, 50.2, 42.1; ^{31}P NMR (202 MHz, $CDCl_3$) δ 5.67 (d, *J* = 10.1 Hz, 1P); IR (KBr) ν 2947, 1723, 1659, 1430, 1272, 1102, 746 cm^{-1}. HRMS (ESI) calcd for $C_{33}H_{26}ClO_5PNa$ $[M+Na]^+$: 591.1104, found: 591.1110.



Dimethyl 4-(2-(4-fluorophenyl)-2-oxoethyl)-1,1-diphenyl-1λ^5-phosphinoline-2,3-dicarboxylate (**5b**)

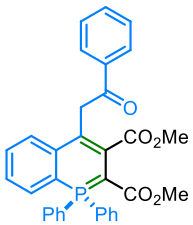
Yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 5:1); 74.5 mg, 67% yield; reaction time = 15 min; mp 222.1-222.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01-7.97 (m, 2H), 7.62 (dd, J_1 = 16.0 Hz, J_2 = 8.0 Hz, 4H), 7.55-7.52 (m, 2H), 7.47-7.43 (m, 4H), 7.38 (t, *J* = 8.0 Hz, 1H), 7.31-7.24 (m, 2H), 7.06 (t, *J* = 8.0 Hz, 1H), 6.96 (t, *J* = 8.0 Hz, 2H), 4.16 (s, 2H), 3.82 (s, 3H), 3.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.5, 171.5 (d, *J* = 15.0 Hz, 1C), 165.3

(d, *J* = 252.0 Hz, 1C), 140.9 (d, *J* = 5.0 Hz, 1C), 133.2 (d, *J* = 3.0 Hz, 1C), 133.1, 133.0, 132.5 (d, *J* = 8.0 Hz, 1C), 131.9, 131.8, 130.8 (d, *J* = 9.0 Hz, 1C), 128.6, 128.5, 124.5, 124.4, 124.3, 115.3 (d, *J* = 22.0 Hz, 1C), 111.4, 110.5, 105.4 (d, *J* = 9.0 Hz, 1C), 52.2, 50.2, 41.8; ^{19}F NMR (375 MHz, $CDCl_3$) δ -105.75; ^{31}P NMR (202 MHz, $CDCl_3$) δ 5.69; IR (KBr) ν 2948, 1724, 1663, 1432, 1271, 1104, 749 cm^{-1}. HRMS (ESI) calcd for $C_{33}H_{26}FO_5PNa$ $[M+Na]^+$: 575.1400, found: 575.1404.



Dimethyl 4-(2-(4-bromophenyl)-2-oxoethyl)-1,1-diphenyl-1λ^5-phosphinoline-2,3-dicarboxylate (**5c**)

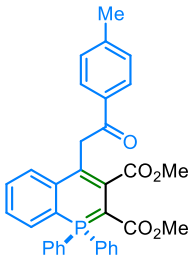
Yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 5:1); 88.8 mg, 72% yield; reaction time = 15 min; mp 203.2-204.1 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 8.0 Hz, 2H), 7.64-7.54 (m, 6H), 7.49-7.44 (m, 4H), 7.42-7.38 (m, 3H), 7.32-7.23 (m, 2H), 7.08 (t, *J* = 8.0 Hz, 1H), 4.16 (s, 2H), 3.83 (s, 3H), 3.38 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.3, 171.4 (d, *J* = 16.0 Hz, 1C), 166.7, 140.8 (d, *J* = 6.0 Hz, 1C), 135.5, 133.1, 133.0, 132.5 (d, *J* = 8.0 Hz, 1C), 131.9 (d, *J* = 3.0 Hz, 1C), 131.8 (d, *J* = 2.0 Hz, 1C), 131.5, 129.7, 128.6, 128.5, 127.7, 124.5 (d, *J* = 12.0 Hz, 1C), 124.3 (d, *J* = 9.0 Hz, 1C), 111.4, 110.5, 105.2 (d, *J* = 9.0 Hz, 1C), 52.3, 50.2, 42.1; ^{31}P NMR (202 MHz, $CDCl_3$) δ 5.71 (d, *J* = 10.1 Hz, 1P); IR (KBr) ν 2981, 1729, 1664, 1433, 1271, 1106, 755 cm^{-1}. HRMS (ESI) calcd for $C_{33}H_{26}BrO_5PNa$ $[M+Na]^+$: 635.0599, found: 635.0601.



Dimethyl 4-(2-oxo-2-phenylethyl)-1,1-diphenyl-1λ^5-phosphinoline-2,3-dicarboxylate (**5d**)

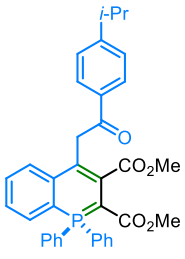
Yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 5:1); 95.0 mg, 89% yield; reaction time = 15 min; mp 183.1-183.7 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (dd, J_1 = 8.0 Hz, J_2 = 4.0 Hz, 2H), 7.67 (dd, J_1 = 12.0 Hz, J_2 = 4.0 Hz, 4H), 7.54-7.44 (m, 7H), 7.38 (dd,

J_1 = 12.0 Hz, J_2 = 8.0 Hz, 3H), 7.33-7.27 (m, 2H), 7.06 (t, J = 8.0 Hz, 1H), 4.22 (s, 2H), 3.77 (s, 3H), 3.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.3, 171.4 (d, J = 16.0 Hz, 1C), 166.8, 141.1 (d, J = 5.0 Hz, 1C), 136.9, 133.2, 133.1, 132.7, 132.6 (d, J = 8.0 Hz, 1C), 131.8, 131.7, 128.6, 128.4 (d, J = 4.0 Hz, 1C), 128.0, 124.5, 124.4, 124.3, 111.4, 110.6, 105.1 (d, J = 9.0 Hz, 1C), 52.1, 50.1, 41.2; ^{31}P NMR (202 MHz, $CDCl_3$) δ 5.76; IR (KBr) ν 2992, 1727, 1664, 1433, 1270, 1103, 753 cm^{-1}. HRMS (ESI) calcd for $C_{33}H_{27}O_5PNa$ [M+Na]$^+$: 557.1494, found: 557.1490.



Dimethyl 4-(2-oxo-2-(*p*-tolyl)ethyl)-1,1-diphenyl-1λ^5-phosphinoline-2,3-dicarboxylate (**5e**)

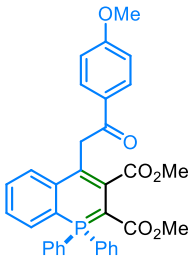
Yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 5:1); 78.9 mg, 72% yield; reaction time = 15 min; mp 176.2-176.7 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, J = 8.0 Hz, 2H), 7.67 (dd, J_1 = 16.0 Hz, J_2 = 8.0 Hz, 4H), 7.55-7.51 (m, 2H), 7.48-7.44 (m, 4H), 7.38-7.27 (m, 3H), 7.18 (d, J = 8.0 Hz, 2H), 7.06 (t, J = 8.0 Hz, 1H), 4.20 (s, 2H), 3.77 (s, 3H), 3.37 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.9, 171.5 (d, J = 15.0 Hz, 1C), 166.8, 143.4, 141.2 (d, J = 5.0 Hz, 1C), 134.4, 133.2, 133.1, 132.5 (d, J = 9.0 Hz, 1C), 131.7 (d, J = 2.0 Hz, 1C), 131.7 (d, J = 4.0 Hz, 1C), 129.1, 128.5, 128.4, 128.2, 124.5 (d, J = 8.0 Hz, 1C), 124.3 (d, J = 12.0 Hz, 1C), 111.4, 110.5, 105.4 (d, J = 10.0 Hz, 1C), 52.1, 50.3, 41.1, 21.6; ^{31}P NMR (202 MHz, $CDCl_3$) δ 5.79 (d, J = 10.1 Hz, 1P); IR (KBr) ν 2946, 1728, 1664, 1436, 1268, 1106, 748 cm^{-1}. HRMS (ESI) calcd for $C_{34}H_{29}O_5PNa$ [M+Na]$^+$: 571.1650, found: 571.1645.



Dimethyl 4-(2-(4-isopropylphenyl)-2-oxoethyl)-1,1-diphenyl-1λ^5-phosphinoline-2,3-dicarboxylate (**5f**)

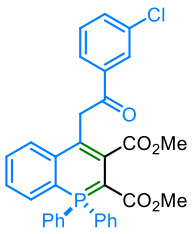
Yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 5:1); 85.6 mg,

74% yield; reaction time = 15 min; mp 197.3-197.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.0 Hz, 2H), 7.70 (dd, J_1 = 12.0 Hz, J_2 = 8.0 Hz, 4H), 7.55-7.45 (m, 6H), 7.38-7.31 (m, 2H), 7.29-7.23 (m, 3H), 7.06 (t, *J* = 8.0 Hz, 1H), 4.22 (s, 2H), 3.78 (s, 3H), 3.37 (s, 3H), 3.00-2.89 (m, 1H), 1.26 (d, *J* = 8.0 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.6, 171.4 (d, *J* = 16.0 Hz, 1C), 166.7, 154.2, 141.2 (d, *J* = 5.0 Hz, 1C), 134.7, 133.2, 133.1, 132.6 (d, *J* = 8.0 Hz, 1C), 131.8, 131.7 (d, *J* = 3.0 Hz, 1C), 128.6, 128.4, 128.4, 126.5, 124.5 (d, *J* = 8.0 Hz, 1C), 124.3 (d, *J* = 12.0 Hz, 1C), 111.5, 110.6, 105.5 (d, *J* = 10.0 Hz, 1C), 52.1, 50.2, 41.1, 34.1, 23.6; ^{31}P NMR (202 MHz, $CDCl_3$) δ 5.81 (d, *J* = 8.1 Hz, 1P); IR (KBr) ν 2959, 1730, 1674, 1433, 1265, 1100, 754 cm^{-1}. HRMS (ESI) calcd for $C_{36}H_{33}O_5PNa$ $[M+Na]^+$: 599.1963, found: 599.1956.



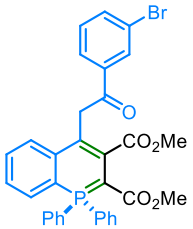
Dimethyl 4-(2-(4-methoxyphenyl)-2-oxoethyl)-1,1-diphenyl-1λ^5-phosphinoline-2,3-dicarboxylate (**5g**)

Yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 4:1 to 3:1); 96.9 mg, 86% yield; reaction time = 15 min; mp 161.4-162.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.0 Hz, 2H), 7.65 (dd, J_1 = 12.0 Hz, J_2 = 8.0 Hz, 4H), 7.54-7.50 (m, 2H), 7.47-7.43 (m, 4H), 7.36 (t, *J* = 8.0 Hz, 1H), 7.31-7.28 (m, 2H), 7.05 (t, *J* = 8.0 Hz, 1H), 6.84 (d, *J* = 8.0 Hz, 2H), 4.16 (s, 2H), 3.82 (s, 3H), 3.79 (s, 3H), 3.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.0, 171.5 (d, *J* = 15.0 Hz, 1C), 166.8, 163.1, 141.2 (d, *J* = 5.0 Hz, 1C), 133.2, 133.1, 132.5 (d, *J* = 8.0 Hz, 1C), 131.8, 131.8, 131.7, 130.4, 129.9, 128.5 (d, *J* = 13.0 Hz, 1C), 124.5 (d, *J* = 8.0 Hz, 1C), 124.3 (d, *J* = 12.0 Hz, 1C), 113.5, 111.4, 110.5, 105.8, 55.3, 52.1, 50.1, 41.2; ^{31}P NMR (202 MHz, $CDCl_3$) δ 5.72 (d, *J* = 10.1 Hz, 1P); IR (KBr) ν 2944, 1727, 1657, 1433, 1260, 1106, 749 cm^{-1}. HRMS (ESI) calcd for $C_{34}H_{29}O_6PNa$ $[M+Na]^+$: 587.1599, found: 5587.1601.



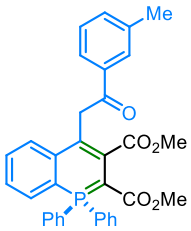
Dimethyl 4-(2-(3-chlorophenyl)-2-oxoethyl)-1,1-diphenyl-1λ^5-phosphinoline-2,3-dicarboxylate (**5h**)

Yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 4:1); 58.0 mg, 51% yield; reaction time = 15 min; mp 190.1-190.5 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (t, *J* = 4.0 Hz, 1H), 7.87 (d, *J* = 8.0 Hz, 1H), 7.66 (dd, J_1 = 12.0 Hz, J_2 = 8.0 Hz, 4H), 7.54-7.52 (m, 2H), 7.49-7.43 (m, 5H), 7.39 (t, *J* = 8.0 Hz, 1H), 7.33-7.24 (m, 3H), 7.08 (t, *J* = 8.0 Hz, 1H), 4.18 (s, 2H), 3.81 (s, 3H), 3.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.3, 171.3 (d, *J* = 15.0 Hz, 1C), 166.7 (d, *J* = 10.0 Hz, 1C), 140.9 (d, *J* = 5.0 Hz, 1C), 138.4, 134.7, 133.2, 133.1, 132.7, 132.7, 131.9, 131.9, 129.7, 128.6, 128.5, 128.2, 126.2, 124.5 (d, *J* = 12.0 Hz, 1C), 124.3 (d, *J* = 9.0 Hz, 1C), 111.5, 110.6, 105.2, 52.3, 50.3, 41.6; ^{31}P NMR (202 MHz, $CDCl_3$) δ 5.77 (d, *J* = 10.1 Hz, 1P); IR (KBr) ν 2948, 1727, 1629, 1434, 1269, 1100, 756 cm^{-1}. HRMS (ESI) calcd for $C_{33}H_{26}ClO_5PNa$ $[M+Na]^+$: 591.1104, found: 591.1101.



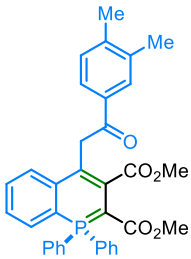
Dimethyl 4-(2-(3-bromophenyl)-2-oxoethyl)-1,1-diphenyl-1λ^5-phosphinoline-2,3-dicarboxylate (**5i**)

Yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 5:1); 48.5 mg, 40% yield; reaction time = 15 min; mp 200.7-201.5 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (s, 1H), 7.92 (d, *J* = 8.0 Hz, 1H), 7.65 (dd, J_1 = 16.0 Hz, J_2 = 8.0 Hz, 4H), 7.59 (d, *J* = 8.0 Hz, 1H), 7.55-7.51 (m, 2H), 7.49-7.45 (m, 4H), 7.39 (t, *J* = 8.0 Hz, 1H), 7.31 (t, *J* = 4.0 Hz, 1H), 7.27-7.20 (m, 2H), 7.08 (t, *J* = 8.0 Hz, 1H), 4.17 (s, 2H), 3.81 (s, 3H), 3.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.3, 171.4 (d, *J* = 16.0 Hz, 1C), 166.7, 140.9 (d, *J* = 6.0 Hz, 1C), 138.6, 135.6, 133.2, 133.1, 132.7, 132.6, 131.9, 131.8, 131.1, 130.0, 128.5 (d, *J* = 13.0 Hz, 1C), 126.7, 124.4 (d, *J* = 13.0 Hz, 1C), 124.3 (d, *J* = 8.0 Hz, 1C), 122.7, 111.5, 110.6, 104.8 (d, *J* = 9.0 Hz, 1C), 52.3, 50.2, 41.6; ^{31}P NMR (202 MHz, $CDCl_3$) δ 5.76 (d, *J* = 10.1 Hz, 1P); IR (KBr) ν 2947, 1727, 1625, 1434, 1267, 1096, 755 cm^{-1}. HRMS (ESI) calcd for $C_{33}H_{26}BrO_5PNa$ $[M+Na]^+$: 635.0599, found: 635.0594.



Dimethyl 4-(2-oxo-2-(*m*-tolyl)ethyl)-1,1-diphenyl-1λ^5-phosphinoline-2,3-dicarboxylate (**5j**)

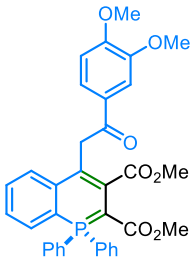
Yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 5:1); 90.5 mg, 83% yield; reaction time = 15 min; mp 183.9-184.7 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, J = 8.0 Hz, 2H), 7.67 (dd, J_1 = 16.0 Hz, J_2 = 8.0 Hz, 4H), 7.53-7.50 (m, 2H), 7.47-7.43 (m, 4H), 7.37-7.24 (m, 5H), 7.05 (t, J = 8.0 Hz, 1H), 4.22 (s, 2H), 3.78 (s, 3H), 3.36 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.3, 171.4 (d, J = 15.0 Hz, 1C), 166.7, 141.1 (d, J = 5.0 Hz, 1C), 138.1, 136.8, 133.5, 133.1, 133.0, 132.5 (d, J = 5.0 Hz, 1C), 131.7, 131.7, 128.6, 128.5, 128.4, 128.2, 125.2, 124.4 (d, J = 8.0 Hz, 1C), 124.2, 111.4, 110.5, 105.2 (d, J = 9.0 Hz, 1C), 52.1, 50.1, 41.2, 21.2; ^{31}P NMR (202 MHz, $CDCl_3$) δ 5.77 (d, J = 10.1 Hz, 1P); IR (KBr) ν 2942, 1726, 1665, 1432, 1273, 1103, 751 cm^{-1}. HRMS (ESI) calcd for $C_{34}H_{29}O_5PNa$ $[M+Na]^+$: 571.1650, found: 571.1649.



Dimethyl 4-(2-(3,4-dimethylphenyl)-2-oxoethyl)-1,1-diphenyl-1λ^5-phosphinoline-2,3-dicarboxylate (**5k**)

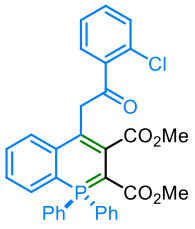
Yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 5:1 to 4:1); 71.6 mg, 64% yield; reaction time = 15 min; mp 205.4-205.9 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (s, 1H), 7.76 (d, J = 8.0 Hz, 1H), 7.67 (dd, J_1 = 12.0 Hz, J_2 = 8.0 Hz, 4H), 7.54-7.51 (m, 2H), 7.48-7.43 (m, 4H), 7.37-7.25 (m, 3H), 7.14 (d, J = 8.0 Hz, 1H), 7.05 (t, J = 8.0 Hz, 1H), 4.20 (s, 2H), 3.78 (s, 3H), 3.37 (s, 3H), 2.28 (s, 3H), 2.25 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.9, 171.4 (d, J = 15.0 Hz, 1C), 166.8, 142.1, 141.1 (d, J = 5.0 Hz, 1C), 136.7, 134.7, 133.2, 133.1, 132.5 (d, J = 8.0 Hz, 1C), 131.7 (d, J = 4.0 Hz, 1C), 131.7, 129.6, 129.3, 128.5, 128.4, 125.8, 124.5 (d, J = 8.0 Hz, 1C), 124.2 (d, J = 12.0 Hz, 1C), 111.4, 110.5, 105.5 (d, J = 9.0 Hz, 1C), 52.1,

50.1, 41.1, 19.9, 19.6; ^{31}P NMR (202 MHz, $CDCl_3$) δ 5.77 (d, *J* = 10.1 Hz, 1P); IR (KBr) ν 2946, 1724, 1662, 1432, 1271, 1103, 752 cm^{-1}. HRMS (ESI) calcd for $C_{35}H_{31}O_5PNa$ $[M+Na]^+$: 585.1807, found: 585.1803.



Dimethyl 4-(2-(3,4-dimethoxyphenyl)-2-oxoethyl)-1,1-diphenyl-1λ^5-phosphinoline-2,3-dicarboxylate (**5l**)

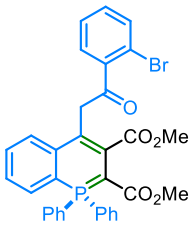
Yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 4:1 to 3:1); 97.5 mg, 82% yield; reaction time = 15 min; mp 104.8-105.7 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69-7.61 (m, 5H), 7.55-7.51 (m, 3H), 7.48-7.43 (m, 4H), 7.40-7.24 (m, 3H), 7.06 (t, *J* = 8.0 Hz, 1H), 6.79 (d, *J* = 8.0 Hz, 1H), 4.17 (s, 2H), 3.91 (s, 3H), 3.81 (s, 6H), 3.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.4, 171.5 (d, *J* = 14.0 Hz, 1C), 166.8, 152.9, 148.7, 141.1 (d, *J* = 5.0 Hz, 1C), 133.2, 133.0, 132.5 (d, *J* = 8.0 Hz, 1C), 131.8, 131.8, 130.0, 128.6, 128.5, 124.6, 124.5, 124.4, 122.7, 111.3, 110.5, 110.4, 109.9, 55.9, 55.9, 52.2, 50.1, 41.5; ^{31}P NMR (202 MHz, $CDCl_3$) δ 5.69 (d, *J* = 10.1 Hz, 1P); IR (KBr) ν 2944, 1728, 1668, 1432, 1265, 1100, 755 cm^{-1}. HRMS (ESI) calcd for $C_{35}H_{31}O_7PNa$ $[M+Na]^+$: 617.1705, found: 617.1705.



Dimethyl 4-(2-(2-chlorophenyl)-2-oxoethyl)-1,1-diphenyl-1λ^5-phosphinoline-2,3-dicarboxylate (**5m**)

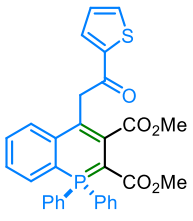
Yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 4:1); 101.6 mg, 89% yield; reaction time = 15 min; mp 87.6-87.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (dd, J_1 = 12.0 Hz, J_2 = 8.0 Hz, 4H), 7.54-7.43 (m, 8H), 7.33-7.28 (m, 3H), 7.22 (t, *J* = 8.0 Hz, 1H), 7.12-7.05 (m, 2H), 4.15 (s, 2H), 3.82 (s, 3H), 3.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.7, 171.1 (d, *J* = 15.0 Hz, 1C), 166.6, 140.8 (d, *J* = 5.0 Hz, 1C), 139.2, 133.1, 133.0, 132.7 (d, *J* = 8.0

Hz, 1C), 131.9 (d, J = 2.0 Hz, 1C), 131.8 (d, J = 3.0 Hz, 1C), 130.9, 130.1, 129.9, 129.3 (d, J = 13.0 Hz, 1C), 128.6, 128.4, 126.4, 124.7 (d, J = 8.0 Hz, 1C), 124.5 (d, J = 12.0 Hz, 1C), 111.4, 110.5, 104.3 (d, J = 9.0 Hz, 1C), 52.2, 50.2, 45.1; ^{31}P NMR (202 MHz, $CDCl_3$) δ 5.67 (d, J = 10.1 Hz, 1P); IR (KBr) ν 2946, 1726, 1665, 1432, 1266, 1099, 754 cm^{-1}. HRMS (ESI) calcd for $C_{33}H_{26}ClO_5PNa$ $[M+Na]^+$: 591.1104, found: 591.1101.



Dimethyl 4-(2-(2-bromophenyl)-2-oxoethyl)-1,1-diphenyl-1λ^5-phosphinoline-2,3-dicarboxylate (**5n**)

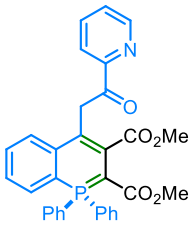
Yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 5:1); 115.5 mg, 94% yield; reaction time = 15 min; mp 69.4-70.2 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (dd, J_1 = 16.0 Hz, J_2 = 8.0 Hz, 4H), 7.56-7.52 (m, 3H), 7.49-7.43 (m, 6H), 7.31 (t, J = 8.0 Hz, 1H), 7.28-7.24 (m, 1H), 7.14-7.06 (m, 3H), 4.14 (s, 2H), 3.84 (s, 3H), 3.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.4, 171.1 (d, J = 16.0 Hz, 1C), 166.6, 141.2, 140.7 (d, J = 5.0 Hz, 1C), 133.1, 133.0, 132.7 (d, J = 8.0 Hz, 1C), 131.9 (d, J = 2.0 Hz, 1C), 131.8 (d, J = 3.0 Hz, 1C), 130.9, 129.2 (d, J = 13.0 Hz, 1C), 128.6, 128.5, 128.4, 126.8, 124.8 (d, J = 9.0 Hz, 1C), 124.5 (d, J = 12.0 Hz, 1C), 118.2, 111.4, 110.5, 103.9 (d, J = 9.0 Hz, 1C), 52.3, 50.2, 44.9; ^{31}P NMR (202 MHz, $CDCl_3$) δ 5.63 (d, J = 10.1 Hz, 1P); IR (KBr) ν 2945, 1726, 1668, 1433, 1268, 1101, 755 cm^{-1}. HRMS (ESI) calcd for $C_{33}H_{26}BrO_5PNa$ $[M+Na]^+$: 635.0599, found: 635.0595.



Dimethyl 4-(2-oxo-2-(thiophen-2-yl)ethyl)-1,1-diphenyl-1λ^5-phosphinoline-2,3-dicarboxylate (**5o**)

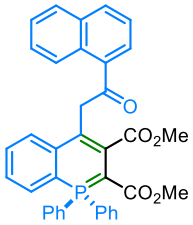
Yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 3:1); 107.5 mg, 99% yield; reaction time = 15 min; mp 187.4-188.2 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, J = 4.0 Hz, 1H), 7.66 (dd, J_1 = 12.0 Hz, J_2 = 8.0 Hz, 4H), 7.55-7.44 (m, 7H), 7.41-7.36 (m, 2H), 7.30 (t, J = 8.0 Hz, 1H), 7.08-7.04 (m, 1H), 6.94 (t, J = 4.0 Hz, 1H), 4.11 (s, 2H), 3.83 (s, 3H), 3.38 (s,

3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.8, 171.3 (d, *J* = 15.0 Hz, 1C), 166.8, 143.4, 141.0 (d, *J* = 5.0 Hz, 1C), 133.2, 133.1, 132.6 (d, *J* = 8.0 Hz, 1C), 132.3, 131.9 (d, *J* = 2.0 Hz, 1C), 131.8 (d, *J* = 3.0 Hz, 1C), 128.6, 128.5, 127.9, 124.6, 124.5, 124.4 (d, *J* = 5.0 Hz, 1C), 111.4, 110.5, 105.1 (d, *J* = 10.0 Hz, 1C), 52.2, 50.2, 42.7; ^{31}P NMR (202 MHz, $CDCl_3$) δ 5.68 (d, *J* = 10.1 Hz, 1P); IR (KBr) ν 2944, 1726, 1658, 1428, 1270, 1102, 751 cm^{-1}. HRMS (ESI) calcd for $C_{31}H_{25}O_5PSNa$ $[M+Na]^+$: 563.1058, found: 563.1061.



Dimethyl 4-(2-oxo-2-(pyridin-2-yl)ethyl)-1,1-diphenyl-1λ^5-phosphinoline-2,3-dicarboxylate (**5p**)

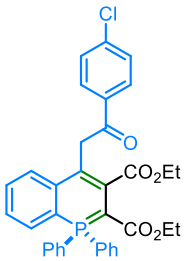
Yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 3:1 to 2:1); 86.8 mg, 81% yield; reaction time = 15 min; mp 125.4-126.2 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71 (d, *J* = 4.0 Hz, 1H), 8.02 (d, *J* = 8.0 Hz, 1H), 7.84-7.80 (m, 1H), 7.72 (dd, J_1 = 16.0 Hz, J_2 = 8.0 Hz, 4H), 7.55-7.46 (m, 7H), 7.39-7.32 (m, 3H), 7.09-7.05 (m, 1H), 4.53 (s, 2H), 3.72 (s, 3H), 3.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.4, 171.2 (d, *J* = 15.0 Hz, 1C), 166.7, 153.5, 148.8, 141.4 (d, *J* = 5.0 Hz, 1C), 136.8, 133.3, 133.2, 132.7 (d, *J* = 8.0 Hz, 1C), 131.7 (d, *J* = 2.0 Hz, 1C), 131.7 (d, *J* = 3.0 Hz, 1C), 128.5, 128.4, 127.0, 124.5 (d, *J* = 9.0 Hz, 1C), 124.2 (d, *J* = 12.0 Hz, 1C), 121.9, 111.5, 110.6, 105.4 (d, *J* = 9.0 Hz, 1C), 52.0, 50.1, 39.1; ^{31}P NMR (202 MHz, $CDCl_3$) δ 5.96 (d, *J* = 10.1 Hz, 1P); IR (KBr) ν 2973, 1728, 1266, 1098, 756 cm^{-1}. HRMS (ESI) calcd for $C_{32}H_{26}NO_5PNa$ $[M+Na]^+$: 558.1446, found: 558.1445.



Dimethyl 4-(2-(naphthalen-1-yl)-2-oxoethyl)-1,1-diphenyl-1λ^5-phosphinoline-2,3-dicarboxylate (**5q**)

Yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 4:1); 97.5 mg, 83% yield; reaction time = 15 min; mp 214.6-214.9 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.42-8.39 (m, 1H), 7.88 (dd, J_1 = 12.0 Hz, J_2 = 8.0 Hz, 2H), 7.82-7.79 (m, 1H), 7.59 (dd, J_1 = 12.0 Hz, J_2 =

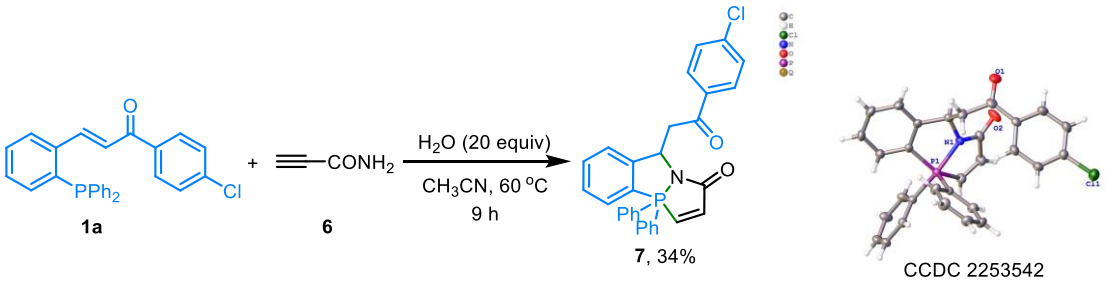
8.0 Hz, 4H), 7.51 (t, *J* = 8.0 Hz, 3H), 7.47-7.40 (m, 7H), 7.36 (t, *J* = 8.0 Hz, 1H), 7.29-7.24 (m, 1H), 7.06 (t, *J* = 8.0 Hz, 1H), 4.30 (s, 2H), 3.71 (s, 3H), 3.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.8, 171.4 (d, *J* = 16.0 Hz, 1C), 166.7, 141.1 (d, *J* = 5.0 Hz, 1C), 135.9, 133.7, 133.1, 133.0, 132.6 (d, *J* = 8.0 Hz, 1C), 131.8, 131.8 (d, *J* = 2.0 Hz, 1C), 131.7 (d, *J* = 3.0 Hz, 1C), 130.0, 128.5, 128.4, 128.1, 127.4, 126.7, 126.1, 125.7, 124.5 (d, *J* = 8.0 Hz, 1C), 124.4 (d, *J* = 12.0 Hz, 1C), 124.2, 111.5, 110.6, 105.3 (d, *J* = 9.0 Hz, 1C), 52.1, 50.2, 44.5; ^{31}P NMR (202 MHz, $CDCl_3$) δ 5.62 (d, *J* = 10.1 Hz, 1P); IR (KBr) ν 2946, 1727, 1664, 1432, 1273, 1102, 751 cm^{-1}. HRMS (ESI) calcd for $C_{37}H_{29}O_5PNa$ $[M+Na]^+$: 607.1650, found: 607.1653.



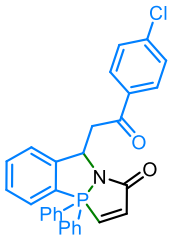
Diethyl 4-(2-(4-chlorophenyl)-2-oxoethyl)-1,1-diphenyl-1λ^5-phosphinoline-2,3-dicarboxylate (**5r**)

Yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 5:1); 89.1 mg, 75% yield; reaction time = 15 min; mp 201.5-202.3 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 8.0 Hz, 2H), 7.63-7.52 (m, 6H), 7.46-7.40 (m, 4H), 7.37 (t, *J* = 8.0 Hz, 1H), 7.29 (dd, J_1 = 8.0 Hz, J_2 = 4.0 Hz, 1H), 7.22-7.17 (m, 3H), 7.05 (t, *J* = 8.0 Hz, 1H), 4.32 (q, *J* = 8.0 Hz, 2H), 4.16 (s, 2H), 3.89 (q, *J* = 8.0 Hz, 2H), 1.25 (t, *J* = 8.0 Hz, 3H), 0.77 (br, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.2, 170.9 (d, *J* = 15.0 Hz, 1C), 166.2, 140.8 (d, *J* = 5.0 Hz, 1C), 138.8, 135.0, 133.1, 133.0, 132.4 (d, *J* = 8.0 Hz, 1C), 131.8 (d, *J* = 3.0 Hz, 1C), 131.7 (d, *J* = 2.0 Hz, 1C), 129.6, 128.6, 128.5, 128.5, 124.4 (d, *J* = 12.0 Hz, 1C), 124.2 (d, *J* = 8.0 Hz, 1C), 111.3, 110.4, 105.7, 61.2, 58.9, 42.4, 14.0, 14.0; ^{31}P NMR (202 MHz, $CDCl_3$) δ 5.65 (d, *J* = 10.1 Hz, 1P); IR (KBr) ν 2979, 1721, 1660, 1259, 1102, 751 cm^{-1}. HRMS (ESI) calcd for $C_{35}H_{30}ClO_5PNa$ $[M+Na]^+$: 619.1417, found: 619.1412.

4. Experimental data for the formation of 7



General procedure for the preparation of 7: To a solution of functionalized organic phosphine **1a** (85.4 mg, 0.20 mmol) in CH_3CN (1.0 mL) was added propiolamide **6** (28.0 mg, 0.40 mmol) and water (4.0 mmol, 20 equiv). After being stirred at 60 °C for 9 h, the mixture was concentrated in vacuum. The residue was purified via flash column chromatography on silica gel (petroleum ether / ethyl acetate = 5:1) to afford the corresponding product **7** as white solid in 34% yield.

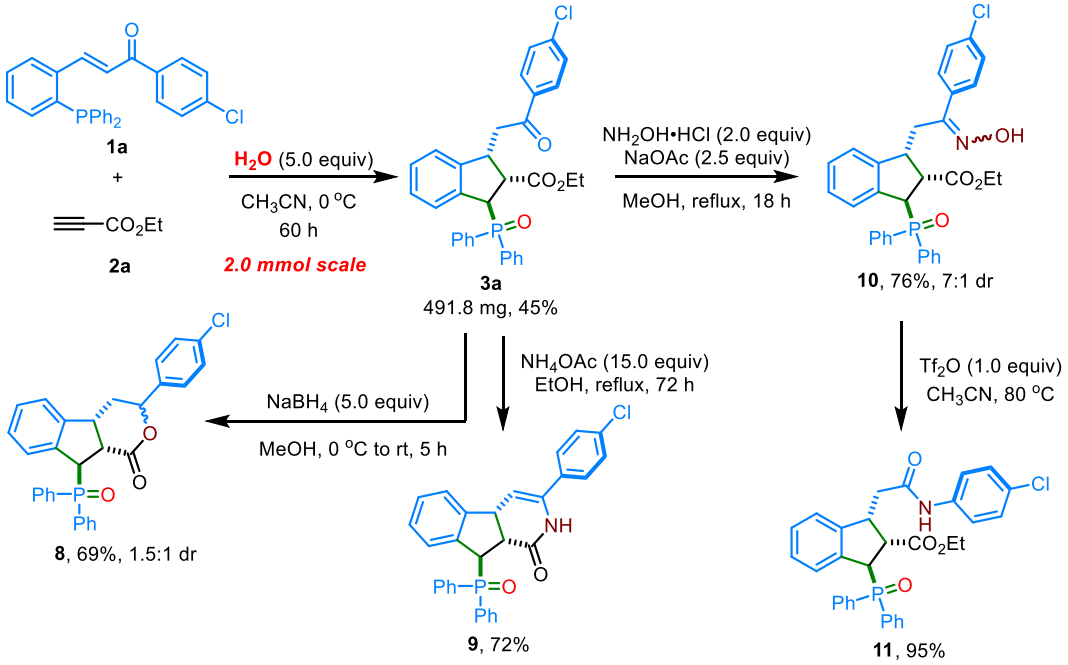


5-(2-(4-Chlorophenyl)-2-oxoethyl)-10,10-diphenyl-5,10-dihydro-3*H*-10λ^5-[1,2]azaphospholo[1,2-*a*]benzo[*c*][1,2]azaphosphol-3-one (**7**)

White solid obtained by column chromatography (petroleum ether/ethyl acetate = 5:1); 33.5 mg, 34% yield; reaction time = 9 h; mp 224.7-224.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, J = 8.0 Hz, 2H), 7.54 (d, J = 8.0 Hz, 1H), 7.48-7.43 (m, 4H), 7.41 (d, J = 8.0 Hz, 1H), 7.37 (d, J = 4.0 Hz, 1H), 7.30 (t, J = 8.0 Hz, 5H), 7.18-7.14 (m, 1H), 7.10 (t, J = 8.0 Hz, 2H), 6.96 (dd, J_1 = 48.0 Hz, J_2 = 4.0 Hz, 1H), 6.70 (d, J = 4.0 Hz, 1H), 6.67 (dd, J_1 = 48.0 Hz, J_2 = 4.0 Hz, 1H), 5.39 (t, J = 4.0 Hz, 1H), 3.12 (dd, J_1 = 12.0 Hz, J_2 = 4.0 Hz, 1H), 2.60 (dd, J_1 = 12.0 Hz, J_2 = 4.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 197.2, 163.8 (d, J = 27.5 Hz, 1C), 149.2 (d, J = 27.5 Hz, 1C), 148.0 (d, J = 35.0 Hz, 1C), 147.0, 146.0, 142.8, 129.3, 135.9 (d, J = 17.5 Hz, 1C), 135.2, 134.9, 134.0, 132.6 (d, J = 2.5 Hz, 1C), 130.6 (d, J = 9.0 Hz, 1C), 130.2 (d, J = 3.75 Hz, 1C), 129.8, 129.5 (d, J = 10.0 Hz, 1C), 128.7 (d, J = 14.0 Hz, 1C), 128.6, 128.0 (dd, J_1 = 9.0 Hz, J_2 = 1.3 Hz, 1C), 127.5 (d, J = 16.3 Hz, 1C), 126.7 (d, J = 11.3 Hz, 1C), 47.4 (d, J = 10.0 Hz, 1C), 44.7; ^{31}P NMR (202 MHz, $CDCl_3$) δ -69.47; IR (KBr) ν 3059, 1673, 1582, 1388, 1083, 757 cm^{-1}. HRMS (ESI) calcd for $C_{30}H_{24}ClNO_2P$ $[M+H]^+$: 496.1228, found: 496.1229.

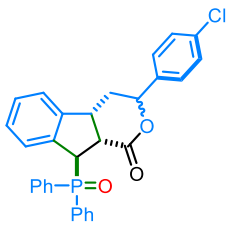
5. Synthetic utility

5.1 Scalable preparation of 3a and its derivation



General procedure for scalable preparation of 3a: To a solution of functionalized organic phosphine **1a** (853.8 mg, 2.0 mmol) and ethyl propargynate **2a** (410 μL, 4.0 mmol) in extra dry CH_3CN (8.0 mL) was added water (180 μL, 10.0 mmol). After being stirred at 0 °C for 60 h, the mixture was concentrated in vacuum. The residue was purified via flash column chromatography on silica gel (petroleum ether / ethyl acetate = 4:1 to 2:1) to afford the corresponding product **3a** as white solid in 45% yield (491.8 mg).

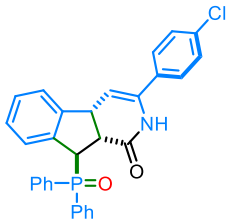
General procedure for the formation of 8: A solution of **3a** (81.5 mg, 0.15 mmol) in 1.0 mL of MeOH was cooled to 0 °C, and then $NaBH_4$ (28.4 mg, 0.75 mmol) was added successively. The reaction mixture was stirred at 0 °C for 5 h until the complete consumption of **3a** as monitored by thin layer chromatography. Then, saturated aq. NH_4Cl solution was added. The mixture was extracted with CH_2Cl_2. The combined organic phase was dried over $MgSO_4$, filtered, concentrated and purified with silica gel column chromatography to obtain **8** in 69% yield with 1.5:1 dr.



3-(4-Chlorophenyl)-9-(diphenylphosphoryl)-4,4a,9,9a-tetrahydroindeno[2,1-*c*]pyran-1(3*H*)-one (**8**)

Light red solid obtained by column chromatography (dichloromethane/methanol = 200:1); 51.4 mg, 69% yield, 1.5:1 dr (inseparable isomer); reaction time = 5 h; mp 202.4-205.3 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) for major isomer δ 8.04-7.99 (m, 2H), 7.66-7.64 (m, 2H), 7.58-7.52 (m, 4H), 7.46 (dd, J_1 = 8.0 Hz, J_2 = 4.0 Hz, 2H), 7.35-7.27 (m, 4H), 7.18 (d, *J* = 8.0 Hz, 1H), 7.08 (d, *J* = 8.0 Hz, 1H), 6.93 (t, *J* = 8.0 Hz, 1H), 6.22 (d, *J* = 8.0 Hz, 1H), 5.32 (d, *J* = 8.0 Hz, 1H), 5.07 (d, *J* = 4.0 Hz, 1H), 4.27 (q, *J* = 8.0 Hz, 1H), 3.73-3.66 (m, 1H), 2.77-2.71 (m, 1H), 1.87-1.78 (m, 1H); ^{1}H NMR (400 MHz, $CDCl_3$) for minor isomer δ 8.11-8.06 (m, 2H), 7.70-7.67 (m, 2H), 7.58-7.52 (m, 4H), 7.43 (d, *J* = 4.0 Hz, 2H), 7.34-7.27 (m, 4H), 7.24 (d, *J* = 8.0 Hz, 1H), 7.08 (d, *J* = 8.0 Hz, 1H), 7.00 (t, *J* = 8.0 Hz, 1H), 6.31 (d, *J* = 8.0 Hz, 1H), 5.04 (d, *J* = 4.0 Hz, 1H), 4.66 (d, *J* = 4.0 Hz, 1H), 4.09-4.05 (m, 1H), 3.65-3.60 (m, 1H), 2.49-2.44 (m, 1H), 2.37-2.29 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) for major isomer δ 172.5 (d, *J* = 12.0 Hz, 1C), 145.9 (d, *J* = 5.0 Hz, 1C), 136.8, 135.7 (d, *J* = 6.0 Hz, 1C), 134.5, 131.6-131.4 (m, 1C), 131.1 (d, *J* = 9.0 Hz, 1C), 130.4 (d, *J* = 17.0 Hz, 1C), 129.0 (d, *J* = 11.0 Hz, 1C), 128.9, 128.4 (d, *J* = 12.0 Hz, 1C), 127.4, 127.0 (d, *J* = 2.0 Hz, 1C), 125.5 (d, *J* = 2.0 Hz, 1C), 123.6 (d, *J* = 2.0 Hz, 1C), 78.2, 46.4, 46.3 (d, *J* = 69.0 Hz, 1C), 41.3, 37.3; ^{13}C NMR (100 MHz, $CDCl_3$) for minor isomer δ 173.2 (d, *J* = 14.0 Hz, 1C), 143.7 (d, *J* = 5.0 Hz, 1C), 137.5, 137.3 (d, *J* = 6.0 Hz, 1C), 134.2, 132.2-132.1 (m, 1C), 131.1 (d, *J* = 9.0 Hz, 1C), 130.4 (d, *J* = 17.0 Hz, 1C), 128.9 (d, *J* = 11.0 Hz, 1C), 128.9, 128.3 (d, *J* = 3.0 Hz, 1C), 127.2 (d, *J* = 3.0 Hz, 1C), 127.0, 126.0 (d, *J* = 3.0 Hz, 1C), 122.9 (d, *J* = 3.0 Hz, 1C), 77.6, 49.4 (d, *J* = 69.0 Hz, 1C), 45.0, 40.6, 32.2; ^{31}P NMR (202 MHz, $CDCl_3$) for major isomer δ 33.77; ^{31}P NMR (202 MHz, $CDCl_3$) for minor isomer δ 33.16; IR (KBr) ν 3058, 1733, 1191, 753 cm^{-1}. HRMS (ESI) calcd for $C_{30}H_{25}ClO_3P$ $[M+H]^+$: 499.1224, found: 499.1226.

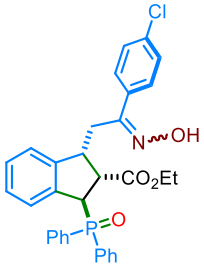
General procedure for the formation of 9: To a solution of **3a** (81.5 mg, 0.15 mmol) in ethanol (1.0 mL) was added NH_4OAc (173.4 mg, 2.25 mmol). The resulting reaction mixture was stirred at 80 ^{o}C for 72 h until complete consumption of **3a** as monitored by thin layer chromatography. Then, the reaction mixture was directly subjected to column chromatography on silica gel (petroleum ether/ethyl acetate = 4:1 to 1:1) to afford **9** as yellow solid in 72% yield.



3-(4-Chlorophenyl)-9-(diphenylphosphoryl)-2,4a,9,9a-tetrahydro-1*H*-indeno[2,1-*c*]pyridin-1-one (**9**)

Yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 4:1 to 1:1); 53.6 mg, 72% yield, >20:1 dr; reaction time = 72 h; mp 153.9-154.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.85 (s, 1H), 8.04-8.00 (m, 2H), 7.70-7.65 (m, 2H), 7.55-7.38 (m, 8H), 7.33 (d, *J* = 8.0 Hz, 2H), 7.18 (q, *J* = 8.0 Hz, 2H), 6.90 (t, *J* = 8.0 Hz, 1H), 6.24 (d, *J* = 8.0 Hz, 1H), 5.71 (d, *J* = 4.0 Hz, 1H), 4.93 (d, *J* = 4.0 Hz, 1H), 4.44 (t, *J* = 8.0 Hz, 1H), 3.55 (dd, J_1 = 16.0 Hz, J_2 = 12.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.6 (d, *J* = 13.0 Hz, 1C), 145.6 (d, *J* = 4.0 Hz, 1C), 135.5 (d, *J* = 6.0 Hz, 1C), 135.3, 134.6, 133.4, 132.6, 131.8 (dd, J_1 = 8.0 Hz, J_2 = 3.0 Hz, 1C), 131.3 (dd, J_1 = 22.0 Hz, J_2 = 9.0 Hz, 1C), 128.7, 128.5 (dd, J_1 = 32.0 Hz, J_2 = 9.0 Hz, 1C), 128.0 (d, *J* = 3.0 Hz, 1C), 126.9, 126.7 (d, *J* = 3.0 Hz, 1C), 125.2 (d, *J* = 3.0 Hz, 1C), 123.5 (d, *J* = 3.0 Hz, 1C), 102.4, 47.7 (d, *J* = 68.0 Hz, 1C), 45.7, 41.8; ^{31}P NMR (202 MHz, $CDCl_3$) δ 33.27; IR (KBr) ν 3064, 2924, 1673, 1185, 1108, 756 cm^{-1}. HRMS (ESI) calcd for $C_{30}H_{24}ClNO_2P$ $[M+H]^+$: 496.1228, found: 496.1226.

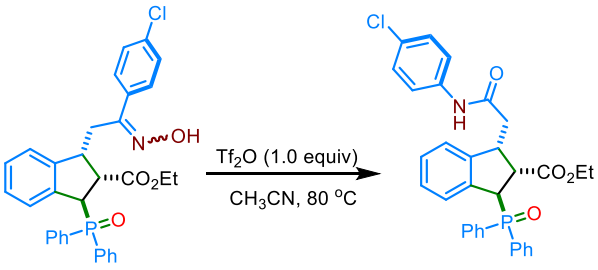
General procedure for the formation of 10: To a solution of **9a** (81.5 mg, 0.15 mmol) and hydroxylamine hydrochloride (20.9 mg, 0.30 mmol) in methanol (1.0 mL) was added NaOAc (30.8 mg, 0.375 mmol). The resulting reaction mixture was stirred at 65 °C for 18 h until complete consumption of **9a** as monitored by thin layer chromatography. Then, the reaction mixture was directly subjected to column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1 to 1:1) to afford **15** as white solid in 76% yield with 7:1 dr.



Ethyl

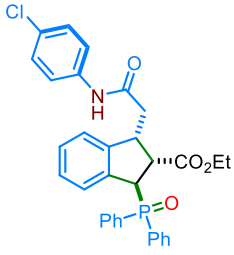
1-(2-(4-chlorophenyl)-2-(hydroxyimino)ethyl)-3-(diphenylphosphoryl)-2,3-dihydro-1*H*-indene-2-carboxylate (**10**)

White solid obtained by column chromatography (petroleum ether/ethyl acetate = 5:1 to 1:1); 63.4 mg, 76% yield, 7:1 dr; reaction time = 18 h; mp 109.2-109.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.41 (br, 1H), 7.94 (dd, J_1 = 12.0 Hz, J_2 = 8.0 Hz, 2H), 7.83 (dd, J_1 = 12.0 Hz, J_2 = 8.0 Hz, 2H), 7.60 (t, J = 8.0 Hz, 1H), 7.54-7.47 (m, 3H), 7.44-7.40 (m, 2H), 7.12 (s, 4H), 6.96-6.90 (m, 3H), 6.61 (d, J = 4.0 Hz, 1H), 4.83 (t, J = 4.0 Hz, 1H), 4.16-4.10 (m, 1H), 4.03-3.95 (m, 1H), 3.76-3.64 (m, 2H), 2.82 (dd, J_1 = 12.0 Hz, J_2 = 4.0 Hz, 1H), 2.66 (dd, J_1 = 12.0 Hz, J_2 = 8.0 Hz, 1H), 1.01 (t, J = 8.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 172.2 (d, J = 3.0 Hz, 1C), 154.7, 145.2 (d, J = 5.0 Hz, 1C), 135.7 (d, J = 4.0 Hz, 1C), 135.1, 134.3, 132.1 (dd, J_1 = 68.0 Hz, J_2 = 3.0 Hz, 1C), 131.7 (t, J = 9.0 Hz, 1C), 131.3, 130.7 (d, J = 34.0 Hz, 1C), 128.6 (dd, J_1 = 58.0 Hz, J_2 = 11.0 Hz, 1C), 128.1, 127.7, 127.3, 125.3, 124.8 (d, J = 3.0 Hz, 1C), 60.8, 48.6, 46.1 (d, J = 70.0 Hz, 1C), 42.3 (d, J = 6.0 Hz, 1C), 29.2, 14.0; ^{31}P NMR (202 MHz, $CDCl_3$) δ 32.58; IR (KBr) ν 3055, 2950, 1728, 1185, 1112, 756 cm^{-1}. HRMS (ESI) calcd for $C_{32}H_{30}ClNO_4P$ $[M+H]^+$: 558.1595, found: 558.1602.



10 **11**, 95%

General procedure for the formation of 11: To a solution of **10** (214.8 mg, 0.385 mmol) in CH_3CN (1.0 mL) was added Tf_2O (65 μL, 108.6 mg, 0.385 mmol). The resulting reaction mixture was stirred at 80 °C for 15 h until complete consumption of **10** as monitored by thin layer chromatography. Then, the reaction mixture was directly subjected to column chromatography on silica gel (petroleum ether/ethyl acetate = 3:1 to 2:1) to afford **11** as white solid in 95% yield.

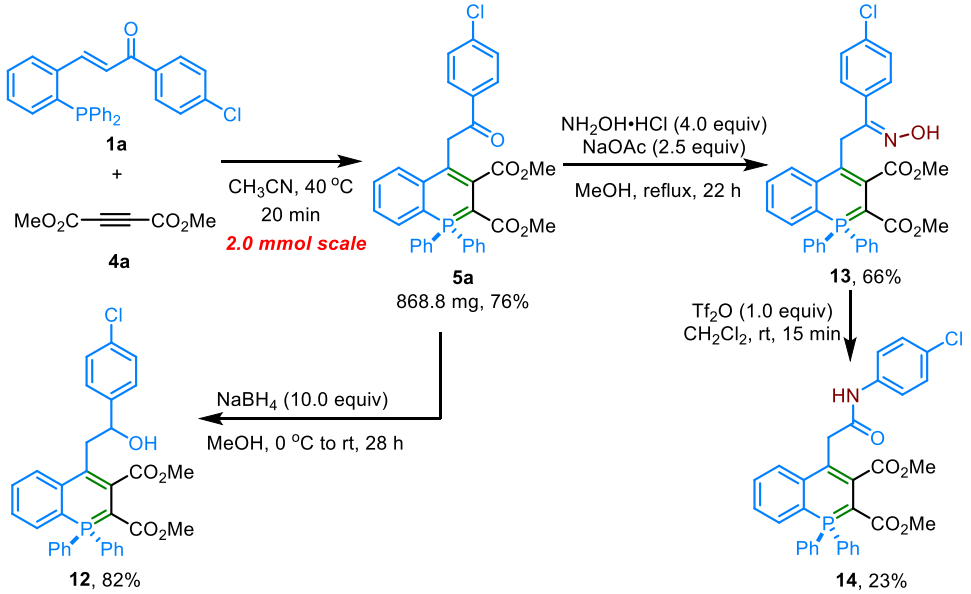


Ethyl

1-(2-((4-chlorophenyl)amino)-2-oxoethyl)-3-(diphenylphosphoryl)-2,3-dihydro-1*H*-indene-2-carb oxylate (**11**)

White solid obtained by column chromatography (petroleum ether/ethyl acetate = 3:1 to 2:1); 203.1 mg, 95% yield, >20:1 dr; reaction time = 15 h; mp 125.4-125.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.91 (s, 1H), 7.69-7.59 (m, 4H), 7.53 (t, J = 8.0 Hz, 1H), 7.47 (d, J = 8.0 Hz, 1H), 7.39-7.36 (m, 6H), 7.12 (dd, J_1 = 16.0 Hz, J_2 = 4.0 Hz, 3H), 7.01 (d, J = 8.0 Hz, 1H), 6.95 (t, J = 8.0 Hz, 1H), 6.68 (d, J = 8.0 Hz, 1H), 4.65-4.61 (m, 1H), 4.01 (q, J = 8.0 Hz, 1H), 3.87-3.80 (m, 1H), 3.75 (q, J = 8.0 Hz, 2H), 2.65-2.55 (m, 2H), 0.98 (t, J = 8.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.6 (d, J = 7.0 Hz, 1C), 169.4, 144.9 (d, J = 6.0 Hz, 1C), 137.1, 136.3 (d, J = 5.0 Hz, 1C), 132.1 (dd, J_1 = 16.0 Hz, J_2 = 3.0 Hz, 1C), 131.6 (t, J = 9.0 Hz, 1C), 131.2 (d, J = 28.0 Hz, 1C), 130.2 (d, J = 28.0 Hz, 1C), 128.6 (dd, J_1 = 14.0 Hz, J_2 = 3.0 Hz, 1C), 128.4, 128.0 (d, J = 2.0 Hz, 1C), 127.3 (d, J = 1.0 Hz, 1C), 125.2 (d, J = 3.0 Hz, 1C), 124.0, 120.9, 61.0, 48.5, 47.5 (d, J = 70.0 Hz, 1C), 42.9 (d, J = 4.0 Hz, 1C), 39.3, 13.8; ^{31}P NMR (202 MHz, $CDCl_3$) δ 32.72; IR (KBr) ν 3433, 3057, 2981, 1727, 1182, 1108, 702 cm^{-1}. HRMS (ESI) calcd for $C_{32}H_{30}ClNO_4P$ $[M+H]^+$: 558.1595, found: 558.1599.

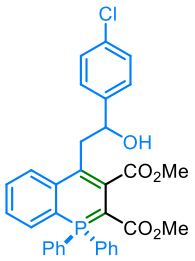
5.2 Scalable preparation of 5a and its derivation



General procedure for scalable preparation of 5a: To a solution of functionalized organic phosphine **1a** (853.8 mg, 2.0 mmol) in extra dry CH_3CN (10.0 mL), diethyl but-2-ynedioate **4a** (270 μL, 2.2 mmol) was added. After being stirred at 40 °C for 20 min, the mixture was concentrated in vacuum. The residue was purified via flash column chromatography on silica gel

(petroleum ether / ethyl acetate = 5:1 to 4:1) to afford the corresponding product **5a** as yellow solid in 76% yield (868.8 mg).

General procedure for the formation of 12： A solution of **5a** (85.4 mg, 0.15 mmol) in 1.0 mL of MeOH was cooled to 0 °C, and then $NaBH_4$ (56.7 mg, 1.50 mmol) was added successively. The reaction mixture was stirred at 0 °C for 15 min and then at room temperature until the complete consumption of **5a** as monitored by thin layer chromatography. Then, saturated aq. NH_4Cl solution was added. The mixture was extracted with CH_2Cl_2. The combined organic phase was dried over $MgSO_4$, filtered, concentrated and purified with silica gel column chromatography to obtain **12** in 82% yield.

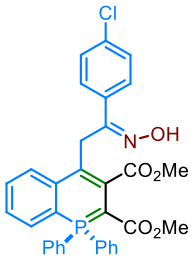


Dimethyl 4-(2-(4-chlorophenyl)-2-hydroxyethyl)-1,1-diphenyl-1λ^5-phosphinoline-2,3-dicarboxylate (**12**)

Yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 5:1); 70.3 mg, 82% yield; reaction time = 28 h; mp 112.4-113.1 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74-7.65 (m, 5H), 7.58-7.51 (m, 7H), 7.42 (dd, J_1 = 12.0 Hz, J_2 = 8.0 Hz, 1H), 7.35 (d, J = 8.0 Hz, 2H), 7.28 (s, 3H), 7.17 (t, J = 8.0 Hz, 1H), 4.93-4.90 (m, 1H), 3.95 (s, 3H), 3.40 (s, 3H), 3.09 (dd, J_1 = 16.0 Hz, J_2 = 4.0 Hz, 1H), 2.73 (t, J = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.7, 144.1, 140.4 (d, J = 5.0 Hz, 1C), 133.3 (d, J = 4.0 Hz, 1C), 133.2, 133.1, 132.6, 131.9 (d, J = 3.0 Hz, 1C), 131.8 (d, J = 3.0 Hz, 1C), 131.9, 128.7, 128.5, 128.4, 126.9, 124.6 (d, J = 12.0 Hz, 1C), 124.2 (d, J = 9.0 Hz, 1C), 112.2, 111.3, 106.5 (d, J = 9.0 Hz, 1C), 72.1, 52.8, 50.2, 40.7; ^{31}P NMR (202 MHz, $CDCl_3$) δ 5.73; IR (KBr) ν 3433, 2938, 1725, 1660, 1435, 1267, 1104, 753 cm^{-1}. HRMS (ESI) calcd for $C_{33}H_{29}ClO_5P$ $[M+Na]^+$: 571.1436, found: 571.1439.

General procedure for the formation of 13: To a solution of **5a** (85.4 mg, 0.15 mmol) and hydroxylamine hydrochloride (41.8 mg, 0.60 mmol) in methanol (1.0 mL) was added NaOAc (30.8 mg, 0.375 mmol). The resulting reaction mixture was stirred at 65 °C for 22 h until complete consumption of **5a** as monitored by thin layer chromatography. Then, the reaction mixture was

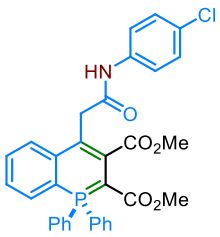
directly subjected to column chromatography on silica gel (petroleum ether/ethyl acetate = 6:1 to 5:1) to afford **13** as yellow solid in 66% yield.



Dimethyl 4-(2-(4-chlorophenyl)-2-(hydroxyimino)ethyl)-1,1-diphenyl-1λ^5-phosphinoline-2,3-dicarboxylate (**13**)

White solid obtained by column chromatography (petroleum ether/ethyl acetate = 6:1 to 5:1); 57.5 mg, 66% yield; reaction time = 22 h; mp 122.3-123.3 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.30 (br, 1H), 7.44-7.41 (m, 2H), 7.33-7.28 (m, 8H), 7.22 (d, *J* = 8.0 Hz, 1H), 7.19-7.16 (m, 3H), 7.00-6.95 (m, 1H), 6.92-6.89 (m, 1H), 6.76 (d, *J* = 8.0 Hz, 2H), 3.99 (br, 2H), 3.89 (s, 3H), 3.26 (br, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.6 (d, *J* = 15.0 Hz, 1C), 166.8 (d, *J* = 11.0 Hz, 1C), 159.5, 140.0 (d, *J* = 5.0 Hz, 1C), 134.0, 133.5, 132.8 (d, *J* = 10.0 Hz, 1C), 132.3 (d, *J* = 8.0 Hz, 1C), 131.8 (d, *J* = 3.0 Hz, 1C), 131.7 (d, *J* = 2.0 Hz, 1C), 129.1, 128.9, 128.5 (d, *J* = 13.0 Hz, 1C), 127.9, 127.7, 124.5 (d, *J* = 12.0 Hz, 1C), 124.0 (d, *J* = 8.0 Hz, 1C), 111.3, 110.4, 106.3 (d, *J* = 9.0 Hz, 1C), 52.4, 50.1, 28.1; ^{31}P NMR (202 MHz, $CDCl_3$) δ 5.36; IR (KBr) ν 3056, 2949, 1727, 1671, 1436, 1272, 1103, 754 cm^{-1}. HRMS (ESI) calcd for $C_{33}H_{28}ClNO_5P$ $[M+H]^+$: 584.1388, found: 584.1389.

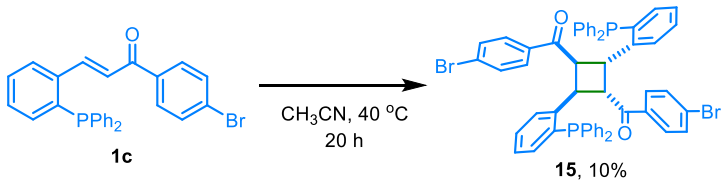
General procedure for the formation of 14: To a solution of **13** (87.6 mg, 0.15 mmol) in CH_2Cl_2 (1.0 mL) was added Tf_2O (25.2 μL, 42.3 mg, 0.15 mmol). The resulting reaction mixture was stirred at room temperature for 15 min until complete consumption of **13** as monitored by thin layer chromatography. Then, the reaction mixture was directly subjected to column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford **14** as yellow solid in 23% yield.



Dimethyl

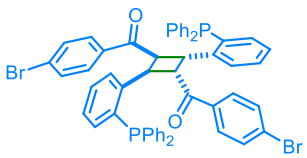
4-(2-((4-chlorophenyl)amino)-2-oxoethyl)-1,1-diphenyl-1λ^5-phosphinoline-2,3-dicarboxylate (**12**) Yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 5:1); 20.0 mg, 23% yield; reaction time = 15 min; mp 117.2-117.9 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.97 (s, 1H), 7.81 (t, *J* = 8.0 Hz, 1H), 7.54-7.48 (m, 4H), 7.43-7.30 (m, 9H), 7.25-7.20 (m, 1H), 7.11 (s, 1H), 7.05 (d, *J* = 8.0 Hz, 2H), 3.84 (s, 3H), 3.36 (s, 2H), 3.24 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.4, 166.7 (d, *J* = 10.0 Hz, 1C), 140.7 (d, *J* = 5.0 Hz, 1C), 137.2, 133.2, 133.1, 132.8 (d, *J* = 2.0 Hz, 1C), 132.7, 132.7, 132.2 (d, *J* = 3.0 Hz, 1C), 128.8, 128.7, 128.6, 128.4, 127.8, 125.4, 125.3 (d, *J* = 3.0 Hz, 1C), 120.8, 111.7, 110.9, 53.1, 50.4, 41.5; ^{31}P NMR (202 MHz, $CDCl_3$) δ 5.82; IR (KBr) ν 2949, 1676, 1436, 1268, 1103, 753 cm^{-1}. HRMS (ESI) calcd for $C_{33}H_{28}ClNO_5P$ $[M+H]^+$: 584.1388, found: 584.1390.

6. Experimental data for the [2+2] cycloaddition between bimolecular 1c



1c **15**, 10%

General procedure：To a 5.0 mL vial were successively added functionalized organic phosphine **1c** (0.20 mmol) and 1.0 mL of extra dry CH_3CN. The resulting mixture was stirred at 40 °C for 20 h. And then, the reaction mixture was directly subjected to flash column chromatography on silica gel (petroleum ether/ethyl acetate) to afford the corresponding product **15**.



2,4-Bis(2-(diphenylphosphanyl)phenyl)cyclobutane-1,3-diyl)bis((4-bromophenyl)methanone) (**15**) White solid obtained by column chromatography (petroleum ether/ethyl acetate = 80:1); 9.4 mg, 10% yield; reaction time = 20 h; mp 230.8-231.2 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (d, *J* =

8.0 Hz, 4H), 7.32 (d, *J* = 8.0 Hz, 6H), 7.23 (d, *J* = 8.0 Hz, 6H), 7.19 (s, 12H), 7.01 (t, *J* = 8.0 Hz, 2H), 6.88 (t, *J* = 8.0 Hz, 4H), 6.71 (t, *J* = 8.0 Hz, 2H), 5.47 (q, *J* = 8.0 Hz, 2H), 4.82 (t, *J* = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.7, 143.2 (d, *J* = 24.0 Hz, 1C), 136.1-135.8 (m, 1C), 134.8, 133.7 (d, *J* = 7.0 Hz, 1C), 133.6 (d, *J* = 4.0 Hz, 1C), 133.5, 131.4, 129.8 (d, *J* = 2.0 Hz, 1C), 129.2, 128.8, 128.5 (q, *J* = 3.0 Hz, 1C), 127.8, 127.1, 126.8 (d, *J* = 5.0 Hz, 1C), 50.0 (d, *J* = 4.0 Hz, 1C), 40.6 (d, *J* = 26.0 Hz, 1C); ^{31}P NMR (162 MHz, $CDCl_3$) δ -15.48; IR (KBr) ν 3444, 1672, 1582, 1219, 744 cm^{-1}. HRMS (ESI) calcd for $C_{54}H_{41}Br_2O_2P_2$ $[M+H]^+$: 941.0949, found: 941.0945.

7. Photophysical and electrochemical studies

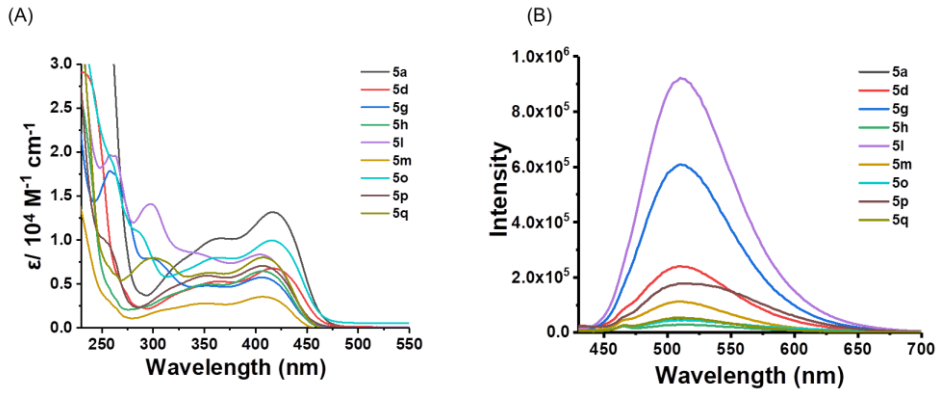


Figure S1. (A) UV-Vis absorption of **5a**, **5d**, **5g**, **5h**, **5l**, **5m**, **5o**, **5p** and **5q** in CH_2Cl_2 at room temperature ([C] = 1 × 10^{-5} M) (left) and (B) Fluorescence absorption spectra in dichloromethane at room temperature (λ_{ex} = 420 nm, slit: 5/5 nm) (right).

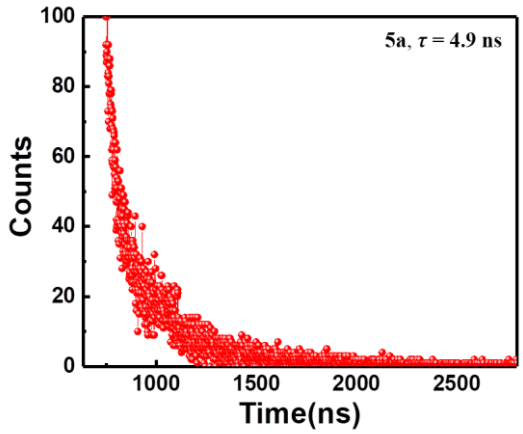


Figure S2. Time-resolved fluorescence decay plot of compound **5a** (λ_{ex} = 512 nm, [C] = 1 × 10^{-5} M) in dichloromethane at room temperature using a nano-LED of 370 nm as the light source.

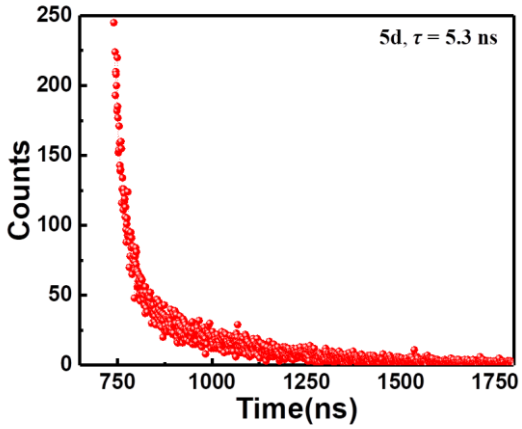


Figure S3. Time-resolved fluorescence decay plot of compound **5d** (λ_{ex} = 512 nm, [C] = 1 × 10^{-5} M) in dichloromethane at room temperature using a nano-LED of 370 nm as the light source.

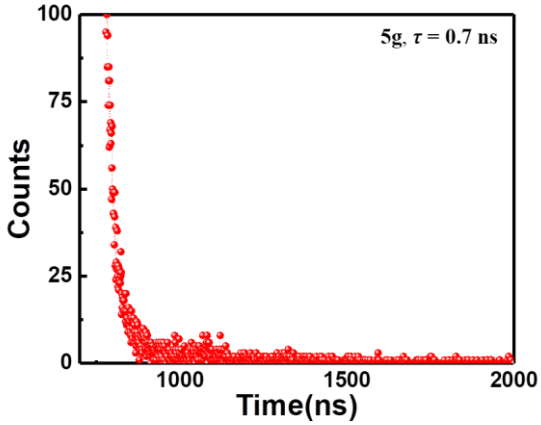


Figure S4. Time-resolved fluorescence decay plot of compound **5g** (λ_{ex} = 510 nm, [C] = 1 × 10^{-5} M) in dichloromethane at room temperature using a nano-LED of 370 nm as the light source.

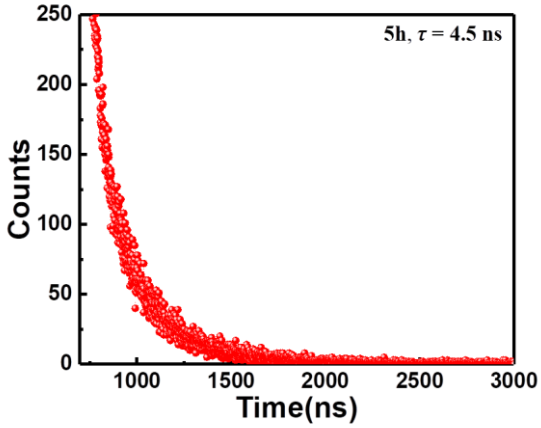


Figure S5. Time-resolved fluorescence decay plot of compound **5h** (λ_{ex} = 517 nm, [C] = 1 × 10^{-5} M) in dichloromethane at room temperature using a nano-LED of 370 nm as the light source.

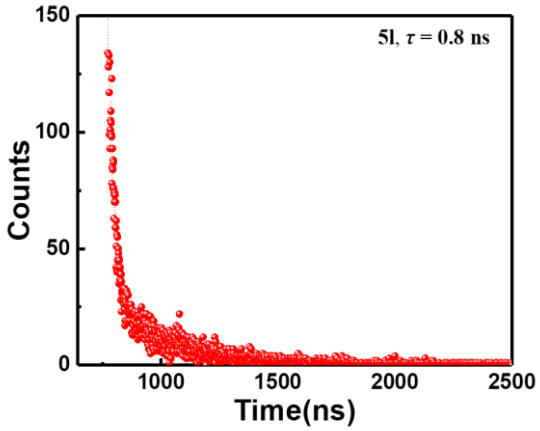


Figure S6. Time-resolved fluorescence decay plot of compound **5l** (λ_{ex} = 513 nm, [C] = 1 × 10^{-5} M) in dichloromethane at room temperature using a nano-LED of 370 nm as the light source.

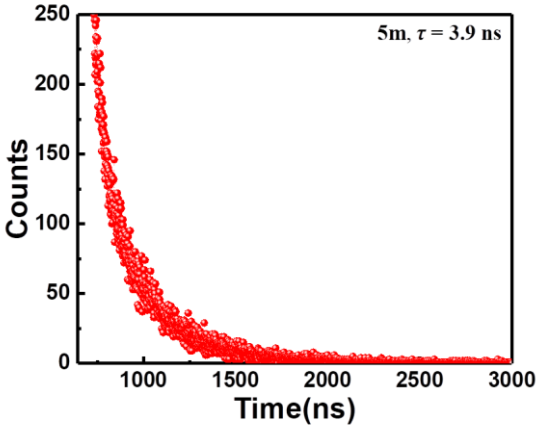


Figure S7. Time-resolved fluorescence decay plot of compound **5m** (λ_{ex} = 510 nm, [C] = 1 × 10^{-5} M) in dichloromethane at room temperature using a nano-LED of 370 nm as the light source.

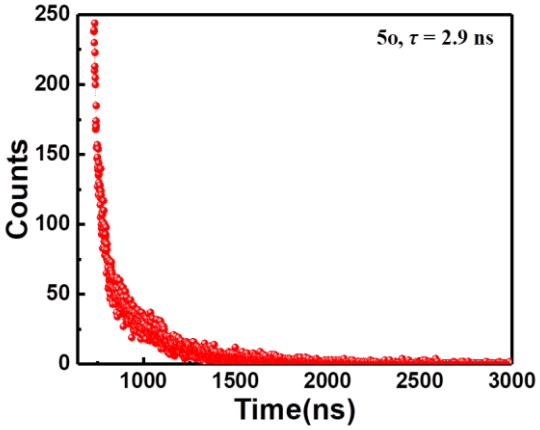


Figure S8. Time-resolved fluorescence decay plot of compound **5o** (λ_{ex} = 514 nm, [C] = 1 × 10^{-5} M) in dichloromethane at room temperature using a nano-LED of 370 nm as the light source.

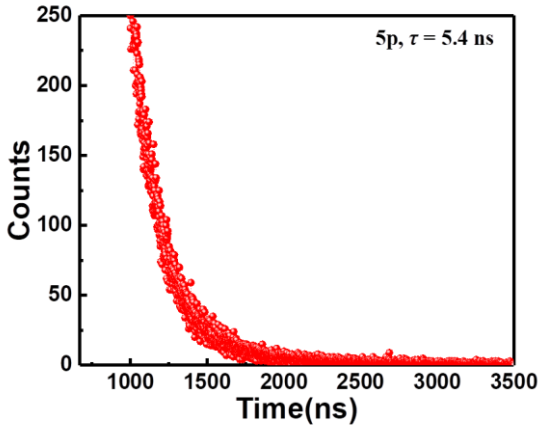


Figure S9. Time-resolved fluorescence decay plot of compound **5p** (λ_{ex} = 518 nm, [C] = 1 × 10^{-5} M) in dichloromethane at room temperature using a nano-LED of 370 nm as the light source.

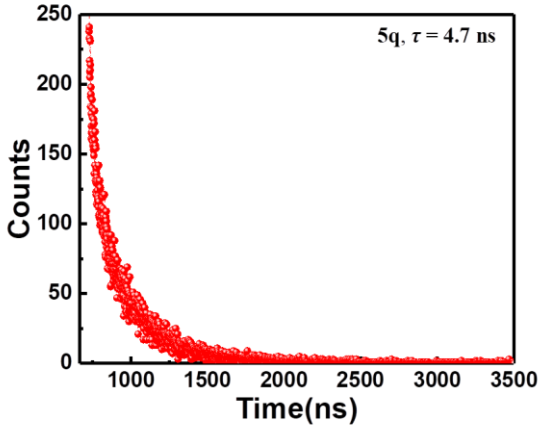


Figure S10. Time-resolved fluorescence decay plot of compound **5q** (λ_{ex} = 511 nm, [C] = 1 × 10^{-5} M) in dichloromethane at room temperature using a nano-LED of 370 nm as the light source.

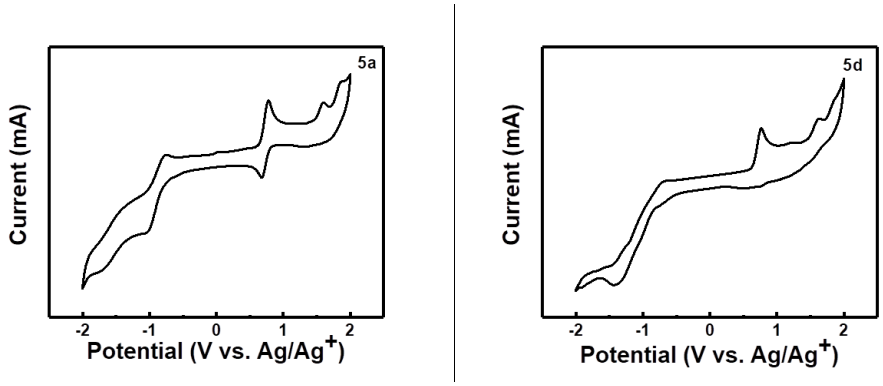


Figure S11. Cyclic voltammograms of **5a** and **5d** in CH_2Cl_2 ([C] = 1×10^{-3} M) at a scan rate of 100 mV/s with tetrabutylammonium hexafluorophosphate (0.1 M) as the supporting electrolyte.

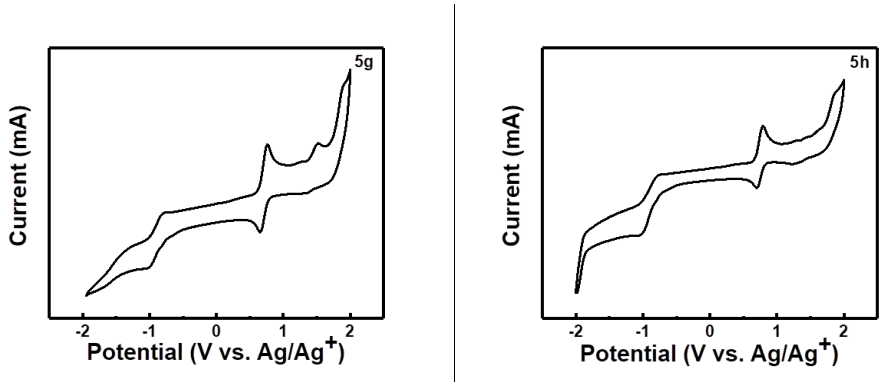


Figure S12. Cyclic voltammograms of **5g** and **5h** in CH_2Cl_2 ([C] = 1×10^{-3} M) at a scan rate of 100 mV/s with tetrabutylammonium hexafluorophosphate (0.1 M) as the supporting electrolyte.

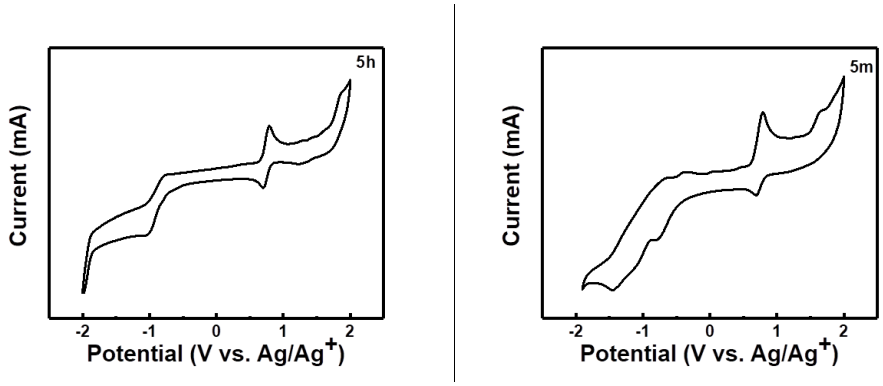


Figure S13. Cyclic voltammograms of **5h** and **5m** in CH_2Cl_2 ([C] = 1×10^{-3} M) at a scan rate of 100 mV/s with tetrabutylammonium hexafluorophosphate (0.1 M) as the supporting electrolyte.

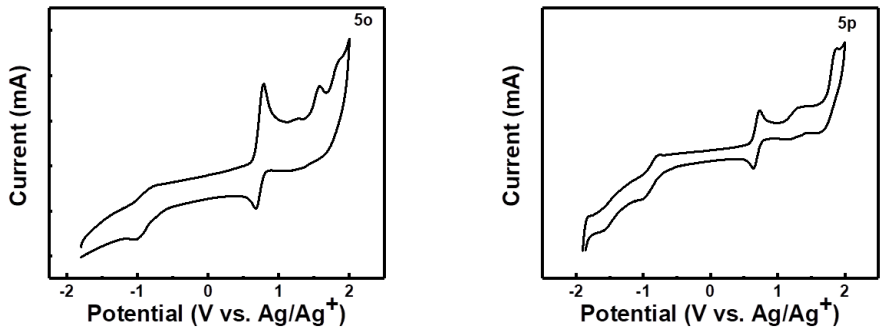


Figure S14. Cyclic voltammograms of **5o** and **5p** in CH_2Cl_2 ([C] = 1×10^{-3} M) at a scan rate of 100 mV/s with tetrabutylammonium hexafluorophosphate (0.1 M) as the supporting electrolyte.

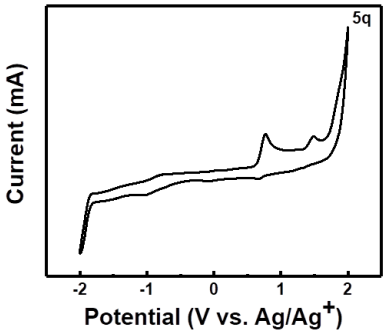


Figure S15. Cyclic voltammogram of **5q** in CH_2Cl_2 ([C] = 1×10^{-3} M) at a scan rate of 100 mV/s with tetrabutylammonium hexafluorophosphate (0.1 M) as the supporting electrolyte.

8. Mechanistic studies

8.1 Deuterium scrambling experiment

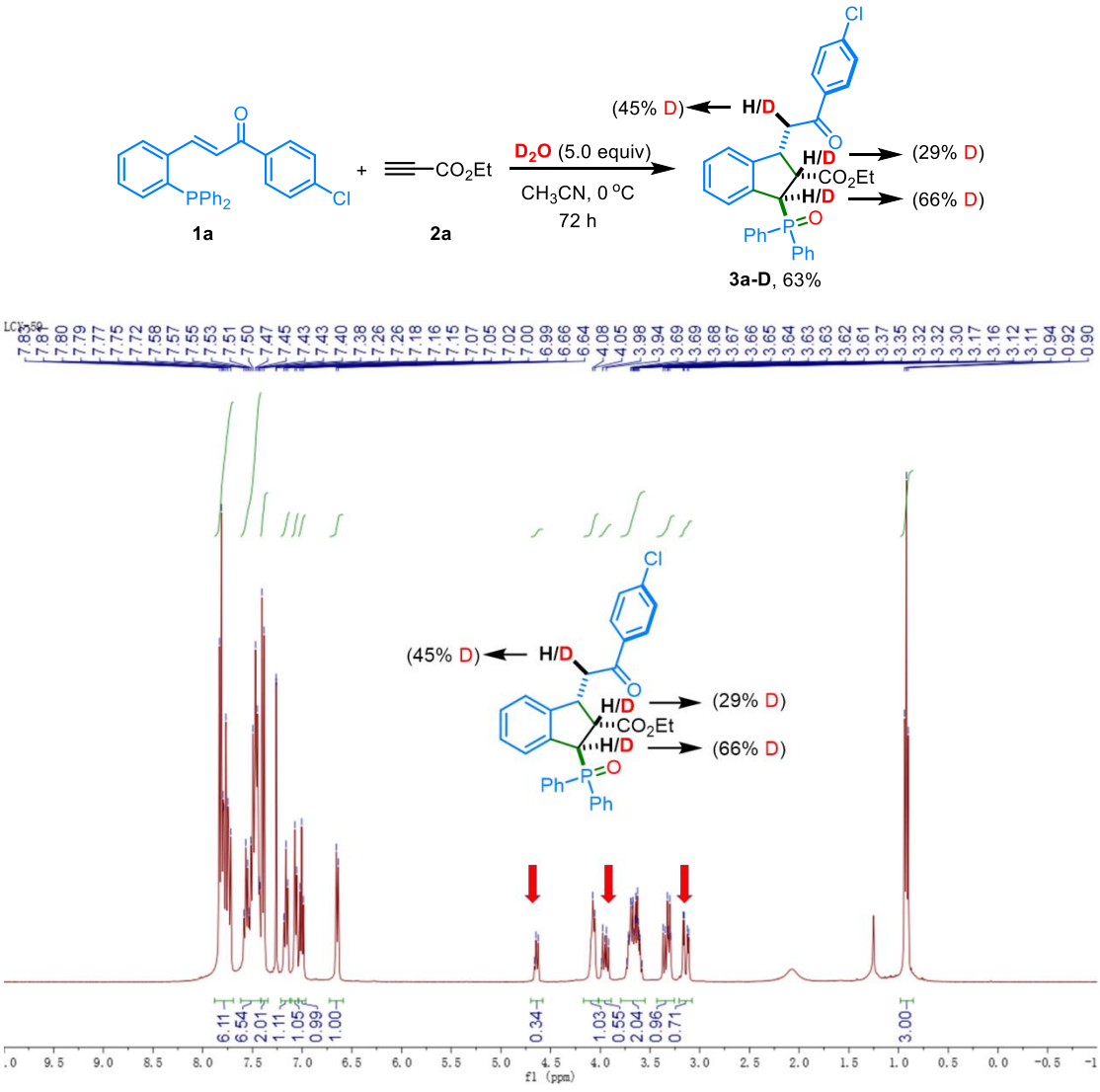
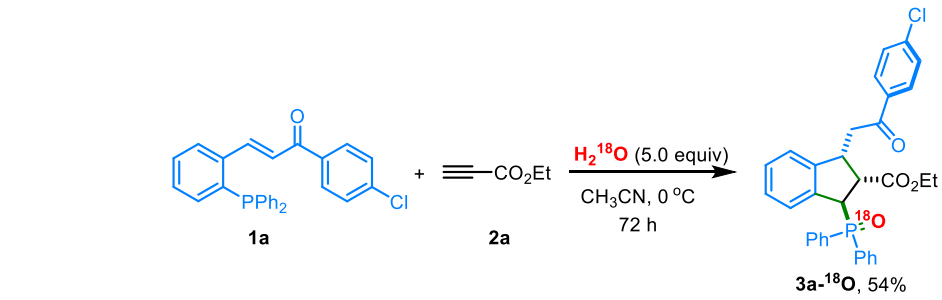


Figure S16. ^{1}H NMR spectrum of **3a-D**



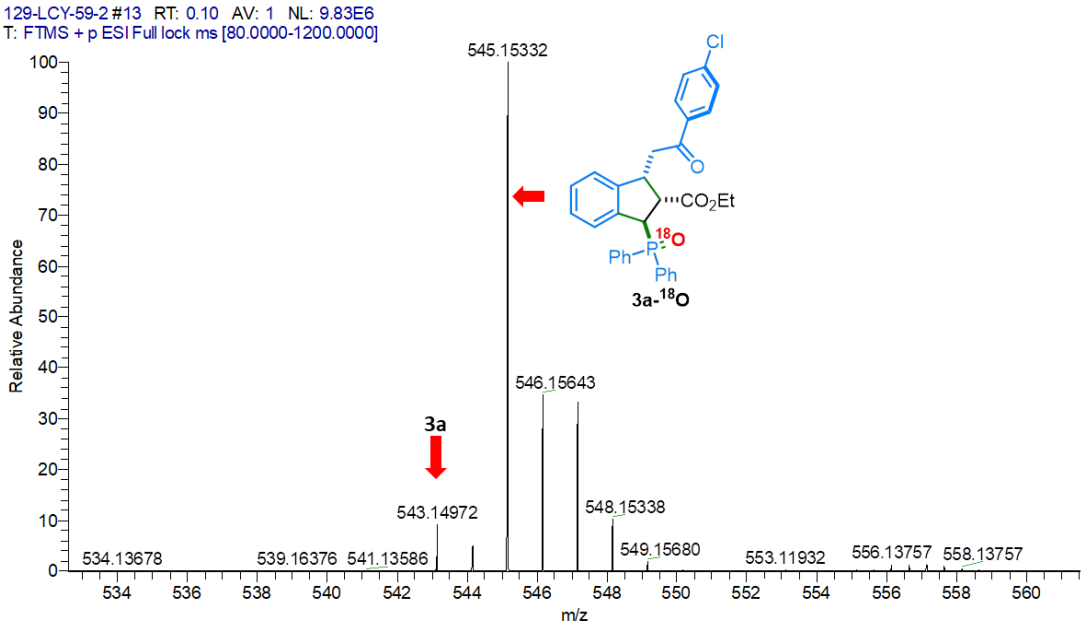
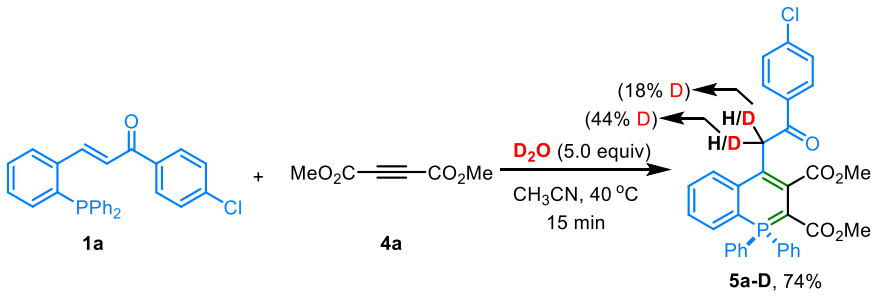


Figure S17. HRMS spectrum of **3a-^{18}O** (^{18}O:^{16}O = 11:1)



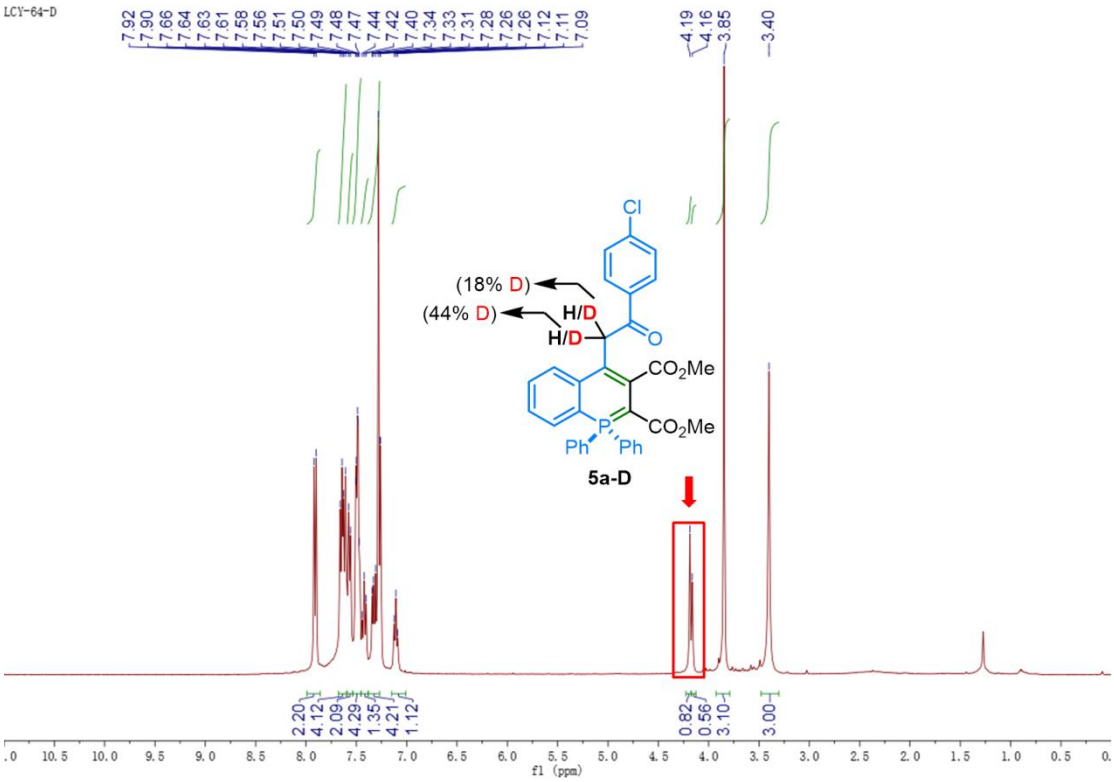


Figure S18. ^{1}H NMR spectrum of **5a-D**

8.2 DFT calculations

8.2.1 Method

The density functional theory (DFT)[1] calculations were performed by using the *Gaussian 09* program.[2] The geometric structures of all involved transition states were optimized by using the M06-2X density functional,[3] combined with the 6-31G(d, p)[4-5] basis set. The solvent effects of acetonitrile were simulated by the SMD model.[6] The harmonic frequency calculations were conducted at the same level to corroborate each transition state has one and only one imaginary frequency and other structures have no imaginary frequency. Natural bond orbital (NBO)[7] analyses were performed at the same level to assign the atomic charges. For the global reactivity index (GRI)[8-9] analysis, the relevant parameters for computing the electrophilicity index ω and nucleophilicity index N were also obtained by the same level of calculations. The thermo corrections to Gibbs free energies were calculated at the experimental temperature, i.e. 0 ℃ for **2a**, 40 ℃ for **4b** and 60 ℃ for **6**. Based on the optimized structures, all energies were refined by conducting single point energy calculations at the M06-2X/6-311++G(d, p)/SMD_{CH_3CN} level of theory, with the empirical dispersion corrections using the original D3 damping function added.[10-11]

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8.2.2 Results for reaction mechanism

Figure S19 gives the calculated Gibbs free energy profiles for the reaction of **1a** and **2a**. The Michael addition proceeds via transition state **TS1-2a** and the barrier is 22.2 kcal/mol. The given zwitterionic intermediate **Int1-2a** locates 11.3 kcal/mol higher than the initial reactants, indicating

an endothermic process. The direct water addition is excluded because the barrier via **TS6-2a** is too high to be overcome. While the stepwise addition going through the proton abstraction via **TS2-2a** and the following barrierless hydroxyl ion addition to the phosphorus center deserves a total barrier of 2.8 kcal/mol. Noteworthy, trimer of the water is used to assist the addition since the released hydroxyl ion could be well stabilized by the remaining water dimer. In addition, the generated phosphorus hydroxyl compound **Int4-2a** is 2.7 kcal/mol lower than **Int1-2a**, indicating the water addition slightly stabilizes the system. As an inherent driving force, construction of the P=O bond facilitates the aryl group. On account of the lower barrier via **TS3-2a** than that via **TS10-2a**, the ring-contraction strategy is indicated to be more favor than the exocyclic phenyl group migration. As a result, the release of the P-Ar bond facilitates enhancement of the P-OH bond, which can be demonstrated from the significant shortening of the bond length from 1.77 Å in **Int4-2a** to 1.58 Å in **Int5-2a**. Subsequently, the second Michael addition occurs via **TS4-2a** to construct the indene backbone, and the water-trimer-assisted proton transfer promotes the formation of the final product **3a**. The barriers for these two processes are respectively 6.5 and 9.5 kcal/mol, both are reasonable values for the experimental conditions.

In addition to the affinity of the P^V toward oxygen, the vinylic anion in **Int1-2a** has potential to attack the vinyl group of the chalcone moiety. This Michael addition proceeds via transition state **TS7-2a**, locating 3.7 kcal/mol higher than **TS2-2a** which corresponds to the water addition mechanism. The following water-trimer-assisted water addition via **TS8-2a** goes fast since the barrier is 8.5 kcal/mol only, but the subsequent aryl migration via **TS9-2a** deserves a barrier as high as 32.6 kcal/mol, which is difficult to be overcome under the experimental conditions. The reason for this extremely high obstacle could be mainly attributed to the significant ring strain stemming from the fused-ring structure in **TS9-2a**. Consequently, this ‘double Michael addition-aryl migration’ mechanism could be excluded.

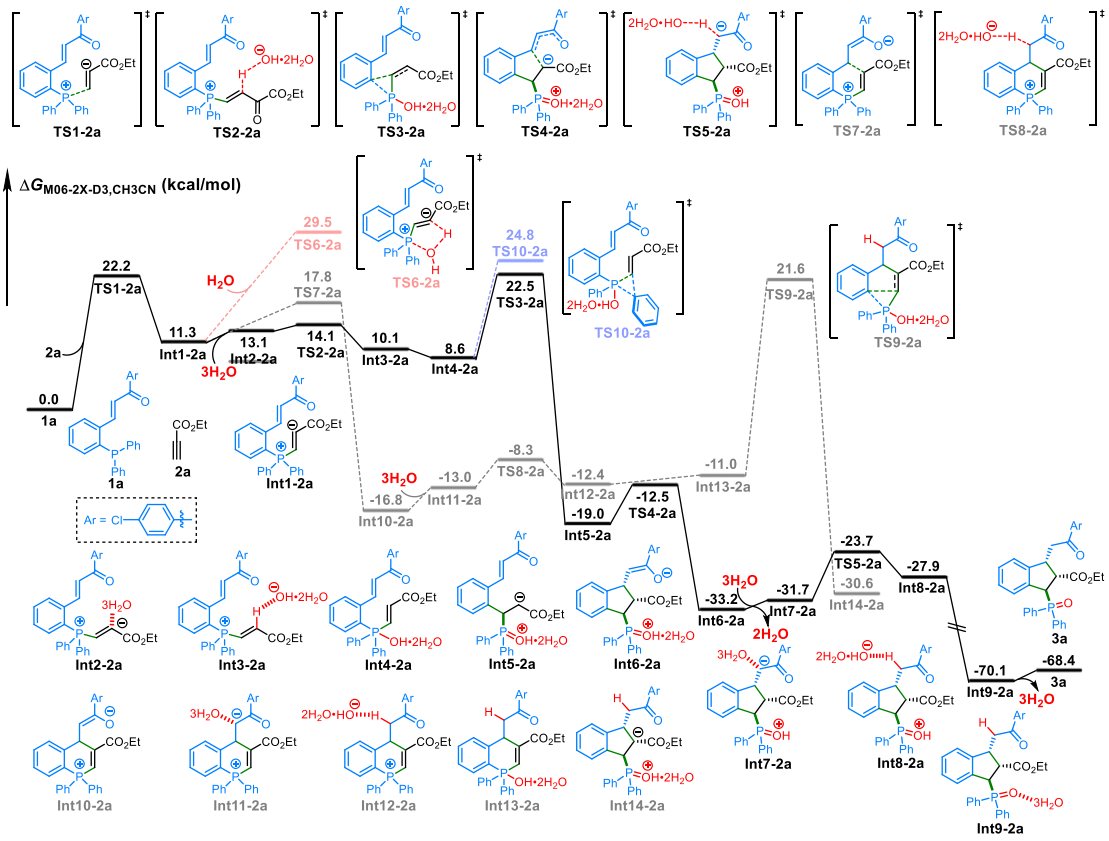

Figure S19. Free-energy profiles for the mechanism of organophosphine **1a** and ethyl propionate **2a** in the acetonitrile solvent. Free energies are given in kcal/mol and represent relative free energies calculated by the M06-2X-D3 functional in acetonitrile at 0 ^{o}C.

For the reaction of organophosphine **1a** with diethyl acetylenedicarboxylate **4b**, the barrier of the Michael addition is 15.1 kcal/mol, obviously lower than that of reaction with **2a** (Figure S20). This should benefit from ability of the ester group to disperse the negative charge on the vinyl group. The total barrier for the water addition via **TS2-4b** and aryl migration via **TS3-4b** is 26.1 kcal/mol, significantly higher than that for the pathway involving cyclization via the second Michael addition and the aromatization via water-trimer-assisted 1,2-proton transfer.

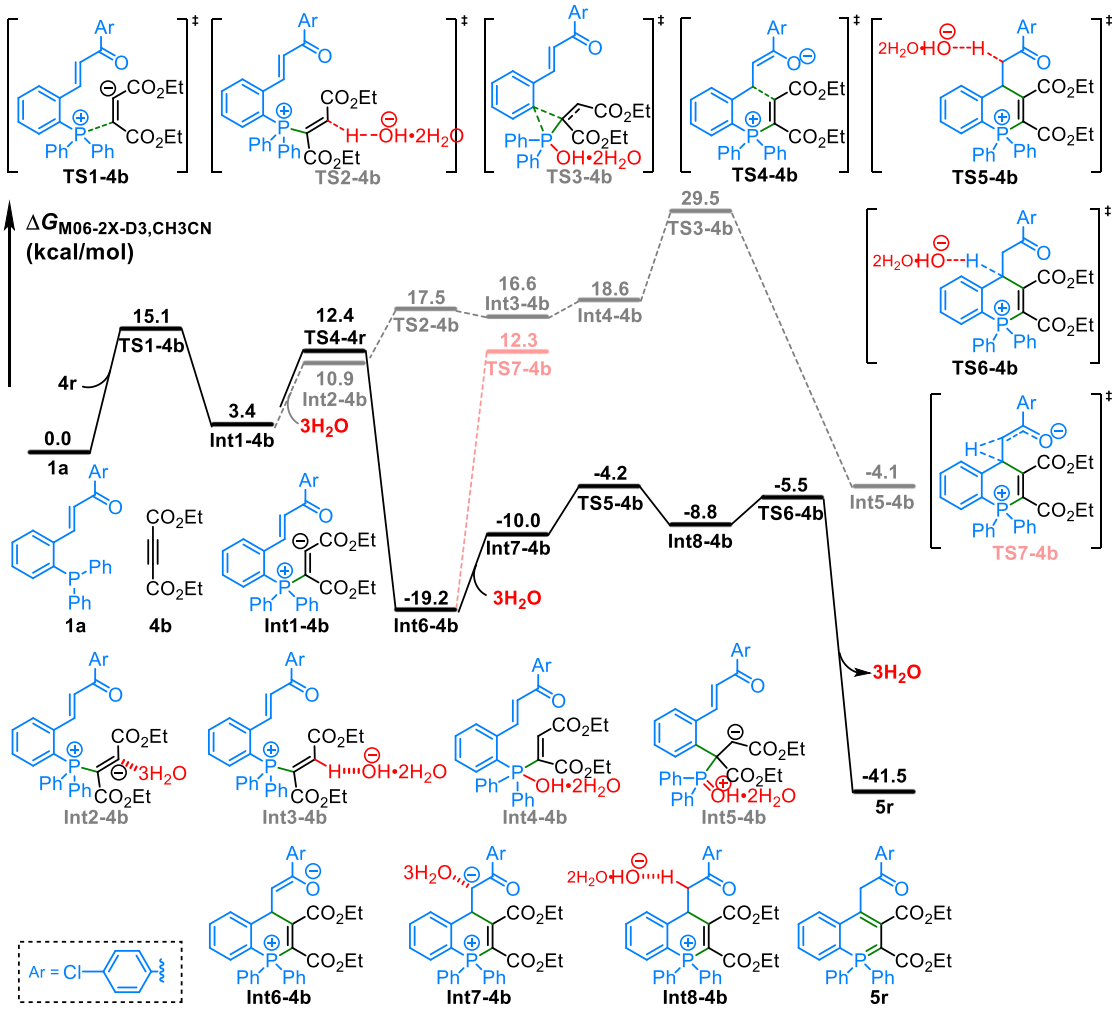

Figure S20. Free-energy profiles for the mechanism of organophosphine **1a** and diethyl acetylenedicarboxylate **4b** in the acetonitrile solvent. Free energies are given in kcal/mol and represent relative free energies calculated by the M06-2X-D3 functional in acetonitrile at 40 °C.

As shown in Figure S21, the barrier of the Michael addition of organophosphine **1a** with propiolamide **6** is 27.5 kcal/mol. This relatively higher barrier should be mainly on account of the poor electrophilicity of the propiolamide. The GRI analysis listed in **Table S1** provides the quantitative evaluation as well. For complexation of the Michael adduct **Int1-6** with the water trimer, the *trans* conformation (water trimer *vs* amino group, as in **Int2-6**) facilitates the aryl migration. The aryl migration transition state **TS3-6** locates 35.1 kcal/mol higher than the initial reactants, indicating that the strategy of water addition followed by aryl migration is difficult to be accomplished. While the *cis* conformation, as in **Int6-6**, drives the 1,3-proton transfer via **TS4-6**

to yield the amide anion in **Int8-6**. Subsequently, the aza-Michael addition of the nitrogen anion towards the vinyl group in chalcone yields the eight-membered heterocyclic intermediate **Int9-6**. Finally, the water-trimer-assisted 1,3-proton transfer occurs to generate the desired benzo[c][1,2]azaphosphol-3-one **7**. The rate-determining step for formation of **7** is the initial Michael addition of **1a** to **6**, and the total barrier is 27.5 kcal/mol. This is obviously lower than the aryl migration tactic and reasonable values for the experimental conditions.

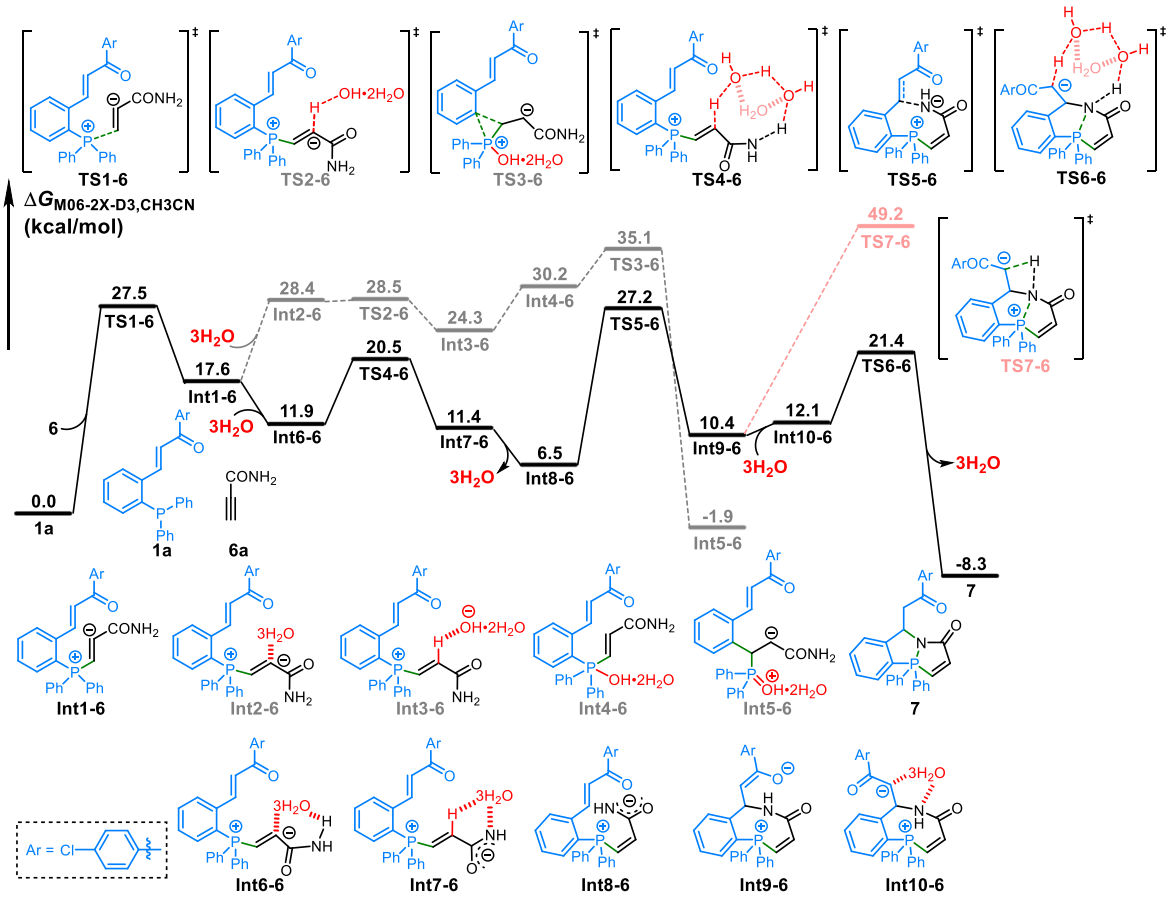

Figure S21. Free-energy profiles for the mechanism of organophosphine **1a** and propiolamide **6** in the acetonitrile solvent. Free energies are given in kcal/mol and represent relative free energies calculated by the M06-2X-D3 functional in acetonitrile at 60 °C.

Table S1. Energy of HOMO (E_H), LUMO (E_L), electronic chemical potential (μ), chemical hardness (η), global electrophilicity (ω) and global nucleophilicity (N) of reactants.

Reactants	E_H **(a.u.)**	E_L **(a.u.)**	μ **(a.u.)**	η **(a.u.)**	ω **(eV)**	N^a **(eV)**
1a	–0.26533	–0.04924	–0.15729	0.21609	1.558	2.819
2a	–0.35079	0.00217	–0.17431	0.35296	1.171	0.494

4b	–0.35507	–0.03619	–0.19563	0.31888	1.633	0.377
6a	–0.33400	0.18480	–0.07460	0.51880	0.146	0.951

[a] E_H (TCE) = –0.36894 a.u. (calculated at the M06-2X-D3/6-31G(d, p)/SMD_{CH_3CN} level)

8.2.3 Energies of all the optimized structures.

Table S2. Absolute Energies, Thermal Corrections to Free Energies and Imaginary Frequency of the Transition State.

Geometry	***E*(elec-M06-2X)[1]**	***G*(corr-M06-2X)[2]**	***E*(elec-M06-2X-D3)[3]**	**Imaginary Frequency[4]**
1a	-1917.20116	0.33772	-1917.52609	
2a	-344.38770	0.07162	-344.48855	
H_2O	-76.39189	0.00514	-76.42970	
$2H_2O$	-152.79352	0.02349	-152.86652	
$3H_2O$	-229.19308	0.04153	-229.30219	
TS1-2a	-2261.57381	0.43306	-2262.00291	264.7*i*
Int1-2a	-2261.59491	0.43592	-2262.02323	
Int2-2a	-2490.82087	0.50303	-2491.34808	
TS2-2a	-2490.81592	0.50027	-2491.34371	1119.8*i*
Int3-2a	-2490.82303	0.50520	-2491.35513	
Int4-2a	-2490.84062	0.50797	-2491.36018	
TS3-2a	-2490.81350	0.50298	-2491.33305	283.9*i*
Int5-2a	-2490.88084	0.50630	-2491.40247	
TS4-2a	-2490.87048	0.50372	-2491.38963	56.8*i*
Int6-2a	-2490.90666	0.50786	-2491.42681	
Int7-2a	-2567.30774	0.52904	-2567.86325	
TS5-2a	-2567.29370	0.52785	-2567.84920	1091.9*i*
Int8-2a	-2567.29950	0.53194	-2567.85995	
Int9-2a	-2567.37331	0.53034	-2567.92566	
TS6-2a	-2337.98087	0.45571	-2338.43851	1059.6*i*

TS7-2a	-2261.58420	0.43613	-2262.01310	177.0*i*
Int10-2a	-2261.64776	0.44092	-2262.07298	
Int11-2a	-2490.86635	0.50673	-2491.39341	
TS8-2a	-2490.85542	0.50341	-2491.38266	1052.0*i*
Int12-2a	-2490.86167	0.50714	-2491.39286	
Int13-2a	-2490.87181	0.50890	-2491.39233	
TS9-2a	-2490.81842	0.50764	-2491.33913	457.2*i*
Int14-2a	-2490.90751	0.50954	-2491.42433	
TS10-2a	-2490.80946	0.50207	-2491.32854	330.0*i*
3a	-2338.15569	0.46537	-2338.60421	
TS4-2a-RR	-2490.87048	0.50372	-2491.38963	56.8*i*
TS4-2a-SS	-2490.86922	0.50979	-2491.38799	226.0*i*
TS4-2a-RS	-2490.86847	0.50742	-2491.38512	249.1*i*
TS4-2a-SR	-2490.86431	0.50285	-2491.38460	193.6*i*
4b	-611.477193	0.129944	-611.6545524	
TS1-4b	-2528.677033	0.481937	-2529.182583	130.7*i*
Int1-4b	-2528.699284	0.486394	-2529.20566	
Int2-4b	-2757.924421	0.552787	-2758.526594	
TS2-4b	-2757.912283	0.552378	-2758.515627	629.1*i*
Int3-4b	-2757.913943	0.555796	-2758.517384	
Int4-4b	-2757.927718	0.558606	-2758.520102	
TS3-4b	-2757.90775	0.556922	-2758.501111	162.7*i*
Int5-4b	-2757.962063	0.55817	-2758.555946	
TS4-4b	-2528.687585	0.48733	-2529.192311	161.0*i*
Int6-4b	-2528.740508	0.488546	-2529.243901	
Int7-4b	-2757.959553	0.556189	-2758.563355	
TS5-4b	-2757.948278	0.554647	-2758.552435	1037.0*i*
Int8-4b	-2757.954117	0.556812	-2758.562059	
TS6-4b	-2757.953272	0.559307	-2758.559263	85.6*i*

TS7-4b	-2528.68949	0.484857	-2529.189942	1375.7*i*
5r	-2528.783053	0.491219	-2529.282008	
6	-245.947026	0.023497	-246.0253218	
TS1-6	-2163.130609	0.380653	-2163.535505	284.6*i*
Int1-6	-2163.145977	0.382329	-2163.553045	
Int2-6	-2392.368089	0.449479	-2392.870717	
TS2-6	-2392.365113	0.446641	-2392.867691	1114.2*i*
Int3-6	-2392.371745	0.449425	-2392.877102	
Int4-6	-2392.372924	0.451765	-2392.870124	
TS3-6	-2392.365386	0.451004	-2392.861432	125.4*i*
Int5-6	-2392.424331	0.453927	-2392.923314	
Int6-6	-2392.373442	0.447792	-2392.87486	
TS4-6	-2392.380791	0.448017	-2392.881766	71.3*i*
Int7-6	-2392.395596	0.449969	-2392.898269	
Int8-6	-2163.175549	0.386403	-2163.574799	
TS5-6	-2163.136211	0.38672	-2163.541989	310.8*i*
Int9-6	-2163.167158	0.388466	-2163.570557	
Int10-6	-2392.39922	0.455743	-2392.902938	
TS6-6	-2392.383934	0.453246	-2392.885616	1127.8*i*
TS7-6	-2163.106508	0.38372	-2163.504075	1800.2*i*
7	-2163.207457	0.390141	-2163.602038	

[1]Electronic energy calculated by M06-2X in CH_3CN as the solvent. [2]Thermal correction to Gibbs free energy calculated by M06-2X in CH_3CN as the solvent. [3]Electronic energy calculated by M06-2X-D3 in CH_3CN as the solvent. [4]Imaginary frequency for each transition state calculated by M06-2X in CH_3CN as the solvent.

8.2.4 Cartesian coordinates of all structures involved.

1a

0 1

P	–2.35397600	0.07061200	–0.84589100
C	–1.86979200	–1.27440800	0.33544200
C	–0.51585400	–1.38501000	0.73522500
C	–2.78116200	–2.24060600	0.76905000
C	–0.13227800	–2.44078800	1.57304700
C	–2.38008400	–3.29308800	1.59085700
H	–3.82095400	–2.17761200	0.46485900
C	–1.05293200	–3.39220600	1.99702000
H	0.89727500	–2.50029600	1.91302200
H	–3.10975300	–4.02679400	1.91877200
H	–0.73570900	–4.20058500	2.64782000
C	–4.15167400	–0.25438000	–1.07464100
C	–5.14994000	0.22914000	–0.22130800
C	–4.51922500	–1.03762400	–2.17589300
C	–6.48885600	–0.07003600	–0.46433000
H	–4.88332000	0.83932000	0.63696100
C	–5.85719300	–1.34531700	–2.41233100
H	–3.75306300	–1.40921400	–2.85214700
C	–6.84431100	–0.85920300	–1.55720900
H	–7.25536200	0.31236400	0.20271500
H	–6.12797100	–1.95633000	–3.26777300
H	–7.88830700	–1.09090300	–1.74402200
C	–2.37010200	1.54887000	0.25664600
C	–2.33075800	2.80329200	–0.36494500
C	–2.42008600	1.48422900	1.65414600
C	–2.35618500	3.97124900	0.39359900
H	–2.27753900	2.86543800	–1.44930700
C	–2.43595700	2.65333600	2.41269000
H	–2.45095400	0.51913600	2.15265300
C	–2.40664700	3.89725600	1.78434000

H	–2.32756300	4.93721600	–0.10091200
H	–2.47381200	2.59166700	3.49600000
H	–2.41864800	4.80640500	2.37743800
C	0.48516200	–0.39902300	0.29604900
C	1.79928300	–0.63459900	0.16691100
H	2.21288900	–1.62044300	0.34785100
C	2.69907800	0.46176900	–0.27410300
O	2.25608600	1.54679200	–0.62121500
C	4.17842700	0.21941600	–0.30359200
C	4.78564200	–0.86690800	0.33353800
C	4.97549500	1.14891100	–0.98165600
C	6.16739100	–1.02737200	0.29363800
H	4.19926200	–1.59234400	0.88620000
C	6.35354300	0.99807300	–1.03917600
H	4.49835400	1.99350600	–1.46702200
C	6.93175500	–0.09392700	–0.39647800
H	6.64214800	–1.86477100	0.79239000
H	6.97174100	1.71327300	–1.57044200
Cl	8.66721100	–0.29327800	–0.45544300
H	0.14321200	0.60691500	0.05633000

2a

0 1

C	–2.95359200	–0.92754800	–0.00000800
C	–1.90857700	–0.32830900	0.00025600
H	–3.88269400	–1.46186000	–0.00117200
C	–0.66897600	0.43883700	0.00011000
O	–0.63125100	1.64663900	–0.00008100
O	0.39233900	–0.36102400	0.00010500
C	1.67480900	0.30797900	–0.00010300

C	2.73854200	–0.76336700	–0.00002100
H	1.73247800	0.94537400	0.88627500
H	1.73233600	0.94509700	–0.88669000
H	3.72448000	–0.29254800	–0.00017700
H	2.65580100	–1.39312700	0.88899600
H	2.65565600	–1.39341300	–0.88882400

H_2O

0 1

H	0.75842200	–0.47702600	0.00000000
O	0.00000000	0.11922200	0.00000000
H	–0.75842200	–0.47675200	0.00000000

$2H_2O$

0 1

O	1.34680300	–0.00810600	–0.11356500
H	–0.51533200	0.00594000	0.05173200
H	1.69941100	–0.73667000	0.41363800
H	1.70405700	0.78576800	0.30502100
O	–1.48567800	0.00890100	0.11709100
H	–1.77713700	–0.06139400	–0.79860100

$3H_2O$

0 1

H	–0.01846700	1.64829000	–0.77189300
O	–0.00185700	1.06014800	–0.00405700
H	1.59992300	0.01095200	0.00103600
H	–1.49937200	–0.13130800	–0.01297900
H	–0.02101100	1.64865700	0.76343200
O	–2.27562100	–0.71302500	–0.01604700

H	–3.01437600	–0.11377900	0.13740600
O	2.39179800	–0.54924100	0.00471500
H	2.03874300	–1.44586900	0.00610300

TS1-2a

0 1

P	1.78365800	–0.36460600	–0.21730400
C	2.41280600	0.95949600	0.88138800
C	1.58624000	1.99780100	1.37419400
C	3.78895800	1.00381900	1.14545700
C	2.18540200	3.06525100	2.06000200
C	4.35420700	2.04935900	1.86838000
H	4.43294000	0.21316900	0.77492000
C	3.54981200	3.09312200	2.31615200
H	1.55225100	3.87593900	2.40914200
H	5.42154200	2.05246300	2.06339200
H	3.98216100	3.92668400	2.85991400
C	3.26271700	–1.01920000	–1.05763700
C	3.84747000	–2.24437800	–0.72161800
C	3.80733200	–0.25460800	–2.09922800
C	4.96838300	–2.69485300	–1.41651700
H	3.43509600	–2.84546800	0.08314500
C	4.93072600	–0.70599900	–2.78464000
H	3.35412600	0.69598300	–2.37018000
C	5.51068300	–1.92788000	–2.44528500
H	5.41879100	–3.64565700	–1.14998000
H	5.34936400	–0.10671000	–3.58672900
H	6.38373000	–2.28223000	–2.98417100
C	1.21507300	–1.74236500	0.83157000
C	0.48118500	–2.76500900	0.21537500

C	1.46541200	–1.79577500	2.20636300
C	0.00932000	–3.83505400	0.96973600
H	0.27907500	–2.72294700	–0.85279000
C	0.98547200	–2.86760300	2.95660400
H	2.02974800	–1.00309700	2.68972600
C	0.25971700	–3.88541400	2.34082000
H	–0.55844100	–4.62490300	0.48833700
H	1.18073900	–2.90605000	4.02354700
H	–0.11382900	–4.71718500	2.92966500
C	0.12134500	2.05869800	1.26058800
C	–0.73747700	1.03195800	1.23030000
H	–0.41705500	–0.00148200	1.28579100
C	–2.20165500	1.28782500	1.17522600
O	–2.68681000	2.33139400	1.58433700
C	–3.07349700	0.20059600	0.63279100
C	–2.55420100	–0.82947400	–0.15605000
C	–4.44337400	0.23622900	0.91017800
C	–3.38926500	–1.82124100	–0.65986200
H	–1.49665100	–0.85610000	–0.40329700
C	–5.28940200	–0.75034400	0.42104100
H	–4.83737100	1.04208900	1.52131500
C	–4.74601400	–1.76873000	–0.35864300
H	–2.99230800	–2.62005200	–1.27698800
H	–6.35134800	–0.73502300	0.63985200
Cl	–5.80142700	–3.01771500	–0.97738300
C	0.62863000	0.21878300	–2.01782900
C	–0.01731200	1.28832100	–2.19354100
H	0.93304600	–0.64150500	–2.60039500
C	–0.48581800	2.54930500	–1.72927400
O	0.17505300	3.57615300	–1.67366200

O	–1.81059900	2.51480700	–1.44188100
C	–2.40477500	3.77756400	–1.10535200
C	–3.90423000	3.58619700	–1.11418400
H	–2.08793600	4.52597100	–1.83704000
H	–2.04917600	4.09118800	–0.11831100
H	–4.39615600	4.52662200	–0.85094200
H	–4.24992100	3.28088400	–2.10545800
H	–4.19663500	2.82672700	–0.38517900
H	–0.30074700	3.06373600	1.25840900

Int1-2a

0 1

P	1.57394900	–0.60145300	–0.42821100
C	2.03138400	0.70591500	0.76102700
C	1.20740300	0.98667800	1.87102200
C	3.26523700	1.35230800	0.62851000
C	1.66389400	1.89169500	2.83461100
C	3.69253000	2.26557100	1.58728400
H	3.90353800	1.13826000	–0.22172400
C	2.89172000	2.53148800	2.69448700
H	1.03992800	2.09295900	3.70050300
H	4.65242400	2.75727000	1.47094900
H	3.22281400	3.23331300	3.45323600
C	3.05303800	–1.03622200	–1.38906300
C	3.79994900	–2.18879800	–1.13040000
C	3.41938200	–0.17633100	–2.43456600
C	4.91691800	–2.47533100	–1.91243700
H	3.51480100	–2.86780200	–0.33374500
C	4.54306300	–0.46645100	–3.20125600
H	2.83641300	0.72164600	–2.63224800

C	5.28962100	–1.61582500	–2.94272900
H	5.49273300	–3.37348500	–1.71463600
H	4.83135300	0.20176100	–4.00614900
H	6.16092600	–1.84338000	–3.54876900
C	1.09188400	–2.03243600	0.57405900
C	–0.09972000	–2.71558900	0.31442400
C	1.89534200	–2.40562300	1.65931900
C	–0.47841100	–3.77593000	1.13419500
H	–0.74635900	–2.41398900	–0.50309300
C	1.51129400	–3.46864000	2.47045600
H	2.81140100	–1.86168000	1.87649600
C	0.32485400	–4.15267700	2.20809700
H	–1.40715700	–4.30094200	0.93635500
H	2.13395300	–3.75606500	3.31122100
H	0.02303400	–4.97652000	2.84697400
C	–0.10645200	0.33187800	2.09448500
C	–1.19979800	0.56933500	1.36390500
H	–1.17574700	1.28649400	0.55109500
C	–2.45546600	–0.17312800	1.66789600
O	–2.58868900	–0.79211700	2.71183400
C	–3.55844500	–0.15756000	0.65545700
C	–3.37128400	0.28280900	–0.65899000
C	–4.81273900	–0.63675200	1.05059200
C	–4.42536700	0.24762400	–1.56751300
H	–2.40521800	0.63924600	–1.00587600
C	–5.87500700	–0.66671300	0.15897500
H	–4.94523500	–0.98277700	2.07019100
C	–5.66311200	–0.22202700	–1.14414000
H	–4.28457600	0.58019100	–2.59001500
H	–6.85074200	–1.02825800	0.46400100

Cl	–6.99225300	–0.25944900	–2.27866700
C	0.28567100	–0.12183900	–1.60498400
C	–0.00256600	1.12758400	–1.98796800
H	–0.17249000	–1.00321200	–2.06022900
C	0.68363000	2.28433800	–1.47582400
O	1.74693000	2.73284000	–1.89555400
O	–0.04281500	2.94223500	–0.53162400
C	0.60676500	4.05538300	0.09281200
C	–0.28529900	4.52149700	1.22109700
H	0.76805700	4.84602800	–0.64699900
H	1.58711200	3.73547600	0.46117900
H	0.18970600	5.35116500	1.75158400
H	–1.25205200	4.86163000	0.83998900
H	–0.45906800	3.70917300	1.93350800
H	–0.17337700	–0.37512700	2.92242000

Int2-2a

0 1

P	–1.45280900	0.97436300	–0.08460400
C	–2.16519400	0.24934600	1.42627300
C	–1.53999900	–0.76438700	2.18605700
C	–3.44590700	0.69550200	1.78716700
C	–2.24961500	–1.32877600	3.25391500
C	–4.11369900	0.14688300	2.87629800
H	–3.93668400	1.46790700	1.20437300
C	–3.51511000	–0.87628400	3.60650200
H	–1.78044600	–2.12799600	3.81917800
H	–5.10254300	0.50726500	3.13832300
H	–4.03420100	–1.32603500	4.44665400
C	–2.82259300	1.65623100	–1.05701300

C	–3.15490700	3.01240000	–0.98545700
C	–3.56250300	0.78076300	–1.86092400
C	–4.23462700	3.49339100	–1.72207600
H	–2.57834300	3.68838900	–0.36045800
C	–4.64148000	1.27331600	–2.58872300
H	–3.30401200	–0.27434700	–1.93467100
C	–4.97646400	2.62530600	–2.52111400
H	–4.49355300	4.54588100	–1.67204200
H	–5.21577300	0.59750700	–3.21455300
H	–5.81599400	3.00444300	–3.09538900
C	–0.34267100	2.34252800	0.31631800
C	0.37082800	2.94057400	–0.73145600
C	–0.16470200	2.77767600	1.63227200
C	1.27935300	3.95650700	–0.45147600
H	0.22069100	2.61658900	–1.75825900
C	0.75124500	3.79191700	1.90310900
H	–0.72478500	2.31885600	2.44233400
C	1.47576200	4.37438000	0.86531600
H	1.83497800	4.41943500	–1.26039500
H	0.89715500	4.12479600	2.92532300
H	2.19106200	5.16171700	1.08075800
C	–0.19539900	–1.32420700	1.93020500
C	0.93676800	–0.61765900	1.87380500
H	0.93737200	0.45918900	2.00348300
C	2.21254900	–1.30878200	1.55287400
O	2.36635500	–2.50016600	1.77113300
C	3.30900500	–0.50617800	0.92118400
C	3.11192200	0.79810400	0.45644500
C	4.56187300	–1.10938100	0.76474600
C	4.14935300	1.49436100	–0.15602700

H	2.14702400	1.28710400	0.55009000
C	5.60884200	–0.42618700	0.16182100
H	4.70459600	–2.12349900	1.12345600
C	5.38484600	0.87200800	–0.29172200
H	3.99710800	2.50419600	–0.52182700
H	6.58265900	–0.88830100	0.04308000
Cl	6.69517400	1.74172000	–1.05430100
C	–0.58865600	–0.22904800	–1.08812600
C	–0.96674500	–1.51167700	–1.04110700
H	0.21121800	0.20888600	–1.69339800
C	–0.23234600	–2.45273600	–1.88320900
O	–0.70474900	–3.07923200	–2.82543800
O	1.02669900	–2.64649800	–1.45481100
C	1.77525100	–3.69116000	–2.09831900
C	3.15088400	–3.69584800	–1.47065900
H	1.81832100	–3.49493700	–3.17351500
H	1.25499500	–4.64266500	–1.94905900
H	3.74612200	–4.51180900	–1.88886800
H	3.66798300	–2.75302800	–1.67036200
H	3.07600800	–3.82718600	–0.38775100
H	–0.16293600	–2.40915600	1.82136800
O	–3.21286800	–2.61870900	0.11893300
H	–2.35315800	–2.16931900	–0.22990400
H	–3.67040500	–1.93429600	0.62743600
H	–3.64098800	–2.60518300	–1.75819800
O	–3.55513600	–2.46494900	–2.71617500
H	–2.61582000	–2.65734300	–2.87643100
H	–2.30740400	–3.69562700	1.26828100
O	–1.71826100	–4.20405900	1.86121000
H	–2.18758800	–4.22050700	2.70291300

TS2-2a

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P	1.44881200	–0.97076700	–0.09260300
C	2.15021600	–0.33910400	1.45963400
C	1.54170500	0.66770200	2.23912100
C	3.40599000	–0.84475900	1.82747100
C	2.24617300	1.17069100	3.33986200
C	4.06709900	–0.35720400	2.94834700
H	3.88038800	–1.61327100	1.22601300
C	3.48726300	0.66127300	3.70084000
H	1.79267100	1.96517400	3.92428100
H	5.03713400	–0.75985800	3.21880400
H	4.00361300	1.06338600	4.56647800
C	2.80959800	–1.63581900	–1.08392200
C	3.09094200	–3.00543700	–1.08135600
C	3.59841500	–0.74273300	–1.81917600
C	4.17063700	–3.48322400	–1.81979100
H	2.47591400	–3.69369500	–0.50865400
C	4.67551300	–1.23419700	–2.55026000
H	3.38718800	0.32554700	–1.83764500
C	4.96084800	–2.59920100	–2.55203200
H	4.39169200	–4.54540100	–1.82307500
H	5.28830800	–0.54572700	–3.12341400
H	5.80022400	–2.97583700	–3.12812000
C	0.27778200	–2.30936000	0.21846000
C	–0.43952700	–2.83000200	–0.86715100
C	0.07050600	–2.80423700	1.50883300
C	–1.38274300	–3.82908000	–0.64942600
H	–0.26641700	–2.45845100	–1.87412600

C	–0.88031400	–3.80089500	1.71699300
H	0.63421200	–2.40427800	2.34714300
C	–1.60912900	–4.30614300	0.64232700
H	–1.94315400	–4.23161400	–1.48680100
H	–1.05040900	–4.17974900	2.71921000
H	–2.35234700	–5.07939400	0.80877900
C	0.22111100	1.27425300	1.96629100
C	–0.92876100	0.60022000	1.87208200
H	–0.96265500	–0.47741000	1.99089700
C	–2.18153500	1.32872900	1.53993800
O	–2.29212700	2.52948300	1.73141100
C	–3.31112700	0.55229900	0.93485200
C	–3.15502800	–0.75365700	0.45958800
C	–4.55414700	1.18375400	0.81409500
C	–4.22194900	–1.42178800	–0.13355700
H	–2.19964300	–1.26495100	0.52798800
C	–5.63031200	0.52818400	0.23265200
H	–4.66687700	2.19747100	1.18425800
C	–5.44593700	–0.77082700	–0.23616800
H	–4.10084000	–2.43203700	–0.50984100
H	–6.59629600	1.01240200	0.14186000
Cl	–6.79282700	–1.60450500	–0.97472300
C	0.62528700	0.31016200	–1.03824500
C	1.08237600	1.56541700	–1.00810000
H	–0.24311200	–0.03837100	–1.60093300
C	0.34940500	2.56976800	–1.80922700
O	0.86966900	3.30760900	–2.62942300
O	–0.94907400	2.62582500	–1.49693800
C	–1.72950700	3.64806600	–2.14531200
C	–3.14635400	3.49684500	–1.64215700

H	–1.65949400	3.51627800	–3.22872400
H	–1.30666500	4.62465300	–1.89153000
H	–3.77659800	4.28142500	–2.06844000
H	–3.55707700	2.52616100	–1.93362300
H	–3.16956200	3.57402200	–0.55150600
H	0.23001700	2.36100100	1.86499800
O	3.23691800	2.45673500	0.16010800
H	2.16571800	1.98507300	–0.35395200
H	3.65856800	1.74368100	0.65797000
H	3.73854700	2.55722300	–1.50341700
O	3.75167100	2.52477800	–2.48845000
H	2.85168100	2.80615000	–2.71199700
H	2.44839600	3.45671500	1.23565300
O	1.90287900	4.01280000	1.85690900
H	2.36627000	3.94576100	2.69886700

Int3-2a

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P	–1.33204100	1.04300600	–0.11153100
C	–2.03167200	0.53593900	1.48009700
C	–1.44735600	–0.48948200	2.25124100
C	–3.23782700	1.12648800	1.87996600
C	–2.13442800	–0.93679000	3.38402900
C	–3.87798500	0.69631700	3.03649400
H	–3.68717700	1.91071800	1.27874200
C	–3.32971100	–0.34647500	3.78014100
H	–1.71022000	–1.75112500	3.96380500
H	–4.81059900	1.15910600	3.34012300
H	–3.83728600	–0.70626600	4.66928200
C	–2.64099600	1.80965300	–1.09479400

C	–2.70545200	3.20228700	–1.20530000
C	–3.61059400	0.99337500	–1.69137100
C	–3.74853600	3.78286600	–1.92213700
H	–1.95280700	3.83032400	–0.73804800
C	–4.64653000	1.59031900	–2.40302900
H	–3.58513200	–0.09513100	–1.62086800
C	–4.71600700	2.97834300	–2.52006900
H	–3.80148400	4.86263100	–2.01310200
H	–5.39949100	0.96317100	–2.86966200
H	–5.52654700	3.43456100	–3.07963600
C	0.00476700	2.23425800	0.08196600
C	0.79853400	2.53941400	–1.03067200
C	0.20992000	2.87815700	1.30551500
C	1.81177900	3.48464000	–0.90694400
H	0.62596600	2.04874700	–1.98509900
C	1.22997100	3.82019800	1.41881300
H	–0.41398200	2.64239900	2.16315600
C	2.02858100	4.12028400	0.31619300
H	2.43341000	3.72209200	–1.76389600
H	1.39789800	4.31915800	2.36729100
H	2.82277000	4.85445800	0.40880100
C	–0.17032400	–1.15855200	1.90855400
C	1.02823600	–0.56742400	1.89465400
H	1.14795800	0.48270300	2.14054000
C	2.20997200	–1.37087000	1.47401600
O	2.20874400	–2.58810000	1.56793800
C	3.39323200	–0.66280100	0.88863400
C	3.41567300	0.71744700	0.66690400
C	4.50360200	–1.43463200	0.52623100
C	4.52955100	1.32265200	0.09244100

H	2.56979800	1.34304100	0.93262900
C	5.62240300	–0.84625500	–0.04546400
H	4.47765300	–2.50522300	0.70030000
C	5.61792600	0.53118800	–0.25494000
H	4.54779600	2.39303200	–0.08276800
H	6.48488200	–1.44100500	–0.32522600
Cl	7.02032000	1.28345300	–0.97707000
C	–0.70702300	–0.41082600	–0.95968400
C	–1.40895400	–1.54320400	–0.93255100
H	0.26326900	–0.31919700	–1.44281000
C	–0.89814900	–2.78290600	–1.58229800
O	–1.60662300	–3.56859400	–2.17561100
O	0.41767700	–2.91059100	–1.44531300
C	1.01241300	–4.09919100	–2.00228700
C	2.47510100	–4.07319100	–1.62416900
H	0.86327600	–4.09345600	–3.08596100
H	0.49642200	–4.97020800	–1.58884400
H	2.96987500	–4.96927700	–2.00688500
H	2.96902800	–3.19567100	–2.05043200
H	2.58421000	–4.04262100	–0.53703800
H	–0.26668200	–2.21201500	1.64060900
O	–3.97811300	–2.23567500	0.61392000
H	–2.37231200	–1.65595100	–0.42037400
H	–3.96804700	–1.37586500	1.05182600
H	–4.27112100	–2.17042000	–0.88349500
O	–4.32267400	–2.14614900	–1.90822800
H	–3.57494100	–2.70127100	–2.16739700
H	–2.79441000	–3.02465300	0.95545100
O	–1.91943500	–3.58077400	1.10143800
H	–1.92411000	–3.80887200	2.03791400

Int4-2a

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P	2.02878700	–0.76374700	0.16980300
C	1.28398800	–0.72694300	1.85987500
C	–0.02272700	–0.28414600	2.14916200
C	2.10617900	–1.17653400	2.89802200
C	–0.45229100	–0.28546800	3.48665400
C	1.66752500	–1.15534800	4.21780200
H	3.09958700	–1.55208400	2.67219100
C	0.38142300	–0.70705100	4.51264100
H	–1.44832400	0.07826700	3.71883100
H	2.32781800	–1.49095500	5.01100400
H	0.03100300	–0.68220800	5.53928100
C	3.86032800	–0.77274300	–0.04127600
C	4.43114200	–1.55757000	–1.05024800
C	4.68720800	–0.00904000	0.78685100
C	5.81092800	–1.56193300	–1.23586200
H	3.80264600	–2.16076800	–1.70259100
C	6.07072900	–0.04669600	0.62244000
H	4.25351500	0.61390700	1.56391500
C	6.63347600	–0.81410600	–0.39447600
H	6.24361400	–2.15797800	–2.03320900
H	6.70589500	0.53451400	1.28341000
H	7.70994700	–0.82898900	–0.53302300
C	1.06997500	–0.91880700	–1.39366500
C	1.54165900	–0.35157200	–2.58153200
C	–0.11670600	–1.66094600	–1.41114800
C	0.83126200	–0.52026700	–3.76904700
H	2.47646100	0.20098300	–2.59716500

C	–0.84213100	–1.79519200	–2.59106400
H	–0.47828700	–2.13517200	–0.50439600
C	–0.36673100	–1.22955600	–3.77346400
H	1.21658000	–0.09177800	–4.68879600
H	–1.77244100	–2.35460700	–2.58840000
H	–0.92522100	–1.34833900	–4.69667900
C	–0.93825800	0.18015300	1.09481700
C	–2.27732900	0.12129900	1.15197600
H	–2.78828000	–0.30775300	2.00653000
C	–3.07361700	0.64471700	0.01384600
O	–2.54426200	1.24669200	–0.90922800
C	–4.55871100	0.43687400	0.00973900
C	–5.20521500	–0.46983700	0.85514400
C	–5.31451500	1.17820000	–0.90569200
C	–6.58589600	–0.63281800	0.79306700
H	–4.64685000	–1.07561900	1.56006600
C	–6.69291200	1.03477200	–0.97353600
H	–4.80524000	1.87407500	–1.56375100
C	–7.31110800	0.12645100	–0.11766900
H	–7.08924100	–1.34003600	1.44275800
H	–7.28084700	1.61433100	–1.67666300
Cl	–9.04693900	–0.06561900	–0.19240900
C	2.06015400	1.16698900	0.03281100
C	1.83588000	2.08789100	0.97681200
H	2.37345700	1.55170400	–0.93906900
C	1.97812400	3.55023300	0.76270300
O	1.81404000	4.36944200	1.64393700
O	2.30563700	3.88452500	–0.49254600
C	2.45373000	5.29203200	–0.74627900
C	2.76118900	5.45665500	–2.21643100

H	3.25860600	5.68191500	–0.11587800
H	1.52771300	5.80135100	–0.46444300
H	2.88532600	6.51755400	–2.44745900
H	3.68420600	4.93469200	–2.48138600
H	1.94681700	5.06166500	–2.82903300
H	–0.50417400	0.60024000	0.19098900
O	2.02177100	–2.52279000	0.36927800
H	1.54051200	1.83827700	1.99275300
H	2.31193600	–2.98234200	–0.44385000
H	0.67130800	–3.74612700	0.43499100
O	0.12225500	–4.46064500	0.05046900
H	0.26487700	–5.22807200	0.61872800
H	1.28795100	–4.42064200	–1.42317500
O	2.09900000	–4.15693400	–1.90155400
H	2.69724700	–4.90875600	–1.80326300

TS3-2a

0 1

P	2.09905800	–0.92319200	0.11792300
C	1.51022400	1.04673900	1.31559000
C	0.26338600	1.70544100	1.29634600
C	2.40590100	1.39620000	2.33051500
C	–0.06892800	2.62710800	2.30813900
C	2.07169600	2.29123100	3.34599800
H	3.40414300	0.95657400	2.32569000
C	0.81930000	2.90840100	3.33737800
H	–1.02361000	3.14560100	2.26304400
H	2.78694200	2.51973200	4.13185500
H	0.55055100	3.62153800	4.11053700
C	2.72871200	–2.26052200	–0.99806500

C	2.55101200	–3.60416900	–0.63561700
C	3.32526900	–1.96443200	–2.22697000
C	2.97965800	–4.62609600	–1.47583900
H	2.06911800	–3.85816400	0.30660300
C	3.75032900	–2.99044900	–3.07231700
H	3.46425600	–0.93117400	–2.52922500
C	3.58196500	–4.31965900	–2.69696500
H	2.83933600	–5.66183100	–1.18256700
H	4.21370100	–2.74688100	–4.02331500
H	3.91389100	–5.11738500	–3.35423300
C	0.34601400	–1.35938600	0.14552100
C	–0.34656100	–1.53364600	–1.05667700
C	–0.28739700	–1.58885300	1.36983300
C	–1.69168400	–1.89084500	–1.03041600
H	0.15832200	–1.38078600	–2.00758000
C	–1.62479200	–1.97466200	1.38655600
H	0.25378600	–1.45237900	2.30308200
C	–2.32883000	–2.11331800	0.18972900
H	–2.24031000	–1.99765400	–1.96071100
H	–2.12104500	–2.15863700	2.33427600
H	–3.37581200	–2.40045100	0.20849300
C	–0.70487800	1.46274400	0.21426400
C	–2.04198400	1.47012500	0.34048100
H	–2.51469300	1.62516800	1.30547800
C	–2.88735100	1.20283200	–0.84501500
O	–2.44641600	1.28438000	–1.98330900
C	–4.31961400	0.80769200	–0.63285900
C	–4.79976200	0.35483500	0.59983700
C	–5.18446800	0.85311400	–1.73109600
C	–6.12596800	–0.04319900	0.73922900

H	–4.14105100	0.28216900	1.45879300
C	–6.51326100	0.47050500	–1.60664000
H	–4.80130400	1.19519600	–2.68669400
C	–6.96528500	0.02494300	–0.36710100
H	–6.49961800	–0.40309000	1.69129500
H	–7.18890500	0.51264400	–2.45377900
Cl	–8.63465400	–0.46862400	–0.19923300
C	2.61196500	0.59895700	–0.60420600
C	3.91645100	1.00044400	–0.60579000
H	1.83554100	1.15574500	–1.12042900
C	4.31607300	2.33031600	–1.03779200
O	5.46738700	2.73072800	–1.08766300
O	3.26867500	3.10609600	–1.39884500
C	3.59634000	4.42430500	–1.85473000
C	2.29747600	5.11842000	–2.19590800
H	4.25681600	4.35123500	–2.72441000
H	4.14082600	4.95132600	–1.06516900
H	2.50147700	6.13569900	–2.53951700
H	1.76856800	4.58451400	–2.98981000
H	1.64721400	5.17232000	–1.31869300
H	–0.30796500	1.24260600	–0.77554500
O	2.87518800	–1.27502400	1.46633500
H	4.71188300	0.37192900	–0.21988600
H	2.89022100	–2.25006900	1.76779100
H	2.13912900	–0.71954700	3.46189800
O	1.79735800	–1.37397300	4.09216300
H	1.94719900	–1.00315400	4.97105300
H	2.37058900	–2.93749000	3.43612800
O	2.67266500	–3.47524500	2.67121200
H	3.48913800	–3.91721500	2.94204000

Int5-2a

0 1

P	2.01300400	0.41472400	0.75639000
C	1.50251300	1.63737100	–1.62480800
C	0.10938400	1.65411200	–1.86904100
C	2.23563900	2.81105400	–1.82925800
C	–0.48545400	2.83551100	–2.34161000
C	1.62527400	3.98158400	–2.27055800
H	3.30632200	2.79854700	–1.65300400
C	0.25670700	3.99192300	–2.53469500
H	–1.54563000	2.83619200	–2.57586800
H	2.21976700	4.87782000	–2.41989800
H	–0.22665300	4.89249800	–2.89928600
C	2.71143800	–1.09529300	1.43645500
C	3.59231800	–1.01412600	2.51785800
C	2.37105600	–2.33862800	0.88973200
C	4.13341100	–2.18015500	3.05375500
H	3.86232300	–0.04711100	2.93192300
C	2.91700400	–3.49834000	1.43114900
H	1.69798100	–2.40012800	0.03947900
C	3.79776900	–3.41832800	2.51024600
H	4.82125100	–2.11977000	3.89073700
H	2.65829700	–4.46375100	1.00714000
H	4.22461100	–4.32504300	2.92718100
C	0.32875800	0.62454800	1.37241000
C	–0.45460100	–0.48575400	1.70941600
C	–0.22924200	1.91151800	1.38692700
C	–1.79236500	–0.31043500	2.04993000
H	–0.02673400	–1.48368500	1.70598000

C	–1.56659400	2.07685200	1.73035500
H	0.37009300	2.77951900	1.12117800
C	–2.34905800	0.96761200	2.05532400
H	–2.40008900	–1.17224500	2.30700300
H	–2.00003000	3.07184300	1.74239700
H	–3.39418100	1.10041800	2.31825800
C	–0.72306100	0.46916900	–1.61700400
C	–2.04343300	0.48059700	–1.37475900
H	–2.60541900	1.40694500	–1.34627900
C	–2.73802600	–0.79919300	–1.09631300
O	–2.15968500	–1.87335300	–1.18564500
C	–4.18481000	–0.77055800	–0.69784200
C	–4.85433600	0.40045000	–0.32829800
C	–4.87576800	–1.98720300	–0.68078900
C	–6.19304900	0.36066500	0.04997300
H	–4.34258600	1.35633100	–0.30929800
C	–6.21324400	–2.04328600	–0.31478600
H	–4.34809100	–2.89210000	–0.96227000
C	–6.85529400	–0.86167500	0.04653600
H	–6.71269600	1.26624400	0.34235900
H	–6.75131200	–2.98465900	–0.30854000
Cl	–8.53972300	–0.91850800	0.51037500
C	2.21969700	0.41055400	–1.08101900
C	3.68566500	0.28204600	–1.31495600
H	1.72952100	–0.50623500	–1.41745600
C	4.28727500	–0.93828600	–1.63889900
O	5.49816000	–1.19843800	–1.71514100
O	3.36629500	–1.94835200	–1.93347000
C	3.91986300	–3.24338900	–2.09908600
C	2.77509400	–4.20440900	–2.34334700

H	4.48575000	–3.52637100	–1.20236000
H	4.62489900	–3.25021900	–2.93801700
H	3.15699100	–5.21946700	–2.48442700
H	2.08346700	–4.21193600	–1.49508400
H	2.21485800	–3.91926100	–3.23846000
H	–0.23884600	–0.50459500	–1.59341000
O	2.85704100	1.66281700	1.24237800
H	4.35028300	1.07697100	–1.00119600
H	2.61164900	2.08751500	2.15622400
H	2.43656000	3.89873100	0.47357100
O	1.96991100	4.46772700	1.10413800
H	2.09557800	5.37225600	0.78991300
H	2.11037900	3.76022500	2.73964000
O	2.22920700	2.94893700	3.28038400
H	2.96130700	3.12454700	3.89048200

TS4-2a

0 1

P	2.44281900	0.62960700	0.01975200
C	0.91820000	–1.57342500	–0.51507300
C	–0.14328200	–1.86380100	0.35837200
C	1.71497500	–2.60710300	–1.00492100
C	–0.38884400	–3.19734200	0.70270900
C	1.46839200	–3.93172700	–0.64621200
H	2.52457500	–2.37264300	–1.69288300
C	0.40967000	–4.22728000	0.20763700
H	–1.21163500	–3.42063100	1.37598800
H	2.09156300	–4.72631200	–1.04459800
H	0.20062200	–5.25530800	0.48675300
C	3.91637000	–0.40090500	0.06819000

C	4.88810100	–0.29416700	–0.93216500
C	4.03489500	–1.36830200	1.07249300
C	5.97882200	–1.15871500	–0.92531700
H	4.79447300	0.45847200	–1.71048800
C	5.13060700	–2.22782000	1.07281400
H	3.27203900	–1.45637800	1.84188600
C	6.09979900	–2.12173300	0.07567200
H	6.73522900	–1.07807700	–1.69883400
H	5.22376700	–2.98358200	1.84709700
H	6.95168400	–2.79430700	0.07776800
C	2.91502300	2.23110400	–0.64996700
C	3.83502300	2.99771900	0.07763700
C	2.41440900	2.69321600	–1.87127900
C	4.24663900	4.22967800	–0.41845400
H	4.22459400	2.63565300	1.02659000
C	2.83981800	3.92488200	–2.36260900
H	1.68439400	2.10848000	–2.42263100
C	3.75130700	4.69016900	–1.63826600
H	4.95515800	4.82821100	0.14439900
H	2.45440600	4.28732700	–3.30976900
H	4.07701600	5.65094700	–2.02434300
C	–1.00477600	–0.78900800	0.90627500
C	–2.35831800	–0.82007800	0.85917800
H	–2.87977800	–1.56226300	0.26180800
C	–3.12501300	0.25255500	1.48392800
O	–2.63704400	1.06088200	2.27299500
C	–4.59172500	0.34327200	1.16317400
C	–5.08976400	0.00541300	–0.09806000
C	–5.46609900	0.81202800	2.14661800
C	–6.45027000	0.11508300	–0.37096500

H	–4.39557800	–0.28523000	–0.88125800
C	–6.82978700	0.91229600	1.89562300
H	–5.06779800	1.09299500	3.11646300
C	–7.30215000	0.55761000	0.63556100
H	–6.84332500	–0.13125600	–1.35145300
H	–7.51530200	1.26092300	2.66030200
Cl	–9.01805200	0.68473400	0.30446600
C	1.13383500	–0.13059500	–0.97703500
C	–0.09309400	0.73624400	–0.90047000
H	1.58147400	–0.17825600	–1.98480700
C	–1.23430900	0.42714600	–1.64012700
O	–2.35910700	0.94764000	–1.56510800
O	–1.03249900	–0.65809200	–2.48240300
C	–2.19338000	–1.21140300	–3.08149200
C	–1.76465600	–2.47614500	–3.79644600
H	–2.64243100	–0.49326300	–3.77853900
H	–2.94538200	–1.43301200	–2.31511600
H	–2.62228800	–2.95418300	–4.27758000
H	–1.01831800	–2.25270900	–4.56393600
H	–1.32620700	–3.18279000	–3.08504200
H	–0.53148900	–0.02855400	1.52122600
O	1.88748400	0.75708100	1.48957400
H	–0.13577800	1.59103600	–0.23782300
H	2.61099200	1.00429400	2.20869200
H	5.85120300	–0.84209800	3.29798800
O	5.22271800	–0.58031600	3.98722800
H	4.75839500	–1.39507200	4.22492800
H	4.23982800	0.61712800	3.43695100
O	3.68828500	1.35971300	3.07115700
H	3.44729100	1.93742400	3.80836900

Int6-2a

0 1

P	2.53398900	0.45107500	0.23262200
C	0.92769000	–1.46844900	–0.90751000
C	–0.28040200	–1.69910100	–0.24901800
C	1.67478900	–2.51208800	–1.44428900
C	–0.75884800	–2.99831900	–0.12111500
C	1.19372500	–3.81573300	–1.30695000
H	2.60644100	–2.31767400	–1.96955900
C	–0.01300600	–4.05513100	–0.64733200
H	–1.70994400	–3.17785400	0.37338300
H	1.75627100	–4.64448500	–1.72514600
H	–0.38025500	–5.07284000	–0.55404200
C	4.01659700	–0.52466500	–0.03837000
C	4.98801200	–0.10652800	–0.95381800
C	4.14947100	–1.74482200	0.63505100
C	6.09438600	–0.91518600	–1.19510200
H	4.88356600	0.84372800	–1.47033600
C	5.26225100	–2.54507400	0.38962200
H	3.38677100	–2.06930100	1.33795600
C	6.23073500	–2.12994400	–0.52394800
H	6.85182600	–0.59470200	–1.90238400
H	5.36901000	–3.49420700	0.90605100
H	7.09637200	–2.75639000	–0.71420500
C	2.95064300	2.19432700	0.09375200
C	3.79375900	2.73997000	1.07174500
C	2.46498500	2.99103600	–0.94835800
C	4.14665500	4.08254200	1.00186800
H	4.16828200	2.12163100	1.88463200

C	2.82769300	4.33419700	–1.01007900
H	1.80536400	2.58057700	–1.70716400
C	3.66509400	4.87716100	–0.03864900
H	4.79665700	4.50864100	1.75873700
H	2.45179700	4.95480400	–1.81652100
H	3.94311700	5.92502900	–0.09036000
C	–0.92689400	–0.41899600	0.24294600
C	–2.41515100	–0.33954600	0.13018900
H	–2.87576300	–0.63233500	–0.80820900
C	–3.17277300	0.03308600	1.22666800
O	–2.73329900	0.32617100	2.38237100
C	–4.68555100	0.06546800	1.05915700
C	–5.34637000	0.13944600	–0.17338400
C	–5.46328200	0.04114200	2.22124300
C	–6.73629100	0.16188500	–0.24909500
H	–4.77530800	0.20304700	–1.09445600
C	–6.85373100	0.05744700	2.17109400
H	–4.94214200	0.01304600	3.17232100
C	–7.47471800	0.11394400	0.92874100
H	–7.23919100	0.22537100	–1.20841700
H	–7.44744400	0.02957800	3.07907600
Cl	–9.22874400	0.13932000	0.84432200
C	1.22814600	0.01577000	–0.95093700
C	–0.11486500	0.68695500	–0.52981100
H	1.59166500	0.33527600	–1.93491700
C	–0.88341000	1.14946300	–1.74748200
O	–1.34294200	2.25923200	–1.89341000
O	–1.01255700	0.17374500	–2.65425500
C	–1.81012800	0.48929100	–3.80992000
C	–1.93009400	–0.77255700	–4.63163500

H	–1.32321200	1.29597800	–4.36586100
H	–2.78598800	0.85090200	–3.47266600
H	–2.53439700	–0.57479700	–5.52047000
H	–0.94571800	–1.12291800	–4.95262200
H	–2.41237200	–1.56476300	–4.05300700
H	–0.69266900	–0.29257900	1.30778600
O	1.96252600	0.10401600	1.65438600
H	0.02122500	1.57384100	0.09335100
H	2.66820700	0.12471900	2.44306600
H	5.91725400	–1.90059800	2.96741300
O	5.26637200	–1.87518200	3.68312300
H	4.82726100	–2.73810700	3.65558200
H	4.26281100	–0.59843000	3.51975700
O	3.69042800	0.20841200	3.39920300
H	3.40039000	0.49815600	4.27546300

Int7-2a

0 1

P	3.05453800	–0.50523300	–0.48339100
C	1.53842700	1.47466900	0.68582400
C	0.31974300	1.77869000	0.07685400
C	2.35817300	2.46909000	1.20961800
C	–0.09810700	3.10268000	–0.00990600
C	1.93868800	3.79708300	1.11495900
H	3.29912900	2.21854700	1.69259400
C	0.72073800	4.10780800	0.50897000
H	–1.05163100	3.36237200	–0.46243900
H	2.55933200	4.58827700	1.52333900
H	0.39935600	5.14344300	0.44704200
C	4.53289400	0.48795600	–0.32502600

C	5.51211900	0.12755600	0.60866500
C	4.64871000	1.66807500	–1.06874000
C	6.61184800	0.95786400	0.79549300
H	5.41821300	–0.79044600	1.18194100
C	5.75869100	2.48496800	–0.87931800
H	3.88056200	1.94670400	–1.78389800
C	6.73375300	2.13178500	0.05222000
H	7.37533300	0.68593700	1.51632600
H	5.85905000	3.39811100	–1.45606000
H	7.59593700	2.77436500	0.19938100
C	3.48100600	–2.23854900	–0.35320900
C	4.56491500	–2.70532200	–1.11140400
C	2.75283100	–3.11199300	0.46336000
C	4.90948700	–4.05034800	–1.05564600
H	5.13701900	–2.02400600	–1.73647900
C	3.11395400	–4.45466200	0.51673200
H	1.91123000	–2.76125300	1.05325300
C	4.18584100	–4.92124200	–0.24125700
H	5.74506600	–4.41683300	–1.64208900
H	2.55566800	–5.13484600	1.15075500
H	4.46118800	–5.97002800	–0.19590500
C	–0.39201800	0.54366600	–0.42104300
C	–1.88103500	0.51612000	–0.21515100
H	–2.53729100	1.68994500	–1.64653900
C	–2.60941600	–0.49146500	–0.82717400
O	–2.12273000	–1.34774500	–1.63841100
C	–4.09198600	–0.59463900	–0.53957100
C	–4.86111800	0.46813500	–0.04989100
C	–4.72720100	–1.81186500	–0.80122000
C	–6.22296700	0.31690100	0.19387600

H	–4.40378600	1.43750000	0.12604000
C	–6.08573600	–1.98674200	–0.55766200
H	–4.13026800	–2.62271600	–1.20478400
C	–6.81738000	–0.91505600	–0.05833900
H	–6.81607700	1.14558300	0.56563200
H	–6.57135900	–2.93675900	–0.75436600
Cl	–8.53292200	–1.11582800	0.24820400
C	1.76683000	–0.02440700	0.69902800
C	0.38601300	–0.62444900	0.28376000
H	2.12309000	–0.38355800	1.67292700
C	–0.35691700	–1.09945200	1.51304800
O	–0.78155100	–2.22151400	1.67267100
O	–0.48682000	–0.12458800	2.41842000
C	–1.29734100	–0.43574000	3.56648500
C	–1.41142600	0.82491900	4.39078200
H	–0.82560800	–1.24975400	4.12434400
H	–2.27377100	–0.78303000	3.21482200
H	–2.02711500	0.63137200	5.27266500
H	–0.42650600	1.16305700	4.72297900
H	–1.87859700	1.62435500	3.80965500
H	–0.19297000	0.43317700	–1.49588100
O	2.36856600	–0.17081000	–1.89397600
H	0.45486000	–1.48305500	–0.38599300
H	2.89203700	–0.42937800	–2.67608400
O	–2.81442000	2.27490000	–2.40204100
H	–3.70244700	1.96249500	–2.63002200
H	–2.95503700	3.91514200	–1.57325400
O	–2.96170200	4.70158600	–0.99709300
H	–3.31211000	4.36942400	–0.16202700
H	–1.65661500	1.01755400	–3.47660100

O	–1.17499400	0.21493600	–3.72361700
H	–1.46645000	–0.42942100	–3.04489400
H	–2.30070300	1.08897900	0.60669800

TS5-2a

0 1

P	3.00271600	–0.55604600	–0.47054000
C	1.53380800	1.44134400	0.71014700
C	0.38869900	1.85033200	0.02569500
C	2.37033100	2.35720800	1.34048800
C	0.06353800	3.20160900	–0.03982800
C	2.04331800	3.71242600	1.27304500
H	3.25269800	2.02586400	1.88164100
C	0.90152000	4.12698100	0.58561900
H	–0.82615800	3.54112900	–0.56321100
H	2.67780200	4.44395400	1.76333600
H	0.65397300	5.18379200	0.54077000
C	4.53249100	0.30152400	–0.12704600
C	5.40898500	–0.21020500	0.83726200
C	4.79191200	1.52205200	–0.76079700
C	6.55161400	0.51091000	1.16652000
H	5.20266800	–1.15961100	1.32398200
C	5.94387700	2.22802000	–0.42998000
H	4.10156400	1.91647700	–1.50039400
C	6.81728600	1.72476500	0.53289500
H	7.23668400	0.12297000	1.91261700
H	6.15622000	3.17115700	–0.92188700
H	7.71287000	2.28133200	0.79021100
C	3.29074200	–2.32244400	–0.45770600
C	4.34929900	–2.81921900	–1.23216000

C	2.48862600	–3.18885400	0.29358300
C	4.59319900	–4.18683300	–1.25890600
H	4.98202700	–2.14475500	–1.80438800
C	2.74907000	–4.55550400	0.26529400
H	1.66866500	–2.81304900	0.89746400
C	3.79518000	–5.05144100	–0.50959100
H	5.40902400	–4.57660900	–1.85801200
H	2.13307500	–5.23074500	0.84912200
H	3.99310200	–6.11833800	–0.52796600
C	–0.36505000	0.68474200	–0.56909500
C	–1.87610600	0.78519300	–0.43726100
H	–2.24942900	1.74847900	–1.23479600
C	–2.59673600	–0.34855800	–0.99363500
O	–2.10927700	–1.11852900	–1.83144100
C	–4.03839300	–0.54422200	–0.59916300
C	–4.79369100	0.46456800	0.00687100
C	–4.63674600	–1.77833200	–0.86606200
C	–6.12521900	0.24598300	0.34726900
H	–4.35456700	1.43846100	0.19849000
C	–5.96114300	–2.01919800	–0.52064000
H	–4.04645800	–2.55097300	–1.34734300
C	–6.68816300	–0.99808000	0.08365300
H	–6.71697500	1.02943000	0.80764700
H	–6.42477500	–2.97974900	–0.71734800
Cl	–8.35958000	–1.28586100	0.51878400
C	1.67008000	–0.06742100	0.65913500
C	0.28776200	–0.56016700	0.12936800
H	1.94222400	–0.49898800	1.63046400
C	–0.57912200	–1.03665500	1.27607000
O	–1.21122100	–2.06863800	1.27422500

O	–0.59637900	–0.16145300	2.28592200
C	–1.49942500	–0.46811700	3.36693700
C	–1.43822000	0.68137100	4.34455000
H	–1.19259000	–1.41332000	3.82343100
H	–2.50295200	–0.59894400	2.95037400
H	–2.11460300	0.48609700	5.18036700
H	–0.42630800	0.80340200	4.73909200
H	–1.74204500	1.61446500	3.86295300
H	–0.12751600	0.61862900	–1.63760900
O	2.44944000	–0.06261200	–1.89264300
H	0.35225700	–1.39531800	–0.57017400
H	3.01546600	–0.28907300	–2.65501200
O	–2.52775100	2.67472500	–2.17251100
H	–3.45683000	2.50824700	–2.38318600
H	–2.43851300	4.23453100	–1.70713100
O	–2.35831300	5.15693300	–1.32700800
H	–2.80481400	5.08225400	–0.47618200
H	–1.66893700	1.64076300	–3.28488500
O	–1.21055500	0.92793700	–3.79253400
H	–1.44761900	0.12985300	–3.29975600
H	–2.20460300	1.05895900	0.56879500

Int8-2a

0 1

P	2.92034600	–0.64345300	–0.49673000
C	1.52278200	1.31556400	0.81702900
C	0.40940400	1.81061600	0.13945200
C	2.38786600	2.16475600	1.50140400
C	0.14631200	3.17663500	0.11936400
C	2.12224400	3.53516900	1.48754700

H	3.24897700	1.77159900	2.03536200
C	1.01598200	4.03312100	0.79584800
H	–0.71347900	3.57073700	–0.41687800
H	2.78245400	4.21460200	2.01749200
H	0.81942400	5.10122400	0.77681700
C	4.46056100	0.18766600	–0.13673400
C	5.35748600	–0.38066100	0.77561500
C	4.71052800	1.44141400	–0.70671200
C	6.51063500	0.31738300	1.11814400
H	5.15899300	–1.35543500	1.21247600
C	5.87309000	2.12375900	–0.36428300
H	4.00447200	1.87959800	–1.40585800
C	6.76668000	1.56420200	0.54788500
H	7.21128700	–0.11429400	1.82469800
H	6.07796800	3.09263100	–0.80679200
H	7.67045600	2.10265000	0.81489600
C	3.19729000	–2.41038700	–0.57164800
C	4.23315300	–2.87355000	–1.39659400
C	2.41106300	–3.30871300	0.15846500
C	4.46872300	–4.23909600	–1.49605900
H	4.85396700	–2.17341000	–1.95115800
C	2.66297800	–4.67360000	0.05666700
H	1.61155000	–2.95840500	0.80403300
C	3.68522100	–5.13569700	–0.76917300
H	5.26666000	–4.60278200	–2.13434500
H	2.05928600	–5.37408700	0.62338400
H	3.87649700	–6.20131700	–0.84474300
C	–0.38240600	0.71166100	–0.52531100
C	–1.89243500	0.87819600	–0.36994700
H	–2.18170100	1.84478100	–0.84486300

C	–2.66294100	–0.19857000	–1.08536900
O	–2.17022600	–0.81873700	–2.01667200
C	–4.07996800	–0.47021700	–0.67875300
C	–4.78224100	0.37433400	0.18556700
C	–4.71390500	–1.60098100	–1.20306900
C	–6.10368700	0.09780500	0.52285000
H	–4.31374200	1.26392000	0.59326400
C	–6.02744200	–1.89821600	–0.86643700
H	–4.16210600	–2.24842600	–1.87636400
C	–6.70545400	–1.03874800	–0.00561500
H	–6.65649400	0.75412600	1.18557500
H	–6.52050600	–2.77859700	–1.26373500
Cl	–8.36262000	–1.39878800	0.42121800
C	1.60159600	–0.19126300	0.66896700
C	0.20504900	–0.59633000	0.10634700
H	1.85166500	–0.69784400	1.60837900
C	–0.71286000	–1.09303200	1.20553800
O	–1.54175100	–1.96115400	1.04785600
O	–0.56114100	–0.41255100	2.34341200
C	–1.48802900	–0.73559300	3.40197300
C	–1.20282200	0.20430800	4.54896200
H	–1.34624300	–1.78310900	3.68168000
H	–2.50564700	–0.61866100	3.01733700
H	–1.88746100	–0.00854400	5.37359700
H	–0.17834800	0.07953900	4.90850200
H	–1.34310400	1.24355000	4.24108000
H	–0.16244900	0.71249100	–1.59733900
O	2.35290600	–0.08098900	–1.88805700
H	0.24222100	–1.39460600	–0.63780000
H	2.91667600	–0.26112700	–2.66434900

O	–2.29122000	3.45909300	–1.95563100
H	–3.22638200	3.49117300	–2.18935400
H	–1.84547800	4.84367400	–1.50801800
O	–1.52186900	5.72637900	–1.09252200
H	–1.98120900	5.74082700	–0.24584600
H	–1.59376100	2.46910000	–2.91621500
O	–1.13158800	1.76413900	–3.49686900
H	–1.54436600	0.93331300	–3.23448400
H	–2.17831500	0.93126100	0.68616600

Int9-2a

0 1

P	–2.35324400	0.22592000	–0.12107600
C	–0.87570400	–2.08851900	–0.32055800
C	0.19856500	–2.01250600	–1.20946000
C	–1.68549400	–3.21858000	–0.26996100
C	0.48065000	–3.07527700	–2.06022400
C	–1.40039200	–4.28596400	–1.12417600
H	–2.51456100	–3.27709700	0.43014200
C	–0.32773800	–4.21361100	–2.01269300
H	1.31758800	–3.02681400	–2.75144500
H	–2.01469100	–5.18023700	–1.09115800
H	–0.11415400	–5.05212000	–2.66831800
C	–3.86728600	–0.71721600	0.17253400
C	–4.36598200	–0.92408300	1.46243100
C	–4.52100900	–1.27023000	–0.93280700
C	–5.51992500	–1.68171000	1.64254100
H	–3.86427500	–0.48660400	2.32200300
C	–5.67574200	–2.02779300	–0.74700900
H	–4.12900300	–1.09600800	–1.93068900

C	–6.17345500	–2.23224900	0.53905300
H	–5.91237200	–1.83896500	2.64198400
H	–6.18611800	–2.45496200	–1.60413800
H	–7.07485100	–2.81949400	0.68350700
C	–2.39078700	1.70724200	0.91744300
C	–2.91811800	2.86664900	0.34010500
C	–1.91317900	1.73864900	2.23281300
C	–2.97838300	4.04682000	1.07367300
H	–3.27545400	2.86236600	–0.68359800
C	–1.97746800	2.92288200	2.96379200
H	–1.48328100	0.85260700	2.69207700
C	–2.51133200	4.07441000	2.38663600
H	–3.38858200	4.93894700	0.61107400
H	–1.60462100	2.94630700	3.98261800
H	–2.55639600	4.99506900	2.96012600
C	0.91567800	–0.68558500	–1.08945300
C	2.43571800	–0.78830700	–1.16431200
C	3.10675200	0.56987300	–1.08924000
O	2.46939500	1.59431900	–1.24762500
C	4.58231200	0.62819100	–0.83523100
C	5.38158700	–0.51784500	–0.80371000
C	5.16604400	1.88200200	–0.62772300
C	6.74934800	–0.41725200	–0.56932800
H	4.95115900	–1.49978900	–0.96958700
C	6.52756000	1.99901700	–0.38522000
H	4.53668700	2.76519900	–0.65560500
C	7.30164500	0.84149300	–0.35967800
H	7.37570900	–1.30200100	–0.54869700
H	6.98410000	2.96844600	–0.21868600
Cl	9.01781800	0.97474300	–0.05436600

C	–0.98163900	–0.81969900	0.49430000
C	0.37362200	–0.10115900	0.25795700
H	–1.17425200	–1.02698900	1.55253500
C	1.35829900	–0.36075900	1.37958100
O	2.13663400	0.46409700	1.80357700
O	1.32229700	–1.62633800	1.80725300
C	2.29698900	–1.98332800	2.80880700
C	2.10891800	–3.45047700	3.11294600
H	2.13752800	–1.35703400	3.69087300
H	3.29496000	–1.76953600	2.41428900
H	2.83307100	–3.76261600	3.86934200
H	1.10335100	–3.64085200	3.49633700
H	2.26304800	–4.05453500	2.21522700
H	0.57375700	–0.01596700	–1.88616500
O	–2.18951300	0.56548200	–1.59069900
H	0.28365800	0.98447700	0.18851200
H	–3.43933300	1.27887300	–2.41006800
O	–4.25472800	1.73286200	–2.74643400
H	–4.49800800	1.30063500	–3.57443800
H	–5.41702000	1.67082200	–1.29015900
O	–5.90454900	1.70259200	–0.44858100
H	–5.97620300	0.77747000	–0.18634000
H	–4.10206900	3.57324500	–2.60083500
O	–3.94224900	4.49762300	–2.33919000
H	–2.99106800	4.60723400	–2.45567800
H	2.82231100	–1.44771300	–0.37838900
H	2.73650300	–1.24734900	–2.11567600

TS6-2a

0 1

P	1.98609500	0.07521400	–0.12180200
C	2.43705400	0.15175800	1.64362800
C	1.48239500	0.52378200	2.60340300
C	3.71202300	–0.25418400	2.04263300
C	1.82812400	0.45594800	3.95813500
C	4.03876300	–0.31773700	3.39312500
H	4.45648600	–0.51844300	1.29830300
C	3.09236100	0.03163600	4.35332100
H	1.09122100	0.74605800	4.70090200
H	5.03189700	–0.63711100	3.69153600
H	3.33885400	–0.01957300	5.40895100
C	3.30050200	–0.43025400	–1.28257900
C	3.96996600	–1.64294300	–1.09129300
C	3.56061100	0.34000300	–2.41974500
C	4.93050200	–2.05646600	–2.01133700
H	3.74326800	–2.26726600	–0.23096800
C	4.50198000	–0.09331300	–3.34905100
H	3.02150200	1.26851000	–2.58380900
C	5.19537200	–1.28420800	–3.14029400
H	5.46082300	–2.98937500	–1.85009400
H	4.69463500	0.50268000	–4.23520100
H	5.93546900	–1.61509600	–3.86193700
C	1.00252300	–1.50568800	–0.15410700
C	0.37616400	–1.85916900	–1.35879900
C	0.90013300	–2.37505300	0.93636100
C	–0.35309800	–3.03976600	–1.46354900
H	0.46217700	–1.21028900	–2.22814600
C	0.16940700	–3.56033500	0.83165700
H	1.38616900	–2.13736000	1.87795000
C	–0.46120200	–3.89257200	–0.36429700

H	–0.83598600	–3.29429100	–2.40196200
H	0.09702500	–4.22245900	1.68881500
H	–1.03028400	–4.81375500	–0.44373900
C	0.12764600	1.01548600	2.23684600
C	–0.96238800	0.24558600	2.22154000
H	–0.90539200	–0.81732500	2.44142100
C	–2.27604800	0.83464600	1.83614400
O	–2.56207300	1.98433500	2.12610000
C	–3.22516700	–0.02154200	1.06102000
C	–2.81181400	–1.21308300	0.45809200
C	–4.54598500	0.41220900	0.90568000
C	–3.70644600	–1.96983500	–0.29224400
H	–1.78532600	–1.55645800	0.55400700
C	–5.45249700	–0.33637800	0.16782100
H	–4.85415500	1.34273200	1.37175300
C	–5.01613800	–1.52131300	–0.42171100
H	–3.38882200	–2.89189200	–0.76728700
H	–6.48001600	–0.01109000	0.04873000
Cl	–6.15047400	–2.47069800	–1.35307300
C	0.72351200	1.20240500	–0.79644100
C	0.99103300	2.50058300	–0.96808200
H	–0.22301400	0.70273300	–1.00443000
C	–0.06257800	3.36887600	–1.53105500
O	0.11292000	4.16713400	–2.43014100
O	–1.25096900	3.20817400	–0.91958700
C	–2.31659800	4.05955000	–1.37424700
C	–3.58741400	3.58542500	–0.70679300
H	–2.38336000	3.99958700	–2.46390200
H	–2.07673000	5.09448900	–1.10881600
H	–4.41669400	4.24108300	–0.98554400

H	–3.82979600	2.56784700	–1.02615600
H	–3.47875800	3.58774100	0.38040500
H	0.03088500	2.06579000	1.96216500
O	3.21254700	2.01806400	–0.00207100
H	3.95518200	2.02508600	–0.61887800
H	2.27378800	2.58511700	–0.52188300

TS7-2a

0 1

P	2.06432900	–0.27904000	–0.23854500
C	2.44380800	0.58280600	1.30777200
C	1.59258500	1.56395200	1.86023900
C	3.68221200	0.31100600	1.90491900
C	2.04457200	2.27248400	2.97967400
C	4.09025200	0.99998500	3.04134800
H	4.33989000	–0.43712600	1.47371500
C	3.27222400	1.99389300	3.57025900
H	1.40521900	3.04458900	3.39782800
H	5.04843200	0.77250100	3.49573700
H	3.58782200	2.55475500	4.44421500
C	3.61190600	–0.90184300	–0.94088800
C	4.01623800	–2.22731700	–0.75652700
C	4.41414000	–0.00972500	–1.66193200
C	5.22832700	–2.65645200	–1.29136100
H	3.39231900	–2.91991700	–0.19893100
C	5.62333000	–0.44720800	–2.19263000
H	4.09228700	1.01812200	–1.80788900
C	6.02905800	–1.76849000	–2.00703500
H	5.54446000	–3.68474900	–1.15030900
H	6.24642400	0.24167400	–2.75331100

H	6.97194500	–2.10768000	–2.42421900
C	1.01333800	–1.72268300	0.06487800
C	0.39981300	–2.33885000	–1.03313500
C	0.81410100	–2.21873100	1.35649700
C	–0.42469200	–3.44210600	–0.83055000
H	0.56019800	–1.96187700	–2.03971300
C	–0.01968600	–3.31763400	1.55050900
H	1.29356300	–1.74096100	2.20651200
C	–0.63959800	–3.92590600	0.46015500
H	–0.90341500	–3.91912000	–1.67960600
H	–0.18335000	–3.69732200	2.55365000
H	–1.28991300	–4.78102400	0.61555700
C	0.22136500	1.88216700	1.38959100
C	–0.79635200	0.98358900	1.40310200
H	–0.59949100	–0.07248700	1.54122200
C	–2.16519400	1.42601700	1.15564100
O	–2.51712000	2.60142300	1.23815600
C	–3.18113800	0.37683900	0.79322900
C	–2.81293900	–0.88619600	0.31961800
C	–4.53803700	0.69848300	0.89626500
C	–3.78056700	–1.81810600	–0.04414800
H	–1.76564700	–1.15102300	0.20455400
C	–5.51772700	–0.22183100	0.54643600
H	–4.81568200	1.68353400	1.25738700
C	–5.12159800	–1.47237400	0.07891000
H	–3.49447400	–2.79492400	–0.42023000
H	–6.57079800	0.02261800	0.63250400
Cl	–6.34675900	–2.63856100	–0.37043400
C	1.27896000	0.83194000	–1.40013700
C	0.85200600	2.01129000	–0.94715800

H	1.13931400	0.39246900	–2.39353700
C	0.05166100	2.91936900	–1.73808000
O	0.43077100	3.94211800	–2.28923100
O	–1.25826000	2.56371300	–1.69110400
C	–2.18509500	3.52599300	–2.20823000
C	–3.57732800	2.99875400	–1.94103500
H	–2.00116800	3.66775100	–3.27830900
H	–2.01949900	4.48845400	–1.71292500
H	–4.32065000	3.68999000	–2.34785100
H	–3.71933400	2.02219800	–2.41328800
H	–3.73639400	2.89660900	–0.86461800
H	–0.03490800	2.93738000	1.35766100

Int10-2a

0 1

P	1.89275900	0.54013400	0.16102100
C	1.93627100	0.80566800	–1.61484700
C	1.25031300	–0.10911200	–2.42772300
C	2.65216500	1.87756300	–2.16092300
C	1.30509200	0.08171400	–3.81097800
C	2.68310700	2.05143400	–3.53877700
H	3.18874700	2.56413700	–1.51168600
C	2.00964400	1.14780500	–4.36098200
H	0.78392600	–0.61872900	–4.45779300
H	3.23396600	2.88100000	–3.96865500
H	2.03791500	1.27292300	–5.43889300
C	3.49946800	0.94472800	0.87742400
C	3.59197800	1.56930500	2.12439400
C	4.65612900	0.54410500	0.19572300
C	4.84644900	1.80358600	2.68255600

H	2.69705800	1.87132300	2.65913900
C	5.90311300	0.78389300	0.76161300
H	4.58404100	0.05161600	–0.77013300
C	5.99765100	1.41524900	2.00192900
H	4.92085300	2.29148900	3.64859800
H	6.80057800	0.47957000	0.23356200
H	6.97317300	1.60277800	2.43926800
C	0.60788800	1.52201000	0.96288900
C	–0.51211000	0.88431100	1.50444400
C	0.72708100	2.91714300	0.99125100
C	–1.51576300	1.65795400	2.08515500
H	–0.62152800	–0.19742500	1.44356000
C	–0.28147200	3.67593500	1.57432600
H	1.60022300	3.40489000	0.56504200
C	–1.40011600	3.04569200	2.12135100
H	–2.39350400	1.17194500	2.49995300
H	–0.19588600	4.75714100	1.60008200
H	–2.18657700	3.64168100	2.57364500
C	0.37483600	–1.22125300	–1.87787300
C	–1.02166000	–0.65190300	–1.65329900
H	–1.35774700	0.09141000	–2.36687300
C	–1.83012900	–1.09436400	–0.63478500
O	–1.55646900	–2.03325700	0.19246100
C	–3.15679600	–0.39468700	–0.42889900
C	–3.41600500	0.91618700	–0.84800300
C	–4.15339800	–1.07427500	0.27829800
C	–4.64281600	1.52359900	–0.59701100
H	–2.64181500	1.48630500	–1.35239800
C	–5.38890200	–0.48809800	0.53662500
H	–3.93470100	–2.07686000	0.63020000

C	–5.61832900	0.80828500	0.08990800
H	–4.83418300	2.54234700	–0.91709400
H	–6.16038600	–1.02468800	1.07900400
Cl	–7.16746600	1.56637200	0.41513000
C	1.57142000	–1.19341600	0.35140900
C	0.88512300	–1.84268100	–0.59893600
H	1.90319100	–1.67311800	1.26594300
C	0.57735900	–3.30566500	–0.43331500
O	0.25069300	–4.02450100	–1.35116400
O	0.78513200	–3.73480400	0.81033800
C	0.46850700	–5.11675000	1.04819000
C	0.72463000	–5.39305200	2.51106100
H	1.09055100	–5.74133900	0.40029600
H	–0.57856900	–5.28266200	0.77773200
H	0.49589000	–6.43870900	2.73153400
H	1.77192400	–5.20735500	2.76311300
H	0.09426300	–4.76034800	3.14092700
H	0.36491200	–2.02462900	–2.62685900

Int11-2a

0 1

P	1.82792200	–1.06845900	–0.23504700
C	2.09584700	–0.24132500	1.33782300
C	1.60693800	1.06757200	1.45167600
C	2.79413000	–0.85429100	2.38154800
C	1.82160600	1.75425000	2.64755400
C	2.98768700	–0.15877700	3.57113700
H	3.18074500	–1.86311900	2.26416200
C	2.50466000	1.14394400	3.69883600
H	1.45235800	2.77351300	2.73751800

H	3.52077100	–0.62777900	4.39099100
H	2.66555100	1.69096700	4.62257800
C	3.20747400	–2.16377800	–0.60675200
C	3.04782600	–3.55149300	–0.58393300
C	4.45386000	–1.58990700	–0.88823500
C	4.14509900	–4.36831500	–0.84767300
H	2.07988000	–3.99236700	–0.36547000
C	5.54077500	–2.41498400	–1.15193400
H	4.57261800	–0.50940300	–0.90211200
C	5.38524200	–3.80165500	–1.13137600
H	4.02744900	–5.44657400	–0.83277200
H	6.50797700	–1.97678400	–1.37409600
H	6.23662800	–4.44203400	–1.33880100
C	0.28296100	–2.00309400	–0.24149500
C	–0.33004600	–2.27615800	–1.46846900
C	–0.28940600	–2.43471700	0.95849200
C	–1.52903000	–2.98378100	–1.48835700
H	0.11413100	–1.92896600	–2.39733900
C	–1.48812800	–3.14121400	0.92518200
H	0.18569000	–2.20634300	1.90899200
C	–2.10768600	–3.41272200	–0.29492500
H	–2.01698300	–3.18799800	–2.43587100
H	–1.94407800	–3.46973800	1.85345700
H	–3.04868500	–3.95408100	–0.31443200
C	0.75435400	1.69646500	0.37018300
C	–0.65469400	1.12342300	0.52622300
H	–1.36174800	2.46534000	1.61379900
C	–1.52642500	1.08595600	–0.55582300
O	–1.32423000	1.62383900	–1.68042000
C	–2.80513900	0.29038100	–0.37584800

C	–3.30740700	–0.10376800	0.87122800
C	–3.49463000	–0.09581900	–1.52832100
C	–4.45416600	–0.88754300	0.96300000
H	–2.80879200	0.19853500	1.78925800
C	–4.63791600	–0.88571600	–1.45796700
H	–3.10532400	0.22820300	–2.48798000
C	–5.09950200	–1.27719000	–0.20626500
H	–4.84062800	–1.19379200	1.92931700
H	–5.16101000	–1.19475400	–2.35693000
Cl	–6.53413400	–2.28128600	–0.09729400
C	1.76613100	0.25732100	–1.42583200
C	1.26630100	1.43488100	–1.02979200
H	2.09379900	0.07586200	–2.44457000
C	1.14916100	2.50758700	–2.07916300
O	1.37445000	2.31741300	–3.25157000
O	0.83204600	3.70495300	–1.57380100
C	0.61619100	4.73918900	–2.55539200
C	0.22507800	5.99878800	–1.81994000
H	–0.17083700	4.40330800	–3.23609000
H	1.53538100	4.87233600	–3.13199300
H	0.04484900	6.79785900	–2.54329300
H	–0.69211000	5.84738400	–1.24373700
H	1.02189900	6.32388300	–1.14504100
H	0.78246600	2.77418100	0.54096500
H	–0.80863500	0.46330700	1.37073700
O	–1.46239500	3.10020800	2.38071000
H	–2.38725700	3.38378700	2.36503800
H	–0.27194500	4.40564300	1.78909700
H	–1.24505300	1.55147800	3.49329600
O	0.45447900	4.93493000	1.41169600

H	0.42745500	4.73100200	0.46822200
O	–1.15508400	0.65354100	3.85713100
H	–0.24209500	0.41575200	3.65051100

TS8-2a

0 1

P	1.83344300	–1.04724700	–0.27956100
C	2.12634300	–0.20984900	1.28433800
C	1.60955100	1.08757500	1.42281400
C	2.84709700	–0.82401700	2.31365100
C	1.81341000	1.75632400	2.63130300
C	3.03671600	–0.14270500	3.51115800
H	3.25486600	–1.82203000	2.17707000
C	2.51947800	1.14401300	3.66461300
H	1.40618800	2.75850200	2.74136900
H	3.58928100	–0.61165400	4.31813900
H	2.67193300	1.67754700	4.59771800
C	3.21308200	–2.12741700	–0.68713700
C	3.04569500	–3.51207600	–0.76071500
C	4.46476300	–1.54113000	–0.91581800
C	4.14256000	–4.31463200	–1.06681000
H	2.07330400	–3.96144800	–0.58346400
C	5.55055100	–2.35214100	–1.22258900
H	4.58699200	–0.46252800	–0.85513300
C	5.38823300	–3.73641200	–1.29734500
H	4.02001600	–5.39081000	–1.12593400
H	6.52237200	–1.90524300	–1.40324400
H	6.23932100	–4.36583700	–1.53695100
C	0.29203400	–1.98780900	–0.22956800
C	–0.50598000	–2.06105100	–1.37511900

C	–0.09378900	–2.62593200	0.95526400
C	–1.69474300	–2.78620000	–1.33414700
H	–0.21403500	–1.54772400	–2.28717200
C	–1.28637200	–3.34154400	0.98510700
H	0.52182300	–2.55604000	1.84792800
C	–2.08408600	–3.42226700	–0.15735400
H	–2.32102600	–2.84042200	–2.21854700
H	–1.59561700	–3.83151800	1.90237300
H	–3.01713500	–3.97660000	–0.12605100
C	0.74692400	1.72435900	0.35175600
C	–0.68730500	1.19261100	0.57803900
H	–1.15668100	1.91859300	1.55102300
C	–1.60462600	1.23593800	–0.54356300
O	–1.43440500	1.90324600	–1.56738600
C	–2.86033700	0.40873700	–0.40648400
C	–3.25763600	–0.15599900	0.81110500
C	–3.61494400	0.16417700	–1.55639200
C	–4.38712600	–0.96779700	0.87302800
H	–2.68798100	0.02381400	1.72110700
C	–4.73890000	–0.65222700	–1.51271600
H	–3.29750800	0.61188400	–2.49261600
C	–5.10528600	–1.21270100	–0.29272500
H	–4.70037800	–1.41156200	1.81203800
H	–5.31832700	–0.85619600	–2.40666800
Cl	–6.50909600	–2.25802300	–0.22512900
C	1.71702100	0.27814500	–1.46867100
C	1.23677600	1.45660000	–1.05274200
H	2.03283200	0.10603500	–2.49312500
C	1.14266800	2.55038300	–2.08692500
O	1.29333300	2.36349200	–3.27240200

O	0.92715100	3.74322200	–1.53891700
C	0.75678300	4.83739400	–2.45910200
C	0.43300000	6.06242500	–1.63736800
H	–0.04981200	4.58311900	–3.15255800
H	1.67926000	4.95983800	–3.03379600
H	0.32503300	6.92791300	–2.29567300
H	–0.50582200	5.92633100	–1.09338500
H	1.23173200	6.27091800	–0.92066500
H	0.75866900	2.80151200	0.52092000
H	–0.68451400	0.20822400	1.04675700
O	–1.40931200	2.59083600	2.67219400
H	–2.35193100	2.80324100	2.64411900
H	–0.51666400	3.91003200	2.27332700
H	–1.20294000	1.07295100	3.39925800
O	0.09441900	4.63681800	1.95923000
H	–0.10890900	4.72316000	1.02013000
O	–1.07113600	0.12303700	3.65571800
H	–0.20106700	–0.08275200	3.29149500

Int12-2a

0 1

P	1.99806500	–0.88248300	–0.30727400
C	2.16998500	–0.07022400	1.28653000
C	1.51411700	1.15846800	1.46544100
C	2.92281700	–0.65292700	2.31163600
C	1.59906000	1.78035200	2.71228800
C	3.00428100	–0.01296600	3.54334000
H	3.43677000	–1.59575100	2.14466700
C	2.33951400	1.19788100	3.73862900
H	1.05289000	2.70940700	2.85861100

H	3.58203800	–0.45791300	4.34627800
H	2.39931300	1.69448900	4.70211500
C	3.48431100	–1.80082200	–0.72479400
C	3.45961700	–3.19317100	–0.83160400
C	4.67124700	–1.08294600	–0.91959300
C	4.63736900	–3.87133900	–1.13717100
H	2.53560300	–3.74256700	–0.67911300
C	5.83858200	–1.77115200	–1.22661900
H	4.67989700	0.00051800	–0.83079400
C	5.81994300	–3.16269800	–1.33433900
H	4.62776400	–4.95273200	–1.22177500
H	6.76216700	–1.22362900	–1.38144100
H	6.73445800	–3.69624800	–1.57316000
C	0.54655900	–1.95652400	–0.32439100
C	–0.21411100	–2.05447100	–1.49519300
C	0.16401900	–2.63216900	0.83946500
C	–1.36160300	–2.84239800	–1.49865400
H	0.07646700	–1.51332100	–2.39136600
C	–0.98602500	–3.41612900	0.82268400
H	0.74345800	–2.53510800	1.75311000
C	–1.74591400	–3.51988100	–0.34210600
H	–1.96102700	–2.91497900	–2.40014800
H	–1.29414700	–3.93442800	1.72457800
H	–2.64902400	–4.12241100	–0.34504500
C	0.61781700	1.75459000	0.39381000
C	–0.75820100	1.07556100	0.58236300
H	–1.21468400	1.46391500	1.51471100
C	–1.73488900	1.20245600	–0.54413200
O	–1.56988800	1.94826600	–1.49634700
C	–2.94638700	0.32200700	–0.46009000

C	–3.22891000	–0.43163800	0.68586000
C	–3.77629700	0.22456900	–1.58064600
C	–4.33359100	–1.27868700	0.70537800
H	–2.59035700	–0.37966000	1.56770800
C	–4.87445000	–0.62517800	–1.57646600
H	–3.54279800	0.81367100	–2.46157300
C	–5.13458900	–1.36867600	–0.42782900
H	–4.56244400	–1.86976900	1.58551600
H	–5.51632100	–0.71426300	–2.44595800
Cl	–6.50697300	–2.45296200	–0.41276600
C	1.75829400	0.46878600	–1.45038400
C	1.15403600	1.57814200	–1.00828600
H	2.11105400	0.37080800	–2.47291500
C	0.98780000	2.69311700	–2.01190800
O	1.12330300	2.54017800	–3.20393300
O	0.72539400	3.85697500	–1.42896300
C	0.48501600	4.96556000	–2.31737800
C	0.15393700	6.16172600	–1.45758200
H	–0.33893700	4.69808000	–2.98519900
H	1.38014000	5.12935600	–2.92383900
H	–0.03823600	7.02777200	–2.09560900
H	–0.73811300	5.96979700	–0.85585400
H	0.98479000	6.40110900	–0.78925300
H	0.49885400	2.81840900	0.59974000
H	–0.62832400	0.00909700	0.78318100
O	–1.82124100	1.80234600	3.38143100
H	–2.75720800	1.77646300	3.14654100
H	–1.24582400	3.06382800	2.84070600
H	–1.31330700	0.38340500	3.36401200
O	–0.81180900	3.90551600	2.41119100

H	–1.27115000	4.00056400	1.56890800
O	–0.97422100	–0.58988600	3.27530400
H	–0.06865200	–0.48280300	2.95976300

Int13-2a

0 1

P	–2.38232300	0.00333900	–0.13104500
C	–1.74440500	–1.05937500	1.33372300
C	–0.35668300	–1.26506400	1.47846700
C	–2.60862400	–1.70053900	2.22724200
C	0.12168500	–2.07048200	2.51410400
C	–2.12693500	–2.51416900	3.25250600
H	–3.68264800	–1.56758200	2.12953600
C	–0.75707800	–2.69171500	3.40055900
H	1.18807800	–2.21898100	2.64578300
H	–2.82151000	–2.99808700	3.93236100
H	–0.36539900	–3.30969000	4.20267500
C	–2.27593900	–1.40297700	–1.30361900
C	–3.05170600	–2.54333400	–1.08170900
C	–1.43282200	–1.34074100	–2.41780700
C	–3.00332300	–3.60324300	–1.98384800
H	–3.70089600	–2.60377000	–0.21205100
C	–1.36164000	–2.41838600	–3.29689500
H	–0.81381000	–0.46304500	–2.59287900
C	–2.15453300	–3.54526200	–3.08735100
H	–3.62314800	–4.47845900	–1.81701100
H	–0.69072100	–2.37283400	–4.14884500
H	–2.10830100	–4.37818900	–3.78179900
C	–3.97454800	0.45605700	0.63131500
C	–5.18784000	0.11828600	0.02871500

C	–3.95876900	1.15686300	1.83958300
C	–6.38489400	0.46525200	0.65276000
H	–5.19969500	–0.39764700	–0.92781900
C	–5.15857000	1.52496300	2.44242400
H	–3.01322900	1.41115300	2.31240500
C	–6.37184100	1.16995400	1.85486200
H	–7.32890700	0.19172500	0.19190600
H	–5.14464200	2.08058900	3.37458300
H	–7.30671500	1.44522300	2.33306800
C	0.59209000	–0.61414000	0.47144400
C	2.06995600	–0.89547900	0.72392300
H	2.40858600	–0.50266200	1.68506200
C	2.94865800	–0.34583400	–0.37898400
O	2.46958500	0.14252200	–1.38862400
C	4.43427200	–0.42637700	–0.21310800
C	5.03026400	–1.07402800	0.87264500
C	5.24052100	0.16949900	–1.18828300
C	6.41556100	–1.12926000	0.98633000
H	4.42407700	–1.54669700	1.63832900
C	6.62408800	0.12799400	–1.08687200
H	4.76794100	0.66844700	–2.02766900
C	7.19247200	–0.52468000	0.00419800
H	6.88443000	–1.63229500	1.82448400
H	7.25365800	0.59232300	–1.83781600
Cl	8.93375000	–0.58528600	0.14364600
C	–1.04066300	1.20761500	0.02313700
C	0.21967900	0.84980500	0.28805500
H	–1.33549600	2.24555100	–0.10361000
C	1.23073400	1.94253600	0.47472100
O	2.16625400	1.88121000	1.24391400

O	0.96062000	3.01303500	–0.27022900
C	1.83626100	4.14441500	–0.08690200
C	1.30932000	5.26084500	–0.95646000
H	2.85059400	3.84656000	–0.36798100
H	1.84031700	4.41625800	0.97206400
H	1.94122600	6.14423400	–0.83725300
H	1.31538400	4.96978800	–2.00973400
H	0.28791300	5.52471900	–0.66958700
H	0.37154600	–1.07572200	–0.50128500
O	–2.98885100	1.05419100	–1.59042300
H	–2.27159300	1.17773700	–2.23230000
H	2.22901200	–1.98103300	0.74458900
H	–4.12530700	0.14704200	–2.69435800
O	–4.74802800	–0.36137000	–3.25097400
H	–5.49313500	0.23982700	–3.36909200
H	–3.28286700	2.74027000	–0.97406800
O	–3.20627400	3.62992300	–0.57403500
H	–2.70856500	4.13495200	–1.22829900

TS9-2a

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P	–2.41933200	0.08934400	–0.52157300
C	–1.58075300	–0.27616400	1.63910600
C	–0.33123600	–0.90883500	1.64478800
C	–2.43864200	–0.40471300	2.72516900
C	0.01838200	–1.72548500	2.71545700
C	–2.05817400	–1.18209100	3.82782300
H	–3.41709300	0.06869700	2.73066900
C	–0.84177500	–1.85207900	3.81304700
H	0.97055800	–2.24839000	2.72855100

H	–2.71971200	–1.26543900	4.68539600
H	–0.54519800	–2.46314700	4.66027900
C	–2.29597800	–1.70493900	–0.75378700
C	–3.00046200	–2.57903000	0.08009900
C	–1.56047600	–2.20503500	–1.83369300
C	–2.96824100	–3.94660400	–0.16921800
H	–3.56782800	–2.19309200	0.92161700
C	–1.51197300	–3.57776400	–2.06084800
H	–1.00512100	–1.54049000	–2.49043400
C	–2.22035500	–4.44649900	–1.23458300
H	–3.52290600	–4.62208400	0.47350100
H	–0.92636300	–3.96348200	–2.88860800
H	–2.19050300	–5.51529900	–1.42089700
C	–4.02561400	0.62669700	0.08538000
C	–5.16597800	0.00383200	–0.43535000
C	–4.15072700	1.69287500	0.98109800
C	–6.42756300	0.44568100	–0.04669800
H	–5.07395800	–0.80727300	–1.15374700
C	–5.41719800	2.13239300	1.35510700
H	–3.27163000	2.16759800	1.40554900
C	–6.55410500	1.50801300	0.84574500
H	–7.31148500	–0.03932300	–0.44762500
H	–5.51239100	2.95965600	2.05050900
H	–7.53964900	1.84984100	1.14545600
C	0.59842100	–0.61886800	0.44378900
C	2.06889100	–0.91108000	0.71991900
H	2.44404200	–0.31498600	1.55298000
C	2.92935300	–0.68869000	–0.50440700
O	2.44933500	–0.64834000	–1.62238100
C	4.41763700	–0.59027900	–0.32641900

C	5.04443900	–0.83487500	0.89794000
C	5.19513600	–0.26675200	–1.44247100
C	6.42951700	–0.75766400	1.01137500
H	4.46399000	–1.09696500	1.77610300
C	6.57707900	–0.17572800	–1.34532600
H	4.70015200	–0.08528800	–2.39061200
C	7.17589600	–0.42512200	–0.11324700
H	6.92069200	–0.95176700	1.95836800
H	7.18243100	0.08104900	–2.20768300
Cl	8.91696700	–0.31951600	0.02238200
C	–1.10666600	1.06805300	0.07176300
C	0.26340100	0.79632900	0.05276700
H	–1.43987000	2.09537300	0.22295500
C	1.18426900	1.89409900	0.15119800
O	2.38827800	1.84767100	0.38057300
O	0.58889600	3.10280900	–0.12706000
C	1.42687500	4.25860900	–0.00361500
C	0.57614200	5.46547900	–0.33158600
H	2.27417800	4.16320200	–0.68877600
H	1.82294000	4.30980400	1.01524000
H	1.17164700	6.37597500	–0.22668600
H	0.20466800	5.41479200	–1.35901300
H	–0.28006600	5.53113500	0.34513100
H	0.29391800	–1.30820000	–0.35606200
O	–2.65532400	0.55770800	–2.12983900
H	–1.83449700	0.46682600	–2.64794100
H	2.18962300	–1.96825800	0.99288300
H	–3.84583900	–0.73392100	–3.07642100
O	–4.44461600	–1.45125000	–3.33160100
H	–5.22627000	–0.99409800	–3.66638400

H	–2.25423900	2.75805000	–2.05846200
O	–1.94238600	3.55588000	–1.61113400
H	–1.02327200	3.36272800	–1.37313400

Int14-2a

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P	–2.41119700	0.52598000	–0.22854300
C	–1.32589500	–1.24650500	1.58615200
C	–0.29729300	–2.06978500	1.12131500
C	–2.35050400	–1.75049300	2.38340800
C	–0.29339800	–3.42320400	1.44756200
C	–2.33772300	–3.10590200	2.71349100
H	–3.14430800	–1.10182300	2.74392800
C	–1.31796600	–3.93641900	2.24366300
H	0.49768600	–4.07553200	1.08610400
H	–3.12421400	–3.51620300	3.33901000
H	–1.32099900	–4.99062200	2.50346100
C	–2.22554500	–0.70094400	–1.52246400
C	–2.67203300	–2.01258700	–1.32124400
C	–1.50698400	–0.36385100	–2.67338400
C	–2.40060800	–2.98340400	–2.28111900
H	–3.22271900	–2.27602700	–0.42162100
C	–1.23915200	–1.34163000	–3.62637000
H	–1.15805500	0.65413800	–2.81873600
C	–1.68408200	–2.64831700	–3.42891100
H	–2.74534000	–4.00080300	–2.12921900
H	–0.68138700	–1.08415200	–4.52061400
H	–1.47123000	–3.40910600	–4.17322000
C	–4.10428400	0.59184400	0.36685700
C	–5.15531200	0.01956000	–0.35975500

C	–4.35276300	1.23072900	1.59043600
C	–6.45155300	0.08311700	0.14310400
H	–4.96416100	–0.45926600	–1.31450500
C	–5.65314000	1.28955600	2.08157200
H	–3.53874200	1.68737700	2.14840300
C	–6.69896100	0.71398000	1.36103500
H	–7.26781800	–0.35965100	–0.41785300
H	–5.84884700	1.78432400	3.02713000
H	–7.71151900	0.75923900	1.74935300
C	0.68932200	–1.31212600	0.25625400
C	2.15474900	–1.50661200	0.68003400
H	2.38081400	–0.86326300	1.53319300
C	3.12429600	–1.26914200	–0.46084200
O	2.84109800	–1.57516500	–1.60407400
C	4.49833200	–0.74224800	–0.15491600
C	5.02843500	–0.71980900	1.13691500
C	5.28000900	–0.29312700	–1.22356500
C	6.32082900	–0.25336500	1.36436600
H	4.44925400	–1.07780000	1.98154400
C	6.56445900	0.18979600	–1.01363200
H	4.86278600	–0.32214200	–2.22458000
C	7.06825300	0.20084300	0.28465700
H	6.73844400	–0.24218000	2.36499400
H	7.16822400	0.55104000	–1.83897200
Cl	8.68787600	0.80326600	0.56251700
C	–1.15362700	0.16225300	1.06569800
C	0.19640300	0.11930400	0.39067300
H	–1.28861800	0.92708000	1.84073300
C	0.96008800	1.19136200	–0.00741000
O	2.10715700	1.24432600	–0.46661400

O	0.25575800	2.46535200	0.13720300
C	1.00066100	3.62353900	–0.28668900
C	0.06847100	4.81612000	–0.27711900
H	1.40349100	3.43692200	–1.28421100
H	1.84118700	3.76530400	0.39754300
H	0.61299500	5.70035300	–0.61823400
H	–0.77771500	4.66071400	–0.95426600
H	–0.31477400	5.02033100	0.72618400
H	0.61180400	–1.69298300	–0.77565700
O	–2.02821600	1.96199800	–0.81528300
H	–1.08495100	2.24466600	–0.52067400
H	2.32130200	–2.54558700	0.99886600
H	–3.29405000	2.17355700	–2.43653000
O	–4.07769300	1.74380100	–2.80502300
H	–4.79919300	2.07819100	–2.25715400
H	–2.34839900	3.62206900	1.28900900
O	–1.81512800	3.28922600	2.02328400
H	–0.97161800	3.05510900	1.60735300

TS10-2a

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P	1.90851000	–0.77952800	0.33306200
C	1.02844000	–1.73549200	1.67447000
C	–0.35726700	–1.56669400	1.91180000
C	1.72473900	–2.66964700	2.44941600
C	–0.98989100	–2.34124100	2.89347600
C	1.08490100	–3.42661800	3.42899300
H	2.78844500	–2.80294800	2.29527300
C	–0.27920600	–3.26759100	3.64726300
H	–2.04796900	–2.18682800	3.08229300

H	1.65642500	–4.13640600	4.01848800
H	–0.78740600	–3.85053800	4.40864900
C	3.19168100	0.80450200	–0.85141300
C	3.01364200	1.00771200	–2.22082900
C	4.37651700	1.25549900	–0.26920400
C	4.01127800	1.61240200	–2.99343600
H	2.10034000	0.68357300	–2.71669400
C	5.38952800	1.83572100	–1.03071000
H	4.50699800	1.16297900	0.81150900
C	5.20661000	2.01564600	–2.40409500
H	3.85414200	1.76131800	–4.05876400
H	6.31127300	2.16435300	–0.55726000
H	5.98430800	2.47932000	–3.00377600
C	1.11996100	–1.30786700	–1.19965900
C	0.04032200	–0.63162500	–1.77915800
C	1.63800100	–2.45652700	–1.80896400
C	–0.51305600	–1.10838200	–2.96500600
H	–0.37979200	0.26007900	–1.32255800
C	1.07664300	–2.92436700	–2.99393800
H	2.47914600	–2.98586400	–1.36825000
C	0.00271800	–2.25170100	–3.57294300
H	–1.35091000	–0.58177900	–3.41113700
H	1.48249500	–3.81388100	–3.46477100
H	–0.43257500	–2.61836200	–4.49715900
C	–1.16173200	–0.58754000	1.16209800
C	–2.43424900	–0.76250600	0.77974500
H	–2.96591700	–1.68540800	0.98882500
C	–3.10782200	0.30985200	0.00426700
O	–2.46584200	1.21613300	–0.51092900
C	–4.59469500	0.26513900	–0.15669100

C	–5.41199800	–0.55245100	0.62931900
C	–5.17698300	1.10486200	–1.11265900
C	–6.79342800	–0.53726600	0.46371200
H	–4.98716800	–1.19595000	1.39189000
C	–6.55190100	1.12420400	–1.29708800
H	–4.53606100	1.74217400	–1.71248800
C	–7.34310700	0.29841500	–0.50179100
H	–7.43198100	–1.16367300	1.07639400
H	–7.00617200	1.76817600	–2.04176000
Cl	–9.07663900	0.31679200	–0.72303000
C	1.66388400	0.91737700	0.71196000
C	2.05248900	1.42647300	1.92510000
H	1.08596300	1.49403800	–0.00434400
C	2.03191000	2.84546500	2.21582900
O	2.33399200	3.34993700	3.28667500
O	1.61925500	3.59614900	1.16464600
C	1.54088400	5.00566800	1.40186600
C	1.09952200	5.65849400	0.11159700
H	2.52108100	5.37136700	1.72325300
H	0.83286900	5.19774300	2.21449900
H	1.03536800	6.74102800	0.24810500
H	1.81403800	5.45277800	–0.68987000
H	0.11709900	5.28928900	–0.19447200
H	–0.69870000	0.36311600	0.90799700
O	3.31950800	–1.49117400	0.54237200
H	2.45957100	0.79062800	2.70463500
H	3.98927900	–1.37762300	–0.22969900
H	3.96233200	–3.63336300	0.45742600
O	4.45798400	–4.03397700	–0.27163000
H	4.86249500	–4.83163500	0.09196700

H	5.22278700	–2.56379400	–1.11024800
O	4.98409300	–1.64414600	–1.33746200
H	5.77148900	–1.08933100	–1.25171800

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P	–2.73268700	0.65083600	–0.74969900
C	–1.52363800	–1.75377600	–0.17474200
C	–0.35818200	–1.98934700	–0.90859900
C	–2.45715400	–2.76483300	0.02793300
C	–0.10672000	–3.24842600	–1.44076700
C	–2.20269500	–4.03041100	–0.50603400
H	–3.36009700	–2.58029000	0.60402400
C	–1.03821400	–4.26954100	–1.23471700
H	0.80001600	–3.44222600	–2.00741400
H	–2.91494200	–4.83406300	–0.34719800
H	–0.85025000	–5.25879600	–1.64053300
C	–4.36787800	–0.03497600	–0.36550200
C	–4.90651800	0.00730900	0.92529100
C	–5.06217900	–0.67722400	–1.39277300
C	–6.13334300	–0.59663800	1.18364100
H	–4.37090500	0.50813700	1.72848300
C	–6.29183500	–1.27902200	–1.13074100
H	–4.63043900	–0.70399700	–2.38907100
C	–6.82415100	–1.24114100	0.15601700
H	–6.55154300	–0.56552500	2.18466500
H	–6.83068700	–1.77939800	–1.92904200
H	–7.77996500	–1.71329800	0.36113800
C	–2.68547900	2.34721700	–0.10062400
C	–2.89345100	3.38012200	–1.02058100

C	–2.44751300	2.65275600	1.24470900
C	–2.87952100	4.70659900	–0.59755800
H	–3.05445600	3.13708300	–2.06690500
C	–2.43266900	3.98106600	1.66313300
H	–2.26741000	1.86342100	1.96948600
C	–2.65082200	5.00652700	0.74404500
H	–3.04079700	5.50480500	–1.31508400
H	–2.24467200	4.21519500	2.70605400
H	–2.63618300	6.04070600	1.07359900
C	0.48043300	–0.73366600	–1.01333700
C	1.98240400	–0.96811500	–0.89768800
C	2.78097200	0.30826800	–1.07508600
O	2.25234300	1.33293400	–1.46451000
C	4.25162900	0.27975100	–0.78671600
C	4.92695700	–0.89822400	–0.45508200
C	4.96222800	1.48163600	–0.86779500
C	6.29619000	–0.88082700	–0.20833300
H	4.39818800	–1.84340300	–0.39157700
C	6.32720000	1.51713400	–0.61963200
H	4.42919900	2.39006400	–1.12771300
C	6.97630000	0.32897100	–0.29338500
H	6.82581000	–1.79229400	0.04533600
H	6.88156500	2.44713400	–0.67851500
Cl	8.69674700	0.36060900	0.01660900
C	–1.57287800	–0.31791700	0.29468800
C	–0.12279600	0.19457600	0.09146000
H	–1.90885300	–0.23601900	1.33404600
C	0.69383800	0.10497700	1.36433500
O	1.49718800	0.93801400	1.72021200
O	0.47342900	–1.03385100	2.02940300

C	1.27000100	–1.24287300	3.21262700
C	0.89107200	–2.59424000	3.77097800
H	1.06591900	–0.43413300	3.91986000
H	2.32716300	–1.19442100	2.93479200
H	1.47424600	–2.79536100	4.67285200
H	–0.17007100	–2.62144000	4.03113700
H	1.09430600	–3.38406100	3.04332600
H	0.27916900	–0.24883700	–1.97527100
O	–2.42148300	0.59370100	–2.21960600
H	–0.07110000	1.23870700	–0.22192700
H	2.23511700	–1.44119400	0.05912300
H	2.31593600	–1.67003700	–1.67354800

TS4-2a-RR

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P	2.44281900	0.62960700	0.01975200
C	0.91820000	–1.57342500	–0.51507300
C	–0.14328200	–1.86380100	0.35837200
C	1.71497500	–2.60710300	–1.00492100
C	–0.38884400	–3.19734200	0.70270900
C	1.46839200	–3.93172700	–0.64621200
H	2.52457500	–2.37264300	–1.69288300
C	0.40967000	–4.22728000	0.20763700
H	–1.21163500	–3.42063100	1.37598800
H	2.09156300	–4.72631200	–1.04459800
H	0.20062200	–5.25530800	0.48675300
C	3.91637000	–0.40090500	0.06819000
C	4.88810100	–0.29416700	–0.93216500
C	4.03489500	–1.36830200	1.07249300
C	5.97882200	–1.15871500	–0.92531700

H	4.79447300	0.45847200	–1.71048800
C	5.13060700	–2.22782000	1.07281400
H	3.27203900	–1.45637800	1.84188600
C	6.09979900	–2.12173300	0.07567200
H	6.73522900	–1.07807700	–1.69883400
H	5.22376700	–2.98358200	1.84709700
H	6.95168400	–2.79430700	0.07776800
C	2.91502300	2.23110400	–0.64996700
C	3.83502300	2.99771900	0.07763700
C	2.41440900	2.69321600	–1.87127900
C	4.24663900	4.22967800	–0.41845400
H	4.22459400	2.63565300	1.02659000
C	2.83981800	3.92488200	–2.36260900
H	1.68439400	2.10848000	–2.42263100
C	3.75130700	4.69016900	–1.63826600
H	4.95515800	4.82821100	0.14439900
H	2.45440600	4.28732700	–3.30976900
H	4.07701600	5.65094700	–2.02434300
C	–1.00477600	–0.78900800	0.90627500
C	–2.35831800	–0.82007800	0.85917800
H	–2.87977800	–1.56226300	0.26180800
C	–3.12501300	0.25255500	1.48392800
O	–2.63704400	1.06088200	2.27299500
C	–4.59172500	0.34327200	1.16317400
C	–5.08976400	0.00541300	–0.09806000
C	–5.46609900	0.81202800	2.14661800
C	–6.45027000	0.11508300	–0.37096500
H	–4.39557800	–0.28523000	–0.88125800
C	–6.82978700	0.91229600	1.89562300
H	–5.06779800	1.09299500	3.11646300

C	–7.30215000	0.55761000	0.63556100
H	–6.84332500	–0.13125600	–1.35145300
H	–7.51530200	1.26092300	2.66030200
Cl	–9.01805200	0.68473400	0.30446600
C	1.13383500	–0.13059500	–0.97703500
C	–0.09309400	0.73624400	–0.90047000
H	1.58147400	–0.17825600	–1.98480700
C	–1.23430900	0.42714600	–1.64012700
O	–2.35910700	0.94764000	–1.56510800
O	–1.03249900	–0.65809200	–2.48240300
C	–2.19338000	–1.21140300	–3.08149200
C	–1.76465600	–2.47614500	–3.79644600
H	–2.64243100	–0.49326300	–3.77853900
H	–2.94538200	–1.43301200	–2.31511600
H	–2.62228800	–2.95418300	–4.27758000
H	–1.01831800	–2.25270900	–4.56393600
H	–1.32620700	–3.18279000	–3.08504200
H	–0.53148900	–0.02855400	1.52122600
O	1.88748400	0.75708100	1.48957400
H	–0.13577800	1.59103600	–0.23782300
H	2.61099200	1.00429400	2.20869200
H	5.85120300	–0.84209800	3.29798800
O	5.22271800	–0.58031600	3.98722800
H	4.75839500	–1.39507200	4.22492800
H	4.23982800	0.61712800	3.43695100
O	3.68828500	1.35971300	3.07115700
H	3.44729100	1.93742400	3.80836900

TS4-2a-SS

0 1

P	1.53299900	–0.26666400	0.14917200
C	1.83195700	2.43853300	0.56030700
C	0.70112600	3.25644800	0.45615300
C	3.05928100	2.87373500	0.05362800
C	0.80807700	4.48767300	–0.19861600
C	3.15925600	4.10715700	–0.58416900
H	3.93990000	2.24673900	0.16943100
C	2.02959000	4.91351800	–0.71485300
H	–0.07316600	5.11629700	–0.29124600
H	4.11740100	4.44092300	–0.96993500
H	2.10111600	5.87730100	–1.20940000
C	3.05023300	–0.24664800	–0.84252500
C	4.21080000	–0.88197600	–0.38879400
C	3.05143400	0.42397700	–2.07117900
C	5.36730600	–0.84824700	–1.16462100
H	4.21329300	–1.41005100	0.56073600
C	4.20829600	0.44974400	–2.84554800
H	2.15492800	0.92543800	–2.42357200
C	5.36541700	–0.18579900	–2.39283000
H	6.26578200	–1.34521500	–0.81437300
H	4.20674000	0.96547200	–3.79994800
H	6.26560700	–0.16678700	–2.99862100
C	1.53429200	–1.85862500	0.98907400
C	1.12694100	–2.98308400	0.26431400
C	2.00355400	–1.99006500	2.29863500
C	1.20723600	–4.24494000	0.84744400
H	0.73401200	–2.88070800	–0.74480500
C	2.07880100	–3.25624500	2.87441800
H	2.29644900	–1.11555100	2.87230500
C	1.68756100	–4.38080800	2.14956900

H	0.89063900	–5.11836600	0.28689500
H	2.44052900	–3.36231400	3.89189700
H	1.75038400	–5.36507900	2.60250100
C	–0.60871200	2.81856200	1.01506000
C	–1.51597100	2.18417000	0.21867300
H	–1.19055100	1.76149800	–0.72362600
C	–2.87960600	1.96773200	0.65781900
O	–3.37544900	2.50036900	1.65365900
C	–3.74660900	1.06292800	–0.18333600
C	–3.21280800	0.10635900	–1.05340300
C	–5.13437100	1.16599100	–0.05399500
C	–4.04903500	–0.72469900	–1.79375900
H	–2.13642200	–0.01912500	–1.13112100
C	–5.98503300	0.35264600	–0.79330700
H	–5.53941400	1.89835000	0.63668500
C	–5.42585400	–0.58368300	–1.65787100
H	–3.63831400	–1.47384200	–2.46204100
H	–7.06225600	0.43980500	–0.70176500
Cl	–6.48425700	–1.61732000	–2.59605500
C	1.66559600	1.12789300	1.32475900
C	0.64174300	1.27609300	2.41284800
H	2.65763900	0.88504300	1.74805900
C	–0.47545300	0.47323900	2.70013400
O	–1.17596600	0.50999200	3.71843600
O	–0.81292400	–0.36223300	1.65601500
C	–1.92409500	–1.22697000	1.86943800
C	–1.58851700	–2.39156600	2.78465600
H	–2.19847100	–1.58710000	0.87394800
H	–2.75799700	–0.64502000	2.27343400
H	–2.47242000	–3.02318800	2.91885700

H	–0.79114900	–3.00554400	2.35667500
H	–1.27079600	–2.02251200	3.76206900
H	–0.96957000	3.30182200	1.92001500
O	0.35855500	–0.14855700	–0.89089700
H	0.97901700	1.89654900	3.23748800
H	0.49175900	–0.71052300	–1.76707100
H	3.14012200	–3.17319700	–1.96386800
O	3.01578500	–2.78589800	–2.84336600
H	3.75643100	–2.16893900	–2.94700700
H	1.55255400	–1.99223000	–2.94727200
O	0.66324100	–1.54912400	–2.91735900
H	0.54306300	–1.09019000	–3.76061400

TS4-2a-RS

0 1

P	2.23287600	0.26225300	–0.11271600
C	0.99991200	–1.98993300	–1.07442200
C	–0.18064700	–2.36306500	–0.41070700
C	1.89971800	–2.96002500	–1.50387000
C	–0.43577400	–3.71683300	–0.18760800
C	1.63533400	–4.31283500	–1.27689400
H	2.79845600	–2.66108400	–2.03855000
C	0.46771100	–4.68918100	–0.62078700
H	–1.34210200	–4.00483600	0.33754900
H	2.33377400	–5.06611500	–1.62754200
H	0.25327600	–5.73930400	–0.44804500
C	3.81826000	–0.60531900	–0.20767100
C	4.77314600	–0.23685300	–1.16162200
C	4.05155800	–1.69898900	0.63299100
C	5.95453000	–0.96331800	–1.27544500

H	4.59696700	0.61484400	–1.81321700
C	5.23673100	–2.42247300	0.51352700
H	3.30758300	–1.99472300	1.36795200
C	6.18591200	–2.05479800	–0.43891200
H	6.69491500	–0.67565000	–2.01444300
H	5.41449800	–3.27722400	1.15944000
H	7.10752400	–2.62073400	–0.53048400
C	2.59055500	1.99020900	–0.47163400
C	3.20911200	2.75565500	0.52086300
C	2.30060000	2.54292500	–1.72221800
C	3.53375200	4.08434200	0.25777000
H	3.43687300	2.32141700	1.49185600
C	2.63906700	3.86850300	–1.97854400
H	1.79446500	1.95294100	–2.48113300
C	3.25257200	4.63799300	–0.99044000
H	4.00896400	4.68464600	1.02674000
H	2.41526900	4.30300100	–2.94734300
H	3.51024100	5.67265700	–1.19352800
C	–1.10469900	–1.30492900	0.06756400
C	–2.46794400	–1.39038400	0.03963100
H	–2.96466300	–2.13015600	–0.57996000
C	–3.25213700	–0.42001900	0.77924900
O	–2.77659400	0.32869500	1.63883000
C	–4.73883600	–0.35776400	0.52566700
C	–5.33362000	–0.84147500	–0.64325600
C	–5.54574800	0.24019400	1.49865700
C	–6.70902700	–0.74402000	–0.83559900
H	–4.72733600	–1.27903000	–1.42931900
C	–6.92117300	0.33819000	1.32951700
H	–5.07482900	0.62791800	2.39586900

C	–7.48518000	–0.15992200	0.15876200
H	–7.16997200	–1.11240000	–1.74548500
H	–7.54720700	0.79306300	2.08950400
Cl	–9.21752700	–0.04114400	–0.07070200
C	1.16040200	–0.49953700	–1.38313300
C	–0.19042600	0.10172600	–1.65333300
H	1.82822700	–0.41772400	–2.25910600
C	–0.84787000	1.17820000	–1.04414400
O	–1.96535300	1.61874700	–1.33901800
O	–0.16159700	1.66723800	0.04997700
C	–0.78754500	2.69743500	0.80236600
C	–0.53298100	4.05882300	0.18097600
H	–0.34169900	2.63521700	1.80033800
H	–1.85483300	2.48048200	0.88369800
H	–1.01868300	4.84481700	0.76773200
H	0.54048900	4.27162800	0.14185200
H	–0.93439700	4.08490900	–0.83567800
H	–0.67995100	–0.56883200	0.74966400
O	1.68894500	0.01773100	1.34172800
H	–0.67713300	–0.29898300	–2.53614300
H	2.38251500	0.17268000	2.11135000
H	5.92592500	–1.21577500	2.77051500
O	5.35150700	–1.19731700	3.55039600
H	5.07783700	–2.11665300	3.67726300
H	4.08742900	–0.17311900	3.28135300
O	3.36098700	0.48303700	3.10729700
H	2.98765200	0.73759700	3.96245100

TS4-2a-SR

0 1

P	1.58049200	–0.73516500	0.49882200
C	1.45334500	1.00616900	–1.61555500
C	0.20025900	1.44538800	–2.05951300
C	2.42863200	0.62996300	–2.54404000
C	–0.06485900	1.45595100	–3.43558400
C	2.16105800	0.66092400	–3.90888400
H	3.40356700	0.30491600	–2.18738400
C	0.90506500	1.06843700	–4.35553800
H	–1.04085900	1.78591400	–3.77993300
H	2.92719500	0.36560400	–4.61895300
H	0.68244900	1.09267000	–5.41778700
C	2.55107900	–1.89968200	–0.47172000
C	3.88869200	–2.15388800	–0.15116500
C	1.97091800	–2.48073100	–1.60538400
C	4.64478900	–2.98929100	–0.96795000
H	4.33660200	–1.70401000	0.73080500
C	2.73557800	–3.31351200	–2.41903300
H	0.93309300	–2.27576600	–1.85545200
C	4.06922100	–3.56714700	–2.09909500
H	5.68151900	–3.19116600	–0.72026800
H	2.29079300	–3.76091100	–3.30278500
H	4.66251900	–4.21669200	–2.73478700
C	2.14077500	–0.82138200	2.20665800
C	1.82347400	–1.96835000	2.94425200
C	2.90148600	0.20321400	2.77995100
C	2.26922400	–2.08622200	4.25708100
H	1.23080000	–2.76402700	2.49826100
C	3.34771900	0.07215800	4.09185000
H	3.13461700	1.10137500	2.21641200
C	3.03125900	–1.06829400	4.82822000

H	2.02164800	–2.97193400	4.83276500
H	3.93722700	0.86489500	4.54027000
H	3.37799200	–1.16288100	5.85244800
C	–0.86375000	1.91302500	–1.12861900
C	–1.98362300	1.16965700	–0.91117100
H	–2.00208700	0.12749000	–1.20909300
C	–3.11840100	1.73448000	–0.19645700
O	–3.10221100	2.85928900	0.30540500
C	–4.36655800	0.90025100	–0.05486700
C	–4.63271300	–0.21802100	–0.85088400
C	–5.30696900	1.28886900	0.90473400
C	–5.81076500	–0.94158400	–0.69000300
H	–3.93571700	–0.52876000	–1.62150000
C	–6.48349600	0.57325500	1.08695700
H	–5.09983800	2.16457500	1.51065000
C	–6.71852200	–0.53793900	0.28236400
H	–6.02134300	–1.80392100	–1.31298700
H	–7.20786800	0.87067800	1.83747600
Cl	–8.19907900	–1.44733700	0.49512500
C	1.72157300	0.96314100	–0.11724300
C	0.83360300	1.84626400	0.70694400
H	2.78586400	1.20336900	0.02986700
C	1.21180900	3.17896900	0.96148000
O	0.66262000	3.99927700	1.70576700
O	2.32202900	3.56174000	0.22255800
C	2.73802200	4.91004600	0.39461800
C	3.94361900	5.13026800	–0.49495900
H	2.98155100	5.09646500	1.44685600
H	1.92054500	5.58964500	0.12874800
H	4.29936700	6.16002400	–0.40288700

H	4.75896400	4.45731700	–0.21502300
H	3.68910200	4.94470000	–1.54217700
H	–0.89965900	2.97046500	–0.87923300
O	0.06706800	–1.15349200	0.37358300
H	0.06172000	1.42780900	1.33886800
H	–0.12635000	–2.17122400	0.52023900
H	1.40590200	–5.22641900	–1.21507700
O	0.44447700	–5.27382000	–1.10500100
H	0.08576100	–5.07451700	–1.98121500
H	–0.03655600	–4.20389100	0.05248400
O	–0.28521400	–3.57280800	0.77956800
H	–1.16095300	–3.82740000	1.10123500

4b

0 1

C	0.56905200	0.19768600	0.08518100
C	–0.56905700	–0.19828200	0.08512300
C	–1.92728600	–0.74283700	0.10306000
O	–2.16171600	–1.91611100	0.26119400
O	–2.82735100	0.21364100	–0.07006400
C	–4.20898600	–0.22300800	–0.05731300
C	–5.06774600	1.00358600	–0.24581100
H	–4.40161300	–0.71970500	0.89711800
H	–4.34564800	–0.95126500	–0.86094400
H	–6.11987600	0.70911500	–0.23803300
H	–4.90320200	1.72120700	0.56137600
H	–4.85101000	1.48808700	–1.20074400
C	1.92716900	0.74251400	0.10326400
O	2.16128000	1.91592700	0.26088100
O	2.82749000	–0.21382100	–0.06917400

C	4.20900500	0.22327400	–0.05684600
C	5.06808800	–1.00292000	–0.24648500
H	4.40194200	0.71943700	0.89780200
H	4.34499700	0.95208100	–0.86008000
H	6.12012600	–0.70811700	–0.23902400
H	4.90417300	–1.72105200	0.56037600
H	4.85105800	–1.48695200	–1.20158300

TS1-4b

0 1

P	–1.50068300	–0.87315000	–0.49970200
C	–1.29211600	0.67120900	–1.45435400
C	–0.24836700	1.54936600	–1.08261400
C	–2.17529200	1.05016800	–2.46830900
C	–0.11940100	2.77828000	–1.73936000
C	–2.03868700	2.27975700	–3.10834600
H	–2.97464700	0.37996300	–2.76882900
C	–1.01186600	3.14654300	–2.74128400
H	0.67445300	3.45484800	–1.43612000
H	–2.73339700	2.55771400	–3.89478600
H	–0.90739100	4.10977700	–3.23122500
C	–2.75200400	–1.84540500	–1.40243300
C	–2.42988700	–2.92880500	–2.22556500
C	–4.09831700	–1.50740700	–1.20294700
C	–3.44146700	–3.65330700	–2.85348100
H	–1.39247800	–3.21079200	–2.37749800
C	–5.10423400	–2.22579600	–1.84215700
H	–4.35859200	–0.67627100	–0.55081700
C	–4.77635900	–3.30133900	–2.66708800
H	–3.18353400	–4.49355900	–3.49048300

H	–6.14325700	–1.95224400	–1.68848900
H	–5.56123300	–3.86687000	–3.15938300
C	0.10455700	–1.72088000	–0.72173900
C	0.68620600	–2.31995300	0.39992400
C	0.81999900	–1.65721400	–1.92476500
C	1.97822200	–2.83838000	0.32523300
H	0.13341500	–2.35610200	1.33520400
C	2.10917300	–2.17601600	–1.99602400
H	0.37669300	–1.18018900	–2.79521600
C	2.69205500	–2.75794000	–0.86847200
H	2.43096900	–3.28985900	1.20235000
H	2.66506000	–2.11624800	–2.92667300
H	3.70550900	–3.14395000	–0.92169500
C	0.70715200	1.17972000	–0.02149100
C	2.03615200	1.31276400	–0.12157100
C	2.89878500	0.84381100	0.99279000
O	2.45390600	0.68140000	2.11907000
C	4.33925800	0.54738600	0.70635800
C	4.81351100	0.32836200	–0.59043900
C	5.21924200	0.44228400	1.78840200
C	6.15126600	0.01337500	–0.80837400
H	4.14320100	0.37660500	–1.44228900
C	6.55958000	0.14306600	1.58657700
H	4.84017600	0.60238500	2.79231800
C	7.00675400	–0.06770200	0.28455600
H	6.52251900	–0.16609700	–1.81106600
H	7.24808700	0.07185000	2.42128900
Cl	8.69210300	–0.44731400	0.01659600
C	–2.35851100	0.14250900	1.52252600
C	–2.32539500	1.38150400	1.55362400

C	–1.98463200	2.73389800	1.20860200
O	–1.00837300	3.31724700	1.64036100
O	–2.89143200	3.28294600	0.38931500
C	–2.66149300	4.66588600	0.05647500
C	–3.73041400	5.07312400	–0.92975400
H	–1.65788300	4.76636200	–0.36514200
H	–2.70739400	5.25944800	0.97483400
H	–3.59471500	6.12278900	–1.20219600
H	–3.66851400	4.46792400	–1.83836900
H	–4.72665100	4.95404800	–0.49623100
H	0.31036800	0.72789600	0.88827900
H	2.49393400	1.70974300	–1.02253000
C	–2.76000600	–1.08618500	2.24563600
O	–2.44971600	–2.21448100	1.93677200
O	–3.50816100	–0.77485800	3.29874700
C	–3.94756200	–1.89334600	4.10345700
C	–4.77093100	–1.32967200	5.23626900
H	–3.06542000	–2.42960600	4.46337600
H	–4.52721900	–2.56949700	3.46922400
H	–5.12424300	–2.14853800	5.86768400
H	–4.17356900	–0.65187200	5.85085400
H	–5.63936500	–0.78807600	4.85373700

Int1-4b

0 1

P	–1.62353700	–0.20997700	–0.58198800
C	–1.36917500	1.59087300	–0.40857800
C	–0.18495800	2.08616600	0.18351300
C	–2.27421300	2.47612000	–0.99866000
C	0.05224200	3.46354000	0.15948300

C	–2.02418000	3.84729700	–1.00263900
H	–3.17537900	2.10304500	–1.47309300
C	–0.85620700	4.33897900	–0.42924300
H	0.95408000	3.84640300	0.62702600
H	–2.73976700	4.52155300	–1.46136200
H	–0.65086200	5.40461700	–0.43408300
C	–2.97549600	–0.46364900	–1.75884600
C	–2.74560800	–0.86888200	–3.07501500
C	–4.28153900	–0.25290400	–1.29885000
C	–3.82611500	–1.05286700	–3.93441100
H	–1.73641300	–1.05232700	–3.42903600
C	–5.35347600	–0.43360400	–2.16701700
H	–4.45728100	0.05611300	–0.27081400
C	–5.12574000	–0.83357700	–3.48326000
H	–3.64971200	–1.37148900	–4.95649900
H	–6.36570700	–0.26772000	–1.81336200
H	–5.96414700	–0.97905200	–4.15695300
C	–0.04168400	–0.79326800	–1.25285300
C	0.70022700	–1.76679000	–0.57907700
C	0.51541000	–0.10908800	–2.34073600
C	1.99927300	–2.05069100	–0.99126500
H	0.28705100	–2.27862300	0.28323600
C	1.81077900	–0.40409900	–2.75171200
H	–0.04800900	0.67078500	–2.84726000
C	2.55564300	–1.36786300	–2.07072300
H	2.58250400	–2.79188300	–0.45444000
H	2.24420400	0.12856300	–3.59187100
H	3.57475700	–1.58083800	–2.37868500
C	0.80267500	1.18638600	0.80840800
C	2.12584400	1.29701200	0.63316800

C	3.02824500	0.29760400	1.26186100
O	2.63362900	–0.44560200	2.14733800
C	4.44294000	0.20142800	0.77790800
C	4.86228100	0.75323900	–0.43659100
C	5.35803600	–0.50628500	1.56429800
C	6.17929900	0.60589900	–0.86092100
H	4.16508000	1.28057100	–1.07921300
C	6.67826400	–0.65136800	1.16129500
H	5.02137600	–0.93944200	2.50021000
C	7.07025200	–0.08984500	–0.05136400
H	6.50772500	1.02391500	–1.80586300
H	7.39293300	–1.19088600	1.77290100
Cl	8.72925500	–0.26799400	–0.57259600
C	–2.10360600	–0.97685200	1.01197200
C	–2.39432400	–0.33731500	2.15194700
C	–2.28385800	1.07230400	2.39715300
O	–1.36669500	1.62822500	2.98883100
O	–3.41390900	1.73179600	2.02507400
C	–3.40042700	3.14686600	2.25020700
C	–4.64337800	3.71532700	1.60428800
H	–2.48963100	3.56903500	1.81325300
H	–3.37981300	3.34509600	3.32704100
H	–4.66468400	4.80107000	1.73088100
H	–4.65694500	3.49058500	0.53386400
H	–5.54513400	3.29623100	2.05885000
H	0.42894900	0.36940100	1.42437200
H	2.54434200	2.07853800	0.00687200
C	–2.31010100	–2.43919400	0.80728400
O	–2.11533400	–2.98180900	–0.26856600
O	–2.72359300	–3.09466800	1.88766500

C	–2.92600300	–4.51100300	1.71824200
C	–3.41105500	–5.05380800	3.04189000
H	–1.98049500	–4.96765000	1.41135500
H	–3.65557700	–4.67069400	0.91942500
H	–3.58291400	–6.12955400	2.95514800
H	–2.67008400	–4.88395600	3.82709700
H	–4.34910600	–4.57592600	3.33528200

Int2-4b

0 1

P	–1.04341200	–0.49062500	0.82135400
C	–0.64638900	–2.04355500	–0.05206100
C	0.50105600	–2.11909500	–0.87396400
C	–1.38222800	–3.19805600	0.22540800
C	0.86690600	–3.36013900	–1.40238200
C	–1.00348700	–4.42505100	–0.31608800
H	–2.24784900	–3.15384100	0.87714800
C	0.12353600	–4.50482700	–1.12741100
H	1.73805400	–3.41687800	–2.04772300
H	–1.58808100	–5.31182200	–0.09480200
H	0.42691700	–5.45740800	–1.54954900
C	–2.32698900	–0.85240900	2.04269400
C	–2.05878700	–0.88226600	3.41148400
C	–3.62585500	–1.07059900	1.56515800
C	–3.09596400	–1.13762800	4.30583200
H	–1.05588700	–0.69567400	3.78231600
C	–4.65317900	–1.32984400	2.46653500
H	–3.82760800	–1.05210200	0.49539800
C	–4.38797000	–1.36087700	3.83564700
H	–2.89190300	–1.15657600	5.37125900

H	–5.65977100	–1.50291400	2.10006100
H	–5.19257700	–1.55666000	4.53713000
C	0.52889800	–0.02295700	1.59224300
C	1.13444600	1.20185800	1.29978000
C	1.22205300	–0.99876800	2.31978700
C	2.43501200	1.44601900	1.73153300
H	0.62032300	1.95017100	0.70648400
C	2.51837700	–0.74370800	2.75379800
H	0.76216500	–1.96264000	2.52457400
C	3.12766000	0.47455300	2.45124000
H	2.91339600	2.38860800	1.48588300
H	3.05729700	–1.50091000	3.31366100
H	4.14785700	0.66315800	2.77100900
C	1.32436700	–0.92929600	–1.15832400
C	2.66216600	–0.92340600	–1.10472300
C	3.39187700	0.35080000	–1.33912500
O	2.83254600	1.31779500	–1.83318300
C	4.83269900	0.44138300	–0.93961700
C	5.43785100	–0.48486500	–0.08439900
C	5.57711500	1.52585900	–1.41602700
C	6.76944600	–0.33419300	0.29023400
H	4.87622200	–1.32022900	0.31986100
C	6.90978700	1.68323500	–1.06204700
H	5.09751700	2.24490400	–2.07159900
C	7.48793100	0.74638300	–0.20900200
H	7.24091800	–1.04455200	0.96006300
H	7.49223100	2.51728700	–1.43736400
Cl	9.16371500	0.93647200	0.25030700
C	–1.72770900	0.78254400	–0.29782000
C	–2.15857600	0.59504900	–1.55434900

C	–1.99429300	–0.63384300	–2.30863200
O	–1.13619100	–0.82977400	–3.15262100
O	–3.00077500	–1.50410400	–2.06683900
C	–2.94668100	–2.73192400	–2.81159100
C	–4.04469000	–3.62605800	–2.28538300
H	–1.95773200	–3.18139700	–2.67859100
H	–3.07831600	–2.51058100	–3.87543800
H	–4.02714200	–4.58182700	–2.81566300
H	–3.90662300	–3.81893400	–1.21755400
H	–5.02559800	–3.16636400	–2.43271800
H	0.81320000	0.00546800	–1.38721600
H	3.21516600	–1.82225100	–0.85120900
C	–1.98764000	2.03300900	0.47587900
O	–1.79583100	2.10584700	1.67627500
O	–2.42825800	3.04943800	–0.26007700
C	–2.88603800	4.20215900	0.47817400
C	–3.70505100	5.05164200	–0.46619600
H	–2.01191100	4.73901800	0.85818200
H	–3.48016700	3.85395700	1.32531600
H	–4.01631100	5.96406500	0.04935600
H	–3.11605400	5.34457600	–1.34117800
H	–4.60519200	4.52308600	–0.79610500
O	–4.02809500	2.45674500	–2.55639500
H	–3.57363300	3.29882900	–2.42158200
H	–3.31827100	1.78457600	–2.31243600
H	–4.51167900	2.04423500	–0.67649200
O	–4.97818200	1.91106300	0.16945800
H	–5.19787300	0.97052200	0.18443100
H	–5.88850000	2.99139600	–2.24356800
O	–6.62385900	3.30993600	–1.69676500

H	–6.40333700	2.90672200	–0.84342400

TS2-4b

0 1

P	–1.08619000	–0.62625000	0.79496900
C	–0.71641400	–2.07402400	–0.24621800
C	0.41132300	–2.06944200	–1.09914800
C	–1.45561900	–3.24599300	–0.06612700
C	0.74677100	–3.25005400	–1.76747700
C	–1.10301900	–4.41156600	–0.74303100
H	–2.30335400	–3.26121900	0.61049300
C	–0.00170300	–4.41125500	–1.59306900
H	1.59971500	–3.24535300	–2.43899000
H	–1.68863600	–5.31327000	–0.59854400
H	0.27826300	–5.31546100	–2.12378900
C	–2.36940900	–1.08578300	1.98023300
C	–2.07042200	–1.34183700	3.31931200
C	–3.68629500	–1.17046900	1.51052900
C	–3.09756600	–1.69452600	4.19107000
H	–1.05301000	–1.25597900	3.68689900
C	–4.70241800	–1.52793900	2.39038100
H	–3.91550300	–0.96610600	0.46699900
C	–4.40800600	–1.78890000	3.72833800
H	–2.87107100	–1.89023100	5.23380800
H	–5.72392300	–1.59666600	2.03145800
H	–5.20468200	–2.06219600	4.41272200
C	0.49333900	–0.21720500	1.57443200
C	1.09789900	1.02732700	1.37622100
C	1.19156900	–1.25193300	2.20962000
C	2.40123400	1.23405900	1.81815000

H	0.59105800	1.82170800	0.83862800
C	2.49077200	–1.03306700	2.65414400
H	0.73670900	–2.23206900	2.33036100
C	3.09720000	0.20686600	2.45194700
H	2.87909800	2.19279200	1.64531100
H	3.03370500	–1.83494500	3.14307200
H	4.11926600	0.36866400	2.78009900
C	1.24584600	–0.86533200	–1.26663300
C	2.58381600	–0.88047200	–1.23076200
C	3.32233400	0.40835900	–1.32388800
O	2.76383600	1.42653600	–1.70209300
C	4.76352800	0.44912500	–0.91933200
C	5.37887900	–0.58594400	–0.20844100
C	5.49852300	1.59689800	–1.23601700
C	6.71133300	–0.48179300	0.17854900
H	4.82601700	–1.47524100	0.07341100
C	6.83118300	1.71177400	–0.86640500
H	5.01093600	2.39952900	–1.77888100
C	7.42007800	0.66519800	–0.16091100
H	7.19035100	–1.27926500	0.73534700
H	7.40577700	2.59649900	–1.11724800
Cl	9.09645300	0.79974100	0.31482700
C	–1.73721100	0.78425400	–0.15000400
C	–2.22227700	0.75093000	–1.39936400
C	–2.16081200	–0.42660500	–2.29545800
O	–1.37699700	–0.53410700	–3.21271800
O	–3.14188400	–1.29632600	–2.03401100
C	–3.18354100	–2.46305600	–2.88422300
C	–4.26340000	–3.37069000	–2.34716400
H	–2.19809800	–2.93770300	–2.86460000

H	–3.39004900	–2.14040400	–3.90861100
H	–4.30625900	–4.28175800	–2.94949500
H	–4.05487100	–3.64997700	–1.31062800
H	–5.23971200	–2.88123700	–2.38888600
H	0.74639200	0.09691000	–1.38047100
H	3.12700700	–1.80925300	–1.08836500
C	–1.92026400	1.98198500	0.73352200
O	–1.88425400	1.89429800	1.94518200
O	–2.07251200	3.11345800	0.06573500
C	–2.50288400	4.24881700	0.84958900
C	–3.07474700	5.27152200	–0.10421900
H	–1.63713500	4.63361300	1.39683700
H	–3.25264400	3.90207200	1.56247700
H	–3.33878600	6.17367200	0.45459300
H	–2.34094900	5.54828300	–0.86722100
H	–3.97662500	4.88911000	–0.59159100
O	–3.75980800	2.72171800	–2.23789200
H	–3.17671500	3.47798800	–2.09080900
H	–2.87331200	1.70605900	–1.86061200
H	–4.35024300	2.46985000	–0.75208100
O	–4.77120600	2.33328000	0.15711000
H	–5.23698800	1.49141900	0.08667100
H	–5.30391500	3.63484800	–2.14957400
O	–6.06788600	4.09156300	–1.73141600
H	–6.02668500	3.68473300	–0.85339700

Int3-4b

0 1

P	–1.07800900	–0.59371600	0.83460700
C	–0.66836600	–2.04208100	–0.18634700

C	0.48966600	–2.04906000	–0.99872600
C	–1.42863100	–3.20451300	–0.02934400
C	0.84854300	–3.24297500	–1.63066500
C	–1.05226500	–4.38150100	–0.67248000
H	–2.31085000	–3.19970700	0.60267900
C	0.09040800	–4.39961800	–1.46621300
H	1.72609800	–3.25202900	–2.26961900
H	–1.65027600	–5.27756900	–0.54542500
H	0.39179900	–5.31396600	–1.96696600
C	–2.34066200	–1.08294600	2.03169000
C	–1.99545500	–1.80648200	3.17704800
C	–3.67681100	–0.76672800	1.76047200
C	–2.99630900	–2.22488800	4.04850300
H	–0.96021800	–2.04246300	3.39918600
C	–4.66704600	–1.19420700	2.64010200
H	–3.94819200	–0.16253400	0.89759800
C	–4.32992600	–1.92405200	3.77814100
H	–2.73108500	–2.78386900	4.93958900
H	–5.70373100	–0.94613900	2.43690900
H	–5.10720500	–2.25279500	4.46052400
C	0.49970600	–0.09536600	1.57258000
C	1.00642700	1.19480500	1.38957500
C	1.29635200	–1.08963200	2.15613300
C	2.30500500	1.48758200	1.79585600
H	0.42638100	1.96483600	0.89316900
C	2.58790100	–0.78426000	2.56894300
H	0.93557900	–2.11017200	2.24734700
C	3.09502300	0.50184300	2.38251200
H	2.70371500	2.48326500	1.63253000
H	3.20517900	–1.55681000	3.01526700

H	4.11272300	0.73131400	2.68266500
C	1.31886900	–0.84266500	–1.18309800
C	2.65677500	–0.84716300	–1.14235600
C	3.38921300	0.44091700	–1.28171200
O	2.82758700	1.44212700	–1.69834700
C	4.83173800	0.49882600	–0.88431500
C	5.44634100	–0.50115700	–0.12409000
C	5.56955600	1.62531100	–1.26371100
C	6.78123700	–0.38309800	0.25011600
H	4.89051300	–1.37203100	0.20599200
C	6.90494100	1.75275000	–0.90802100
H	5.08256200	2.40095900	–1.84501100
C	7.49311700	0.74129000	–0.15261200
H	7.26023400	–1.15227000	0.84547100
H	7.48201900	2.62045300	–1.20766200
Cl	9.17316300	0.89128400	0.30519100
C	–1.78659200	0.77282200	–0.12885800
C	–2.20211500	0.70504300	–1.39892300
C	–2.01748000	–0.44895100	–2.32871600
O	–1.14242900	–0.48888100	–3.16213900
O	–2.97477400	–1.35586100	–2.17577800
C	–2.89401200	–2.50219600	–3.05568500
C	–4.00292000	–3.44727900	–2.66226100
H	–1.90362800	–2.95145900	–2.93888900
H	–2.99655000	–2.15340000	–4.08681500
H	–3.96056800	–4.33883900	–3.29276400
H	–3.89833300	–3.75580100	–1.61866700
H	–4.98011200	–2.97604600	–2.79372400
H	0.81522600	0.11244300	–1.33052100
H	3.20626200	–1.76679000	–0.96800400

C	–2.08958700	1.96869600	0.72539800
O	–2.02812700	1.91249700	1.93734500
O	–2.38024200	3.05531600	0.03421300
C	–2.90500400	4.15595800	0.81284300
C	–3.50561200	5.15577900	–0.14589600
H	–2.08318700	4.58353600	1.39460700
H	–3.65402200	3.75337400	1.49766300
H	–3.82516100	6.03805200	0.41575100
H	–2.76850200	5.47620400	–0.88823200
H	–4.37628200	4.73322500	–0.65491100
O	–4.14314400	2.61887700	–2.29459100
H	–3.57639900	3.38079900	–2.11945600
H	–2.80576800	1.54282600	–1.84105500
H	–4.53604100	2.17002700	–0.93052900
O	–4.87736400	1.86844200	0.01255300
H	–5.56072000	1.21501800	–0.18162100
H	–5.61682000	3.38567700	–2.06102900
O	–6.41500200	3.78441500	–1.61211600
H	–6.30248200	3.38629500	–0.73782700

Int4-4b

0 1

P	–1.61523300	–0.18243800	0.48734000
C	–1.18527100	–1.69041400	–0.67184400
C	0.05761800	–1.79579600	–1.34769600
C	–2.08802100	–2.74639300	–0.83023400
C	0.33763800	–2.92732000	–2.12844900
C	–1.81161400	–3.85536800	–1.63000200
H	–3.03155500	–2.71993000	–0.30155200
C	–0.58910600	–3.95136000	–2.28272500

H	1.29402700	–2.98035400	–2.64043000
H	–2.55284400	–4.64295700	–1.72778400
H	–0.35582300	–4.80979000	–2.90450600
C	–2.50243700	1.22597000	1.42901900
C	–2.21283600	1.39211600	2.79078900
C	–3.48920300	2.03791000	0.86328200
C	–2.86520900	2.35775900	3.55397100
H	–1.46566500	0.76333300	3.26820100
C	–4.15874100	2.99294900	1.62836400
H	–3.74849000	1.93404200	–0.18477600
C	–3.84474100	3.16122100	2.97453900
H	–2.61124600	2.47622400	4.60315500
H	–4.92406500	3.60941100	1.16602400
H	–4.35963600	3.91100900	3.56740000
C	0.02522900	–0.10576300	1.32245200
C	0.80094300	1.04816900	1.45464200
C	0.49589400	–1.31119300	1.85624900
C	2.06230400	0.97922900	2.04399300
H	0.43259600	2.00283100	1.09823500
C	1.74745300	–1.37531400	2.45947400
H	–0.11340500	–2.20716200	1.77974600
C	2.54437600	–0.23245400	2.53356600
H	2.66904000	1.87663600	2.11593700
H	2.10525700	–2.31804300	2.86174900
H	3.53104900	–0.28429400	2.98412400
C	1.11030500	–0.76441800	–1.26793600
C	2.41811300	–1.00654400	–1.09565900
H	2.79599100	–2.01500000	–0.96117500
C	3.34793300	0.14712200	–1.02726800
O	3.00156900	1.26980500	–1.36948800

C	4.73934900	–0.07339100	–0.51288600
C	5.10620500	–1.21600200	0.20472500
C	5.68715600	0.93115000	–0.73481000
C	6.40207700	–1.35867100	0.69145100
H	4.38359400	–1.99729600	0.41426300
C	6.98716200	0.79906300	–0.26661700
H	5.39157300	1.81886800	–1.28381800
C	7.32606700	–0.34986000	0.44346200
H	6.68846300	–2.23893900	1.25602900
H	7.72635800	1.57213500	–0.44452000
Cl	8.95884100	–0.52688800	1.04287500
C	–1.57297400	0.94058900	–1.10956600
C	–2.39152100	0.74653100	–2.15301300
C	–3.51730600	–0.22474000	–2.17524900
O	–3.99945800	–0.69518900	–3.17875700
O	–3.97481800	–0.45201200	–0.93510500
C	–5.11661400	–1.31884400	–0.78605000
C	–6.39458200	–0.51937200	–0.92749100
H	–5.00894200	–1.74205000	0.21450900
H	–5.05152700	–2.12161600	–1.52403300
H	–7.25582500	–1.16878500	–0.75058900
H	–6.41845600	0.29609500	–0.19901400
H	–6.47826800	–0.09831100	–1.93260000
H	0.83049500	0.27870400	–1.36640000
O	–2.48625200	–1.27676200	1.41548000
H	–2.31318400	1.35403500	–3.05201100
H	–3.19409300	–0.85918700	1.96027200
H	–3.37354800	–3.00696800	1.71978900
O	–4.26429400	–3.36954600	1.85809000
H	–4.14737500	–4.18583500	2.36027000

H	–4.92306500	–1.77733900	2.59045200
O	–4.77794900	–0.82933200	2.77203000
H	–5.41310900	–0.35289700	2.22130600
C	–0.72424800	2.17468000	–1.21643700
O	–0.73655800	3.07719300	–0.40774500
O	0.01564200	2.17336700	–2.32625100
C	0.86129100	3.32533200	–2.54342400
C	0.07326600	4.45419300	–3.17312500
H	1.64825000	2.95996600	–3.20269100
H	1.30377600	3.61795600	–1.58972200
H	0.74342100	5.29149100	–3.38608500
H	–0.38176200	4.12901600	–4.11233300
H	–0.71258300	4.80388600	–2.49939500

TS3-4b

0 1

P	1.86393000	–0.41711300	0.03004300
C	0.88532600	1.61516400	1.10913800
C	–0.46397300	2.02887200	1.16371200
C	1.75055100	2.14113900	2.06899400
C	–0.89947300	2.90348200	2.17973500
C	1.31811000	2.97802000	3.09910300
H	2.81428100	1.89413300	2.01573400
C	–0.02297800	3.36170000	3.15414700
H	–1.93205000	3.24465800	2.18374400
H	2.02164400	3.34164200	3.84379600
H	–0.37383800	4.03186200	3.93294400
C	2.60522500	–1.74170800	–1.00750400
C	2.47034500	–3.07672600	–0.60457000
C	3.28173200	–1.44868700	–2.19298400

C	3.03287600	–4.09939000	–1.36232300
H	1.93049500	–3.32313700	0.30821600
C	3.83056700	–2.47477100	–2.96084100
H	3.39487300	–0.41706700	–2.51449400
C	3.71327200	–3.79853700	–2.54264300
H	2.93514400	–5.13026500	–1.03687400
H	4.35403500	–2.23846800	–3.88194500
H	4.14637200	–4.59661000	–3.13766600
C	0.15508700	–1.03518800	0.10899000
C	–0.53878200	–1.44583400	–1.03336800
C	–0.40575900	–1.22461200	1.37618200
C	–1.81379800	–1.99069700	–0.90609000
H	–0.09438300	–1.32205500	–2.01480500
C	–1.66631400	–1.80097300	1.49747100
H	0.13662900	–0.91477200	2.26410100
C	–2.37759500	–2.17080100	0.35640000
H	–2.36405800	–2.28135600	–1.79529700
H	–2.09628200	–1.95149300	2.48274800
H	–3.36827100	–2.60511500	0.45139900
C	–1.43735400	1.57590800	0.15557400
C	–2.75764100	1.41733600	0.35147800
H	–3.20809600	1.57841300	1.32610000
C	–3.61337400	0.96189400	–0.76624300
O	–3.25895500	1.05356700	–1.93381900
C	–4.95416000	0.36723900	–0.44567300
C	–5.28195600	–0.10240800	0.82974700
C	–5.88689600	0.24834900	–1.48098800
C	–6.52584600	–0.67694400	1.07377900
H	–4.56455500	–0.04839200	1.64193600
C	–7.13681200	–0.31093500	–1.25210300

H	–5.61986700	0.60406500	–2.47046500
C	–7.43855600	–0.76633500	0.02880000
H	–6.78146000	–1.04968300	2.05939800
H	–7.86596000	–0.39506700	–2.05048700
Cl	–9.00935000	–1.47276200	0.33129200
C	2.38613400	1.14192400	–0.70563600
C	3.57355500	1.77669300	–0.52487000
C	4.76601600	1.24605900	0.14846600
O	5.59410100	1.93647200	0.71148000
O	4.87642600	–0.08383300	0.03555400
C	5.92035600	–0.70681000	0.79728800
C	5.73705900	–2.20151500	0.66784000
H	5.84730000	–0.37521700	1.83752800
H	6.88824200	–0.38025500	0.40471700
H	6.55173900	–2.71941900	1.18037900
H	4.78943500	–2.51302600	1.11513800
H	5.73883100	–2.50156900	–0.38456600
H	–1.05600600	1.32455800	–0.83176900
O	2.55703500	–0.58959500	1.44906000
H	3.64954700	2.81434500	–0.83364400
H	2.51346000	–1.52346500	1.86978200
H	1.79517800	0.18740500	3.41441500
O	1.63208800	–0.39541700	4.17410000
H	0.79164500	–0.09541000	4.54488700
H	1.93812800	–2.05825100	3.55293100
O	2.22277500	–2.65768400	2.82780600
H	3.00095500	–3.13792400	3.14729300
C	1.38225500	1.69150500	–1.66057800
O	0.68086300	0.96258600	–2.33644500
O	1.37013400	3.01494400	–1.72172500

C	0.45630500	3.60684000	–2.67519600
C	1.04346000	3.58765200	–4.07021700
H	0.31384000	4.62504500	–2.31227300
H	–0.49436800	3.07043100	–2.62723900
H	0.35912000	4.09145500	–4.75792600
H	2.00223400	4.11165400	–4.09092900
H	1.18854600	2.56227100	–4.41761300

Int5-4b

0 1

P	–1.82228600	–0.50968200	–0.36651300
C	–1.10002800	2.10410900	–0.44567700
C	0.30387900	2.28225500	–0.52106200
C	–1.91710000	2.80364300	–1.34154400
C	0.80889800	3.20259300	–1.46016100
C	–1.39461800	3.67759100	–2.28674700
H	–2.98891400	2.64691200	–1.27276700
C	–0.01624700	3.88763000	–2.33741300
H	1.87666800	3.39290800	–1.48594000
H	–2.05870200	4.19769900	–2.97002500
H	0.41017200	4.58844800	–3.04785200
C	–2.67265200	–1.89832300	0.41016300
C	–2.52194300	–3.14141300	–0.21316900
C	–3.48916700	–1.76372400	1.53605900
C	–3.21054400	–4.24802800	0.27918200
H	–1.87782100	–3.25472800	–1.08194300
C	–4.16769100	–2.87463100	2.02380400
H	–3.58986100	–0.79536300	2.01577600
C	–4.03494700	–4.11298900	1.39328600
H	–3.09876500	–5.21120800	–0.20752700

H	–4.80343700	–2.77396300	2.89743800
H	–4.57117500	–4.97522400	1.77710200
C	–0.11193600	–1.05300800	–0.61680000
C	0.57205100	–1.79094200	0.35806100
C	0.51409900	–0.74640100	–1.83131200
C	1.87952700	–2.20145900	0.12047200
H	0.08468700	–2.03550100	1.29558200
C	1.81894300	–1.16851000	–2.06459300
H	–0.00650800	–0.16824500	–2.58800800
C	2.50253500	–1.89145100	–1.08846700
H	2.41289100	–2.76390200	0.87995900
H	2.30184600	–0.93048400	–3.00701100
H	3.52176600	–2.21825500	–1.27101800
C	1.27190900	1.55663500	0.32179000
C	2.57813200	1.39193500	0.05870500
H	3.04080600	1.77105700	–0.84507300
C	3.41039600	0.64393600	1.03354500
O	2.99725600	0.37270800	2.15248300
C	4.79232300	0.22068700	0.63226000
C	5.23547400	0.23167700	–0.69415400
C	5.65265800	–0.23255400	1.63802000
C	6.51866200	–0.20097300	–1.01429200
H	4.58293200	0.55414200	–1.49851500
C	6.93922500	–0.65774100	1.33719800
H	5.29907200	–0.24518900	2.66338200
C	7.35444800	–0.63586200	0.00826400
H	6.86306100	–0.20118400	–2.04236800
H	7.60993300	–1.00172700	2.11677200
Cl	8.97015100	–1.17361400	–0.38653700
C	–1.84378500	1.13898700	0.51262000

C	–3.19297700	1.64972900	0.99217900
C	–4.49365800	1.28896200	0.64156300
O	–5.54799100	1.78300900	1.07217800
O	–4.56188300	0.24828900	–0.27296300
C	–5.84695400	–0.32693000	–0.45989100
C	–5.69970600	–1.49978400	–1.40682700
H	–6.53268900	0.42511700	–0.86512500
H	–6.25676200	–0.65052900	0.50514900
H	–6.68358000	–1.91476900	–1.64351100
H	–5.22297700	–1.18301400	–2.33915100
H	–5.09140600	–2.29116100	–0.95886700
H	0.93969100	1.07959100	1.23571500
O	–2.37015000	–0.20792400	–1.81479700
H	–3.10422100	2.52342600	1.62599900
H	–2.20419200	–0.89840600	–2.57048600
H	–1.69223900	1.32600300	–3.37839500
O	–1.37904200	1.05131200	–4.25462100
H	–0.54039900	1.51653000	–4.37535000
H	–1.60656600	–0.74030000	–4.30844000
O	–1.87019000	–1.56288900	–3.84074400
H	–2.64236200	–1.91655700	–4.30773900
C	–1.16747800	0.91229200	1.85639000
O	–1.00165200	–0.18035000	2.36596800
O	–0.82768400	2.06390500	2.43300800
C	–0.29727500	1.97606800	3.77360900
C	–1.41253300	1.78976100	4.78028200
H	0.22289600	2.92343000	3.92050500
H	0.42834000	1.15953600	3.81009100
H	–0.99496400	1.78002600	5.79062300
H	–2.13195700	2.60982900	4.71141900

H	–1.93436100	0.84465200	4.61226000

TS4-4b

0 1

P	1.18582200	–1.21734500	0.08726400
C	1.28395800	–1.30113300	1.89832700
C	0.70544500	–0.31776100	2.72694700
C	2.04618400	–2.33265600	2.46180900
C	0.95214400	–0.37914200	4.10191200
C	2.24657200	–2.39543600	3.83678100
H	2.49619600	–3.08754600	1.82505400
C	1.71042300	–1.40589300	4.65513200
H	0.52348800	0.38605100	4.74244600
H	2.83434400	–3.20328500	4.25899000
H	1.87923900	–1.43261800	5.72696400
C	2.57959600	–2.18267800	–0.54864400
C	2.39068700	–3.43542100	–1.13358700
C	3.86621100	–1.64675800	–0.41480000
C	3.49568000	–4.15565000	–1.58400800
H	1.39275100	–3.84935100	–1.24105800
C	4.96196300	–2.37251500	–0.86765700
H	4.01008500	–0.66941500	0.03958300
C	4.77659800	–3.62616500	–1.45172700
H	3.35152500	–5.12929500	–2.04064400
H	5.96020800	–1.95945800	–0.76704700
H	5.63424900	–4.18954500	–1.80539800
C	–0.34471200	–1.99057100	–0.49941200
C	–0.89720500	–1.62018200	–1.73028000
C	–0.94361600	–2.99410400	0.27270800
C	–2.04497200	–2.26339300	–2.18809900

H	–0.43118300	–0.84561500	–2.32896000
C	–2.09301400	–3.62669200	–0.19281000
H	–0.52020900	–3.27639100	1.23266700
C	–2.64043900	–3.26542000	–1.42374400
H	–2.47532100	–1.97579200	–3.14183100
H	–2.55876500	–4.40231800	0.40599100
H	–3.53470200	–3.76337700	–1.78537000
C	–0.21428400	0.74279800	2.24698800
C	–1.41720500	0.42003900	1.68682600
C	–2.45467600	1.42645900	1.52188600
O	–2.35479600	2.57205800	1.95859800
C	–3.72125000	1.02840000	0.80661200
C	–3.84418900	–0.16096600	0.08229400
C	–4.80821900	1.90666000	0.85813900
C	–5.02863600	–0.47465300	–0.57718500
H	–3.01406100	–0.85476300	0.00384200
C	–6.00127300	1.60767200	0.21287300
H	–4.70284000	2.83215000	1.41417000
C	–6.09452400	0.41418500	–0.49794600
H	–5.11825900	–1.39547900	–1.14425100
H	–6.84608400	2.28630800	0.25743500
Cl	–7.59256800	0.02452200	–1.31464000
C	1.41100400	0.51809300	–0.39326300
C	1.25770800	1.44465300	0.55934300
C	1.42646300	2.86980300	0.33650700
O	0.53276400	3.64887400	0.05907100
O	2.68894900	3.26363300	0.61240800
C	2.93237400	4.67168700	0.48975400
C	4.40286800	4.90018800	0.75602700
H	2.30389300	5.20999600	1.20640900

H	2.64925200	5.00046100	–0.51511100
H	4.63180300	5.96618900	0.67830800
H	4.67384000	4.56142900	1.75946100
H	5.01597400	4.36093600	0.02896100
H	–0.11105100	1.72134600	2.70695900
H	–1.61164900	–0.60127600	1.38692500
C	1.79054000	0.71233300	–1.81968500
O	1.76408000	–0.17211200	–2.65646800
O	2.16662000	1.96098500	–2.08097600
C	2.52323500	2.24996100	–3.44679400
C	2.87732600	3.71683100	–3.50726600
H	1.67401300	2.00595300	–4.09119500
H	3.36455000	1.61192100	–3.73144100
H	3.15236400	3.98503900	–4.53037700
H	2.02509900	4.33083200	–3.20463200
H	3.72405200	3.93728900	–2.85173800

Int6-4b

0 1

P	2.07879300	–0.81680600	0.15456200
C	1.74791800	–0.96486900	1.91323400
C	0.68829400	–0.23319800	2.46680500
C	2.52338100	–1.83329500	2.69504400
C	0.42465600	–0.39660500	3.83123400
C	2.24208900	–1.97748300	4.04547300
H	3.34653600	–2.38361900	2.24798900
C	1.18885000	–1.25469900	4.61089300
H	–0.39408600	0.16285000	4.27508800
H	2.84086300	–2.64474100	4.65581500
H	0.96710000	–1.35972400	5.66824400

C	3.85507200	–0.86632800	–0.14031300
C	4.38167400	–1.56058700	–1.23298400
C	4.69147100	–0.14086800	0.71725400
C	5.75514700	–1.53680800	–1.45797400
H	3.72910000	–2.10939200	–1.90442900
C	6.06148400	–0.12166300	0.48013600
H	4.27778300	0.40217700	1.56279400
C	6.59144000	–0.82111400	–0.60370500
H	6.16994500	–2.07633100	–2.30274500
H	6.71407200	0.43707500	1.14244400
H	7.66160700	–0.80630200	–0.78396000
C	1.24719200	–2.13942400	–0.74976300
C	0.17938900	–1.84159100	–1.60134200
C	1.64586100	–3.46403300	–0.53502700
C	–0.48676300	–2.88140200	–2.24584400
H	–0.13804000	–0.81392800	–1.75389100
C	0.97571800	–4.49296900	–1.18784900
H	2.47311400	–3.68971100	0.13357800
C	–0.08855900	–4.20090300	–2.04094300
H	–1.31664600	–2.65689100	–2.90789800
H	1.28210400	–5.52130800	–1.02839400
H	–0.61056600	–5.00680900	–2.54678800
C	–0.21607800	0.66711200	1.66531500
C	–1.44582300	–0.05395700	1.14475800
C	–2.62829800	0.65903400	1.04028300
O	–2.78237500	1.86311900	1.41140800
C	–3.83984600	–0.04811000	0.46640100
C	–3.77135000	–1.22025100	–0.29625700
C	–5.09462300	0.52483200	0.69273500
C	–4.92202000	–1.81654000	–0.80293400

H	–2.81039300	–1.67250100	–0.52286600
C	–6.25855200	–0.05724000	0.20029300
H	–5.13565200	1.44651200	1.26343600
C	–6.15518200	–1.22790100	–0.54239100
H	–4.86192300	–2.72152800	–1.39822500
H	–7.22962100	0.39014700	0.38572000
Cl	–7.61058900	–1.97499600	–1.17713300
C	1.38029500	0.75515700	–0.31585100
C	0.36733800	1.26718600	0.42085800
C	–0.42191400	2.44884900	–0.11198900
O	–1.01522900	2.42258800	–1.16242000
O	–0.38639600	3.46421100	0.73631300
C	–1.34734400	4.51073100	0.48151000
C	–1.34483100	5.42026300	1.68621100
H	–2.31547600	4.02757400	0.33300500
H	–1.05843400	5.03988400	–0.43137800
H	–2.06141800	6.23130300	1.53323300
H	–1.63485700	4.86541300	2.58217600
H	–0.35637000	5.85869200	1.84636500
H	–0.56960100	1.49111000	2.29544100
H	–1.32034600	–1.07268200	0.79830800
C	1.84418600	1.28707800	–1.62062500
O	2.25859000	0.57111100	–2.51035100
O	1.79760800	2.61270200	–1.67963100
C	2.06800000	3.20320100	–2.96874800
C	1.80231600	4.68361000	–2.84065000
H	1.41478700	2.73202400	–3.70827700
H	3.10608600	2.99029800	–3.23772700
H	1.98938000	5.17175700	–3.80021200
H	0.76186200	4.86179000	–2.55708300

H	2.45608800	5.13276800	–2.08897600

Int7-4b

0 1

P	1.25376100	–1.16913900	0.53948300
C	1.23417600	–0.29898200	2.10964800
C	0.81121500	1.03742600	2.08119900
C	1.66235200	–0.90877600	3.29190600
C	0.81552100	1.75868000	3.27548800
C	1.64580700	–0.17750000	4.47550800
H	2.00502900	–1.93973700	3.28502200
C	1.22780200	1.15347400	4.46240600
H	0.50098700	2.79951100	3.25776100
H	1.96819600	–0.64120600	5.40141200
H	1.22732700	1.72732700	5.38373700
C	2.62254000	–2.33471500	0.46482700
C	2.39231600	–3.70139500	0.29160000
C	3.92775800	–1.83118200	0.56197500
C	3.47848700	–4.56992100	0.21327700
H	1.37950000	–4.08467000	0.21448100
C	5.00268300	–2.70770800	0.47540400
H	4.10219500	–0.76704400	0.70004500
C	4.77676500	–4.07413600	0.30122400
H	3.30704000	–5.63258200	0.07926900
H	6.01561800	–2.32565600	0.54594000
H	5.61944500	–4.75481600	0.23451900
C	–0.30616600	–2.00876600	0.20545500
C	–0.71463100	–2.20020400	–1.11782400
C	–1.08371000	–2.46413100	1.27563200
C	–1.91892900	–2.85508600	–1.36542900

H	–0.10618200	–1.83171500	–1.94003300
C	–2.28472500	–3.11485400	1.01210600
H	–0.76574800	–2.29737200	2.30119900
C	–2.70178800	–3.30861000	–0.30533700
H	–2.24980000	–2.99854800	–2.38887800
H	–2.89913600	–3.46242200	1.83614700
H	–3.64418500	–3.80963900	–0.50518300
C	0.24628500	1.66266400	0.82350100
C	–1.18427000	1.15426900	0.66413000
C	–1.79238200	1.20352600	–0.58300600
O	–1.30193500	1.76193400	–1.60549000
C	–3.11369200	0.48046100	–0.73553800
C	–3.90616500	0.08142800	0.34811300
C	–3.52975100	0.15470400	–2.02901100
C	–5.07270000	–0.65018500	0.14603200
H	–3.62131000	0.34055500	1.36500400
C	–4.68886600	–0.58221200	–2.25110500
H	–2.91358600	0.47992800	–2.86088400
C	–5.44273200	–0.98243400	–1.15356600
H	–5.68524600	–0.96113300	0.98579800
H	–5.00014700	–0.84638100	–3.25633100
Cl	–6.89913900	–1.92575500	–1.41178100
C	1.57645200	0.13651100	–0.65670700
C	1.05628400	1.35054000	–0.41918400
C	1.22037200	2.40804900	–1.47941900
O	1.59491600	2.16377400	–2.60317900
O	0.96057700	3.63746800	–1.03261000
C	1.00088500	4.67223100	–2.03811100
C	0.57865700	5.96491200	–1.38141900
H	0.32573900	4.38506100	–2.84846300

H	2.01651000	4.72965300	–2.43851100
H	0.61184100	6.77132300	–2.11817300
H	–0.44460100	5.89528500	–1.00137100
H	1.25110900	6.22614600	–0.55942400
H	0.28296000	2.74454300	0.96669700
H	–1.55092400	0.49008000	1.43644900
C	2.39594100	–0.26122300	–1.84973100
O	2.02625500	–1.08086000	–2.66045000
O	3.60146300	0.28870100	–1.82159800
C	4.48978000	–0.09129800	–2.89478000
C	5.82911200	0.54306900	–2.60816300
H	4.05909500	0.25768200	–3.83758200
H	4.55019800	–1.18295300	–2.92269900
H	6.53363900	0.27765800	–3.39998200
H	5.74388100	1.63181700	–2.57057000
H	6.22809300	0.18622900	–1.65487700
H	–2.03077100	2.52534900	1.62562900
O	–2.23142300	3.15461100	2.37506700
H	–3.12427000	3.48669900	2.20590700
H	–0.89876200	4.41318600	2.04795700
H	–2.30326300	1.55930600	3.46479700
O	–0.08639500	4.91603900	1.85327100
H	0.07540000	4.75324600	0.91546300
O	–2.33592400	0.64929000	3.80658700
H	–1.41128900	0.37078700	3.79837000

TS5-4b

0 1

P	1.30866900	–1.15975200	0.49548300
C	1.25504500	–0.33447500	2.08785500

C	0.78770900	0.98873100	2.10985700
C	1.67594400	–0.98569600	3.25208200
C	0.73395700	1.64918600	3.33828200
C	1.60998600	–0.31134500	4.46627000
H	2.05120100	–2.00428900	3.20476400
C	1.14056600	1.00208700	4.50338200
H	0.36215000	2.67059900	3.35965600
H	1.92796500	–0.80657100	5.37730100
H	1.09398500	1.52959900	5.45096900
C	2.70230600	–2.28744400	0.38236500
C	2.50264800	–3.65426100	0.17619400
C	3.99448000	–1.75246100	0.48354100
C	3.60938000	–4.49308100	0.06981700
H	1.49844300	–4.05910300	0.09598100
C	5.08963500	–2.59987700	0.36765100
H	4.14194900	–0.68777200	0.64743100
C	4.89548200	–3.96685100	0.16156500
H	3.46386300	–5.55605400	–0.08959400
H	6.09349300	–2.19511200	0.44039100
H	5.75425700	–4.62437500	0.07245400
C	–0.24215400	–2.00354700	0.12839500
C	–0.71372200	–2.04134000	–1.18748000
C	–0.96333100	–2.59417400	1.17275600
C	–1.91899300	–2.68605300	–1.45660100
H	–0.14884200	–1.57134000	–1.98839900
C	–2.16616300	–3.23254000	0.88846800
H	–0.59946000	–2.54602900	2.19557800
C	–2.64193800	–3.27796200	–0.42279100
H	–2.29633400	–2.71430600	–2.47351900
H	–2.73565600	–3.68656100	1.69252900

H	–3.58567700	–3.77045500	–0.63685600
C	0.23573700	1.66189400	0.86908000
C	–1.22823100	1.19117200	0.73490100
C	–1.85900400	1.34916800	–0.56084800
O	–1.42269200	2.06122400	–1.46909100
C	–3.14540300	0.58941200	–0.76688100
C	–3.84051000	–0.00001500	0.29550600
C	–3.61679500	0.42776200	–2.07193100
C	–4.98602700	–0.75260100	0.05318000
H	–3.49123100	0.11273300	1.32003900
C	–4.75183100	–0.33163800	–2.33092100
H	–3.07065000	0.89328800	–2.88606200
C	–5.41832700	–0.91718200	–1.25855200
H	–5.52845500	–1.21573700	0.87045300
H	–5.11120300	–0.47312500	–3.34444200
Cl	–6.83748300	–1.89490700	–1.56955800
C	1.58221600	0.18970900	–0.66351000
C	1.04761300	1.38607900	–0.37733000
C	1.21823600	2.48802700	–1.39507700
O	1.52039600	2.28194400	–2.54840500
O	1.03499200	3.68993400	–0.86569800
C	1.10062600	4.79992400	–1.78350800
C	0.75182600	6.04382300	–1.00188500
H	0.39626600	4.61372800	–2.59888800
H	2.10999600	4.84582000	–2.20200400
H	0.82914700	6.91769600	–1.65333300
H	–0.27134700	5.98795100	–0.62078600
H	1.43653000	6.17773500	–0.16053600
H	0.24823700	2.73895600	1.04299100
H	–1.36698900	0.18287000	1.12527400

C	2.40140400	–0.14909900	–1.87678300
O	2.03995400	–0.94966800	–2.70927100
O	3.59224800	0.42926400	–1.84039800
C	4.48281900	0.10210100	–2.93063800
C	5.81066300	0.75384400	–2.63100400
H	4.03873300	0.47214900	–3.85891800
H	4.56471800	–0.98659700	–2.99312100
H	6.51500500	0.52553000	–3.43446900
H	5.70480000	1.83906000	–2.56028700
H	6.22206500	0.37599600	–1.69124600
H	–1.88743300	1.87150200	1.62203700
O	–2.39212200	2.47021000	2.70501900
H	–3.30526300	2.69341800	2.47956000
H	–1.43151300	3.79229400	2.54162300
H	–2.34505200	0.89987800	3.35427000
O	–0.76262000	4.51829400	2.38095300
H	–0.78737100	4.65367800	1.42617400
O	–2.27900100	–0.06730500	3.56707000
H	–1.34748600	–0.26621700	3.40933800

Int8-4b

0 1

P	1.52938000	–1.14837900	0.36072100
C	1.36233600	–0.53611300	2.03857100
C	0.70915800	0.69443300	2.21350300
C	1.83982500	–1.27536100	3.12636900
C	0.51106600	1.15847400	3.51505000
C	1.64282400	–0.78934300	4.41367400
H	2.35751100	–2.21688600	2.96525200
C	0.97580700	0.42146000	4.60178600

H	–0.02887900	2.09284900	3.64818000
H	2.00645200	–1.35398900	5.26535700
H	0.81782200	0.79673600	5.60807100
C	3.03425500	–2.09701800	0.11873400
C	2.97537700	–3.42182000	–0.32005800
C	4.26449100	–1.46239600	0.34298000
C	4.16230700	–4.11717500	–0.53714300
H	2.01799000	–3.90370000	–0.49376800
C	5.44062900	–2.16612900	0.11449900
H	4.30214500	–0.43215300	0.68758400
C	5.38752000	–3.49034000	–0.32396700
H	4.12673800	–5.14667300	–0.87660800
H	6.39744000	–1.68250900	0.28056800
H	6.30927300	–4.03547300	–0.50029800
C	0.06526300	–2.07825600	–0.13259600
C	–0.45954300	–1.91024000	–1.41940400
C	–0.57394500	–2.89320000	0.80838000
C	–1.63565000	–2.57064200	–1.76193100
H	0.03969800	–1.26673300	–2.13877600
C	–1.74879600	–3.54755100	0.45038800
H	–0.17466400	–3.00276400	1.81293000
C	–2.27862300	–3.38339300	–0.82885400
H	–2.05728000	–2.43712800	–2.75279100
H	–2.25653000	–4.17261900	1.17711100
H	–3.20392300	–3.88387800	–1.09690100
C	0.11500500	1.47015000	1.05025900
C	–1.29881500	0.88832300	0.82728100
C	–1.99346500	1.29247100	–0.43360400
O	–1.56029700	2.14870000	–1.18897900
C	–3.26961800	0.56912600	–0.74131400

C	–3.85292500	–0.31295000	0.17711800
C	–3.85728300	0.76009400	–1.99498100
C	–5.01620900	–0.99850100	–0.16104300
H	–3.40765100	–0.48458800	1.15726200
C	–5.01290700	0.07511800	–2.34616900
H	–3.39208500	1.44515400	–2.69628800
C	–5.57556900	–0.79827800	–1.41869200
H	–5.47742900	–1.68516500	0.54036800
H	–5.47025500	0.21141700	–3.31989300
Cl	–7.02888900	–1.67062300	–1.85010100
C	1.64472300	0.36101900	–0.61295100
C	0.96939800	1.44200600	–0.19711100
C	1.05206000	2.68071900	–1.05753200
O	1.34448600	2.64638100	–2.23093000
O	0.80289200	3.78585500	–0.37129900
C	0.77288500	5.00688200	–1.14023200
C	0.41551500	6.12556600	–0.19196600
H	0.03269800	4.88813000	–1.93647800
H	1.75413500	5.15354800	–1.59961800
H	0.37221200	7.06750100	–0.74418700
H	–0.56016000	5.94777300	0.26750100
H	1.16450900	6.22091400	0.59793600
H	–0.00560700	2.50896100	1.36119200
H	–1.27957600	–0.20377300	0.86279400
C	2.50467000	0.27237300	–1.84285200
O	2.23627100	–0.45642800	–2.77051900
O	3.61801000	0.97547700	–1.71603800
C	4.54064800	0.89894900	–2.82695700
C	5.79081900	1.63773600	–2.41589700
H	4.05975800	1.34828000	–3.70039800

H	4.73657200	–0.15554400	–3.03960600
H	6.51500000	1.60890900	–3.23359000
H	5.56783100	2.68256900	–2.18687400
H	6.24237600	1.17090400	–1.53651400
H	–1.92700000	1.17543700	1.69543000
O	–2.91617600	1.37651400	3.38519300
H	–3.78090200	1.44989100	2.96177800
H	–2.18821200	2.64879700	3.12251700
H	–2.52310700	–0.08384500	3.28788400
O	–1.63735800	3.49861000	2.88698600
H	–1.89985400	3.70300400	1.98189300
O	–2.25724300	–1.06946100	3.13528400
H	–1.30069100	–1.02943300	3.01424700

TS6-4b

0 1

P	0.11853700	1.47957500	0.36032700
C	0.16480100	0.63468300	1.93349500
C	–0.29446100	–0.68514600	2.02289600
C	0.64291600	1.32650700	3.05773200
C	–0.26939800	–1.29430100	3.28820200
C	0.68601400	0.69257200	4.28854800
H	0.96773300	2.35990500	2.96466600
C	0.22222200	–0.62130700	4.39768500
H	–0.67673400	–2.30079300	3.37985400
H	1.05959000	1.22034200	5.15934900
H	0.22849000	–1.11624500	5.36398000
C	–0.59839500	3.12101200	0.55146200
C	0.01914200	4.25553200	0.01906800
C	–1.83617100	3.20768800	1.20531800

C	–0.60213600	5.49428400	0.15600400
H	0.96967500	4.17806700	–0.49906900
C	–2.44428400	4.45257100	1.32967600
H	–2.32000800	2.30970000	1.59377600
C	–1.82807500	5.59149300	0.81025900
H	–0.12809800	6.38048400	–0.25230800
H	–3.40222000	4.53369000	1.83286100
H	–2.30908800	6.55909200	0.91336700
C	1.74713600	1.59210700	–0.40518100
C	1.98082800	1.00348300	–1.65112800
C	2.77151300	2.26738100	0.27183400
C	3.24328200	1.11294500	–2.22936900
H	1.18838300	0.47180100	–2.16927600
C	4.02827600	2.36538300	–0.31441500
H	2.58997300	2.71929700	1.24325800
C	4.26041900	1.79592400	–1.56681900
H	3.42952300	0.65988600	–3.19755500
H	4.82471700	2.88824900	0.20456500
H	5.24134800	1.87930800	–2.02367600
C	–0.87986600	–1.50160200	0.89829600
C	–0.15222400	–2.86416900	0.66269200
C	0.74312600	–2.85661500	–0.55862600
O	0.30013300	–3.23572800	–1.63105900
C	2.15010000	–2.35659100	–0.46842000
C	2.65411800	–1.73874400	0.67954700
C	2.97338300	–2.50052200	–1.59180500
C	3.95555000	–1.24404900	0.70123100
H	2.04139300	–1.62912700	1.56853400
C	4.28196400	–2.04180500	–1.57500100
H	2.57246600	–2.97901100	–2.47909200

C	4.75249200	–1.40941500	–0.42547600
H	4.34553000	–0.74825300	1.58346400
H	4.92673400	–2.15776300	–2.43933200
Cl	6.39036000	–0.80421700	–0.40227300
C	–0.97114600	0.49864000	–0.65955700
C	–1.22949600	–0.78721300	–0.36122600
C	–2.00984700	–1.57244000	–1.40125300
O	–1.94118000	–1.34830700	–2.58677800
O	–2.74692800	–2.52448700	–0.84819600
C	–3.39940800	–3.43857800	–1.75572500
C	–4.15764000	–4.43001700	–0.90558700
H	–2.62441100	–3.91680100	–2.36132000
H	–4.05851700	–2.86840700	–2.41581300
H	–4.61797500	–5.18484900	–1.54765500
H	–3.48446100	–4.93183300	–0.20525700
H	–4.94886000	–3.93235600	–0.33832300
H	–1.90131700	–1.78879200	1.30742500
H	0.40148000	–3.13329800	1.56285800
C	–1.60314000	1.24107200	–1.79649700
O	–0.98515600	1.91649200	–2.58716600
O	–2.92867600	1.14868400	–1.74317600
C	–3.65169100	1.76229100	–2.83320200
C	–5.11811900	1.49582200	–2.59436400
H	–3.29806700	1.31906500	–3.76837800
H	–3.42085100	2.83084300	–2.84310600
H	–5.70556400	1.94676800	–3.39763700
H	–5.31731200	0.42110300	–2.57932900
H	–5.43998900	1.92925200	–1.64400500
H	–0.90536300	–3.63460000	0.49541200
O	–3.43508800	–2.08426300	2.10594500

H	–3.83267000	–2.43225300	1.29728900
H	–3.40339700	–0.57364000	1.84467300
H	–2.59932300	–3.27611700	2.58983600
O	–3.32597900	0.41715300	1.58190700
H	–3.52965100	0.44002000	0.63914000
O	–1.98849300	–4.05339300	2.85959200
H	–2.25713200	–4.26713000	3.76025400

TS7-4b

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P	2.28216000	–0.79157000	0.03279200
C	1.51991100	–1.39207500	1.54177900
C	0.26497500	–0.87166700	1.91005800
C	2.19365400	–2.32359000	2.34459800
C	–0.28209100	–1.32266600	3.12456900
C	1.61982900	–2.76540300	3.52564300
H	3.16632400	–2.69576800	2.03383400
C	0.37980800	–2.25174100	3.91310400
H	–1.22641900	–0.91731500	3.47277600
H	2.13381000	–3.49245100	4.14483900
H	–0.07030800	–2.57102800	4.84767600
C	4.07243800	–0.74569400	0.25901500
C	4.89917600	–1.65654600	–0.40098900
C	4.61271600	0.19506100	1.14447500
C	6.27393300	–1.62394700	–0.17347100
H	4.47924100	–2.38491200	–1.08801500
C	5.98523200	0.22273500	1.36061400
H	3.96497500	0.90284400	1.65604100
C	6.81458300	–0.68685900	0.70260200
H	6.91951800	–2.33024300	–0.68479600

H	6.40838100	0.95321700	2.04213500
H	7.88585400	–0.66285400	0.87526700
C	1.89962800	–1.89344800	–1.35092800
C	1.92999400	–1.36443200	–2.64609300
C	1.59723100	–3.24040700	–1.13439000
C	1.66061000	–2.19575700	–3.72846000
H	2.16511800	–0.31345200	–2.79656900
C	1.32953200	–4.06366200	–2.22529800
H	1.56583200	–3.64235000	–0.12547300
C	1.36130700	–3.54174800	–3.51728200
H	1.68007800	–1.79306700	–4.73577000
H	1.09094400	–5.10988400	–2.06493800
H	1.14737900	–4.18573600	–4.36445300
C	–0.45912900	0.12760100	1.08138300
C	–1.98213600	–0.08227000	0.99760800
C	–2.75563900	0.27735300	–0.11611100
O	–2.33229200	0.86952200	–1.13623000
C	–4.20399100	–0.14791800	–0.09239000
C	–4.93004700	–0.35069700	1.08634900
C	–4.85239600	–0.31693200	–1.31972000
C	–6.26686900	–0.73572200	1.04501500
H	–4.46170200	–0.18654100	2.05172600
C	–6.18450800	–0.70954500	–1.38123400
H	–4.29214300	–0.13350600	–2.23042900
C	–6.87544400	–0.91759100	–0.19193000
H	–6.82957300	–0.88473100	1.96021800
H	–6.68186200	–0.84946800	–2.33507200
Cl	–8.55722600	–1.40754700	–0.25431700
C	1.60389400	0.81555600	–0.13680000
C	0.26668900	1.00363600	0.22428900

C	–0.39984700	2.24211000	–0.33248300
O	–0.13729200	2.72767700	–1.40577400
O	–1.24770800	2.77385700	0.55089900
C	–2.14201100	3.77663400	0.03530900
C	–3.27515300	3.91318300	1.02520300
H	–2.49353300	3.44145600	–0.94277700
H	–1.59047000	4.71391700	–0.08645600
H	–3.98522700	4.66461300	0.67055100
H	–3.80234900	2.96076800	1.13444100
H	–2.90443900	4.22296800	2.00586400
H	–1.20546500	0.86198700	1.69756600
H	–2.38808900	–0.70621800	1.77728200
C	2.45877300	1.83564100	–0.75497500
O	3.27503400	1.60308400	–1.63143400
O	2.31209700	3.04440200	–0.19771800
C	2.95275500	4.13079500	–0.88629400
C	2.52374000	5.40895100	–0.20457900
H	2.64789700	4.10883500	–1.93689200
H	4.03659400	3.98848800	–0.84314700
H	2.99238400	6.26407500	–0.69796800
H	1.43852600	5.52749400	–0.25949300
H	2.82359000	5.40872900	0.84649300

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P	2.59687400	–0.41694700	0.00047700
C	1.97236100	–1.67058300	1.12360600
C	0.59131800	–1.68006800	1.44103400
C	2.86878300	–2.57727100	1.70582400
C	0.17985700	–2.64469000	2.38741900

C	2.42154000	–3.52772500	2.60978000
H	3.92275100	–2.53098400	1.44354000
C	1.06781700	–3.54642700	2.95265400
H	–0.85231900	–2.67039000	2.71638300
H	3.11553000	–4.23516700	3.05056300
H	0.70234800	–4.26456800	3.68008500
C	4.25957900	0.05783100	0.53947600
C	5.39166700	–0.32323300	–0.18256100
C	4.39095000	0.78818700	1.72642200
C	6.65758600	0.02770100	0.28482700
H	5.29242700	–0.88696000	–1.10509000
C	5.65618000	1.13670800	2.18409700
H	3.50587400	1.08608000	2.28255400
C	6.78950900	0.75614000	1.46361000
H	7.53808900	–0.26653800	–0.27691200
H	5.75949300	1.70621200	3.10199000
H	7.77624500	1.03045600	1.82317400
C	2.74091200	–1.10282800	–1.67777900
C	2.57667800	–0.22551000	–2.75489000
C	2.99986300	–2.45799300	–1.90044900
C	2.68638100	–0.70652200	–4.05637800
H	2.36489800	0.82442900	–2.56695300
C	3.10729900	–2.93168800	–3.20577500
H	3.11213300	–3.14136600	–1.06300300
C	2.95225700	–2.05698400	–4.28029000
H	2.55950000	–0.02946600	–4.89488900
H	3.30659300	–3.98350400	–3.38344900
H	3.03310900	–2.43045700	–5.29630300
C	–0.37042900	–0.72282800	0.87140100
C	–1.83822900	–1.09401800	0.94503600

C	–2.63999000	–0.89887000	–0.33002500
O	–2.11840500	–0.77036500	–1.42082500
C	–4.13631400	–0.88733500	–0.20913600
C	–4.80376100	–1.28205200	0.95434200
C	–4.87651000	–0.43807100	–1.30758100
C	–6.19225400	–1.22358100	1.02553700
H	–4.25373700	–1.64553600	1.81583400
C	–6.26132700	–0.35830400	–1.24718700
H	–4.35051300	–0.14174400	–2.20933000
C	–6.90054100	–0.75397500	–0.07519600
H	–6.71540400	–1.53417900	1.92299100
H	–6.83756800	0.00241800	–2.09193300
Cl	–8.64409300	–0.66210900	0.01318100
C	1.44240500	0.85388400	0.16392000
C	0.06465600	0.46870100	0.34747700
C	–0.92066000	1.43430700	–0.27350800
O	–0.76067000	1.94938100	–1.35470200
O	–2.00327200	1.64763000	0.48624500
C	–3.03038600	2.45211300	–0.12668500
C	–4.17847000	2.55616400	0.84872700
H	–3.32930200	1.97206800	–1.06457400
H	–2.61072800	3.43236600	–0.36925000
H	–4.97636800	3.15746800	0.40527200
H	–4.58238700	1.56795500	1.08722300
H	–3.85745100	3.03777100	1.77601700
H	–2.34348100	–0.56524200	1.75907500
H	–1.94775700	–2.16272300	1.16243500
C	1.86935700	2.20557300	–0.09971900
O	2.88327600	2.53120100	–0.70818200
O	1.04393300	3.12610600	0.45123700

C	1.23081000	4.47547300	0.01013700
C	0.12353300	5.30371100	0.62074500
H	1.19838400	4.50119100	–1.08396300
H	2.21804200	4.82598900	0.32592800
H	0.22344100	6.34648900	0.30894600
H	–0.85456400	4.93721200	0.29634600
H	0.16572200	5.26354000	1.71240400

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C	–2.17350900	–0.06925000	–0.00001200
C	–0.96969000	–0.00286100	–0.00001000
H	–3.24335100	–0.12929600	0.00003100
C	0.49365800	0.13715100	–0.00001300
O	1.02331700	1.23869800	0.00000200
N	1.15846200	–1.03298500	0.00009900
H	0.67546000	–1.91972500	–0.00017600
H	2.16936500	–1.01991300	–0.00035800

TS1-6

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P	2.24161400	–0.26932900	–0.42748700
C	1.74714700	0.61214100	1.09629000
C	0.40777300	0.53837200	1.54627900
C	2.65887200	1.42146600	1.77943100
C	0.03759400	1.26665300	2.68523600
C	2.26779100	2.14940800	2.89968500
H	3.68547000	1.48920300	1.43487500
C	0.95334900	2.07037600	3.35289800
H	–0.97833000	1.18779400	3.05939200

H	2.99162600	2.76864800	3.41930900
H	0.64342000	2.62589900	4.23207300
C	3.93419500	0.28915900	–0.80577000
C	5.04312700	–0.55639500	–0.69519500
C	4.10343500	1.60179800	–1.27301900
C	6.30920400	–0.09512200	–1.05035000
H	4.92474400	–1.57270100	–0.33211200
C	5.37420900	2.05703600	–1.61233000
H	3.24825900	2.27289900	–1.35000600
C	6.47701300	1.20957800	–1.50797700
H	7.16475800	–0.75745000	–0.96355800
H	5.50194300	3.07566800	–1.96536100
H	7.46478200	1.56599300	–1.78293300
C	2.39348400	–2.02887400	0.03302300
C	2.51862600	–2.95853800	–1.00875800
C	2.35256600	–2.47572100	1.35833100
C	2.62028400	–4.31697900	–0.72429800
H	2.54237400	–2.61832900	–2.04146600
C	2.44413700	–3.83793000	1.63598300
H	2.25447000	–1.76340900	2.17225800
C	2.58016500	–4.75772800	0.59811300
H	2.72213000	–5.03159000	–1.53479100
H	2.41341900	–4.17901400	2.66597100
H	2.65200600	–5.81803900	0.81898900
C	–0.59061000	–0.28119000	0.84117600
C	–1.91603300	–0.07238800	0.85889200
H	–2.35357100	0.75680500	1.40533600
C	–2.80982500	–0.98983400	0.10608000
O	–2.39400700	–2.03799400	–0.36451700
C	–4.24937200	–0.61230600	–0.06362800

C	–4.71824500	0.68886400	0.13954700
C	–5.14258300	–1.60869900	–0.47267000
C	–6.06173300	0.99393700	–0.05591700
H	–4.04346500	1.48675800	0.42992700
C	–6.48747800	–1.32349400	–0.66032200
H	–4.76903100	–2.61373500	–0.63776200
C	–6.92871700	–0.01975200	–0.44712500
H	–6.42788500	2.00377900	0.09175800
H	–7.18466600	–2.09501200	–0.96767400
Cl	–8.62027300	0.35157800	–0.68206600
C	0.87546100	0.58926600	–1.99725000
C	0.45930000	1.76192200	–1.79330400
H	0.84290600	–0.21133600	–2.71893600
C	0.52515600	2.90212000	–0.91390800
O	1.49989900	3.66078800	–0.87978000
H	–0.23800900	–1.12254400	0.24603600
N	–0.61178200	3.16136100	–0.19181400
H	–1.27637100	2.40845700	–0.06459400
H	–0.49495100	3.78960800	0.59292600

Int1-6

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P	–2.25439100	0.16983400	–0.37223400
C	–1.71295600	–0.76844700	1.08483300
C	–0.38192800	–0.67859200	1.55525900
C	–2.62096700	–1.62978400	1.70394000
C	–0.01972400	–1.44877000	2.66724500
C	–2.23241300	–2.39813900	2.79778000
H	–3.63562600	–1.71023200	1.32795600
C	–0.93063400	–2.30224700	3.28015800

H	0.98672200	–1.36310100	3.06404700
H	–2.94752500	–3.06250900	3.27084400
H	–0.62288400	–2.88767100	4.14042600
C	–3.98754000	–0.23564900	–0.71824800
C	–5.01695900	0.54035100	–0.17267400
C	–4.28078400	–1.34033200	–1.52612000
C	–6.34213300	0.20893500	–0.43856000
H	–4.78798300	1.39751100	0.45378000
C	–5.61116700	–1.66307500	–1.78220500
H	–3.47321500	–1.95489900	–1.91750800
C	–6.63833000	–0.88990100	–1.24383600
H	–7.14178400	0.81042500	–0.01887000
H	–5.84484900	–2.51976900	–2.40616100
H	–7.67305700	–1.14362300	–1.45209300
C	–2.23019500	1.93728500	0.02959100
C	–2.44207400	2.85132700	–1.01080800
C	–2.03401100	2.39304100	1.33677400
C	–2.44609700	4.21582900	–0.74022000
H	–2.61203500	2.50224600	–2.02591000
C	–2.04135900	3.76112300	1.59821100
H	–1.87576000	1.68843800	2.14818300
C	–2.24431700	4.67027900	0.56248000
H	–2.60767400	4.92330700	–1.54677500
H	–1.88928500	4.11402300	2.61291600
H	–2.24801800	5.73550700	0.77048300
C	0.61898100	0.18503900	0.90558500
C	1.93862800	–0.05426400	0.89414200
H	2.35689900	–0.93919900	1.36250100
C	2.84647000	0.90763900	0.21367500
O	2.44089300	1.99376800	–0.17109100

C	4.28048000	0.52808900	0.00979700
C	4.74444300	–0.78380800	0.14427700
C	5.17502300	1.53844200	–0.36104500
C	6.08376500	–1.08578900	–0.08225700
H	4.07034300	–1.59215700	0.40475100
C	6.51540400	1.25562300	–0.58021400
H	4.80543500	2.55217900	–0.47251500
C	6.95162900	–0.05936300	–0.43631100
H	6.44579400	–2.10334200	0.01306400
H	7.21268100	2.03760400	–0.85953900
Cl	8.63720800	–0.42834900	–0.71356300
C	–1.19001600	–0.17851500	–1.80099000
C	–0.60552500	–1.35041400	–2.07488700
H	–1.11917100	0.70081200	–2.44692500
C	–0.76488700	–2.54922900	–1.27854900
O	–1.78107300	–3.26393500	–1.31314700
H	0.27946200	1.07926900	0.38637900
N	0.35889100	–2.98455000	–0.60014100
H	1.06020000	–2.28767600	–0.38022300
H	0.16903000	–3.64964300	0.13921700

Int2-6

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P	–1.22454900	0.40893200	–0.35447900
C	–1.79837700	0.82388700	1.32774800
C	–1.01169100	1.62870300	2.18071100
C	–3.06326800	0.39457400	1.74965100
C	–1.53890500	2.02210300	3.41371100
C	–3.55100400	0.76435900	2.99999000
H	–3.68117500	–0.23342200	1.11556100

C	–2.79415100	1.58783500	3.82739500
H	–0.94184700	2.66038800	4.05804400
H	–4.52972100	0.41744600	3.31456000
H	–3.17730700	1.89313700	4.79575300
C	–2.64697500	–0.19239100	–1.30948400
C	–3.77495600	0.63128600	–1.41980300
C	–2.59221900	–1.40498500	–2.00109300
C	–4.85002400	0.22933800	–2.20319500
H	–3.81527100	1.58192600	–0.89398500
C	–3.67392100	–1.79782500	–2.78669600
H	–1.71687500	–2.03911900	–1.91835600
C	–4.80009500	–0.98584600	–2.88504700
H	–5.72538200	0.86553700	–2.28179700
H	–3.63227700	–2.74154700	–3.32060000
H	–5.64098600	–1.29730300	–3.49676700
C	–0.73565300	1.96468100	–1.15178800
C	0.11409100	1.90788200	–2.26195500
C	–1.25249700	3.19299200	–0.72565600
C	0.46083200	3.08081100	–2.92744700
H	0.50006500	0.95581300	–2.61484800
C	–0.90205300	4.36021400	–1.39817800
H	–1.92024000	3.24340700	0.12965500
C	–0.04263800	4.30546100	–2.49400600
H	1.12441200	3.03518900	–3.78465400
H	–1.29949000	5.31234900	–1.06248700
H	0.23140100	5.21823400	–3.01339100
C	0.35789600	2.07919500	1.83209400
C	1.38224800	1.23332700	1.68802900
H	1.22518500	0.17094200	1.82693200
C	2.72428900	1.74003500	1.28503500

O	2.97127000	2.93550800	1.28870700
C	3.75038100	0.75320400	0.82213500
C	3.52895800	–0.62725000	0.82914600
C	4.96537400	1.24879400	0.33328800
C	4.49446300	–1.50509100	0.34626100
H	2.61139400	–1.06345300	1.20436700
C	5.94195700	0.38711800	–0.14478300
H	5.13269100	2.32059600	0.32817200
C	5.68924700	–0.98385800	–0.13431200
H	4.29749300	–2.57198200	0.34739900
H	6.88317100	0.76742600	–0.52576600
Cl	6.91132300	–2.07387200	–0.74625400
C	0.16817800	–0.72854400	–0.44590400
C	0.03597200	–2.01785700	–0.09132200
H	1.08827700	–0.22872800	–0.76933500
C	1.26005300	–2.83755800	–0.17744300
O	1.84045900	–3.26670000	0.82612200
H	0.53016200	3.14928100	1.71912000
N	1.71496000	–3.10963200	–1.43331700
H	1.14885300	–2.87963100	–2.23708000
H	2.40348100	–3.84331800	–1.53931200
O	–2.39230300	–2.57650000	0.99719700
H	–1.44969400	–2.49492300	0.56866200
H	–2.31102400	–2.10700200	1.83863400
H	–4.18309600	–1.95842200	0.06523400
O	–5.11405100	–1.95181900	0.33540500
H	–5.13784300	–2.73910700	0.90557700
H	–3.51688500	–3.90942100	1.40115200
O	–4.34868500	–4.36313200	1.65219200
H	–4.35301900	–4.34146200	2.61678700

TS2-6

0 1

P	–1.28924300	0.37950300	–0.33307800
C	–1.83405100	0.75575300	1.36577000
C	–1.06088600	1.58737800	2.20489400
C	–3.07936800	0.28673400	1.80393100
C	–1.58594400	1.97172200	3.44187100
C	–3.56354000	0.65077700	3.05698100
H	–3.67821900	–0.37156600	1.18202400
C	–2.82337700	1.50313400	3.87059900
H	–1.00056900	2.63006100	4.07660400
H	–4.52666600	0.27523600	3.38624300
H	–3.20562100	1.80312000	4.84098800
C	–2.69760400	–0.24767400	–1.28786100
C	–3.84888900	0.54522100	–1.37087800
C	–2.60602000	–1.43553800	–2.01565000
C	–4.91151200	0.13630000	–2.16766600
H	–3.91558400	1.47847500	–0.81723700
C	–3.67373000	–1.83366300	–2.81605600
H	–1.71239100	–2.04634900	–1.95580900
C	–4.82305500	–1.05228300	–2.89107200
H	–5.80532300	0.74853800	–2.22746300
H	–3.60329800	–2.75747200	–3.38095300
H	–5.65225900	–1.36698000	–3.51699900
C	–0.86205400	1.96068500	–1.11996400
C	–0.05728900	1.94369600	–2.26470800
C	–1.39681400	3.16790700	–0.65754100
C	0.23201900	3.13477000	–2.92474100
H	0.33735600	1.00832700	–2.65116700

C	–1.10386500	4.35393800	–1.32495100
H	–2.03472200	3.18848700	0.22121800
C	–0.28585900	4.33912800	–2.45294600
H	0.86116500	3.11881500	–3.80855100
H	–1.51463700	5.28946200	–0.95998600
H	–0.05639500	5.26640000	–2.96819400
C	0.29227200	2.07181500	1.84169100
C	1.32978700	1.24806700	1.66545000
H	1.19487500	0.18099300	1.79048000
C	2.65776300	1.78513600	1.25640000
O	2.87591300	2.98613500	1.25416200
C	3.70762200	0.82113900	0.79841800
C	3.52167800	–0.56443000	0.81374100
C	4.91038300	1.34424900	0.30785100
C	4.51022200	–1.42057000	0.33855700
H	2.61379200	–1.01784800	1.19224700
C	5.90948100	0.50483100	–0.16290200
H	5.05017300	2.41990500	0.29617600
C	5.69210300	–0.87206900	–0.14335700
H	4.34160400	–2.49240200	0.34516200
H	6.84128300	0.90644200	–0.54515800
Cl	6.94241400	–1.93433700	–0.74588300
C	0.15261000	–0.69411800	–0.49187000
C	0.11092000	–1.98757900	–0.14248200
H	1.03567900	–0.16772800	–0.86374400
C	1.36491900	–2.77501400	–0.28659500
O	1.91251400	–3.29743800	0.68632100
H	0.44276800	3.14708700	1.74944600
N	1.86298900	–2.87499700	–1.54249200
H	1.34947700	–2.51845000	–2.33488900

H	2.64105600	–3.49841600	–1.71236300
O	–2.15285500	–2.56297800	0.95221400
H	–1.02938400	–2.42708700	0.42616200
H	–2.07322800	–2.11154000	1.80384400
H	–3.88403100	–2.19639800	0.27330300
O	–4.85293400	–2.24558200	0.38471700
H	–4.90216600	–3.02511100	0.96114200
H	–3.07624500	–3.90826600	1.42372900
O	–3.79002300	–4.52623800	1.73307600
H	–3.77025300	–4.44741900	2.69395000

Int3-6

0 1

P	–1.38956500	0.30016100	–0.31801300
C	–1.85427500	0.66131500	1.40499400
C	–1.05238900	1.49099500	2.21728000
C	–3.10362400	0.22492600	1.86471800
C	–1.54373700	1.88570500	3.46564900
C	–3.55594700	0.60680700	3.12374200
H	–3.72494800	–0.42568000	1.25722800
C	–2.77944600	1.44116000	3.92237600
H	–0.93476100	2.53832400	4.08383500
H	–4.52211800	0.25604000	3.47111500
H	–3.13474000	1.75077900	4.89998900
C	–2.78803300	–0.37154100	–1.25156500
C	–3.92855200	0.42803700	–1.38468200
C	–2.70193700	–1.59779600	–1.91150900
C	–4.98878000	–0.01213200	–2.16906500
H	–3.99034100	1.39019400	–0.88249000
C	–3.76209700	–2.02226800	–2.70623300

H	–1.82067600	–2.21819900	–1.80249300
C	–4.90306700	–1.23420500	–2.83328300
H	–5.87625200	0.60430400	–2.26785400
H	–3.69499300	–2.97336000	–3.22433500
H	–5.72739300	–1.57077600	–3.45436800
C	–1.06344600	1.90807200	–1.10937500
C	–0.39243100	1.92071800	–2.33806100
C	–1.55256800	3.10199500	–0.56965700
C	–0.18556900	3.12517900	–3.00338000
H	–0.03718200	0.99630800	–2.78589000
C	–1.34298800	4.30304300	–1.24296700
H	–2.09427200	3.10295400	0.37118100
C	–0.65575500	4.31666200	–2.45425100
H	0.34036800	3.13023400	–3.95225200
H	–1.71929600	5.22731500	–0.81724400
H	–0.49135600	5.25498200	–2.97423200
C	0.28405600	1.99046500	1.81735700
C	1.33482000	1.19333100	1.60186600
H	1.23192100	0.12128400	1.71375600
C	2.64372200	1.77799700	1.19503000
O	2.80970300	2.98709000	1.17401700
C	3.74416100	0.85501200	0.77472400
C	3.61891000	–0.53649100	0.80049800
C	4.93557100	1.42646800	0.30972400
C	4.65755500	–1.35180200	0.36066500
H	2.71911500	–1.02178100	1.16038500
C	5.98325100	0.62893100	–0.12530100
H	5.02694100	2.50711100	0.28993100
C	5.82596500	–0.75611900	–0.09658900
H	4.53899300	–2.43034400	0.36498300

H	6.90590000	1.06796000	–0.48828800
Cl	7.13449100	–1.76829400	–0.65938300
C	0.12800400	–0.64529000	–0.60242800
C	0.28903100	–1.93932200	–0.31498200
H	0.92720400	–0.04255500	–1.03363700
C	1.59944900	–2.62490600	–0.56298400
O	2.09353900	–3.33969600	0.30466700
H	0.41608000	3.06956200	1.74289300
N	2.18700700	–2.37436300	–1.74942800
H	1.70621500	–1.87510300	–2.48360200
H	3.06062700	–2.83472400	–1.96755000
O	–2.15896600	–2.50532100	0.95787600
H	–0.53130000	–2.48559400	0.19023400
H	–1.96907800	–2.05220300	1.78967900
H	–3.79295400	–2.25239100	0.52656700
O	–4.78628100	–2.28252300	0.56906900
H	–4.87197500	–3.04273700	1.16432400
H	–2.91648000	–3.76232000	1.54885800
O	–3.53566300	–4.45484600	1.96705900
H	–3.49297100	–4.25774800	2.90961900

Int4-6

0 1

P	1.79294400	0.38405400	0.02349400
C	1.92281200	–1.51206400	0.76724800
C	1.10763100	–2.64835500	0.55038000
C	3.05439800	–1.71217700	1.58314600
C	1.52814000	–3.91610600	1.00486500
C	3.43269800	–2.95365000	2.08122700
H	3.68584700	–0.85886200	1.81743900

C	2.67554900	–4.07952200	1.76382900
H	0.90990000	–4.78006600	0.77290600
H	4.32353700	–3.04301700	2.69591400
H	2.96728900	–5.06535100	2.11201800
C	1.88937400	2.22497300	–0.59268600
C	2.48601800	2.48419000	–1.84004400
C	1.25321700	3.30131000	0.03930700
C	2.48745300	3.75642100	–2.40494700
H	2.95549800	1.68130500	–2.40592900
C	1.24398600	4.58001200	–0.52439000
H	0.74625000	3.15891400	0.98659000
C	1.86799700	4.81630800	–1.74418400
H	2.96597100	3.91736000	–3.36668000
H	0.74438500	5.39064400	–0.00186000
H	1.86410100	5.81011500	–2.18131800
C	0.64595100	–0.04689600	–1.32152200
C	–0.58666600	0.59395700	–1.45196000
C	1.03307500	–1.02163700	–2.24009000
C	–1.46320400	0.20756700	–2.46203000
H	–0.86816000	1.38241600	–0.75779700
C	0.16420400	–1.38758800	–3.26701300
H	2.00474300	–1.50127100	–2.14677900
C	–1.08976200	–0.78771500	–3.36616000
H	–2.43450800	0.68553200	–2.54656200
H	0.46441400	–2.14572400	–3.98347200
H	–1.77278500	–1.08730500	–4.15484600
C	–0.23699400	–2.68542100	–0.06805100
C	–1.27432500	–1.90117200	0.25033800
H	–1.16006300	–1.09467700	0.96579800
C	–2.59633900	–2.14117100	–0.37693700

O	–2.79941100	–3.11501300	–1.08838600
C	–3.71612900	–1.17521900	–0.11217000
C	–3.52589900	0.07073800	0.49393600
C	–5.00187700	–1.54635500	–0.52050300
C	–4.60038300	0.93206200	0.69437200
H	–2.53986700	0.39860700	0.80411400
C	–6.08602200	–0.70288600	–0.32093200
H	–5.14097800	–2.51075000	–0.99703400
C	–5.86760200	0.53018200	0.28760000
H	–4.45444100	1.90024200	1.16022600
H	–7.08392500	–0.99360700	–0.63023500
Cl	–7.22397200	1.60192400	0.54833100
C	1.13842400	0.76881800	1.68213400
C	1.83983600	1.47188200	2.57457900
H	0.25141100	0.20622100	1.97291500
C	1.46222400	1.60913200	4.01552400
O	1.73653300	2.62951600	4.63582000
H	–0.42915300	–3.50602200	–0.75957800
O	3.38205100	0.13526200	–0.31615700
H	2.71607600	2.04756800	2.28228900
H	3.82713100	0.76597900	–0.91756200
H	4.04688800	–1.69421100	–0.76734500
O	4.55913600	–2.12944400	–1.46852700
H	4.01632500	–2.87271000	–1.75995400
H	4.87559000	–0.52419400	–2.33757300
O	4.94220300	0.44005800	–2.47718200
H	5.88233900	0.64392900	–2.40199300
N	0.78655000	0.56682900	4.55566400
H	0.78299300	–0.33763600	4.10651100
H	0.56989300	0.60450700	5.54236700

TS3-6

0 1

P	1.71784700	0.83044200	–0.10641200
C	1.83298200	–1.55991900	0.80298900
C	1.23501600	–2.75214900	0.32548000
C	3.03662400	–1.71977100	1.49763700
C	1.90918400	–3.98792900	0.41855400
C	3.68867500	–2.94731000	1.64263700
H	3.50966800	–0.83417800	1.93055000
C	3.13247500	–4.09148200	1.07002000
H	1.44406900	–4.87783900	–0.00136800
H	4.63294100	–3.00880000	2.17799100
H	3.63514200	–5.05087100	1.14552500
C	1.66752400	2.63269300	–0.49116300
C	2.20872400	3.07719900	–1.70603600
C	1.05326200	3.55666300	0.35804000
C	2.14872300	4.42165700	–2.05536100
H	2.67252100	2.37096000	–2.39239200
C	0.99058500	4.90526500	0.00505900
H	0.62695900	3.23001700	1.30117700
C	1.53970200	5.33886500	–1.19765800
H	2.57345700	4.75499700	–2.99698900
H	0.51391500	5.61451400	0.67437300
H	1.49241100	6.38852600	–1.47044300
C	0.60270200	0.19147900	–1.36394300
C	–0.68446000	0.72626100	–1.46333300
C	1.03407100	–0.78952700	–2.25722900
C	–1.55841900	0.23929600	–2.43263500
H	–1.00683900	1.51577300	–0.78821100

C	0.16357700	–1.25396700	–3.23924200
H	2.03173600	–1.20860600	–2.16642000
C	–1.13387900	–0.74902600	–3.31943500
H	–2.56647200	0.63683000	–2.49818400
H	0.49572300	–2.01721100	–3.93562700
H	–1.81479300	–1.12421600	–4.07695500
C	–0.12818000	–2.82190700	–0.22366300
C	–1.15009200	–2.02736800	0.13242900
H	–0.99306800	–1.23666700	0.85633000
C	–2.49047800	–2.23155800	–0.45363700
O	–2.72435900	–3.15448400	–1.22374000
C	–3.60076400	–1.28638300	–0.08299800
C	–3.39917400	–0.11686200	0.65740600
C	–4.88991800	–1.59433400	–0.53050600
C	–4.46379400	0.73087400	0.94822500
H	–2.41185400	0.16121500	1.00908000
C	–5.96463400	–0.76337500	–0.24443500
H	–5.03873500	–2.49980700	–1.10874600
C	–5.73375100	0.39401400	0.49381800
H	–4.30738000	1.64003200	1.51800600
H	–6.96442200	–1.00514200	–0.58802900
Cl	–7.07644200	1.45444200	0.85488200
C	1.22402700	0.69200500	1.58705300
C	2.02044700	1.13745800	2.58479300
H	0.23649200	0.27163700	1.74860600
C	1.73258400	0.88687200	4.01226100
O	2.23482100	1.56401000	4.90554200
H	–0.34510500	–3.63577400	–0.91635000
O	3.25077800	0.49856900	–0.36101100
H	2.93472200	1.68871800	2.38406800

H	3.60922300	0.60906600	–1.31717400
H	3.83543400	–1.75758900	–0.68341000
O	4.21227800	–2.05433300	–1.52922200
H	3.76962600	–2.89331300	–1.71421200
H	4.29833700	–0.61080300	–2.54944400
O	4.15995800	0.35274900	–2.69565200
H	5.03364600	0.74397200	–2.84413900
N	0.84870900	–0.12454600	4.27240600
H	0.73902500	–0.86899100	3.59653500
H	0.74660100	–0.38528600	5.24410600

Int5-6

0 1

P	1.45133800	1.07058500	–0.34837500
C	2.08553300	–0.61359400	1.67792500
C	1.88831400	–1.94969400	1.26541700
C	3.29015400	–0.28001100	2.30606400
C	2.91513200	–2.88551800	1.45739900
C	4.29049600	–1.22587300	2.51937000
H	3.42983400	0.74402100	2.64006900
C	4.10556300	–2.53685900	2.08411200
H	2.76316300	–3.90478400	1.11234700
H	5.21332700	–0.93507900	3.01227800
H	4.88115300	–3.28153800	2.23108400
C	0.23271900	2.26716000	–0.90747200
C	0.55591400	3.06448000	–2.01041600
C	–1.03227000	2.35050700	–0.31567200
C	–0.39080900	3.94623200	–2.52368900
H	1.53908900	3.00034700	–2.46983800
C	–1.97499100	3.22862400	–0.84288200

H	–1.27637100	1.75362500	0.56008200
C	–1.65517200	4.02444400	–1.94237700
H	–0.14166400	4.56845000	–3.37688400
H	–2.95820900	3.29613400	–0.38837000
H	–2.39336900	4.71018100	–2.34621800
C	1.49180300	–0.26312900	–1.56089000
C	0.31595000	–0.63381000	–2.22499100
C	2.66061600	–1.01519900	–1.72498100
C	0.31370900	–1.75209300	–3.05253800
H	–0.59625500	–0.05846000	–2.08721700
C	2.65181200	–2.13036300	–2.55763100
H	3.56946400	–0.73952200	–1.19709400
C	1.48046900	–2.49828700	–3.21903800
H	–0.59795800	–2.04160300	–3.56453800
H	3.55847800	–2.71219300	–2.68779800
H	1.47671500	–3.36997900	–3.86590500
C	0.67149600	–2.42663400	0.57322600
C	–0.59511700	–2.19558500	0.93812700
H	–0.83536100	–1.63370000	1.83576200
C	–1.70549200	–2.66543000	0.06886700
O	–1.56248800	–3.59356000	–0.71170800
C	–3.00829300	–1.92917900	0.13845000
C	–3.13060000	–0.69207700	0.77879800
C	–4.12004200	–2.48639500	–0.50237900
C	–4.34770400	–0.01724500	0.78358500
H	–2.28582600	–0.22365100	1.27664400
C	–5.34350200	–1.83137500	–0.49604000
H	–4.01347000	–3.44172300	–1.00546400
C	–5.43891400	–0.60032800	0.14980500
H	–4.44223200	0.94467700	1.27632400

H	–6.21067200	–2.26306900	–0.98335500
Cl	–6.97576600	0.23239900	0.16270100
C	1.10254900	0.51797600	1.36717000
C	1.10418500	1.74173300	2.22180600
H	0.08822600	0.12240600	1.29687300
C	–0.01682200	2.15966000	2.94985300
O	–0.14619800	3.24533600	3.55907900
H	0.83722600	–3.02962500	–0.32140900
O	2.89013300	1.72738200	–0.28881000
H	1.95349200	2.41442100	2.18338100
H	3.46321200	1.74816300	–1.15513300
H	4.81663400	0.50724000	0.49918600
O	5.54243000	0.30384700	–0.11088900
H	5.70582200	–0.64176400	0.00915800
H	5.10623000	1.07202500	–1.66171100
O	4.47165300	1.59162000	–2.20402100
H	4.91760700	2.41829200	–2.44287400
N	–1.14720700	1.26442300	2.98005000
H	–0.88591500	0.30055500	3.16964300
H	–1.77833700	1.58580600	3.70726000

Int6-6

0 1

P	–2.10673200	0.69930100	–0.17635400
C	–1.57765300	0.21693000	1.49300600
C	–0.21058300	0.23073400	1.85562000
C	–2.53988200	–0.24844000	2.39108200
C	0.14069300	–0.23856400	3.12694600
C	–2.16590400	–0.70992800	3.65067800
H	–3.58662100	–0.26952100	2.10677900

C	–0.82254300	–0.71167100	4.01280000
H	1.18182200	–0.20693500	3.43163700
H	–2.92306500	–1.06814300	4.33978800
H	–0.52115100	–1.06852500	4.99229000
C	–3.85285600	0.25619800	–0.35413400
C	–4.85781700	1.21202200	–0.17534100
C	–4.18001300	–1.07958400	–0.60922300
C	–6.19305300	0.82547500	–0.26179100
H	–4.60475100	2.24798600	0.02963400
C	–5.51645200	–1.45908100	–0.67699700
H	–3.40309700	–1.82720000	–0.73758400
C	–6.52108400	–0.50627600	–0.50999200
H	–6.97553600	1.56579500	–0.13110800
H	–5.75203400	–2.50416800	–0.84669600
H	–7.56387400	–0.80225800	–0.56965600
C	–1.99041200	2.49337000	–0.36914400
C	–2.19855700	3.03465400	–1.64474300
C	–1.73783500	3.32980700	0.72166900
C	–2.14303500	4.41265900	–1.82316800
H	–2.41015300	2.38572700	–2.49079100
C	–1.68366500	4.70878700	0.53231100
H	–1.58116500	2.90999500	1.71124200
C	–1.88437000	5.24781500	–0.73618700
H	–2.30177400	4.83435400	–2.81008400
H	–1.48461000	5.35932900	1.37741800
H	–1.84084300	6.32266300	–0.88006200
C	0.83298800	0.74537700	0.95236900
C	2.11167400	0.34525300	0.95124900
H	2.45146300	–0.45301500	1.60172700
C	3.06508800	0.96427600	–0.00674700

O	2.69482400	1.79458400	–0.82279100
C	4.50213200	0.54269600	0.02867800
C	5.07550300	–0.11237700	1.12253200
C	5.29785200	0.85379600	–1.07966300
C	6.42432400	–0.45487100	1.11254200
H	4.49018000	–0.34691100	2.00485000
C	6.64080000	0.50663100	–1.11103500
H	4.84695400	1.36811300	–1.92155600
C	7.18664200	–0.14505500	–0.00773500
H	6.87531500	–0.95378800	1.96295500
H	7.25670500	0.73671900	–1.97340300
Cl	8.87875700	–0.58229700	–0.03206600
C	–1.10064900	–0.11768800	–1.40924500
C	–0.69580000	–1.38186100	–1.19678900
H	–0.85444600	0.49909300	–2.27935000
C	0.16110900	–1.90129000	–2.32131000
O	0.94783600	–1.20408000	–2.96578500
H	0.55833000	1.51749900	0.23495300
N	0.00611900	–3.22392500	–2.57124900
H	–0.53897400	–3.83480200	–1.96661400
H	0.55936800	–3.63450100	–3.31036800
O	–1.62634000	–2.92728700	0.80239600
H	–1.20085600	–2.28491400	0.05059600
H	–1.21399900	–2.69327300	1.64441900
H	–3.41256800	–3.61248200	0.49169700
O	–4.01600300	–4.17569700	–0.02168700
H	–3.38309600	–4.74696600	–0.48195500
H	–1.35000200	–4.37210200	–0.00092400
O	–1.40403800	–5.04409500	–0.72823800
H	–0.86832000	–5.79692500	–0.45123200

TS4-6

0 1

P	–2.10273900	0.72879800	–0.12743100
C	–1.56803200	0.18577700	1.51638800
C	–0.19957000	0.18789500	1.87124800
C	–2.53281100	–0.27104700	2.41502700
C	0.15253900	–0.28643400	3.14010900
C	–2.15750000	–0.73177700	3.67361700
H	–3.58061700	–0.27895800	2.13521300
C	–0.81283100	–0.74586000	4.03031500
H	1.19536800	–0.26546000	3.43990200
H	–2.91519300	–1.08004100	4.36716000
H	–0.51170700	–1.10261200	5.00993500
C	–3.83535500	0.27969800	–0.37944100
C	–4.81665300	1.26215600	–0.53772600
C	–4.17028000	–1.08061600	–0.40260500
C	–6.14145600	0.87518700	–0.73050000
H	–4.55868300	2.31612800	–0.51163700
C	–5.49755100	–1.45200800	–0.58327900
H	–3.41260300	–1.84391400	–0.23637400
C	–6.48030700	–0.47587200	–0.75362100
H	–6.90717500	1.63337300	–0.85732900
H	–5.73998300	–2.50985500	–0.57303900
H	–7.51565500	–0.76859500	–0.89894400
C	–1.94078000	2.52114700	–0.26430300
C	–2.03234700	3.11430000	–1.53003300
C	–1.76678200	3.30802800	0.87802400
C	–1.94252700	4.49716400	–1.64594200
H	–2.18332700	2.50601000	–2.41773400

C	–1.67614300	4.69159600	0.74967100
H	–1.69757900	2.84763500	1.85917200
C	–1.76231100	5.28349300	–0.50819600
H	–2.01218500	4.95998200	–2.62454400
H	–1.53634700	5.30424800	1.63393400
H	–1.68960900	6.36210500	–0.60407700
C	0.84226500	0.69091800	0.96062100
C	2.11183200	0.26474400	0.93401500
H	2.45101400	–0.53881800	1.57853900
C	3.05445000	0.86382600	–0.04830900
O	2.66641100	1.65599900	–0.89351400
C	4.49741600	0.46724600	–0.00181000
C	5.07791400	–0.15542900	1.10714800
C	5.29066000	0.76786500	–1.11484000
C	6.43182100	–0.47719800	1.10696300
H	4.49370600	–0.38086300	1.99263400
C	6.63900800	0.44184300	–1.13572500
H	4.83373400	1.25722400	–1.96831000
C	7.19194000	–0.17856200	–0.01790700
H	6.88840900	–0.95179300	1.96824200
H	7.25368200	0.66447200	–2.00091400
Cl	8.89044000	–0.59028600	–0.02975600
C	–1.08147200	–0.02896100	–1.39584400
C	–0.73492600	–1.31554300	–1.32247700
H	–0.76516200	0.61107400	–2.21936700
C	0.10689600	–1.87106700	–2.44387900
O	0.67179400	–1.13877200	–3.25394000
H	0.57361400	1.47311900	0.25135100
N	0.17892300	–3.21386600	–2.46714900
H	–0.38401000	–3.81887000	–1.85000700

H	0.68473400	–3.63410500	–3.23554000
O	–1.88026700	–2.93730300	0.76534500
H	–1.11769300	–2.03733600	–0.37761900
H	–1.33534900	–2.98604200	1.55935300
H	–3.43143100	–3.72031900	0.71075700
O	–4.14952500	–4.26220100	0.30472100
H	–3.62651100	–4.76931600	–0.33224700
H	–1.63688600	–4.01627800	–0.13921700
O	–1.45774000	–4.81419400	–0.80746000
H	–0.95343700	–5.45552900	–0.29341200

Int7-6

0 1

P	–2.13608600	0.68785100	–0.12312400
C	–1.58100200	0.23430700	1.53873000
C	–0.21460300	0.29051600	1.89773700
C	–2.53987300	–0.20451400	2.45377700
C	0.14331400	–0.11782400	3.18781300
C	–2.15891500	–0.59646200	3.73378100
H	–3.58484500	–0.25783500	2.16754100
C	–0.81545500	–0.56052800	4.09447700
H	1.18383300	–0.05705300	3.49008400
H	–2.91023900	–0.93364800	4.43943500
H	–0.51010300	–0.86623500	5.08988700
C	–3.82748100	0.10398100	–0.36704900
C	–4.89625100	1.00452400	–0.38691700
C	–4.04455500	–1.27216100	–0.50905200
C	–6.19101300	0.52006400	–0.55957100
H	–4.72528900	2.07049200	–0.27227000
C	–5.34180000	–1.74233700	–0.67674900

H	–3.22759300	–1.98738700	–0.46226800
C	–6.41214400	–0.84767900	–0.70615000
H	–7.02423900	1.21459500	–0.58015400
H	–5.49161800	–2.81173900	–0.78441300
H	–7.42355700	–1.21762800	–0.84272800
C	–2.09369900	2.47825500	–0.33195300
C	–2.32597500	3.01033200	–1.60745500
C	–1.86993200	3.31936500	0.76139800
C	–2.32570900	4.38929600	–1.78216300
H	–2.51241200	2.35491900	–2.45436900
C	–1.87031100	4.69942500	0.57343600
H	–1.69264400	2.90452100	1.74931400
C	–2.09645600	5.23138200	–0.69353100
H	–2.50339100	4.80638700	–2.76765800
H	–1.69268700	5.35593200	1.41848500
H	–2.09497700	6.30726700	–0.83580300
C	0.81596100	0.78147300	0.96766800
C	2.09112600	0.37240000	0.95457100
H	2.43812900	–0.40426200	1.62727600
C	3.02580000	0.94641700	–0.05076800
O	2.62905800	1.71762500	–0.91100400
C	4.46846400	0.54850400	–0.00957500
C	5.05619400	–0.06504800	1.10072100
C	5.25378500	0.83484500	–1.13208100
C	6.40881500	–0.39178300	1.09281100
H	4.47898100	–0.28068500	1.99301300
C	6.60087900	0.50437600	–1.16034900
H	4.79161000	1.31655300	–1.98704800
C	7.16084200	–0.10692800	–0.04097400
H	6.87039200	–0.85997700	1.95494300

H	7.20932100	0.71642800	–2.03255800
Cl	8.85750700	–0.52502500	–0.06259800
C	–1.08124200	–0.04992200	–1.37294100
C	–0.63505600	–1.30237300	–1.28389900
H	–0.83355400	0.56621400	–2.23612700
C	0.19909900	–1.86711500	–2.41093300
O	0.63847700	–1.12686200	–3.29456600
H	0.52941200	1.53392000	0.23310400
N	0.36642000	–3.18723200	–2.31716000
H	–0.18685900	–3.79066900	–1.55738000
H	0.87583800	–3.61418400	–3.08175900
O	–1.89130800	–2.98921200	1.32350400
H	–0.86911100	–1.94403000	–0.43387800
H	–1.21954600	–2.62118400	1.90950000
H	–3.58731900	–3.98530200	0.47801100
O	–3.64828300	–4.43348800	–0.37611800
H	–2.68343500	–4.53003900	–0.59579700
H	–1.41507700	–3.59626200	0.65273900
O	–0.99228700	–4.42852600	–0.55815500
H	–0.59237800	–5.25585300	–0.26613100

Int8-6

0 1

P	2.27667100	–0.14005200	0.34638700
C	1.78656800	–1.22317200	–1.05079400
C	0.50221900	–1.79361100	–1.14874600
C	2.71923000	–1.42419100	–2.07081900
C	0.19449400	–2.56186900	–2.28135600
C	2.38834500	–2.17432600	–3.19499000
H	3.71215500	–0.99366300	–1.98648500

C	1.12267800	–2.74713200	–3.29804700
H	–0.78204000	–3.03201900	–2.34596700
H	3.12255500	–2.31880100	–3.98069800
H	0.86204800	–3.34599000	–4.16460500
C	3.71937400	0.95535500	0.05526300
C	3.77816800	1.73251800	–1.10459100
C	4.72491000	1.06434900	1.01838900
C	4.85266100	2.59464800	–1.31018000
H	2.99006900	1.66535000	–1.84999800
C	5.77584400	1.95721500	0.82659600
H	4.68749900	0.45722100	1.91758500
C	5.84636100	2.71528200	–0.34091600
H	4.90434300	3.17992900	–2.22259400
H	6.54597300	2.05085100	1.58561000
H	6.67433900	3.40009700	–0.49467000
C	1.00596300	1.24045000	0.07095900
C	0.89052800	2.22293800	1.06605300
C	0.24812000	1.40001300	–1.09480900
C	0.02324800	3.30209800	0.92237000
H	1.49331100	2.15485800	1.97001400
C	–0.62151000	2.48096400	–1.24559700
H	0.32500000	0.67944600	–1.90367100
C	–0.74360900	3.42996900	–0.23492700
H	–0.05122900	4.04373800	1.71186000
H	–1.20305500	2.57768700	–2.15759200
H	–1.42460000	4.26754800	–0.34992600
C	–0.52081300	–1.58797800	–0.10976800
C	–1.83171200	–1.45341800	–0.35170200
H	–2.22376500	–1.46069800	–1.36412000
C	–2.76600900	–1.24329000	0.78403700

O	–2.44409700	–1.50972200	1.93213400
C	–4.12386000	–0.68465400	0.49366700
C	–4.40816400	0.00481700	–0.68848800
C	–5.11980900	–0.82903400	1.46515300
C	–5.67373300	0.54132300	–0.90410900
H	–3.64179400	0.15263500	–1.44244300
C	–6.39139300	–0.31272900	1.25864200
H	–4.88627900	–1.35633600	2.38416700
C	–6.64936000	0.36804100	0.07108300
H	–5.89807300	1.08620500	–1.81420200
H	–7.17032000	–0.43201900	2.00362500
Cl	–8.24570900	1.02674300	–0.20026100
C	1.77063200	–0.50442900	2.06428400
C	2.46531800	–1.45034700	2.68915100
H	0.92889000	0.02532500	2.49415300
C	3.55603300	–2.06570600	1.87872900
O	3.61646700	–1.53695700	0.68397600
H	–0.19495900	–1.52553300	0.92717000
N	4.34130900	–2.99571600	2.28596000
H	4.09223400	–3.23027400	3.24788700
H	2.27222900	–1.78054300	3.70570500

TS5-6

0 1

P	2.68174400	0.13447600	0.40181600
C	1.87647900	–1.30807000	–0.38365600
C	0.47965700	–1.56636100	–0.40584300
C	2.76894600	–2.23168400	–0.94455300
C	0.06118400	–2.76666400	–0.98870400
C	2.31722800	–3.41836800	–1.51013100

H	3.83429100	–2.03354400	–0.94449000
C	0.95504800	–3.68547500	–1.52692800
H	–0.99810100	–2.98735800	–1.03422500
H	3.02920200	–4.11802900	–1.93405100
H	0.57999800	–4.60493900	–1.96472000
C	4.34131100	0.31677800	–0.31689400
C	4.55209800	1.13856200	–1.42819200
C	5.41221700	–0.39078400	0.24587100
C	5.82838000	1.24861500	–1.97333700
H	3.73456400	1.70040900	–1.86707100
C	6.68362900	–0.27489800	–0.30645900
H	5.25721700	–1.03619300	1.10567800
C	6.89214400	0.54442800	–1.41449300
H	5.98925500	1.89009800	–2.83328500
H	7.51031600	–0.82362300	0.13211400
H	7.88604300	0.63571900	–1.84071500
C	1.78878200	1.67181200	0.08698900
C	1.64916100	2.60952200	1.11321700
C	1.26138200	1.92250400	–1.18673100
C	0.98061600	3.80515800	0.86058700
H	2.04829200	2.40573600	2.10285200
C	0.59902600	3.12048800	–1.42794300
H	1.34869300	1.17836500	–1.97494400
C	0.45947300	4.05976100	–0.40533000
H	0.86496100	4.53359400	1.65609600
H	0.18386300	3.31669000	–2.41078400
H	–0.06513400	4.99043600	–0.59638500
C	–0.54614800	–0.62562200	0.12782900
C	–1.91025800	–0.80350900	–0.04923100
H	–2.35469400	–1.77234100	–0.23374700

C	–2.75926800	0.32030400	0.21603300
O	–2.34767400	1.41611400	0.62905000
C	–4.24606700	0.16648700	–0.01031300
C	–4.79847200	–0.83693800	–0.81203400
C	–5.09983100	1.09240200	0.59630900
C	–6.17524600	–0.92413700	–0.99881500
H	–4.15791600	–1.55155200	–1.31808000
C	–6.47748700	1.01691400	0.43038800
H	–4.66288400	1.87739600	1.20430300
C	–6.99726700	0.00303900	–0.36833700
H	–6.60260800	–1.69751200	–1.62773700
H	–7.13865500	1.73093800	0.90953800
Cl	–8.73163000	–0.10403700	–0.59054700
C	3.00889300	–0.09118800	2.16164900
C	2.24517700	–0.82155100	2.97896300
H	3.93421000	0.37221200	2.49531500
C	0.96886700	–1.47692800	2.50068600
O	0.93676700	–2.71272100	2.45971500
H	–0.26305100	0.41841100	0.15568800
N	0.00077800	–0.64690200	2.09766800
H	0.25669500	0.32493800	2.26559300
H	2.56087500	–0.98478600	4.00772300

Int9-6

0 1

P	2.71504000	–0.03684000	0.51274800
C	1.67342300	–1.17976600	–0.46978200
C	0.26356100	–1.07752400	–0.60579600
C	2.37471500	–2.16520600	–1.18206400
C	–0.36849700	–1.96519500	–1.47507700

C	1.71061900	–3.04738500	–2.02682900
H	3.45052300	–2.25225800	–1.08702800
C	0.33460300	–2.93766100	–2.18042000
H	–1.44543000	–1.88203900	–1.57825800
H	2.27301300	–3.80518400	–2.56138800
H	–0.19797700	–3.61173100	–2.84415100
C	4.44524100	–0.37400800	0.08736800
C	5.06935300	0.33607000	–0.94255300
C	5.13763400	–1.38158600	0.77100900
C	6.38645100	0.03936900	–1.28269900
H	4.53657600	1.11779000	–1.47541100
C	6.45277400	–1.67170800	0.42295800
H	4.65268600	–1.94527300	1.56352800
C	7.07649800	–0.96099500	–0.60151200
H	6.87269500	0.59297800	–2.07894000
H	6.98909100	–2.45191300	0.95264100
H	8.10377100	–1.18758300	–0.86851600
C	2.38962600	1.67741000	0.04451900
C	2.69547700	2.70185900	0.94726300
C	1.89303700	1.97161800	–1.22922500
C	2.49474400	4.02592300	0.57049900
H	3.07980200	2.46913100	1.93666100
C	1.69656900	3.30112600	–1.59441900
H	1.65974600	1.17368900	–1.92911200
C	1.99544000	4.32398400	–0.69679600
H	2.72597700	4.82394400	1.26802600
H	1.30697100	3.53452400	–2.57959100
H	1.83680000	5.35824500	–0.98468200
C	–0.59078500	–0.02912700	0.12713800
C	–2.05049100	–0.31452600	0.22609100

H	–2.36734800	–1.19631200	0.76852500
C	–2.94313600	0.59013000	–0.32102300
O	–2.64612200	1.67729400	–0.90801000
C	–4.42768000	0.28066900	–0.19522500
C	–4.94900400	–0.98853500	0.08409200
C	–5.32678700	1.33165600	–0.40003000
C	–6.32151100	–1.20133200	0.17757900
H	–4.28286500	–1.83559100	0.21343600
C	–6.70255000	1.14444200	–0.30709400
H	–4.91447800	2.30532800	–0.64234300
C	–7.18333700	–0.12693600	–0.01627500
H	–6.71752500	–2.18914100	0.38851000
H	–7.39166600	1.96825000	–0.46160700
Cl	–8.91618200	–0.38729200	0.09380600
C	2.71297900	–0.22100900	2.32858900
C	1.63016400	–0.52740400	3.04538600
H	3.69289100	–0.11007100	2.78577600
C	0.36300900	–0.77238200	2.28273900
O	–0.20857000	–1.84978000	2.31829800
H	–0.51630800	0.91286700	–0.43286100
N	0.09688500	0.22583600	1.40077000
H	0.39016700	1.16793000	1.62874900
H	1.67890900	–0.71382000	4.11395200

Int10-6

0 1

P	2.93009600	–0.18969600	0.47620000
C	1.81635900	–1.41111300	–0.31869800
C	0.40662600	–1.28554900	–0.41587600
C	2.46065600	–2.49714500	–0.93318000

C	–0.28604000	–2.23819700	–1.16103100
C	1.73918400	–3.44660600	–1.64729600
H	3.53555600	–2.61117700	–0.86261200
C	0.36252000	–3.30722600	–1.77171900
H	–1.36160000	–2.13080400	–1.24609900
H	2.25834000	–4.28016000	–2.10758400
H	–0.21210400	–4.03271600	–2.33907800
C	4.63005700	–0.66075700	0.05045900
C	5.24447900	–0.11752000	–1.08192200
C	5.30577000	–1.60293300	0.83609300
C	6.53493000	–0.51395400	–1.42242900
H	4.72372700	0.61196000	–1.69497800
C	6.59441600	–1.99420200	0.48717100
H	4.82799600	–2.03764500	1.71004400
C	7.20853500	–1.44876400	–0.63954100
H	7.01311800	–0.08871300	–2.29850800
H	7.11803900	–2.72349800	1.09622400
H	8.21539900	–1.75317500	–0.90696900
C	2.68841400	1.45904400	–0.22252600
C	3.26067500	2.55311100	0.43581300
C	2.00926000	1.62934200	–1.43176000
C	3.14249400	3.82350400	–0.11769500
H	3.79035200	2.42017400	1.37511200
C	1.88696900	2.90833400	–1.97254600
H	1.57902800	0.77742800	–1.95073400
C	2.45258500	4.00164400	–1.31780100
H	3.58174300	4.67497000	0.39103400
H	1.35252200	3.04664400	–2.90634500
H	2.35570700	4.99536900	–1.74300100
C	–0.38391700	–0.13263600	0.22381600

C	–1.84402200	–0.38015800	0.47071800
H	–2.12841700	–0.92271800	1.36368900
C	–2.73696500	–0.09349800	–0.54534500
O	–2.39668200	0.34929400	–1.69521900
C	–4.21625600	–0.29802500	–0.30110200
C	–4.78313600	–0.39588500	0.97437400
C	–5.05906200	–0.37439800	–1.41344600
C	–6.15193900	–0.58594400	1.13929200
H	–4.15808200	–0.30607900	1.85759500
C	–6.42930100	–0.56817300	–1.27186400
H	–4.61452900	–0.27541300	–2.39803600
C	–6.95831400	–0.67452500	0.00950700
H	–6.58780800	–0.65515900	2.13018500
H	–7.07745000	–0.63363700	–2.13940200
Cl	–8.68488800	–0.91445700	0.20750600
C	2.99410900	–0.11385000	2.29978300
C	1.93007300	–0.27527500	3.08773300
H	3.99464000	0.02448100	2.70167800
C	0.63287700	–0.58529400	2.40586900
O	0.03432000	–1.62851700	2.61609700
H	–0.32886400	0.70536700	–0.48583300
N	0.37139300	0.28586700	1.39662800
H	0.60076100	1.28331700	1.49000700
H	2.01193100	–0.30775400	4.16995300
O	–2.36963300	2.48039400	1.17676800
H	–2.28706400	1.50598100	1.01873900
H	–2.87206100	2.57118100	1.99740400
H	–0.67473900	3.02092200	1.25638200
O	0.30205100	3.09502500	1.28724200
H	0.56903600	3.36738100	0.39914100

H	–3.29983600	2.91200100	–0.55296100
O	–3.61018500	2.83127500	–1.46641100
H	–3.22460200	1.97173100	–1.72896100

TS6-6

0 1

P	2.90383200	–0.18088200	0.44217800
C	1.71870100	–1.42208000	–0.21031400
C	0.30983800	–1.25087200	–0.24259100
C	2.28895400	–2.59291300	–0.73060900
C	–0.46106400	–2.27029200	–0.79641700
C	1.49276900	–3.59587700	–1.27318700
H	3.36256400	–2.73625900	–0.71647600
C	0.11454600	–3.43120500	–1.30643000
H	–1.53936400	–2.16032000	–0.81581800
H	1.95522000	–4.49542400	–1.66448200
H	–0.52020500	–4.20605000	–1.72456300
C	4.56548100	–0.75131200	–0.02371000
C	5.15239900	–0.31069000	–1.21363200
C	5.23920000	–1.66588000	0.79600700
C	6.41162400	–0.78049800	–1.57752000
H	4.63536100	0.39742000	–1.85414200
C	6.49645700	–2.13116500	0.42428300
H	4.78260500	–2.02266500	1.71561400
C	7.08271000	–1.68721200	–0.76030700
H	6.86784000	–0.43376700	–2.49875500
H	7.01739700	–2.83870700	1.06074700
H	8.06543100	–2.04856900	–1.04605400
C	2.70423200	1.43034500	–0.35017400
C	3.28714300	2.54812400	0.25509000

C	2.03451400	1.54759800	–1.57106000
C	3.18903400	3.79032400	–0.36295400
H	3.80678100	2.45507600	1.20472800
C	1.93217700	2.79866700	–2.17632500
H	1.59514100	0.67549700	–2.04793900
C	2.50759500	3.91651600	–1.57371200
H	3.63650500	4.66060900	0.10529000
H	1.40499800	2.89656500	–3.11938600
H	2.42524500	4.88852200	–2.04930800
C	–0.35531300	0.02014500	0.28817800
C	–1.83774800	–0.03669200	0.59915400
H	–2.11100200	–0.76129000	1.36506700
C	–2.70526200	0.01180400	–0.56083300
O	–2.31314900	0.34371300	–1.68827700
C	–4.17753700	–0.24638500	–0.36330600
C	–4.77941000	–0.24677200	0.89811400
C	–4.96355900	–0.47922800	–1.49467500
C	–6.14477000	–0.47948000	1.03208500
H	–4.19079800	–0.04673800	1.78746000
C	–6.32660300	–0.72498200	–1.37959800
H	–4.48981800	–0.46513600	–2.47067300
C	–6.89882400	–0.72054600	–0.11125100
H	–6.61663200	–0.47086600	2.00842400
H	–6.93686300	–0.91499900	–2.25588600
Cl	–8.61629700	–1.02194400	0.04960900
C	3.05870400	–0.00357900	2.25386100
C	2.02165800	–0.05792700	3.09134700
H	4.08126200	0.09954700	2.60755600
C	0.68373600	–0.32875200	2.47457600
O	0.01572100	–1.30104900	2.78814400

H	–0.23878000	0.78501600	–0.49121900
N	0.47146200	0.47218200	1.39462100
H	0.66863200	1.49253500	1.44256300
H	2.14602500	–0.03490200	4.16969700
O	–2.09362000	2.50093100	1.25096200
H	–2.04807400	1.17900300	1.03892200
H	–2.53083500	2.66486200	2.09595800
H	–0.65013900	3.00498400	1.24747000
O	0.35759900	3.18675600	1.23137600
H	0.57231300	3.40923400	0.31620400
H	–3.08498100	2.88084200	–0.14402700
O	–3.59764200	2.96750100	–0.98087300
H	–3.24605600	2.24905200	–1.52053600

TS7-6

0 1

P	2.62129000	–0.02817300	0.55004100
C	1.77893200	–1.19773400	–0.59140200
C	0.38329700	–1.18044800	–0.83161600
C	2.58254700	–2.12648600	–1.26736700
C	–0.15559700	–2.08868400	–1.73806300
C	2.02023700	–3.03187800	–2.16255700
H	3.65344800	–2.15284500	–1.10450700
C	0.65047500	–3.00999300	–2.40156600
H	–1.22770100	–2.06682500	–1.91261100
H	2.65808800	–3.74661800	–2.67120600
H	0.20696600	–3.71087700	–3.10186000
C	4.40637500	–0.23545200	0.23875700
C	5.07277900	0.59825700	–0.66432900
C	5.10575100	–1.26480000	0.88355000

C	6.42884100	0.40474100	–0.91677400
H	4.54292000	1.39982600	–1.16897100
C	6.45957700	–1.45322500	0.62493700
H	4.59606800	–1.92766100	1.57767200
C	7.12167000	–0.61781800	–0.27361700
H	6.94215400	1.05733300	–1.61525800
H	6.99597800	–2.25188100	1.12647000
H	8.17872300	–0.76445300	–0.47143100
C	2.25846300	1.69338100	0.14527700
C	2.38917200	2.67040200	1.13635300
C	1.92126800	2.04500400	–1.16394500
C	2.17539900	4.00533400	0.81135200
H	2.64692100	2.39092900	2.15429600
C	1.70562100	3.38595700	–1.47741600
H	1.82674600	1.28347000	–1.93380500
C	1.83238700	4.36266300	–0.49289100
H	2.27219100	4.76690700	1.57817900
H	1.43754300	3.66295200	–2.49159300
H	1.66241900	5.40552500	–0.74061800
C	–0.49170400	–0.16325600	–0.14777900
C	–1.96979800	–0.35733800	0.10559400
H	–2.27619300	–1.32135400	0.49850400
C	–2.90829300	0.44324700	–0.61831500
O	–2.59872300	1.31899700	–1.44323600
C	–4.37969900	0.25102800	–0.31393800
C	–4.84432200	–0.44738300	0.80480500
C	–5.30968600	0.80863200	–1.19498400
C	–6.20821900	–0.59819500	1.03674800
H	–4.14105700	–0.86464600	1.51793700
C	–6.67664200	0.66458700	–0.98472400

H	–4.94093700	1.36084300	–2.05287700
C	–7.10742200	–0.04181800	0.13329000
H	–6.56717300	–1.13462300	1.90839000
H	–7.39690000	1.09296700	–1.67347400
Cl	–8.82718200	–0.22932300	0.41442900
C	2.51682900	–0.40015200	2.33074200
C	1.39371500	–0.83831600	2.90052900
H	3.45821300	–0.32439700	2.86780400
C	0.20957300	–1.01321000	1.99401700
O	–0.36838600	–2.08854000	1.93622300
H	–0.39678700	0.78107500	–0.70102300
N	0.01224700	0.12014600	1.21739300
H	–1.26995000	0.26983000	1.28599200
H	1.36306500	–1.17134500	3.93444700

7

0 1

P	2.27311600	0.00029200	0.62894500
C	1.34899600	–1.14430300	–0.50011400
C	0.08916600	–0.68687200	–0.90570300
C	1.87718400	–2.31431600	–1.05789300
C	–0.61525400	–1.37649700	–1.89337800
C	1.15426800	–3.01578100	–2.01747400
H	2.84652900	–2.68733800	–0.75041400
C	–0.08386500	–2.53868000	–2.44392900
H	–1.57781200	–1.00964900	–2.23236000
H	1.56319700	–3.92860900	–2.43813700
H	–0.64083300	–3.07605600	–3.20527100
C	3.88532900	–1.00423700	0.61588500
C	4.88070500	–0.85510800	–0.35573100

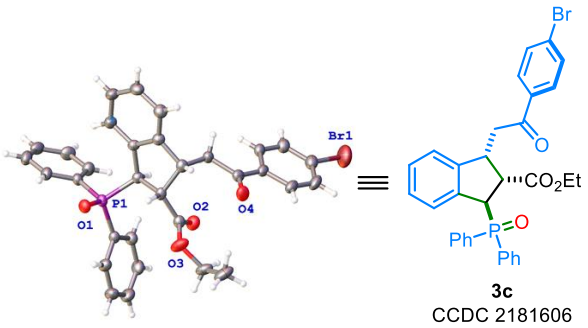
C	4.03958100	–2.01960900	1.56916700
C	6.00096300	–1.68692100	–0.36759600
H	4.78548500	–0.08822700	–1.12021400
C	5.15298700	–2.85690700	1.56013900
H	3.27354000	–2.16846400	2.32909100
C	6.14018700	–2.68901600	0.59000000
H	6.76445400	–1.55193200	–1.12799600
H	5.25048900	–3.63782500	2.30835200
H	7.01187800	–3.33615500	0.58041300
C	2.88009400	1.45090900	–0.31660300
C	3.82889200	2.29659100	0.26779100
C	2.42852300	1.71232300	–1.61260600
C	4.30487300	3.40235900	–0.43135300
H	4.20386900	2.09138100	1.26675100
C	2.91450700	2.81611800	–2.31197700
H	1.70619500	1.05575100	–2.08933000
C	3.84855700	3.66414500	–1.72223200
H	5.03707700	4.05613100	0.03191400
H	2.56105500	3.00963700	–3.31979700
H	4.22403500	4.52399500	–2.26791000
C	–0.45128400	0.54775900	–0.19792400
C	–1.87228100	0.30700400	0.33587900
H	–1.97115200	–0.71375800	0.72094000
C	–2.95660500	0.58010500	–0.68000000
O	–2.71449400	1.07080200	–1.76950100
C	–4.37201400	0.25426400	–0.30411400
C	–4.72326400	–0.20305400	0.96928700
C	–5.36635400	0.42460800	–1.27291200
C	–6.05011300	–0.48757600	1.27524600
H	–3.97096800	–0.33758500	1.73910900

C	–6.69411200	0.14001100	–0.98544500
H	–5.08447000	0.78176800	–2.25764800
C	–7.01674600	–0.31404600	0.29087600
H	–6.32875700	–0.83818100	2.26256100
H	–7.46732400	0.26639200	–1.73518700
Cl	–8.68483200	–0.67722100	0.66647400
C	2.42577500	0.38716100	2.43298100
C	1.45443800	1.14541000	2.92901500
H	3.32943300	0.11843700	2.96804600
C	0.30098100	1.41788800	2.00588200
O	–0.66349300	2.10593400	2.35172400
H	–0.48595400	1.38710200	–0.90725500
N	0.51924200	0.78623200	0.84633200
H	–2.05684300	0.98406500	1.17780200
H	1.43679900	1.56757600	3.92921700

9. Crystal structures

9.1 Crystal structure of 3c

Preparation of the single crystals of **3c**: 10.0 mg of pure compound **3c** was dissolved in the combined solvents of dichloromethane and ethanol (1.5 mL, v/v = 1:2) at room temperature. The bottle was sealed by a piece of plastic film with several tiny holes, thus allowing slow evaporation of the solvents at 4 ^{o}C. After about seven days, several small particles were observed at the bottom of the bottle. The crystals were chosen and subjected to the single crystal X-ray diffraction analysis for the determination of the structure and relative configuration of **3c**. The data were collected on a SuperNova, Dual, Cu at zero, AtlasS2 diffractometer. The crystal was kept at 240.00(10) K during data collection.



3c
CCDC 2181606

Table S3. Crystal data and structure refinement for **3c**.

Bond precision: C-C = 0.0083 A Wavelength=1.54184

Cell: a=21.1054(10) b=11.2350(3) c=24.6803(12)

alpha=90 beta=106.321(5) gamma=90

Temperature: 240 K

	Calculated	Reported
Volume	5616.3(4)	5616.3(4)
Space group	P 2/n	P 1 2/n 1
Hall group	-P 2yac	-P 2yac
Moiety formula	$C_{32}H_{28}BrO_4P$	$C_{32}H_{28}BrO_4P$
Sum formula	$C_{32}H_{28}BrO_4P$	$C_{32}H_{28}BrO_4P$
Mr	587.41	587.42
Dx,g cm-3	1.389	1.389
Z	8	8
Mu (mm-1)	2.819	2.819
F000	2416.0	2416.0
F000'	2418.93	
h,k,lmax	26,13,30	25,13,30
Nref	11342	11000
Tmin,Tmax	0.700,0.776	0.598,1.000
Tmin'	0.624	

Correction method= # Reported T Limits: Tmin=0.598 Tmax=1.000 AbsCorr =

MULTI-SCAN

Data completeness= 0.970 Theta(max)= 73.671

R(reflections)= 0.0807(7356) wR2(reflections)= 0.2568(11000)

S = 1.043 Npar= 727

9.2 Crystal structure of 5a

Preparation of the single crystals of **5a**: 15.0 mg of pure compound **5a** was dissolved in the combined solvents of dichloromethane and methanol (2.0 mL, v/v = 3:1) at room temperature. The bottle was sealed by a piece of plastic film with several tiny holes, thus allowing slow evaporation of the solvents at 25 ^{o}C. After about one day, several small particles were observed at the bottom of the bottle. The crystals were chosen and subjected to the single crystal X-ray diffraction analysis for the determination of the structure and relative configuration of **5a**. The data were collected on a XtaLAB AFC12 (RINC): Kappa single diffractometer. The crystal was kept at 170(2) K during data collection.

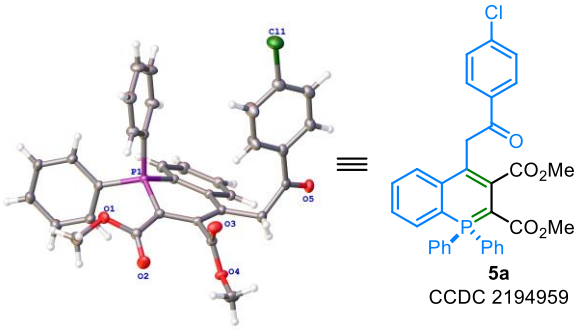


Table S4. Crystal data and structure refinement for **5a**.

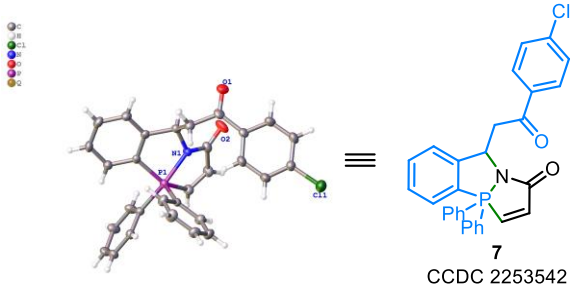
Identification code	**5a**
Empirical formula	$C_{33}H_{26}ClO_5P$
Formula weight	568.96
Temperature/K	170(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	14.9304(2)
b/Å	9.09920(10)

c/Å	21.2031(3)
α/°	90
β/°	106.572(2)
γ/°	90
Volume/Å^3	2760.89(7)
Z	4
ρ_{calc}g/cm^3	1.369
μ/mm^{-1}	2.119
F(000)	1184.0
Crystal size/mm^3	0.15 × 0.12 × 0.1
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	6.176 to 143.3
Index ranges	-18 ≤ h ≤ 17, -5 ≤ k ≤ 10, -18 ≤ l ≤ 25
Reflections collected	13610
Independent reflections	5251 [R_{int} = 0.0275, R_{sigma} = 0.0327]
Data/restraints/parameters	5251/0/363
Goodness-of-fit on F^2	1.053
Final R indexes [I>=2σ (I)]	R_1 = 0.0367, wR_2 = 0.0987
Final R indexes [all data]	R_1 = 0.0399, wR_2 = 0.1008
Largest diff. peak/hole / e Å^{-3}	0.31/-0.39

9.3 Crystal structure of 7

Preparation of the single crystals of **7**: 15.0 mg of pure compound **7** was dissolved in the combined solvents of dichloromethane and ethanol (2.0 mL, v/v = 2:1) at room temperature. The bottle was sealed by a piece of plastic film with several tiny holes, thus allowing slow evaporation of the solvents at 25 ^{o}C. After about three days, several small particles were observed at the bottom of the bottle. The crystals were chosen and subjected to the single crystal X-ray diffraction analysis for the determination of the structure and relative configuration of **7**. The data were collected on a CCD area detector diffractometer. The crystal was kept at 296.15 K during data

collection.



7

CCDC 2253542

Table S5. Crystal data and structure refinement for **7**.

Identification code	**7**
Empirical formula	$C_{30}H_{23}ClNO_2P$
Formula weight	495.91
Temperature/K	296.15
Crystal system	triclinic
Space group	P-1
a/Å	9.7322(16)
b/Å	10.0029(16)
c/Å	12.561(2)
α/°	89.918(4)
β/°	88.573(4)
γ/°	81.090(4)
Volume/Å^3	1207.7(3)
Z	2
ρ_{calc}g/cm^3	1.364
μ/mm^{-1}	0.254
F(000)	516.0
Crystal size/mm^3	0.14 × 0.12 × 0.11
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/ °	4.122 to 50.148
Index ranges	-11 ≤ h ≤ 11, -11 ≤ k ≤ 11, -14 ≤ l ≤ 14

Reflections collected	25964
Independent reflections	4274 [R_{int} = 0.1030, R_{sigma} = 0.0924]
Data/restraints/parameters	4274/0/316
Goodness-of-fit on F^2	1.040
Final R indexes [I>=2σ (I)]	R_1 = 0.0581, wR_2 = 0.0897
Final R indexes [all data]	R_1 = 0.1320, wR_2 = 0.1155
Largest diff. peak/hole / e $Å^{-3}$	0.23/-0.31

9.4 Crystal structure of 15

Preparation of the single crystals of **15**: 15.0 mg of pure compound **15** was dissolved in the combined solvents of dichloromethane and ethanol (2.0 mL, v/v = 2:1) at room temperature. The bottle was sealed by a piece of plastic film with several tiny holes, thus allowing slow evaporation of the solvents at 25 ^{o}C. After about three days, several small particles were observed at the bottom of the bottle. The crystals were chosen and subjected to the single crystal X-ray diffraction analysis for the determination of the structure and relative configuration of **15**. The data were collected on a SuperNova, Dual, Cu at zero, AtlasS2 diffractometer. The crystal was kept at 149.99(10) K during data collection.

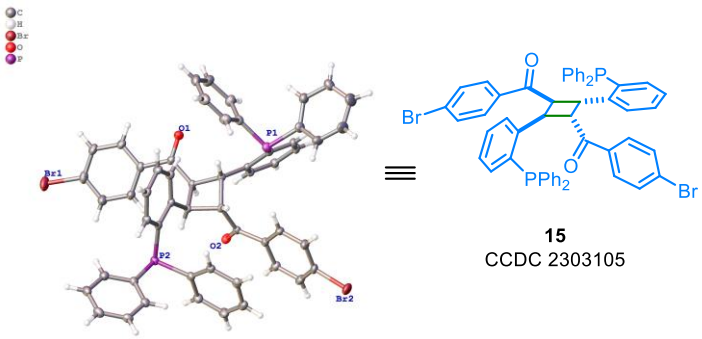


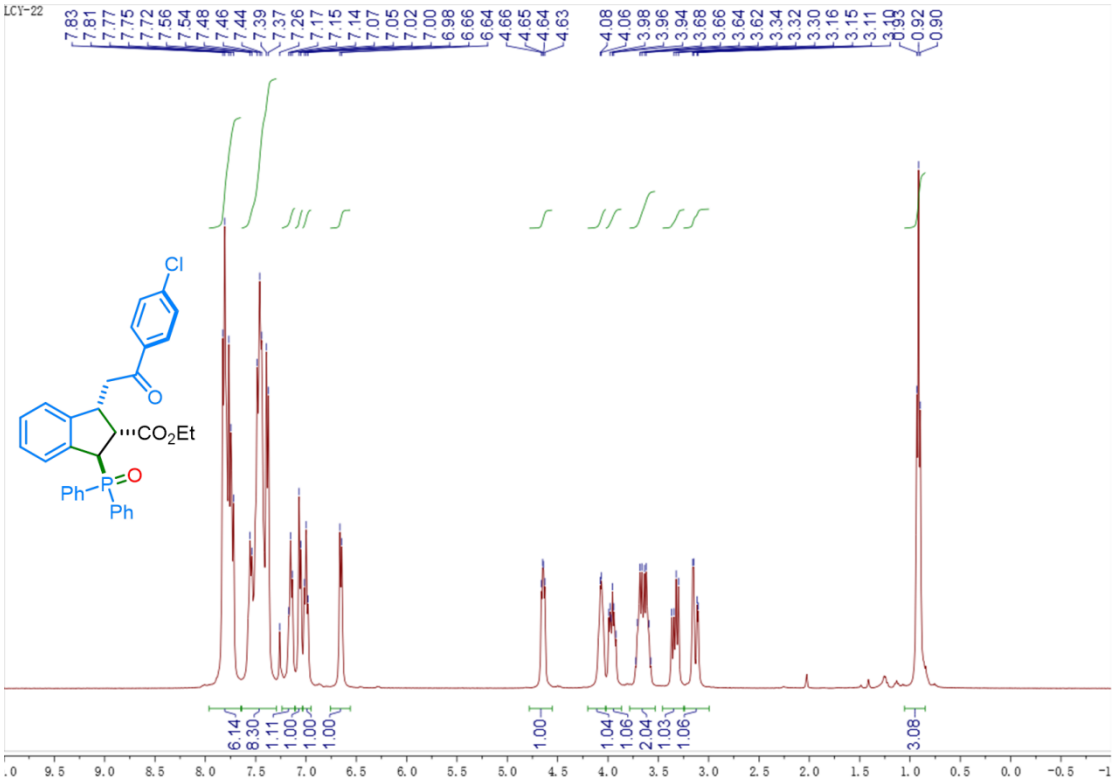
Table S6. Crystal data and structure refinement for **15**.

Identification code	**15**
Empirical formula	$C_{54}H_{40}Br_2O_2P_2$
Formula weight	942.62
Temperature/K	149.99(10)
Crystal system	triclinic

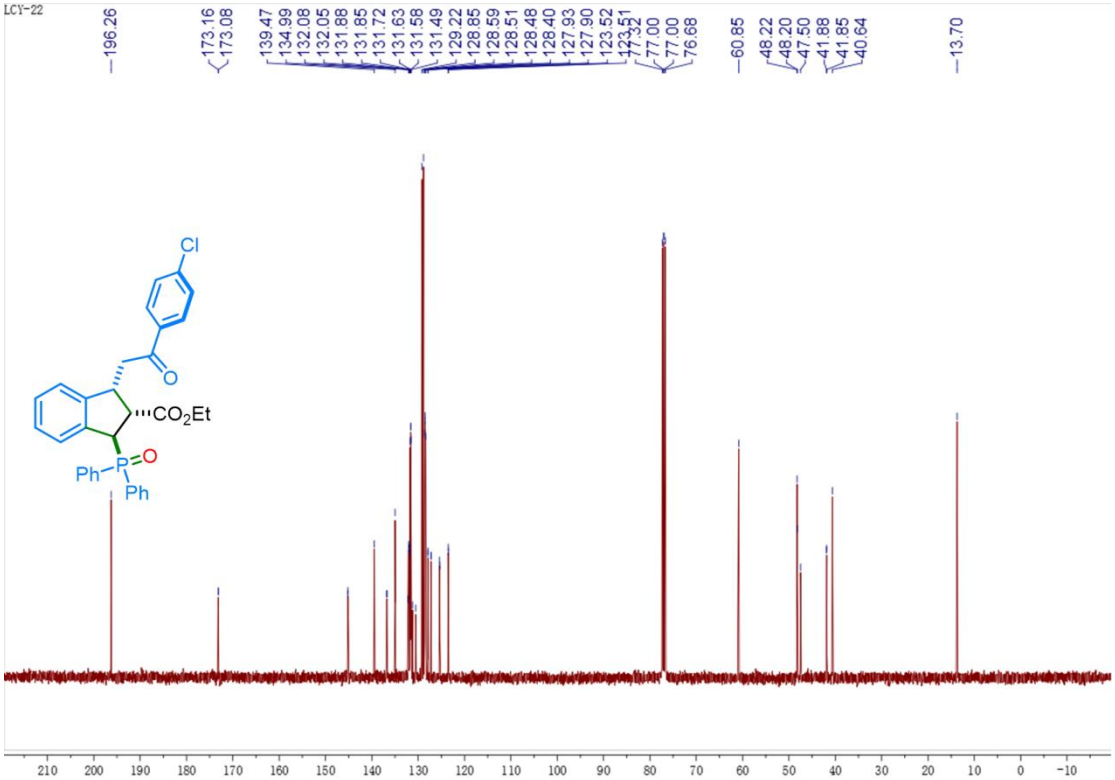
Space group	P-1
a/Å	14.3800(5)
b/Å	15.4793(7)
c/Å	17.3460(6)
α/°	101.507(3)
β/°	108.532(3)
γ/°	108.298(4)
Volume/$Å^3$	3278.1(2)
Z	3
$\rho_{calc}g/cm^3$	1.432
μ/mm^{-1}	3.372
F(000)	1440.0
Crystal size/mm^3	0.14 × 0.12 × 0.11
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	5.698 to 148.9
Index ranges	$-17 \leq h \leq 17$, $-19 \leq k \leq 19$, $-21 \leq l \leq 18$
Reflections collected	23821
Independent reflections	12906 [R_{int} = 0.0417, R_{sigma} = 0.0570]
Data/restraints/parameters	12906/0/830
Goodness-of-fit on F^2	1.038
Final R indexes [I>=2σ (I)]	R_1 = 0.0534, wR_2 = 0.1433
Final R indexes [all data]	R_1 = 0.0753, wR_2 = 0.1573
Largest diff. peak/hole / e $Å^{-3}$	1.42/-1.10

10. NMR spectra

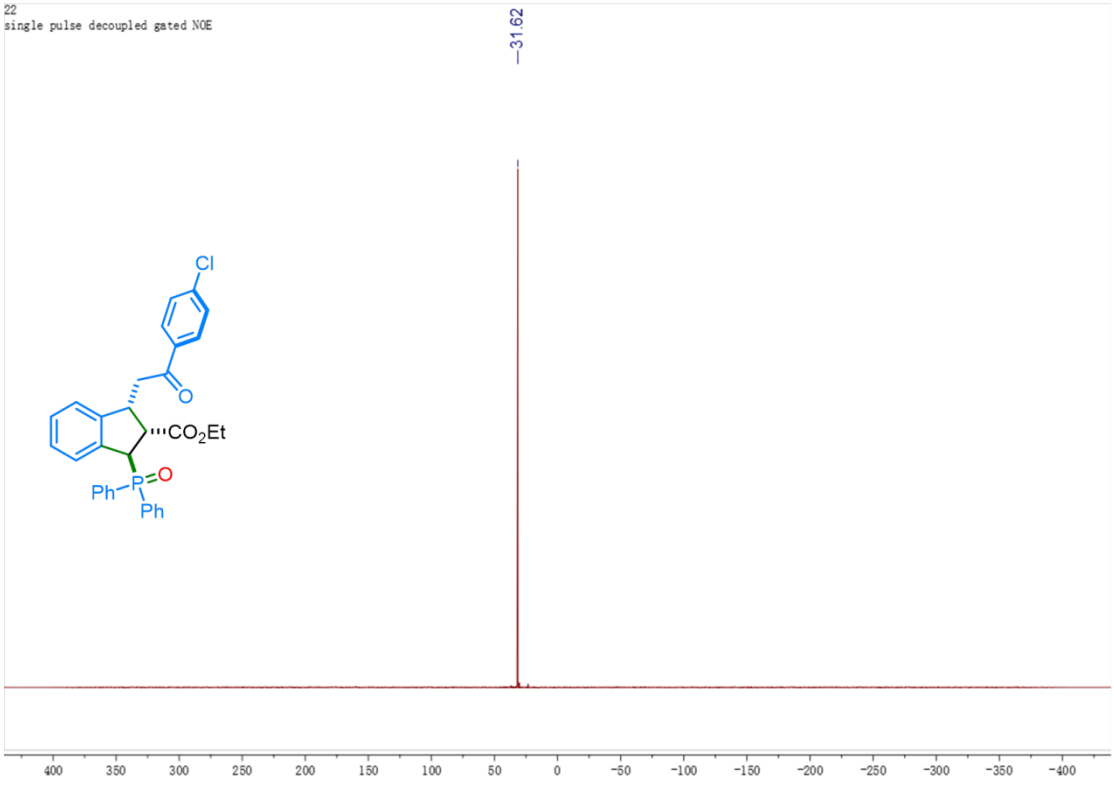
^{1}H NMR spectrum of **3a** (400 MHz, $CDCl_3$)



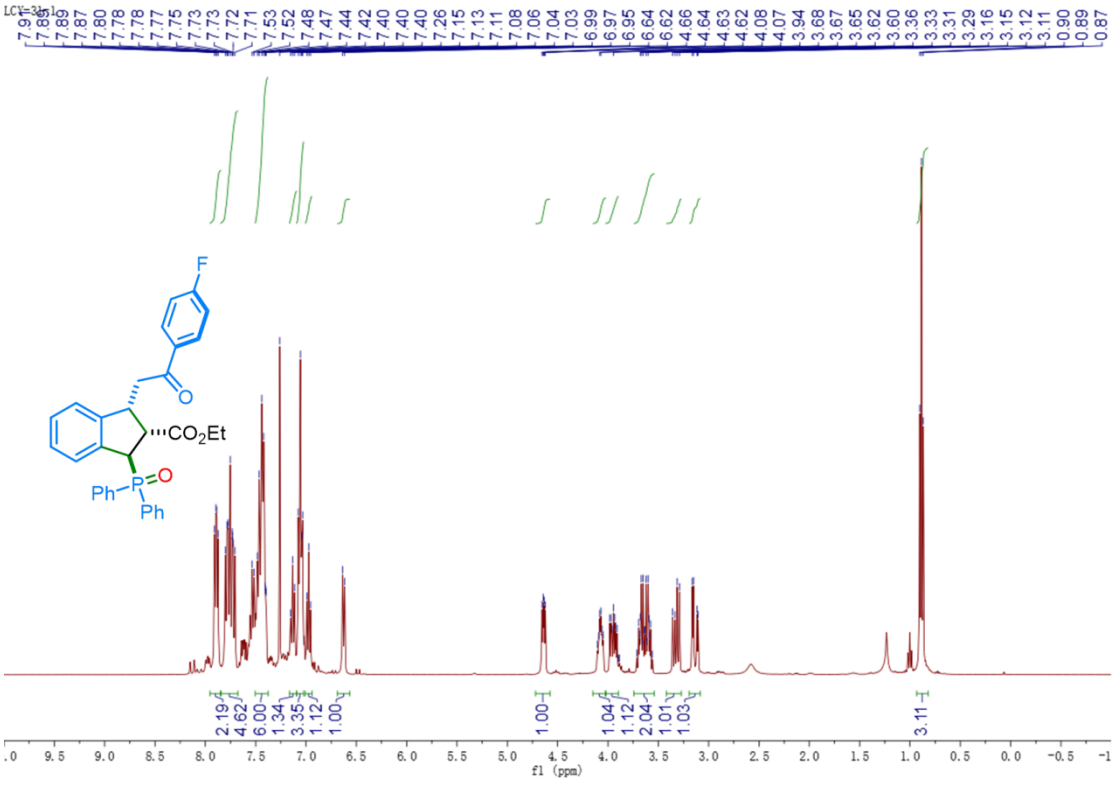
^{13}C NMR spectrum of **3a** (100 MHz, $CDCl_3$)



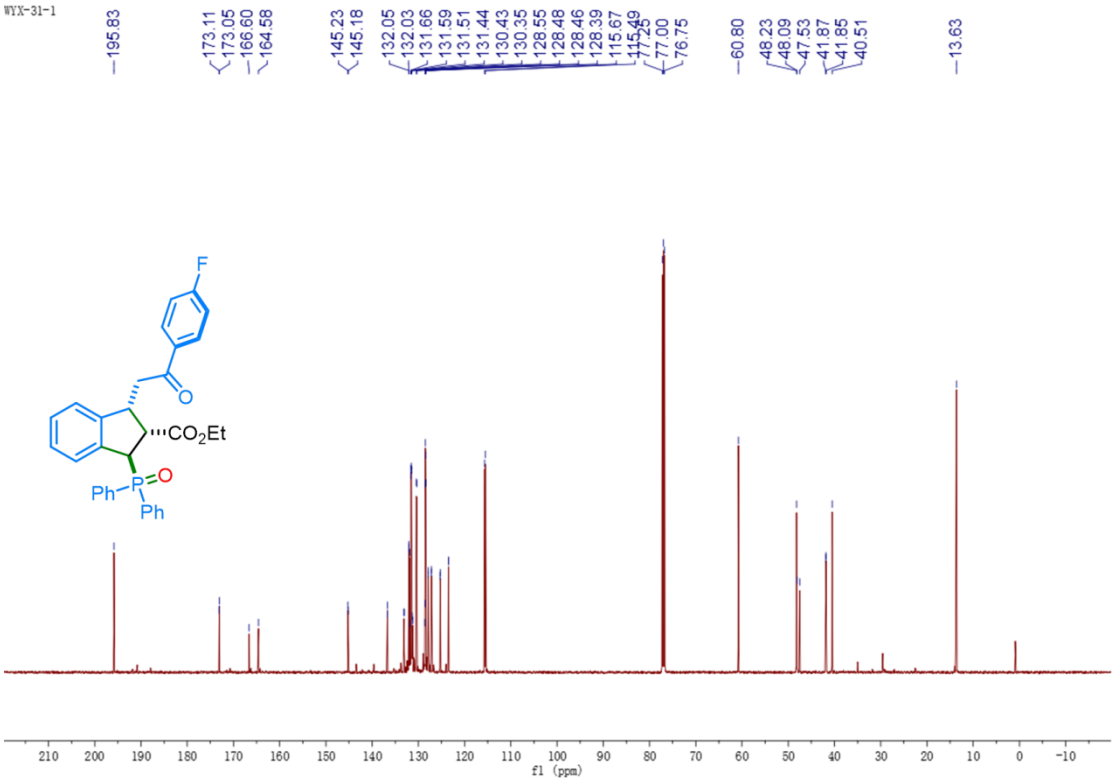
^{31}P NMR spectrum of **3a** (162 MHz, $CDCl_3$)



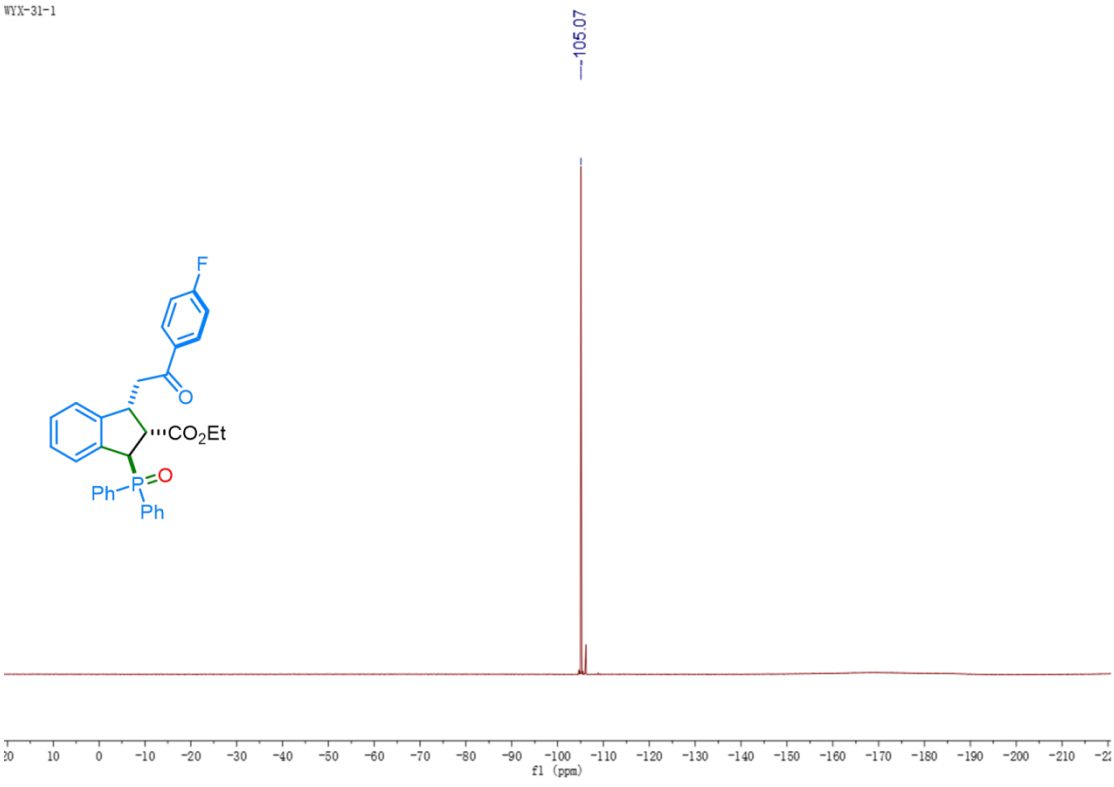
^{1}H NMR spectrum of **3b** (400 MHz, $CDCl_3$)



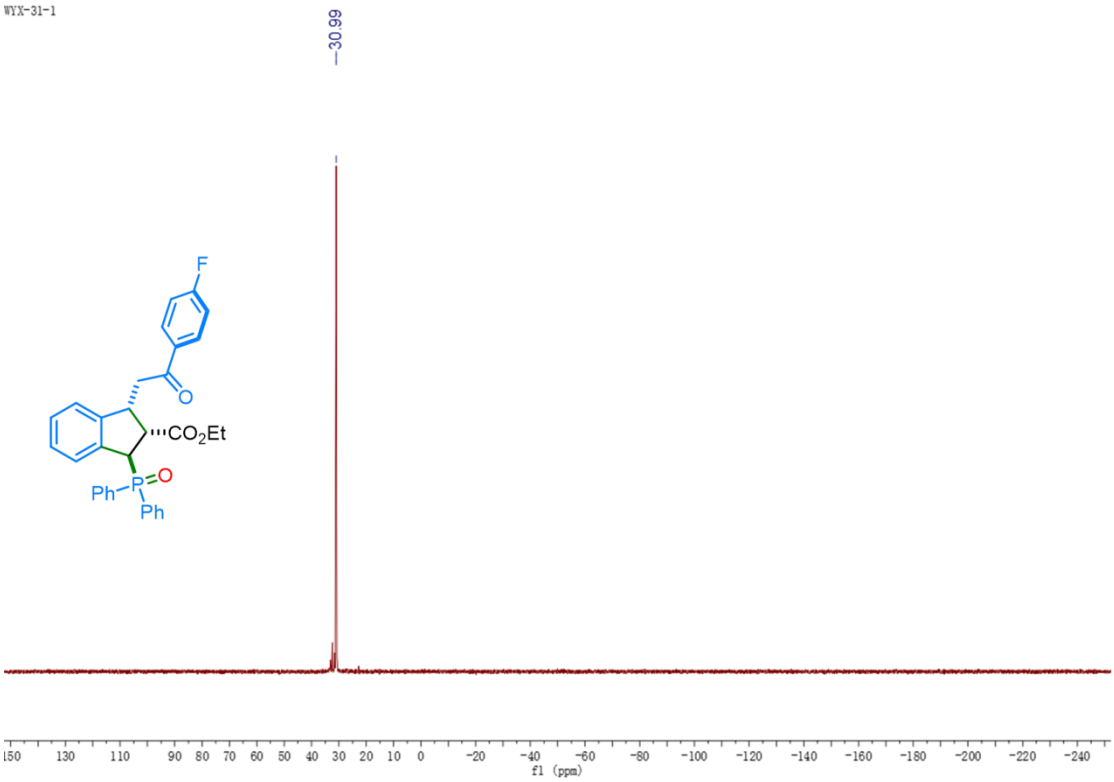
^{13}C NMR spectrum of **3b** (125 MHz, $CDCl_3$)



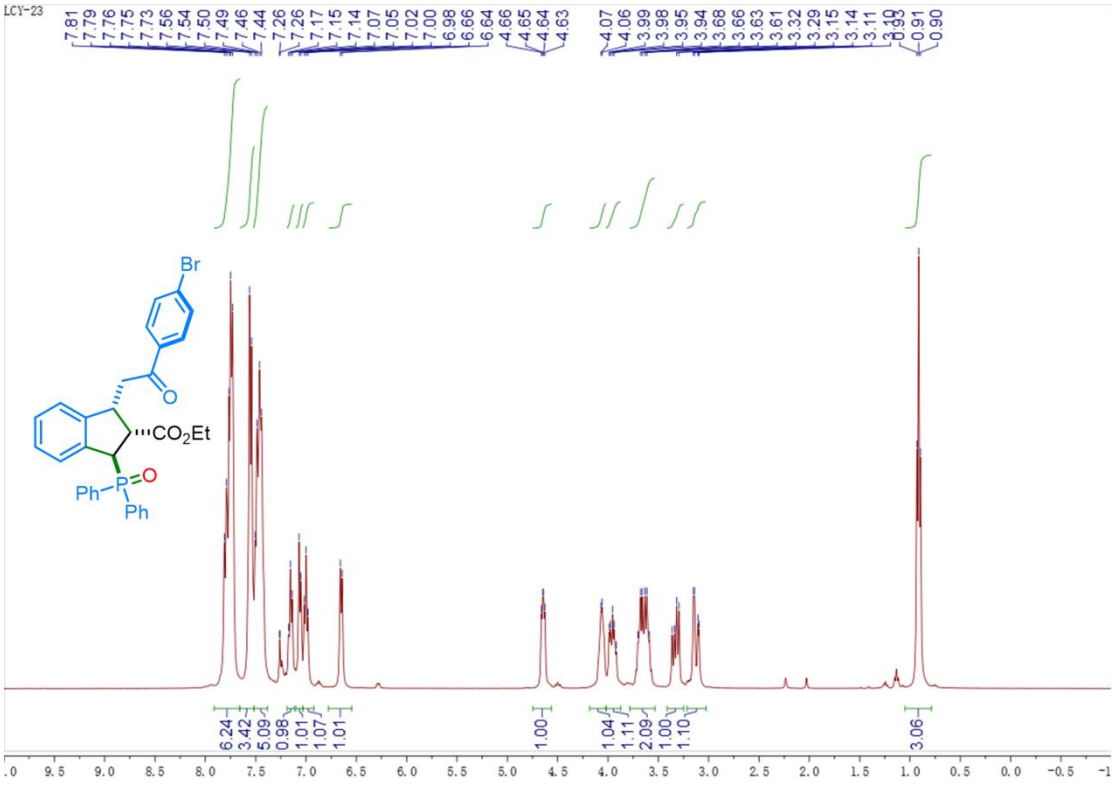
^{19}F NMR spectrum of **3b** (471 MHz, $CDCl_3$)



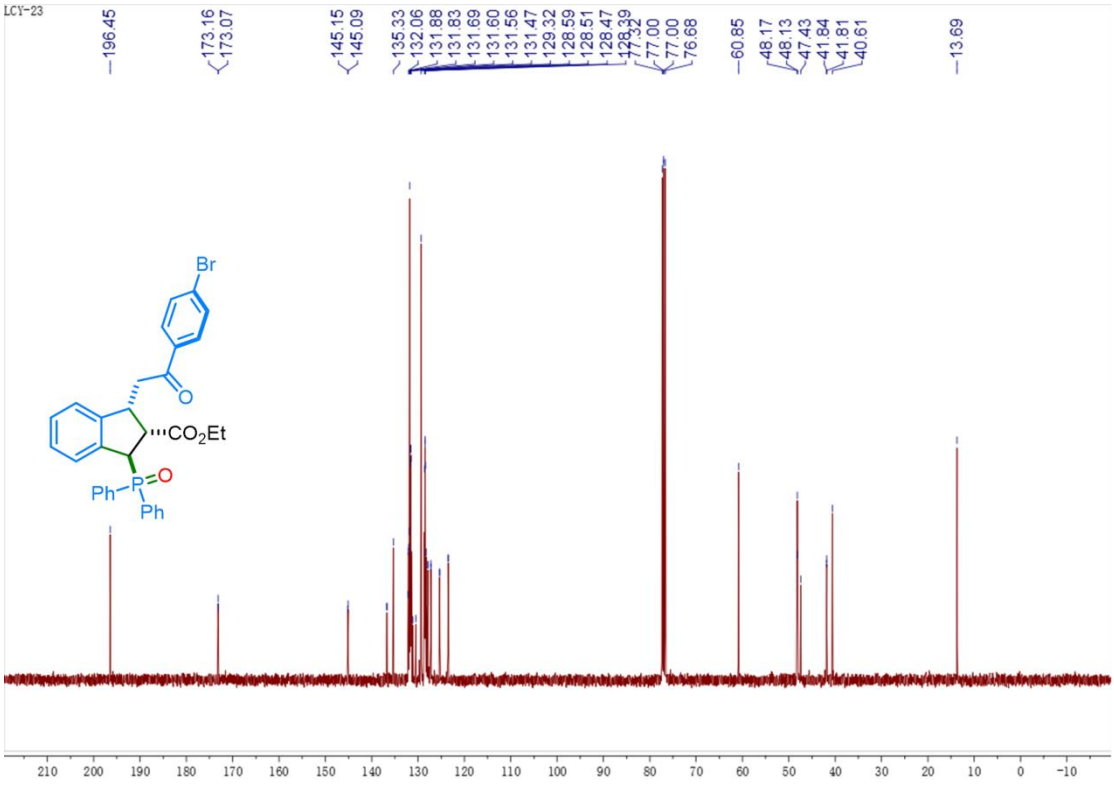
^{31}P NMR spectrum of **3b** (202 MHz, $CDCl_3$)



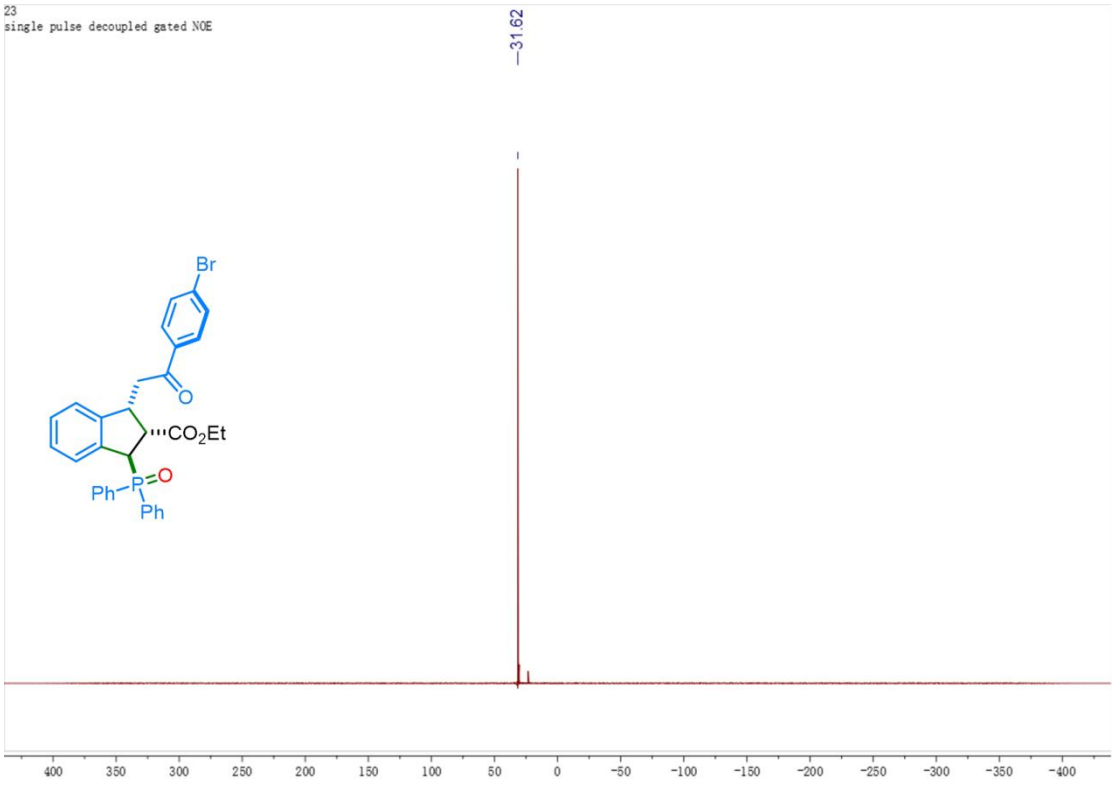
^{1}H NMR spectrum of **3c** (400 MHz, $CDCl_3$)



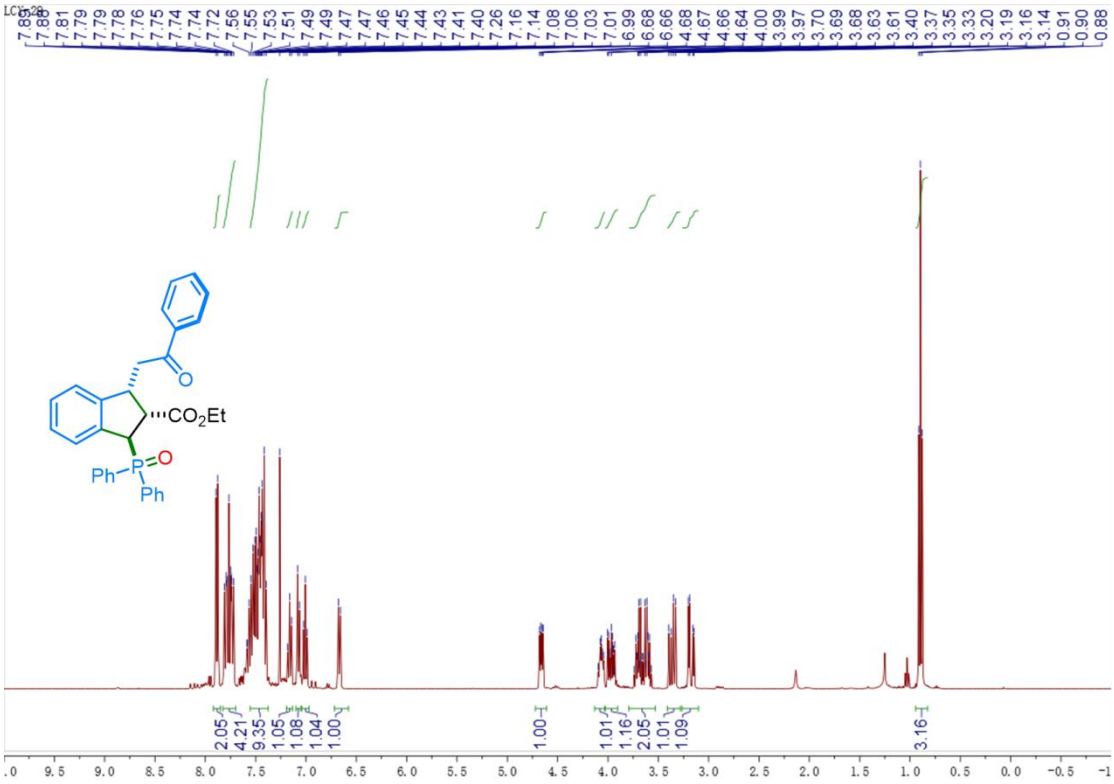
^{13}C NMR spectrum of **3c** (100 MHz, $CDCl_3$)



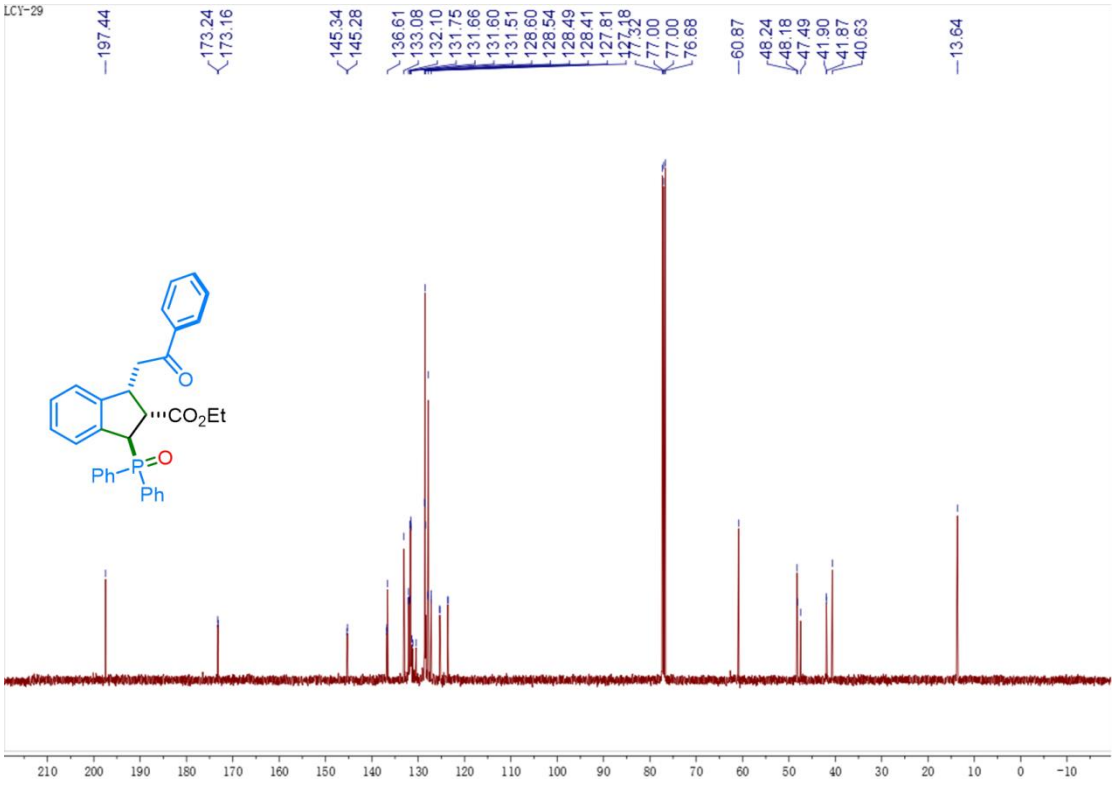
^{31}P NMR spectrum of **3c** (162 MHz, $CDCl_3$)



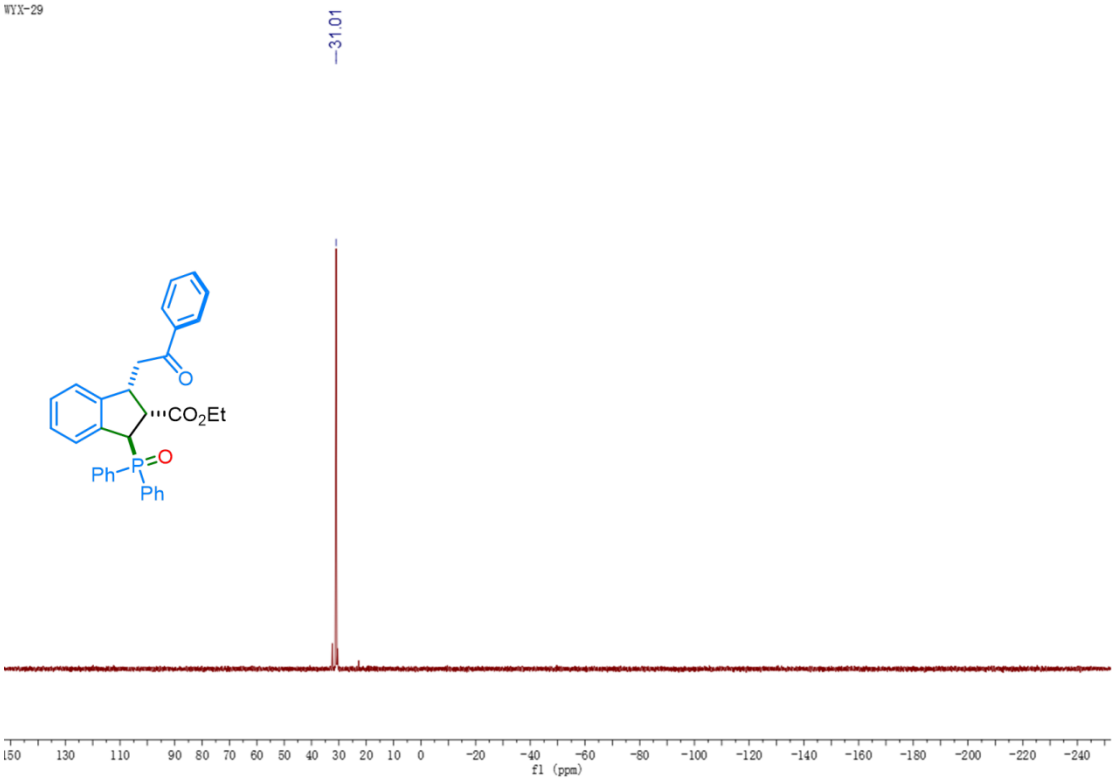
^{1}H NMR spectrum of **3d** (400 MHz, $CDCl_3$)



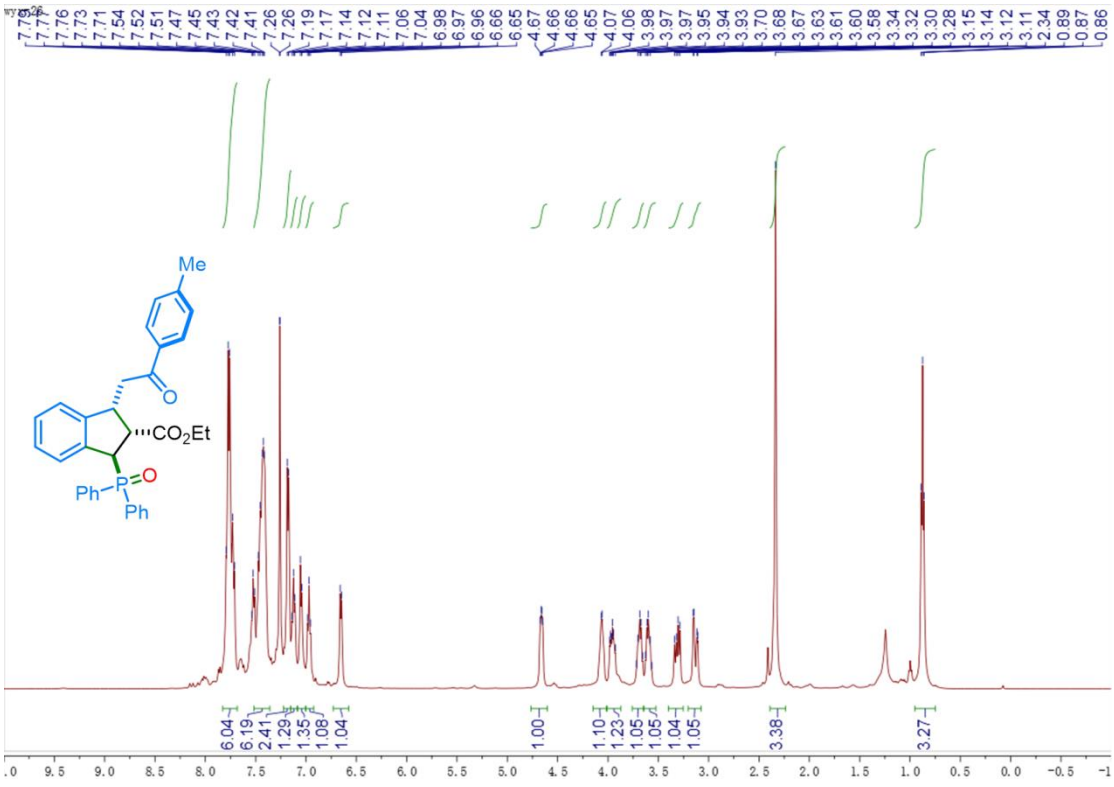
^{13}C NMR spectrum of **3d** (100 MHz, $CDCl_3$)



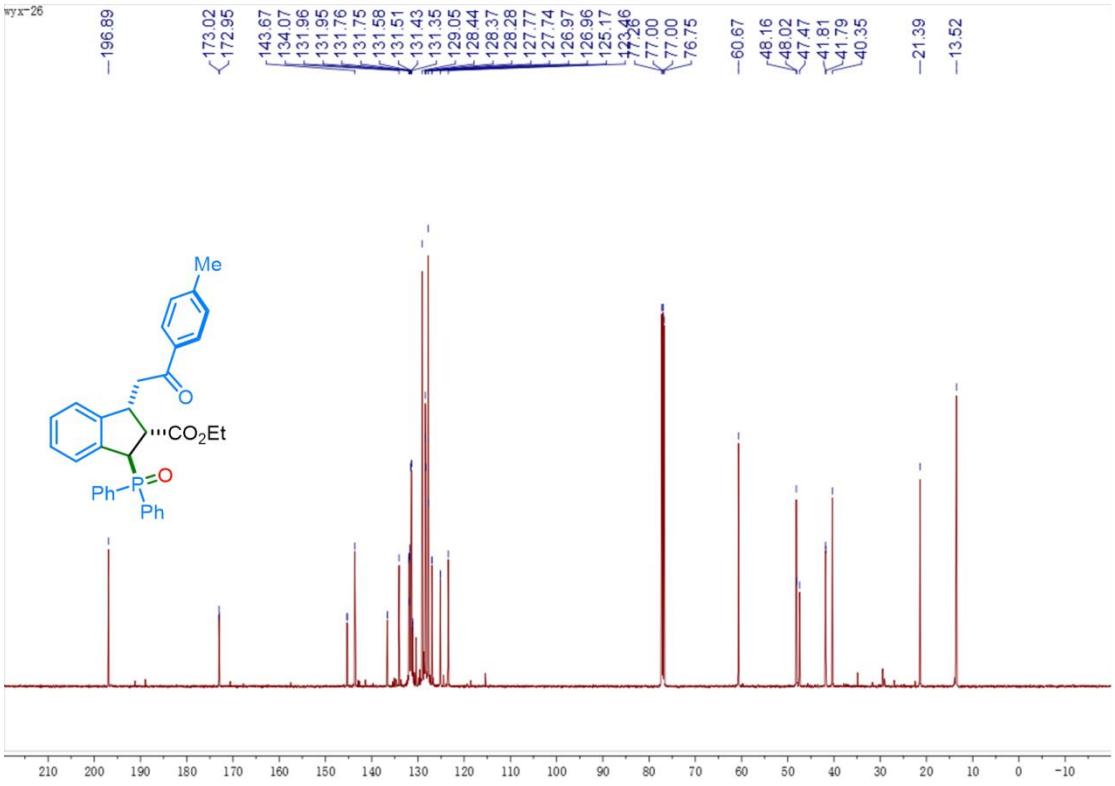
^{31}P NMR spectrum of **3d** (202 MHz, $CDCl_3$)



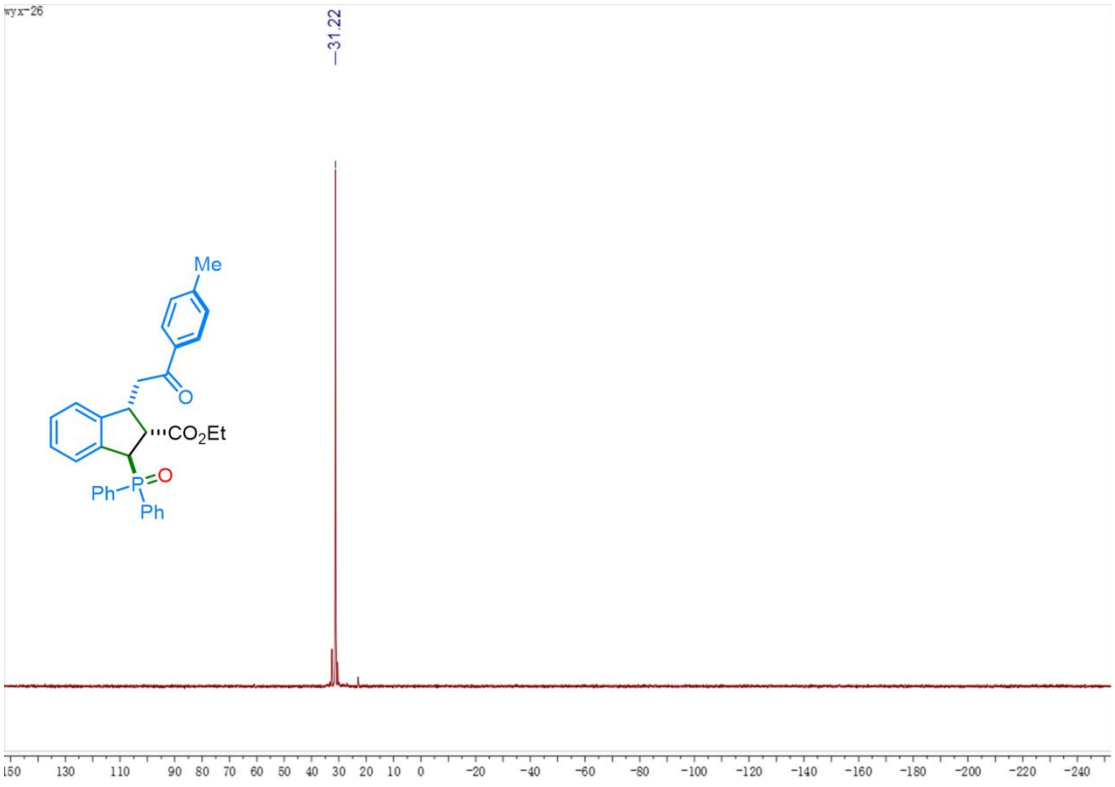
^{1}H NMR spectrum of **3e** (500 MHz, $CDCl_3$)



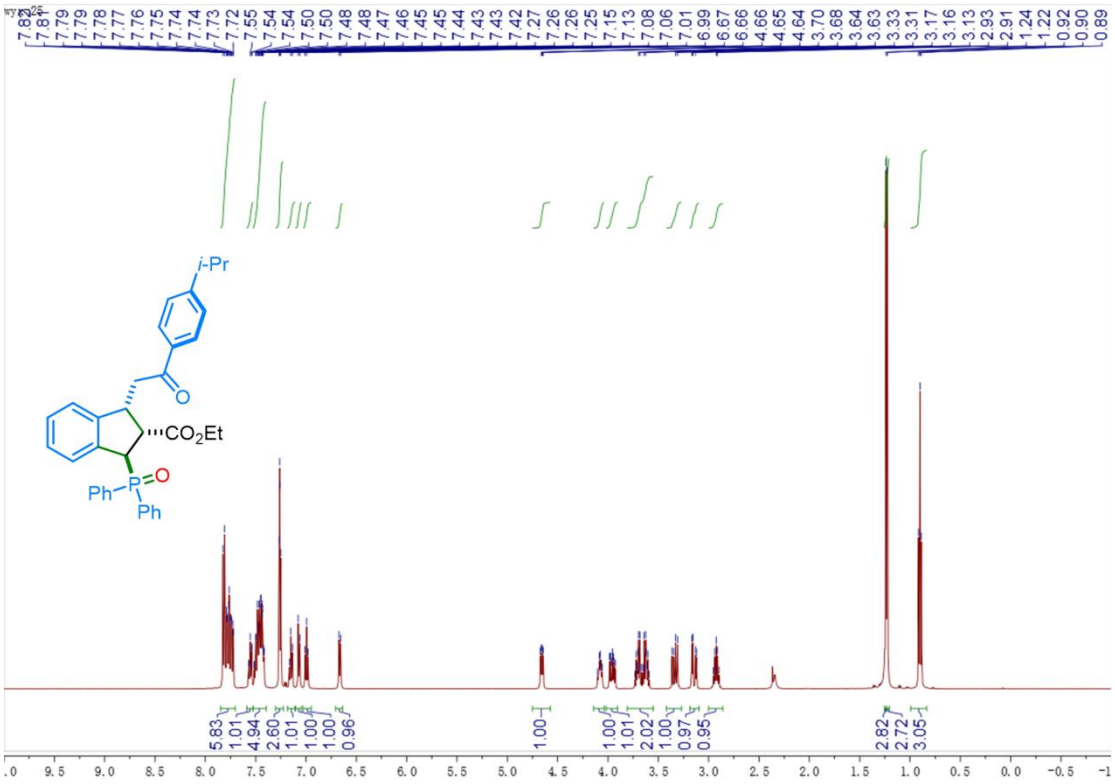
^{13}C NMR spectrum of **3e** (125 MHz, $CDCl_3$)



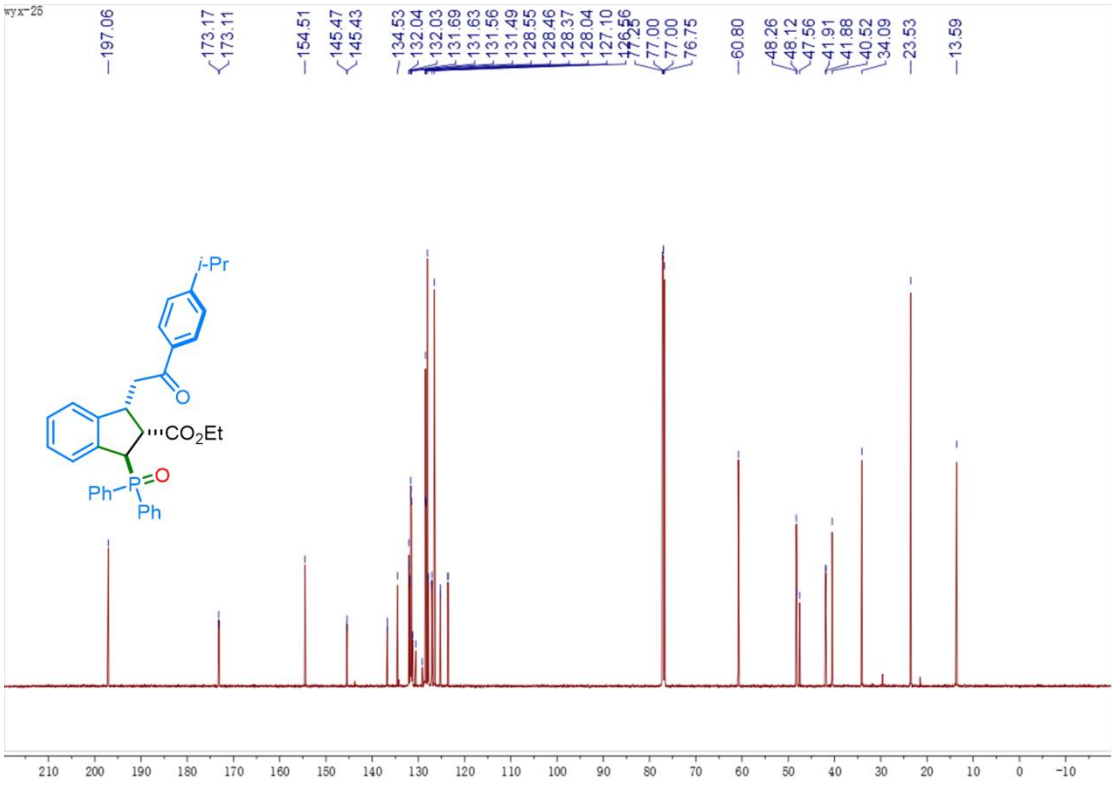
^{31}P NMR spectrum of **3e** (202 MHz, $CDCl_3$)



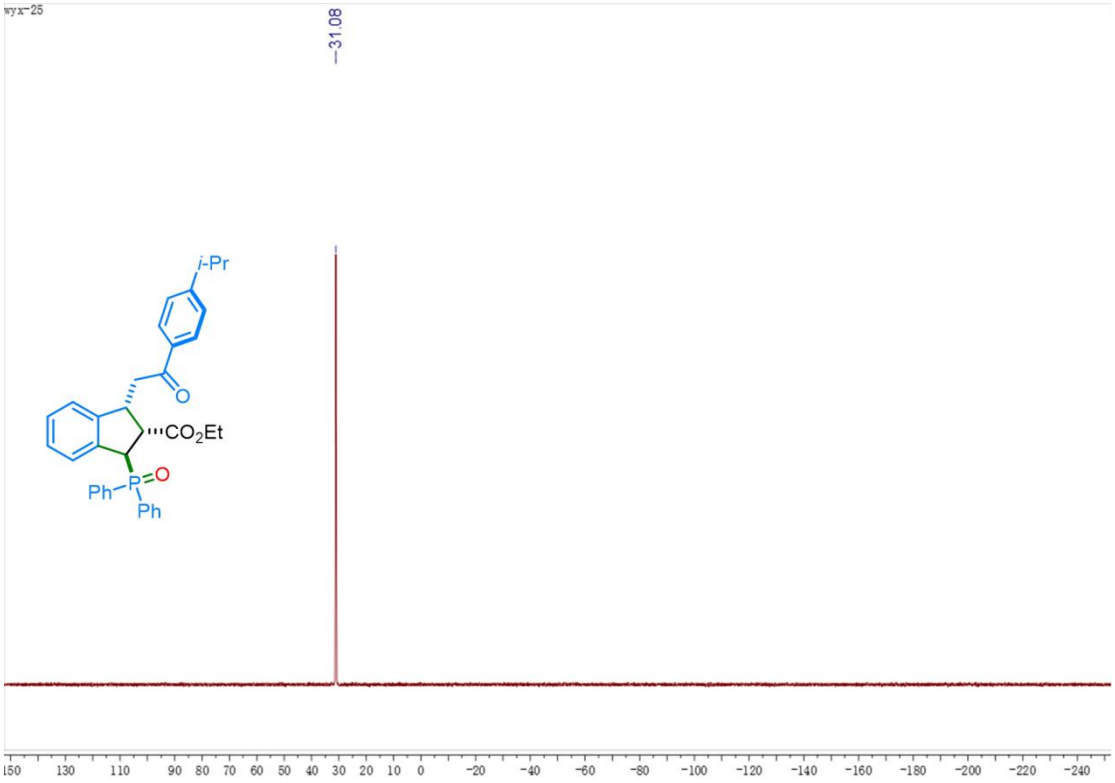
^{1}H NMR spectrum of **3f** (500 MHz, $CDCl_3$)



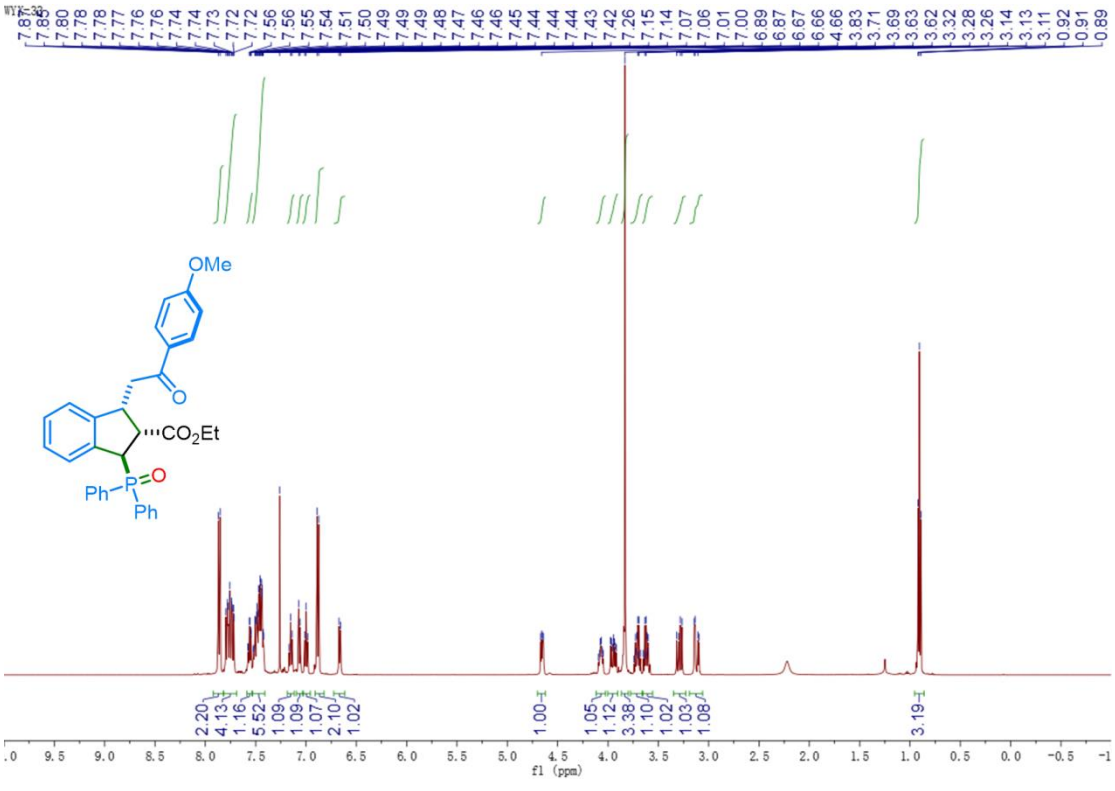
^{13}C NMR spectrum of **3f** (125 MHz, $CDCl_3$)



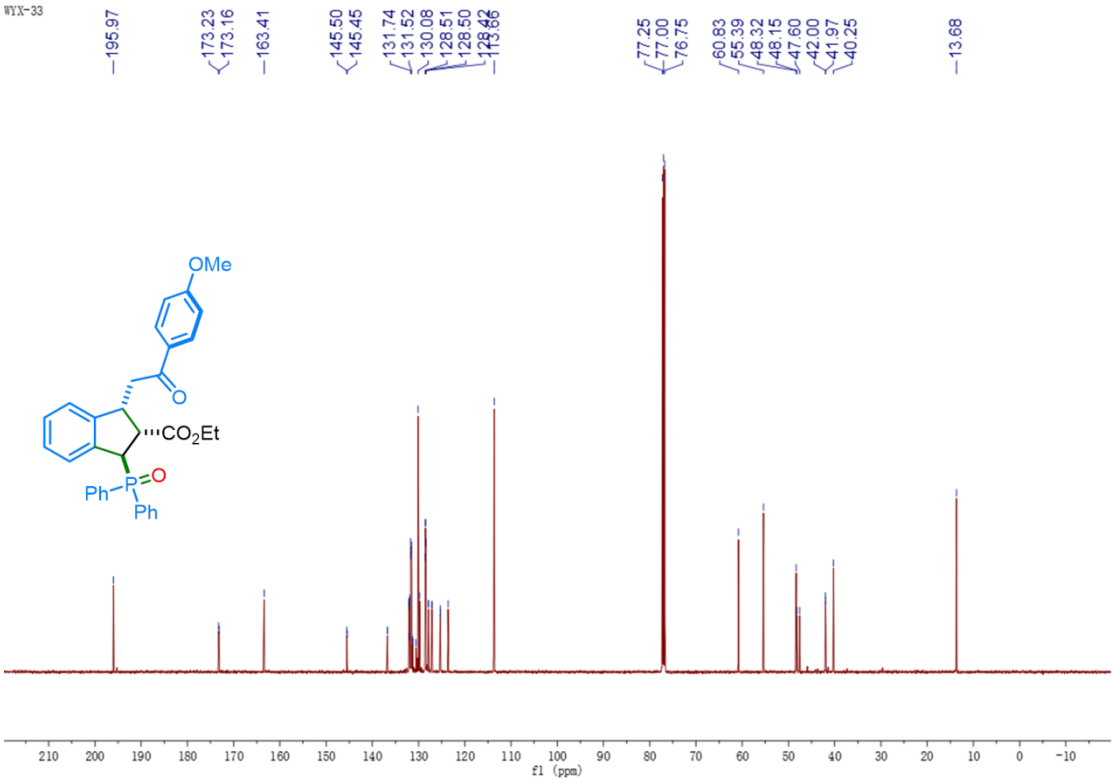
^{31}P NMR spectrum of **3f** (202 MHz, $CDCl_3$)



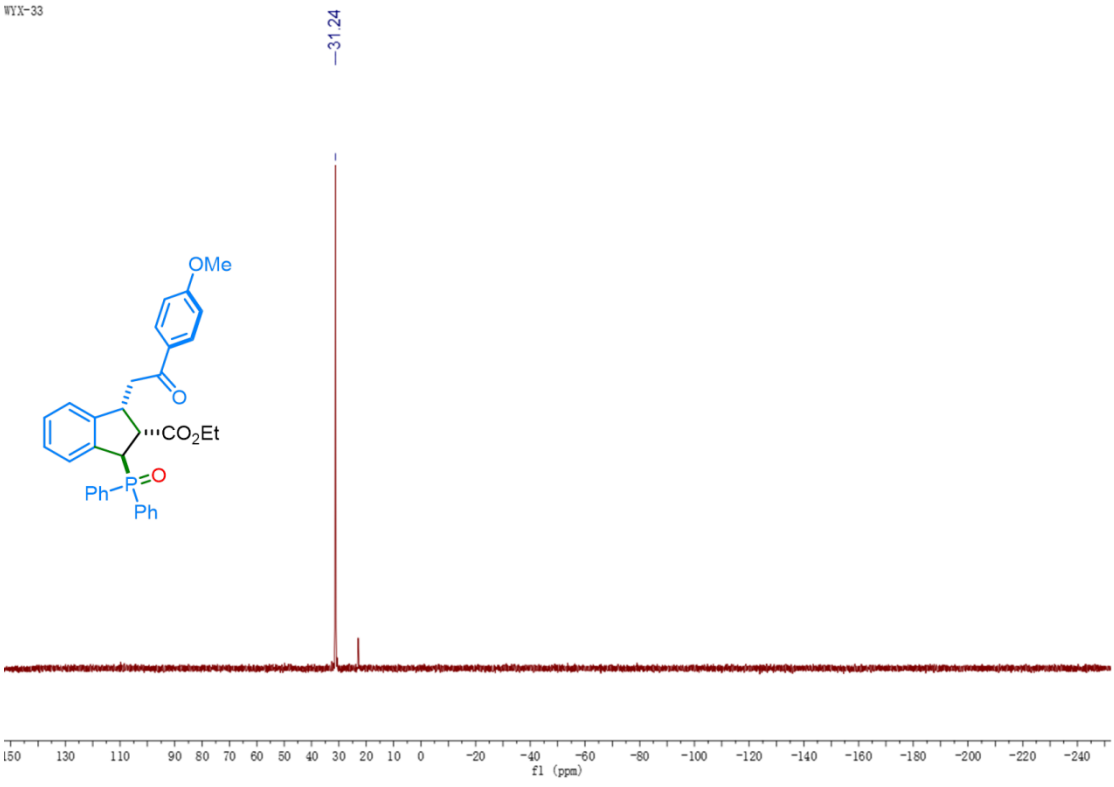
^{1}H NMR spectrum of **3g** (500 MHz, $CDCl_3$)



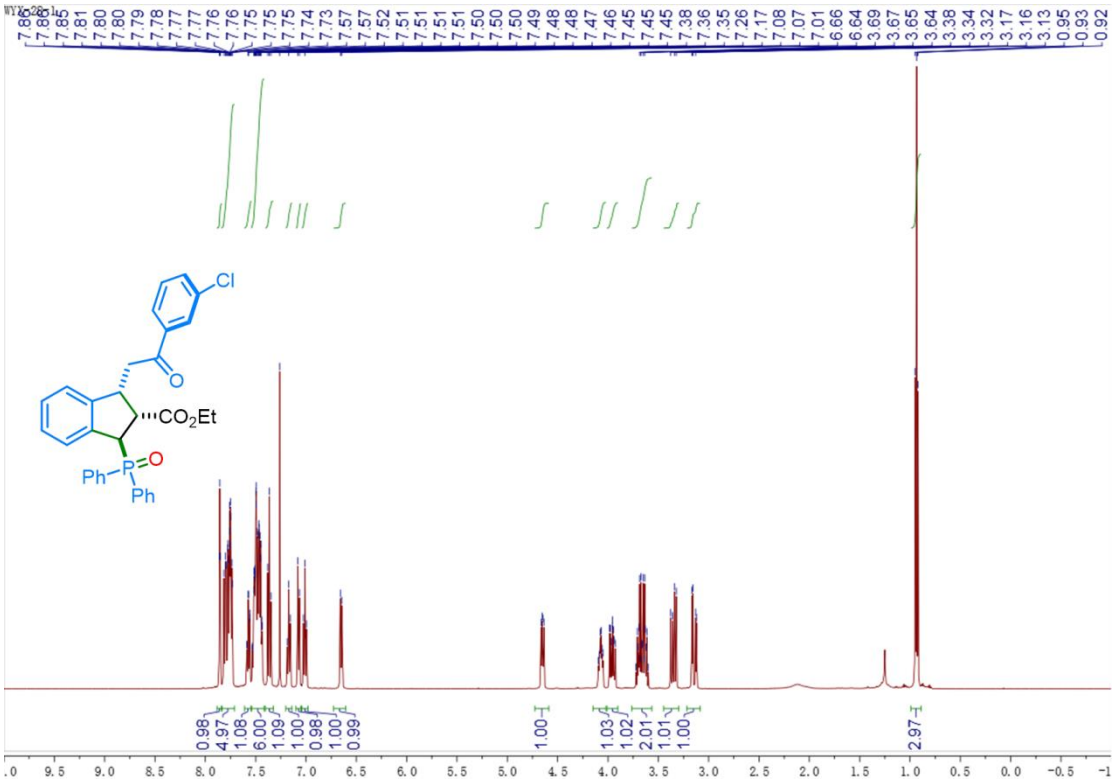
^{13}C NMR spectrum of **3g** (125 MHz, $CDCl_3$)



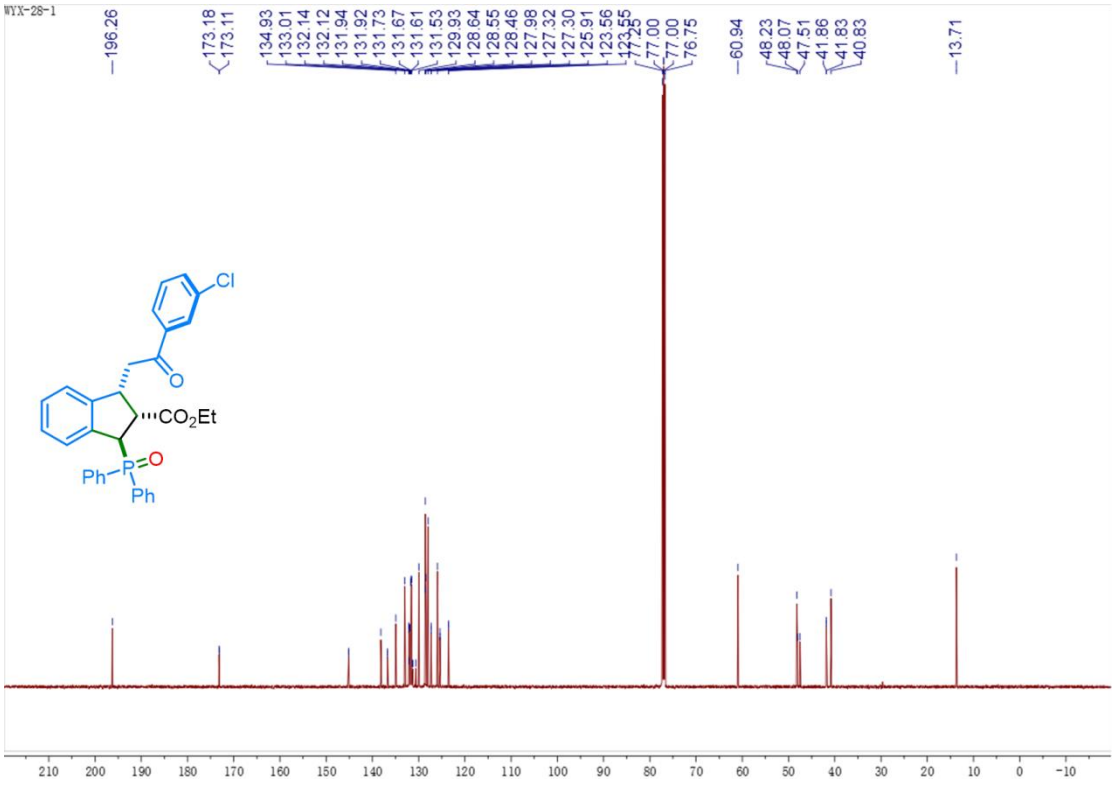
^{31}P NMR spectrum of **3g** (202 MHz, $CDCl_3$)



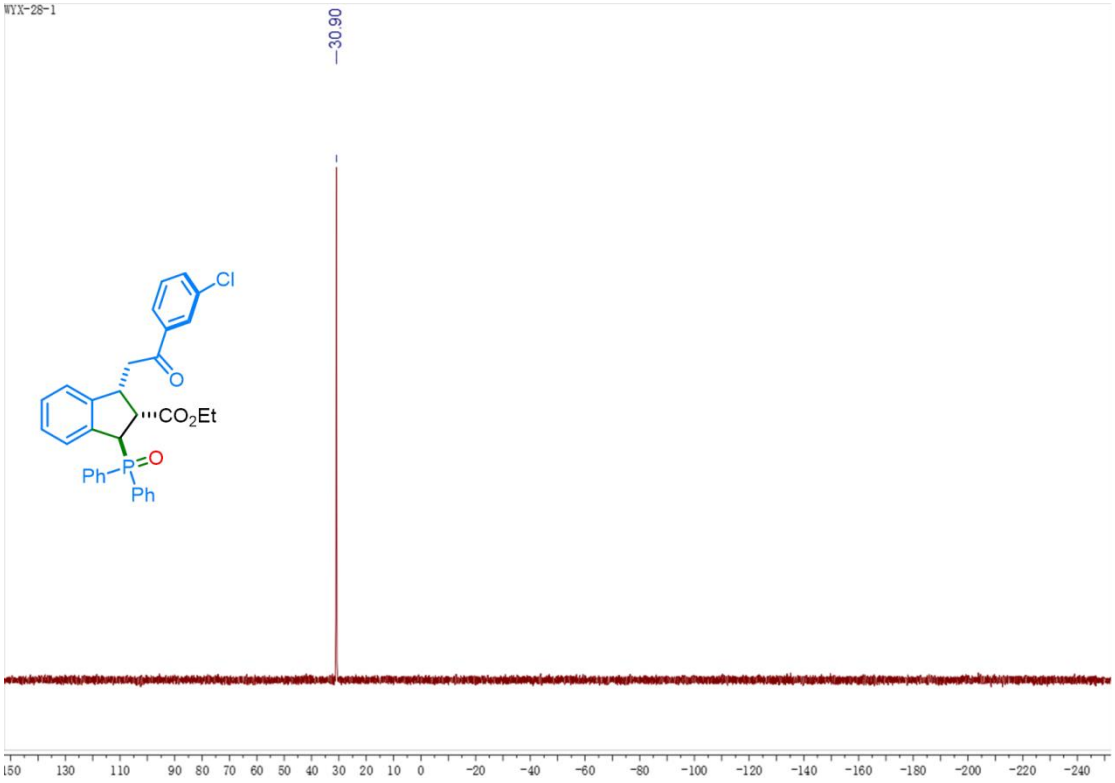
^{1}H NMR spectrum of **3h** (500 MHz, $CDCl_3$)



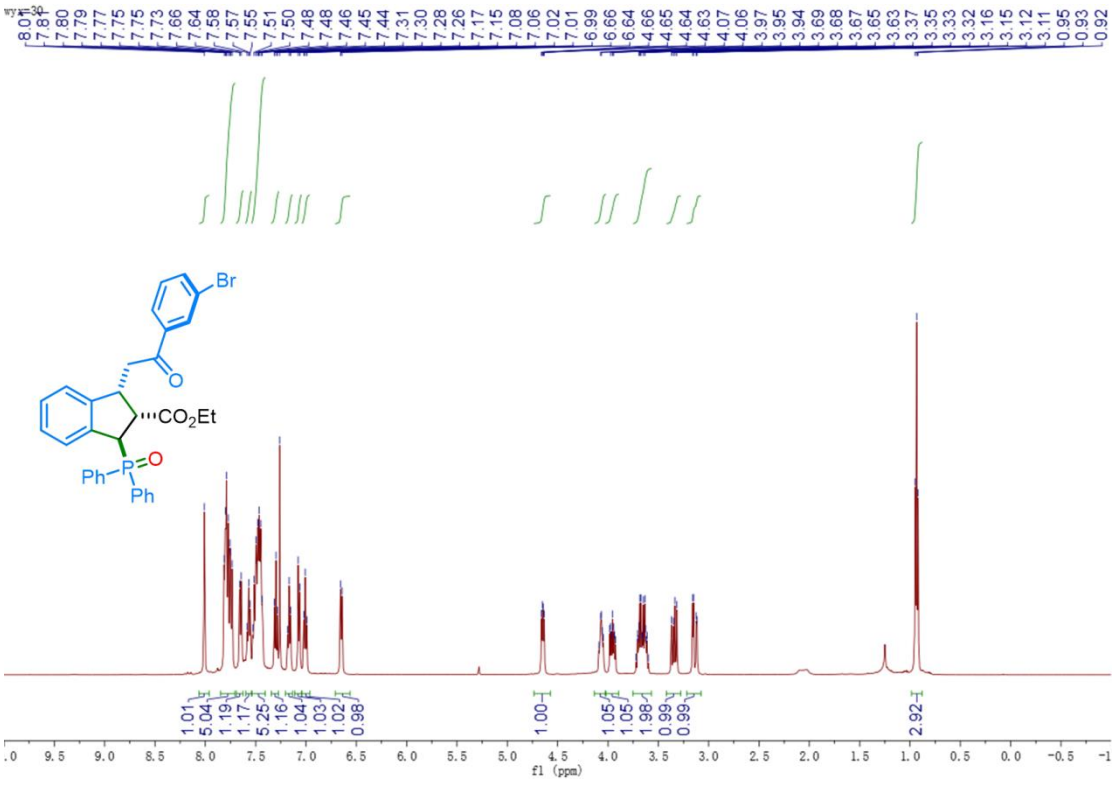
^{13}C NMR spectrum of **3h** (125 MHz, $CDCl_3$)



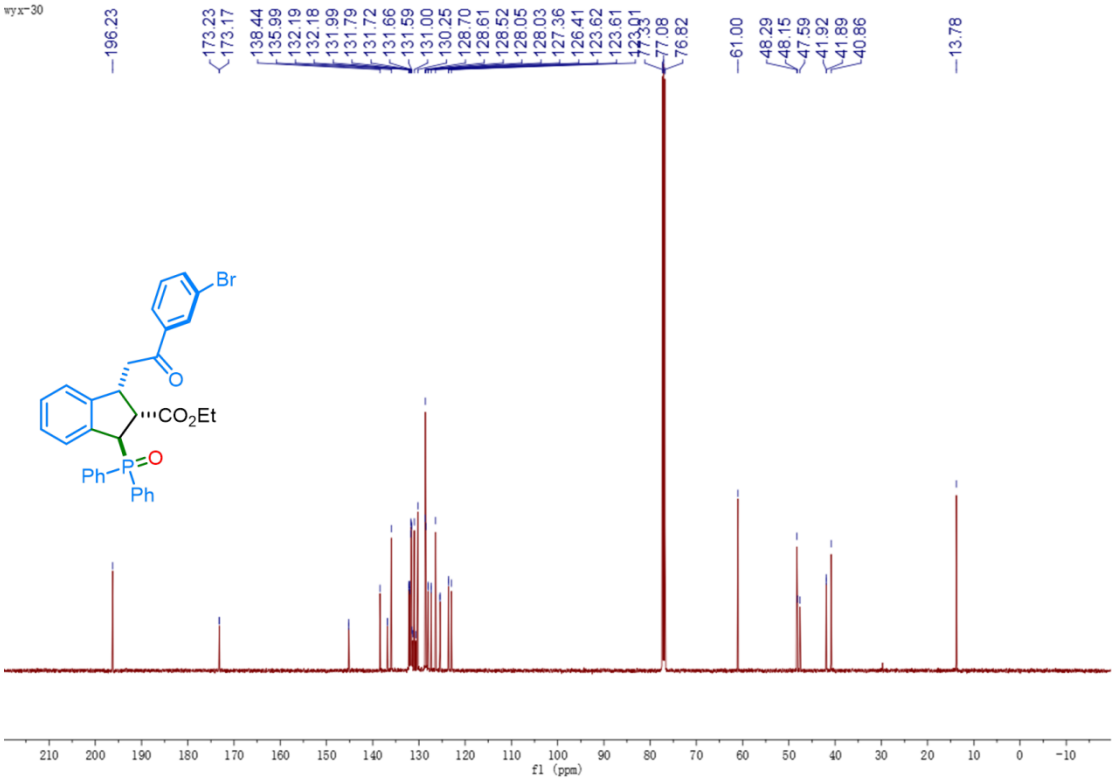
^{31}P NMR spectrum of **3h** (202 MHz, $CDCl_3$)



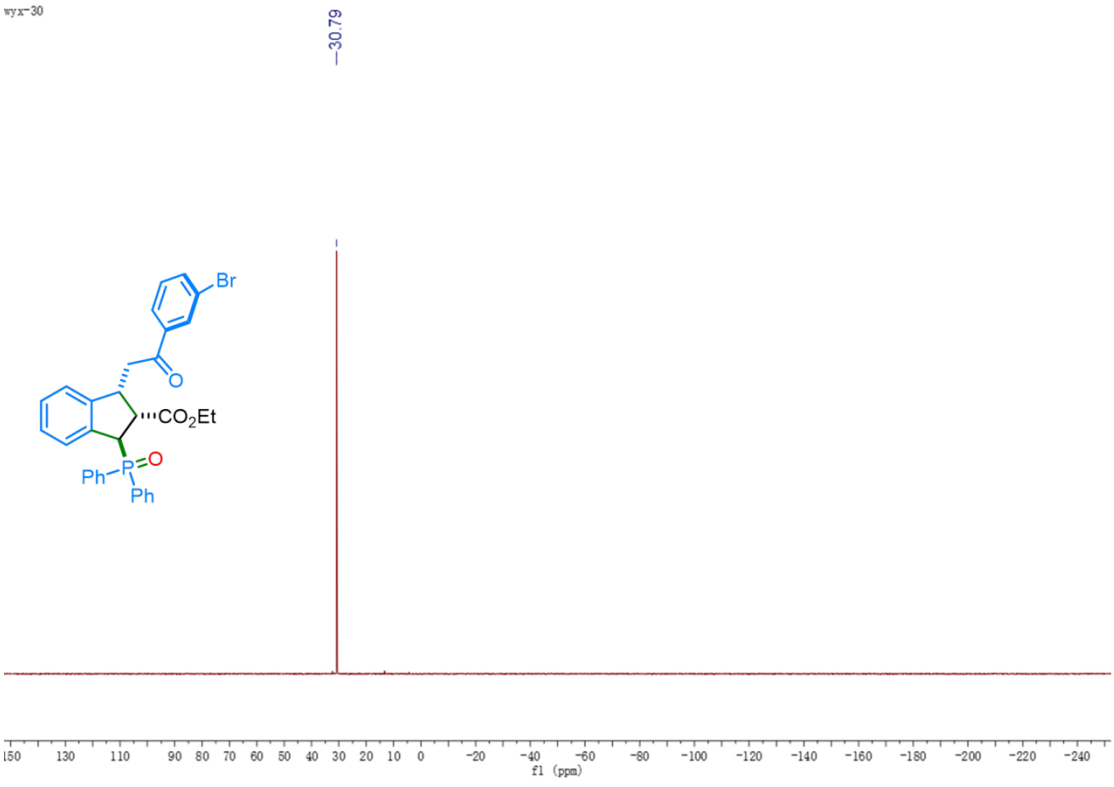
^{1}H NMR spectrum of **3i** (500 MHz, $CDCl_3$)



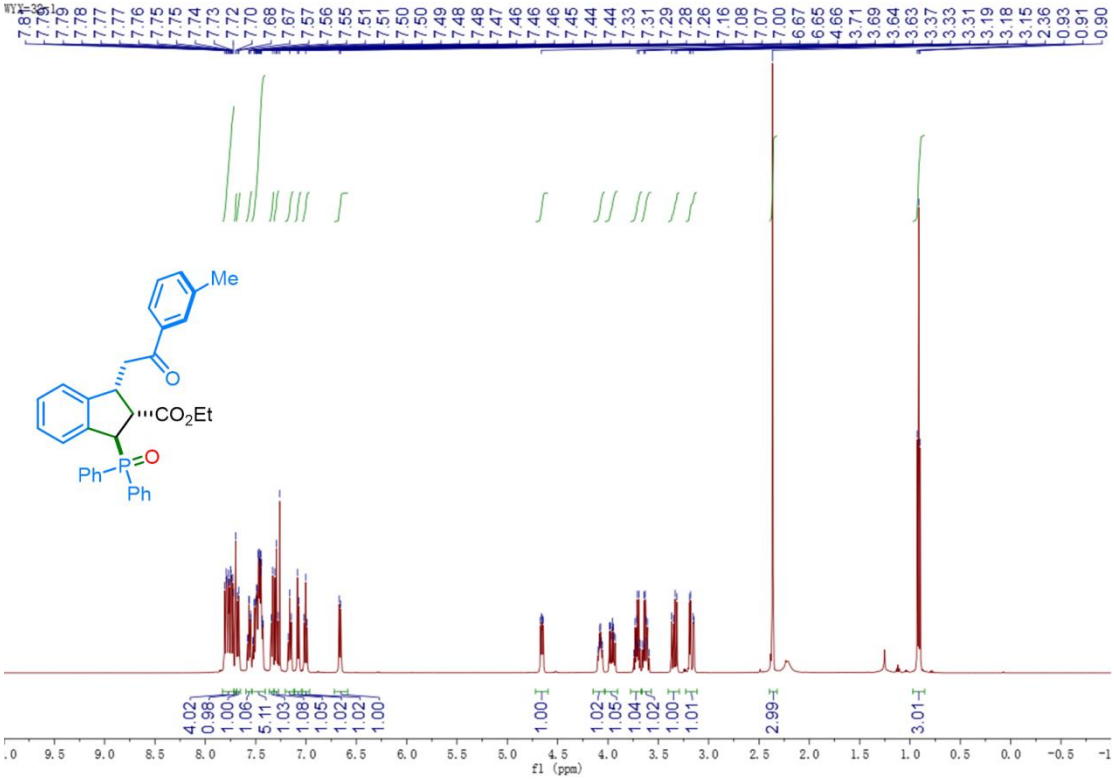
^{13}C NMR spectrum of **3i** (125 MHz, $CDCl_3$)



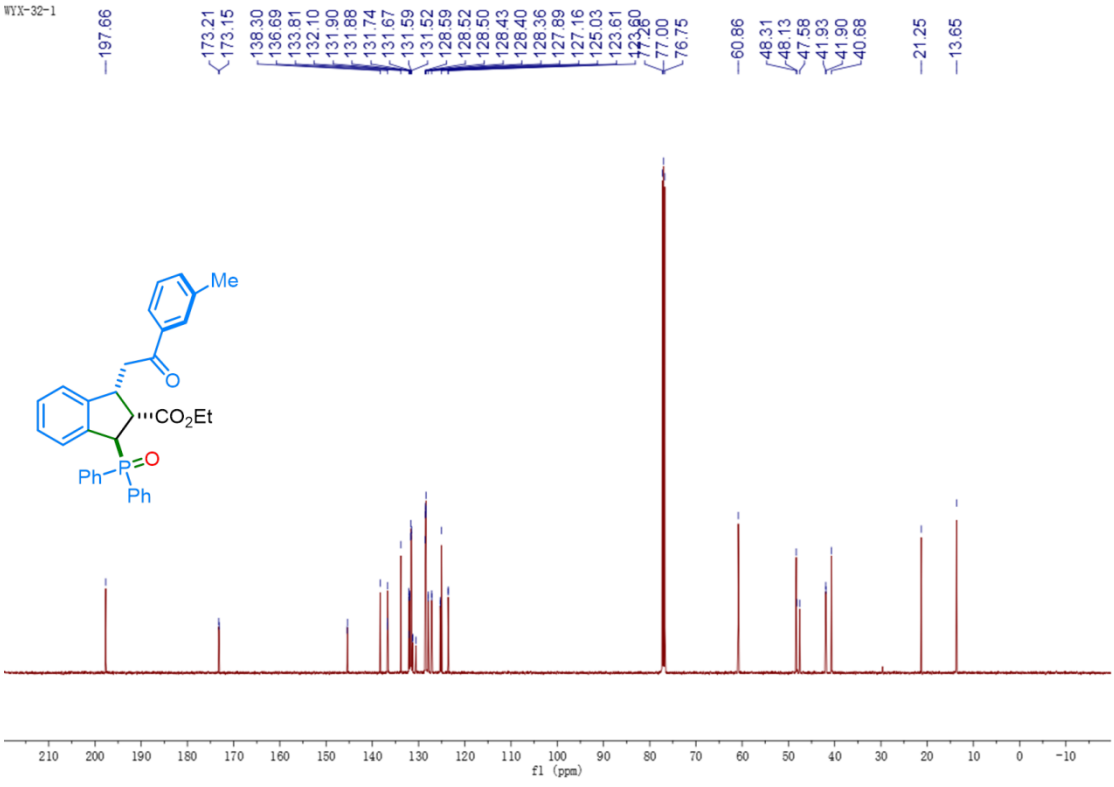
^{31}P NMR spectrum of **3i** (202 MHz, $CDCl_3$)



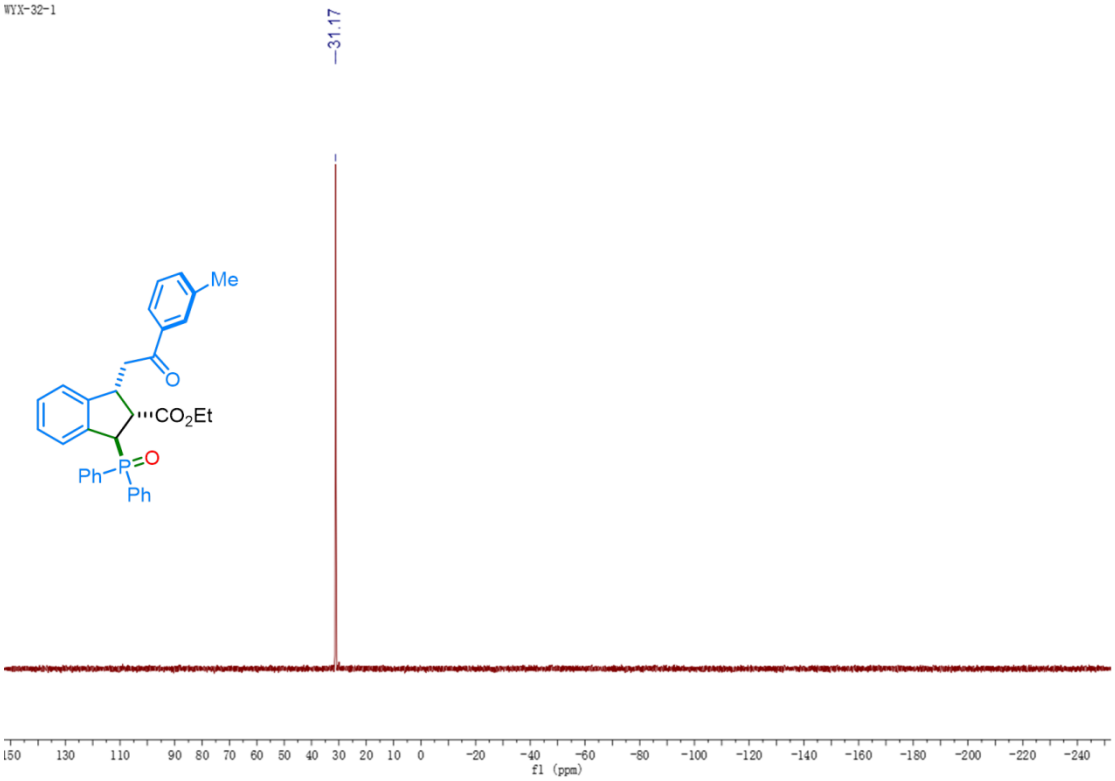
^{1}H NMR spectrum of **3j** (500 MHz, $CDCl_3$)



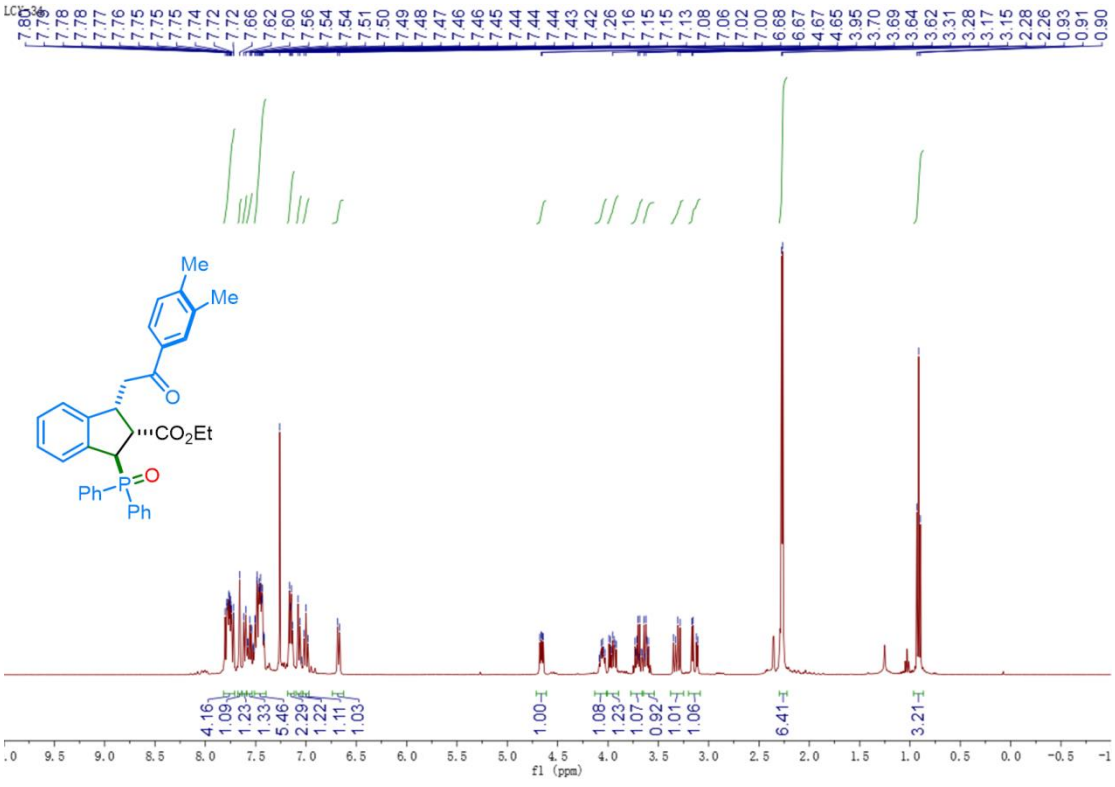
^{13}C NMR spectrum of **3j** (125 MHz, $CDCl_3$)



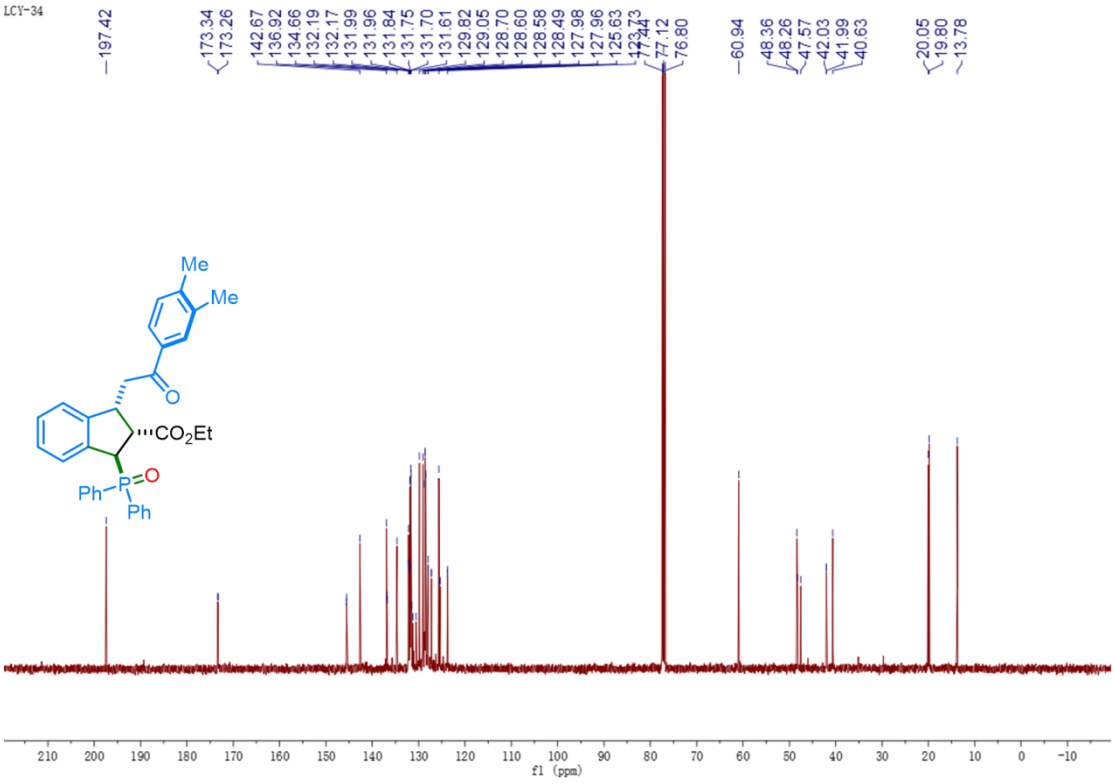
^{31}P NMR spectrum of **3j** (202 MHz, $CDCl_3$)



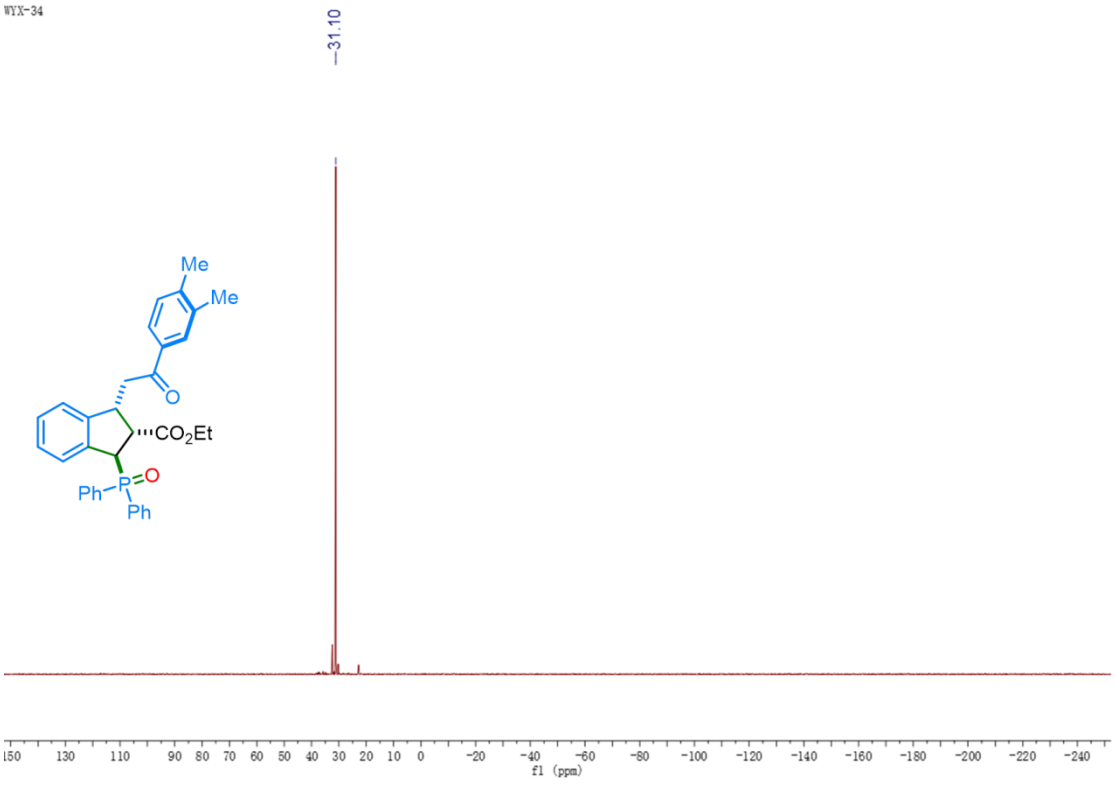
^{1}H NMR spectrum of **3k** (400 MHz, $CDCl_3$)



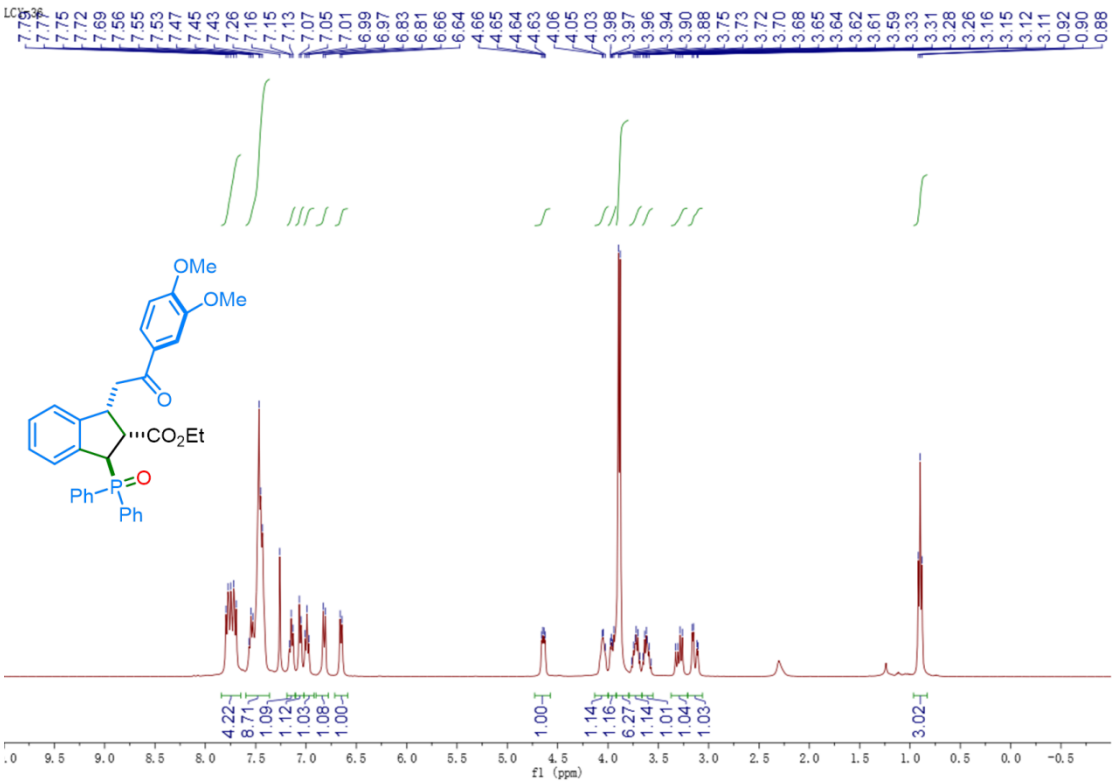
^{13}C NMR spectrum of **3k** (100 MHz, $CDCl_3$)



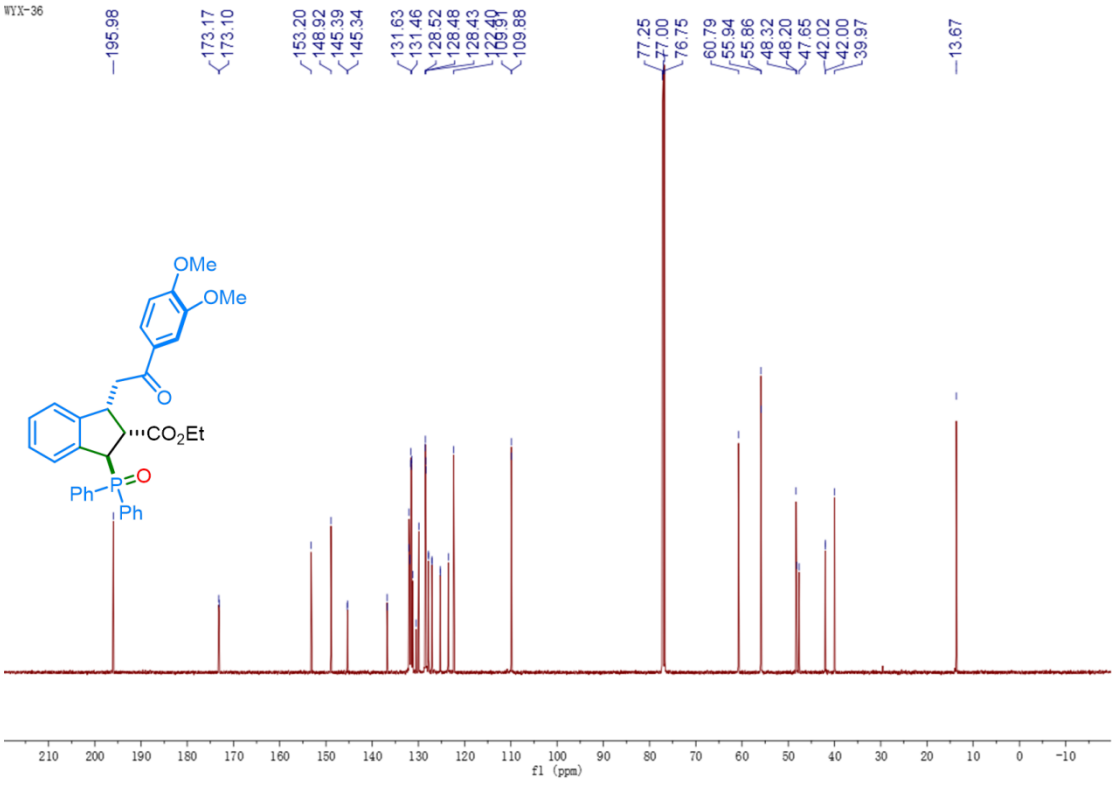
^{31}P NMR spectrum of **3k** (202 MHz, $CDCl_3$)



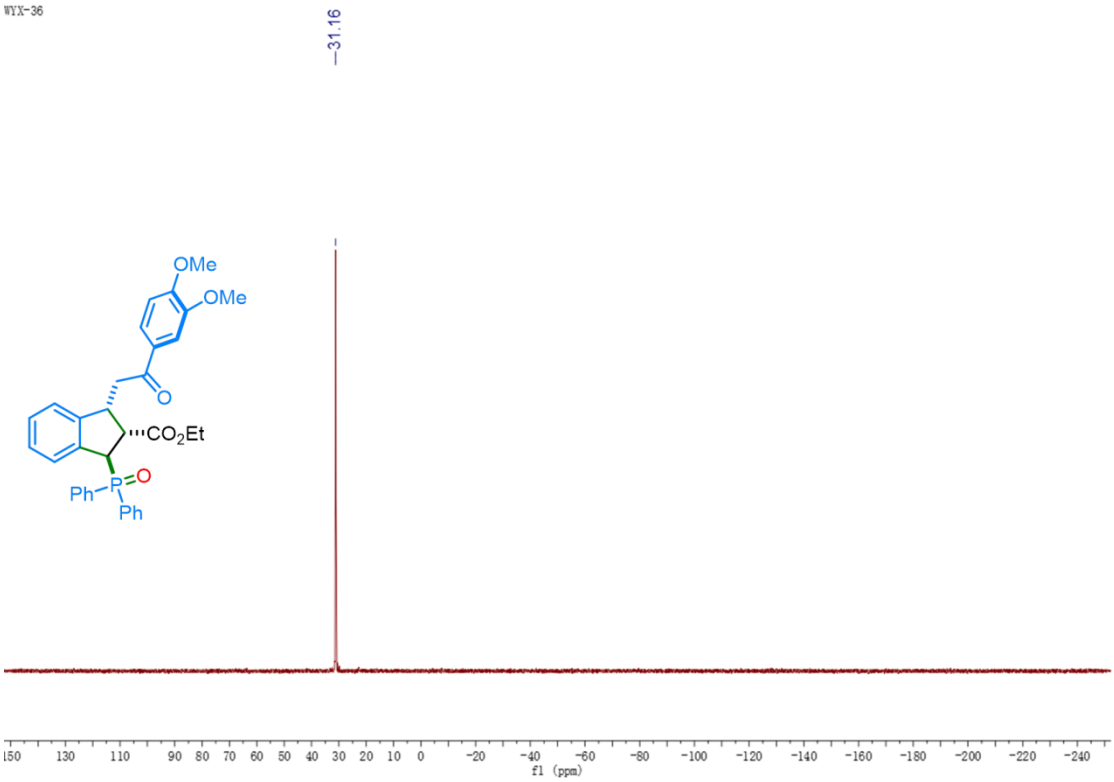
^{1}H NMR spectrum of **3l** (400 MHz, $CDCl_3$)



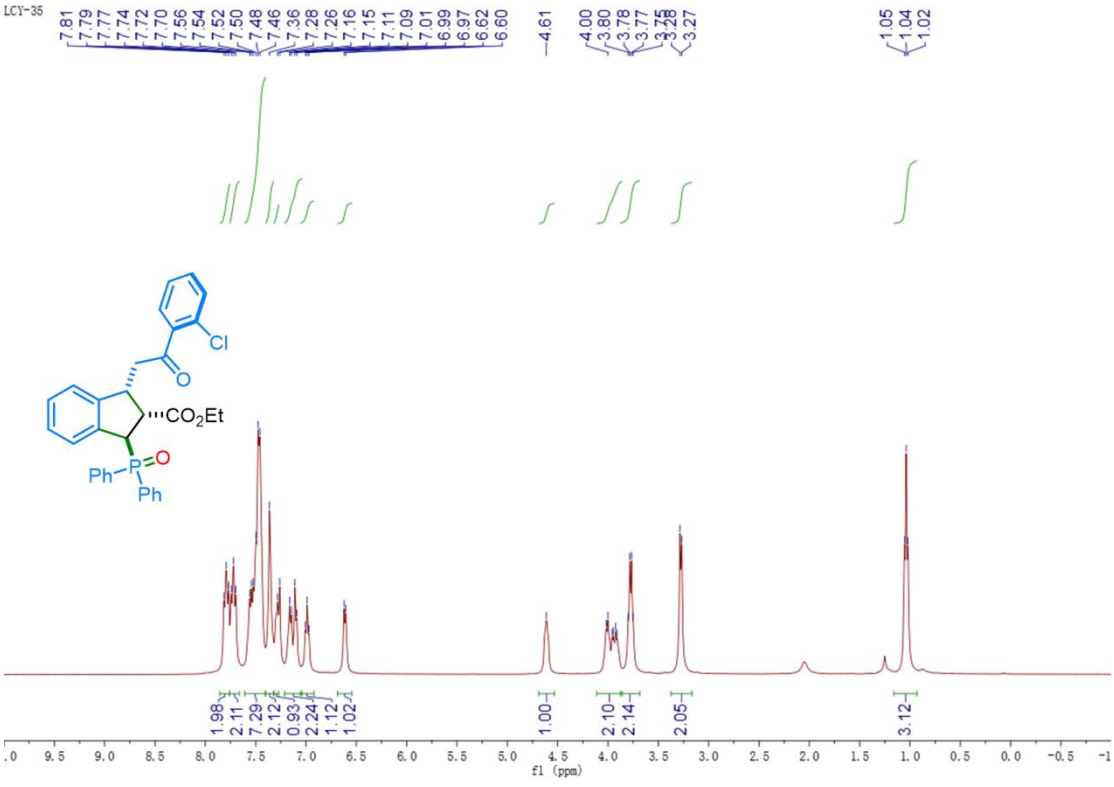
^{13}C NMR spectrum of **3l** (100 MHz, $CDCl_3$)



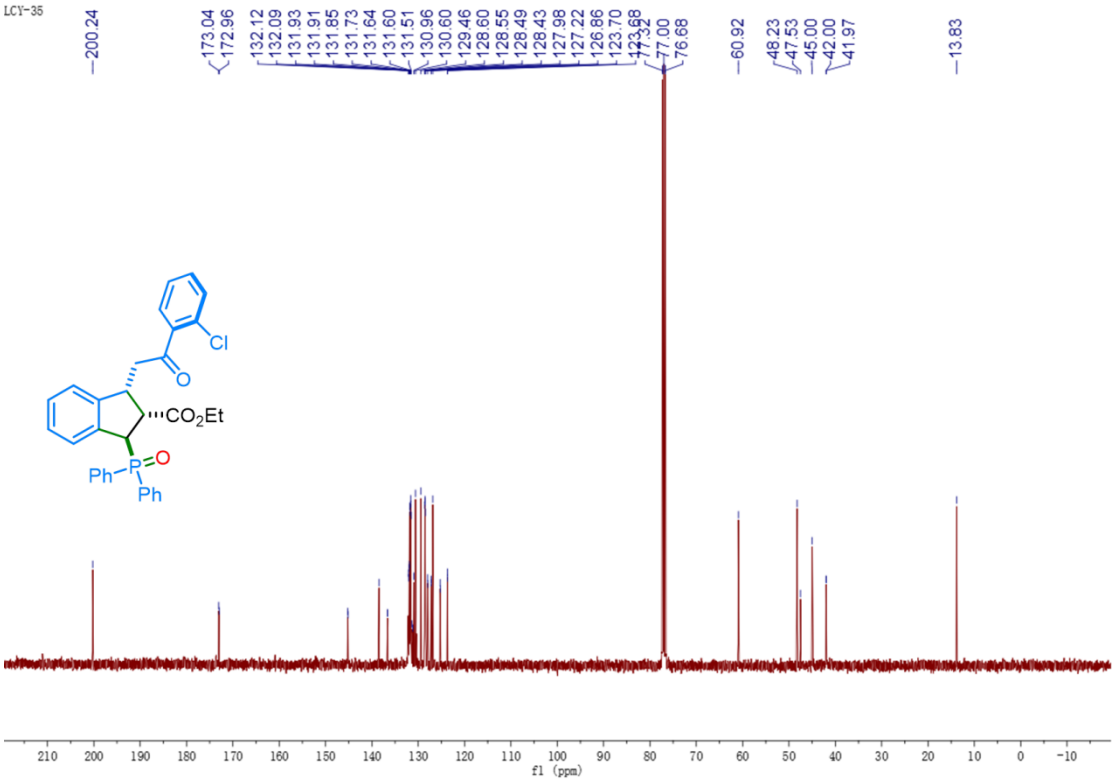
^{31}P NMR spectrum of **3l** (202 MHz, $CDCl_3$)



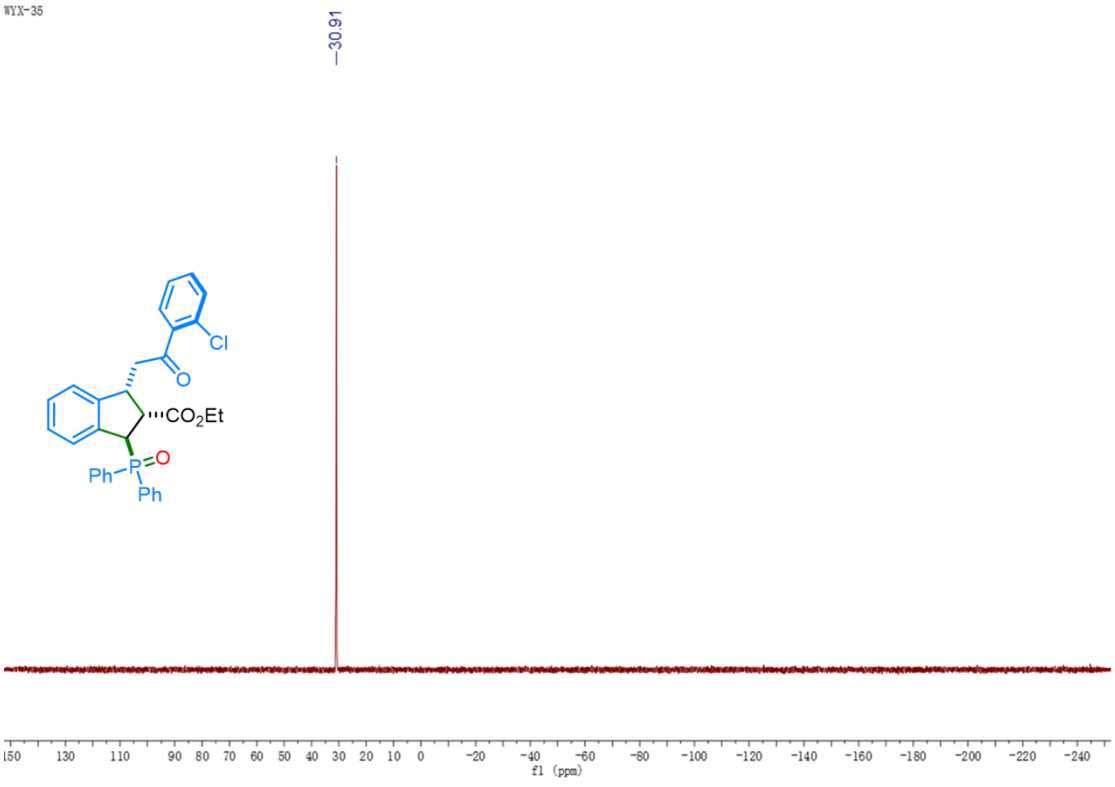
^{1}H NMR spectrum of **3m** (400 MHz, $CDCl_3$)



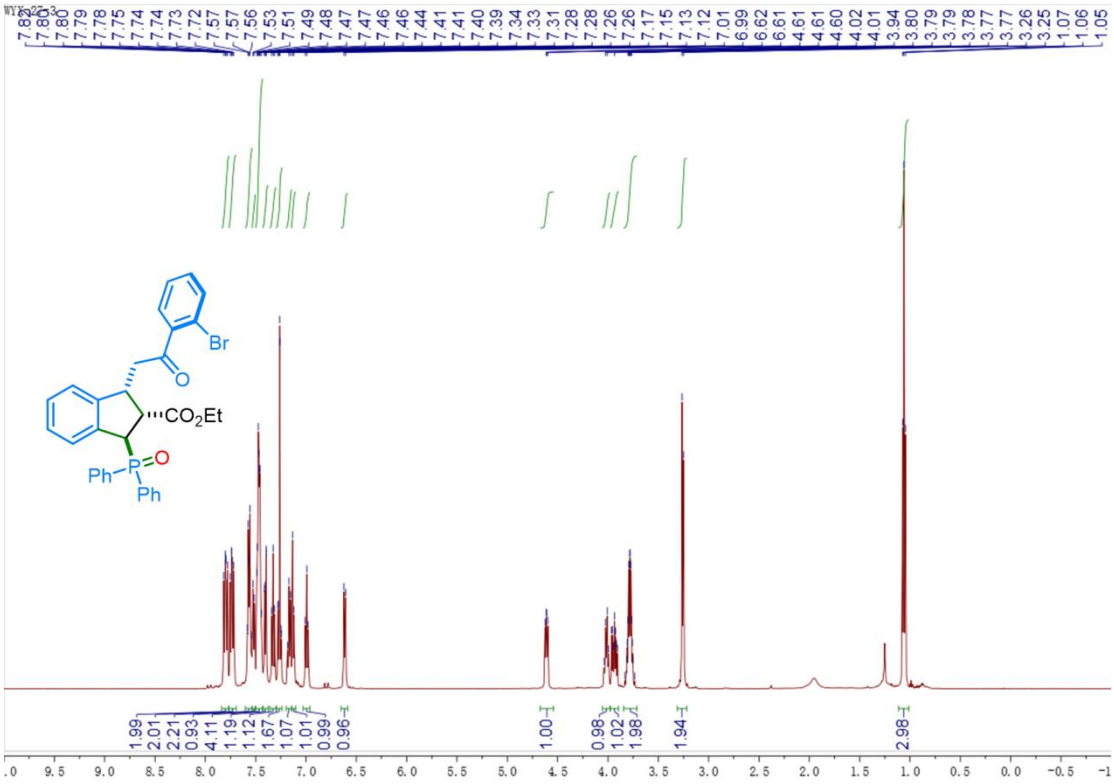
^{13}C NMR spectrum of **3m** (100 MHz, $CDCl_3$)



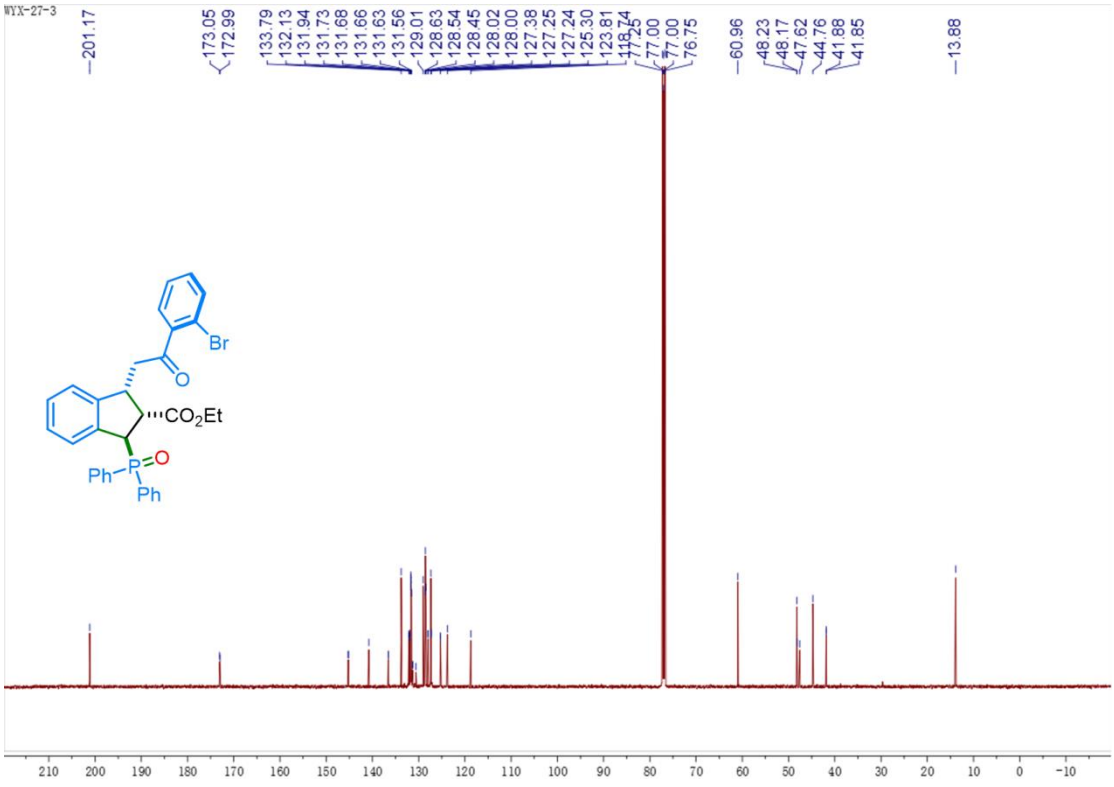
^{31}P NMR spectrum of **3m** (202 MHz, $CDCl_3$)



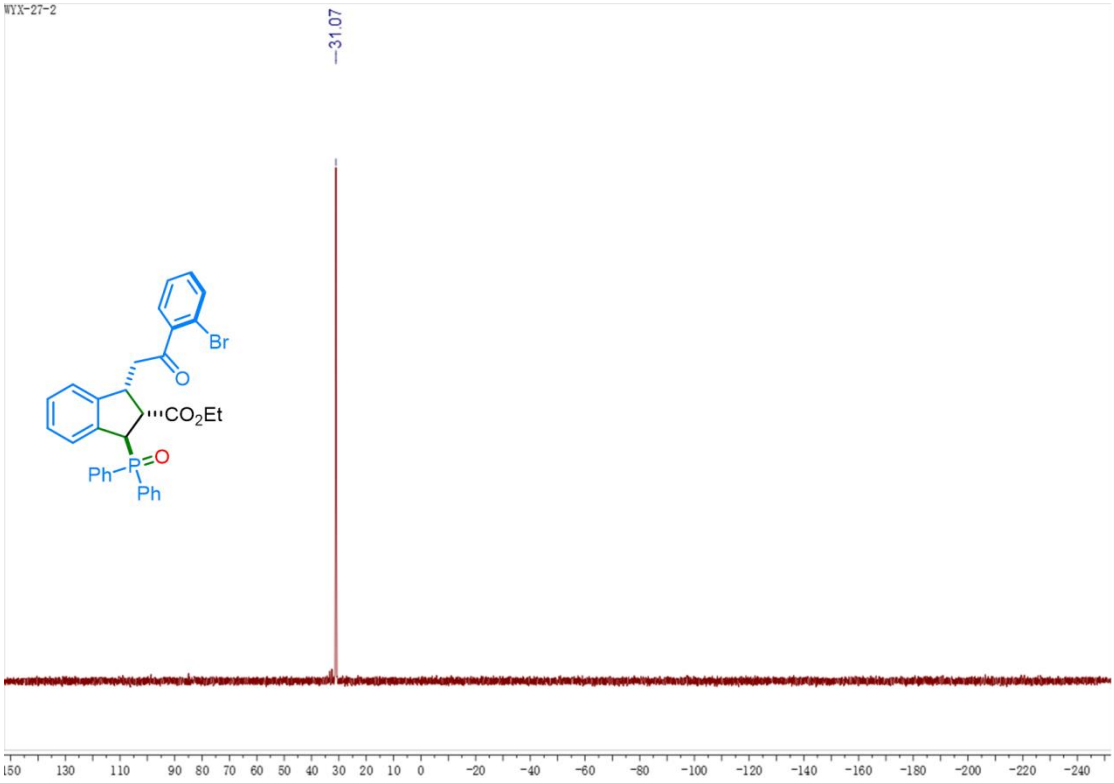
^{1}H NMR spectrum of **3n** (500 MHz, $CDCl_3$)



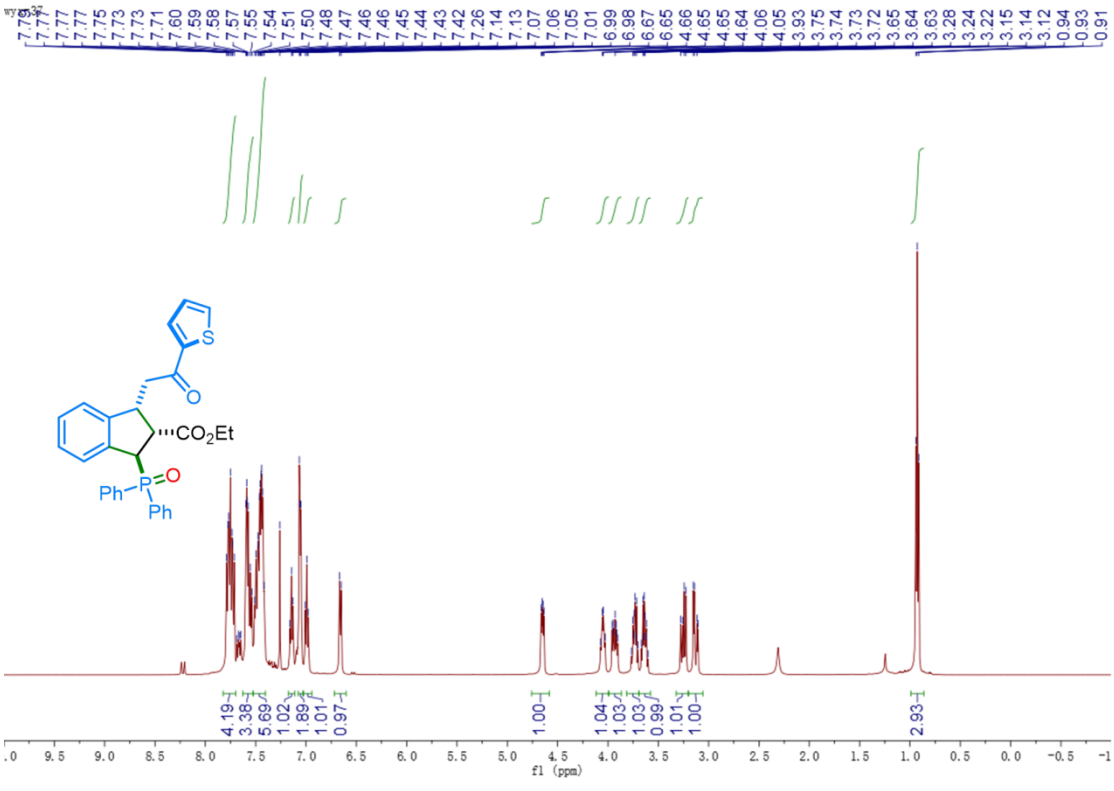
^{13}C NMR spectrum of **3n** (125 MHz, $CDCl_3$)



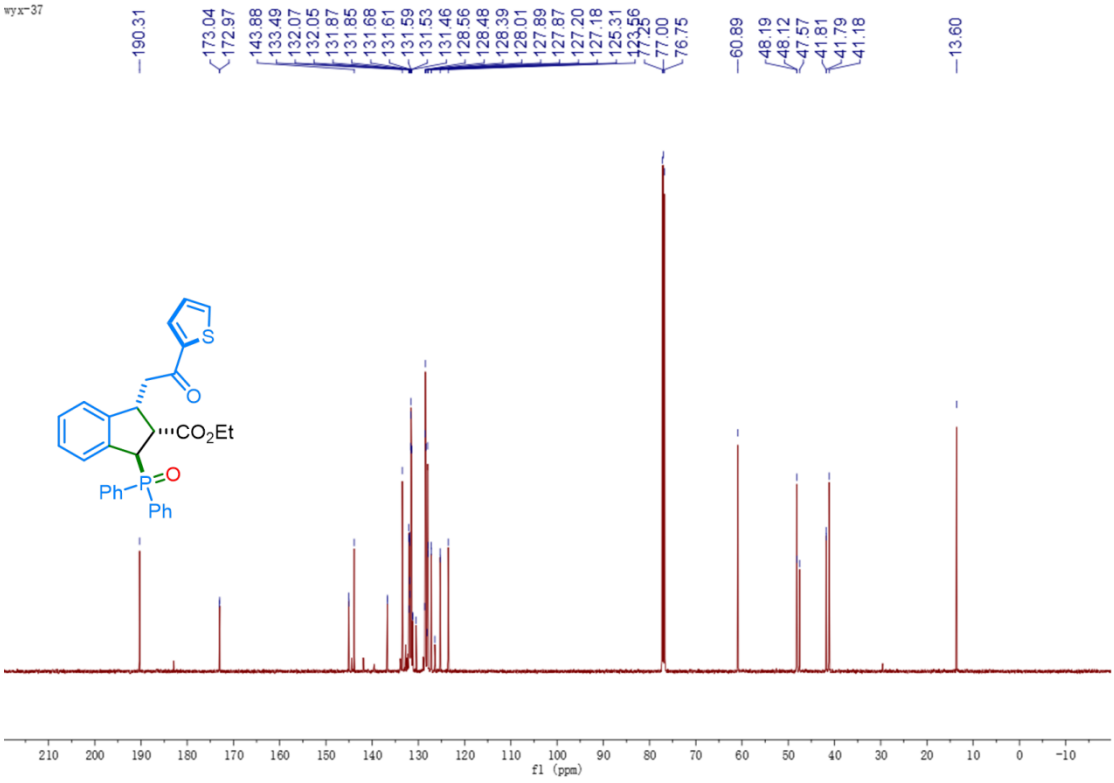
^{31}P NMR spectrum of **3n** (202 MHz, $CDCl_3$)



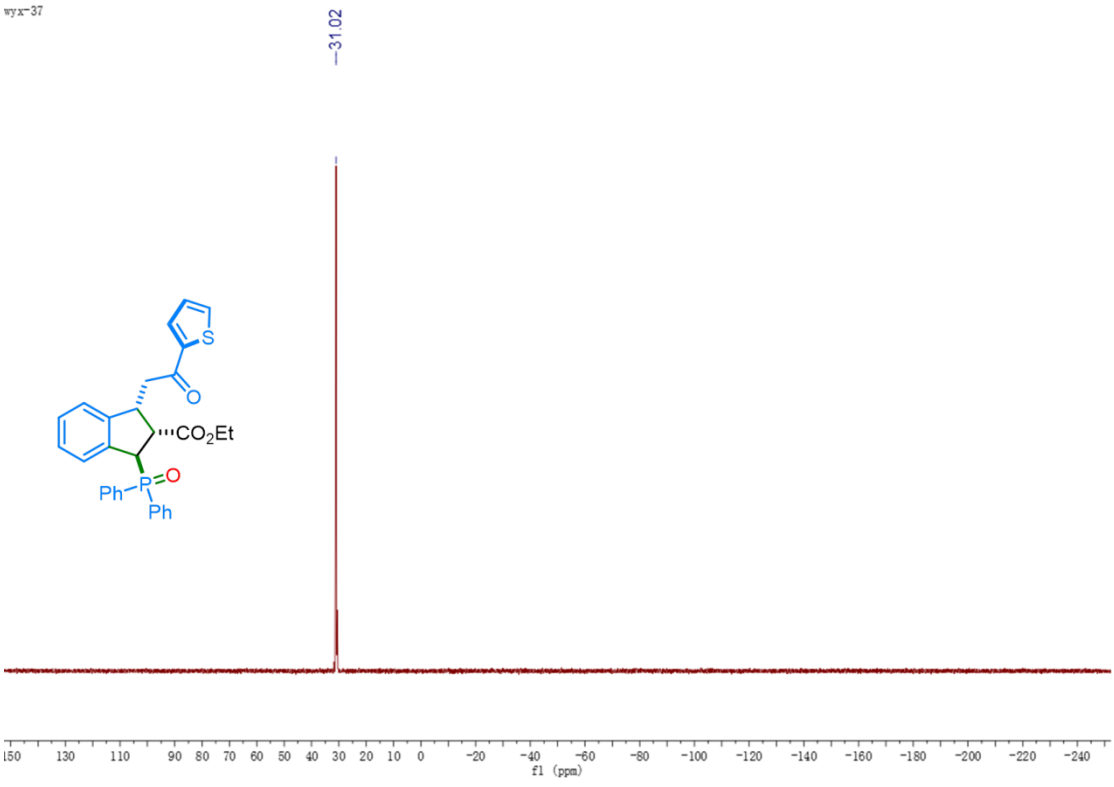
^{1}H NMR spectrum of **3o** (500 MHz, $CDCl_3$)



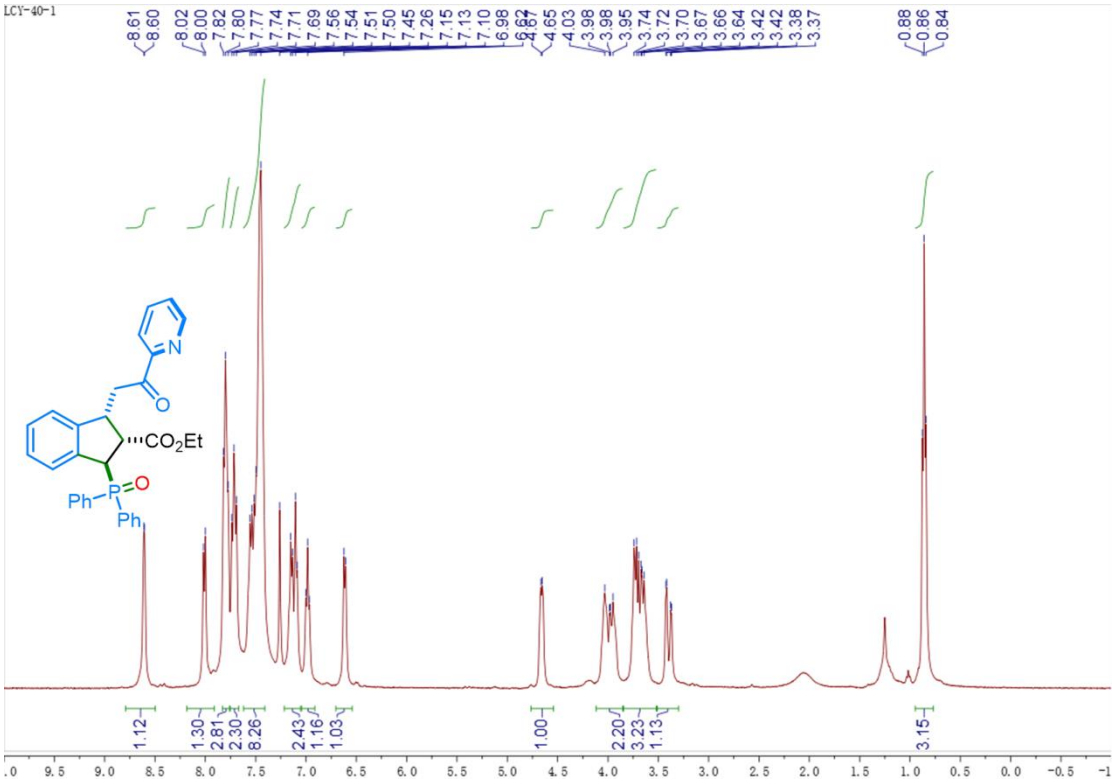
^{13}C NMR spectrum of **3o** (125 MHz, $CDCl_3$)



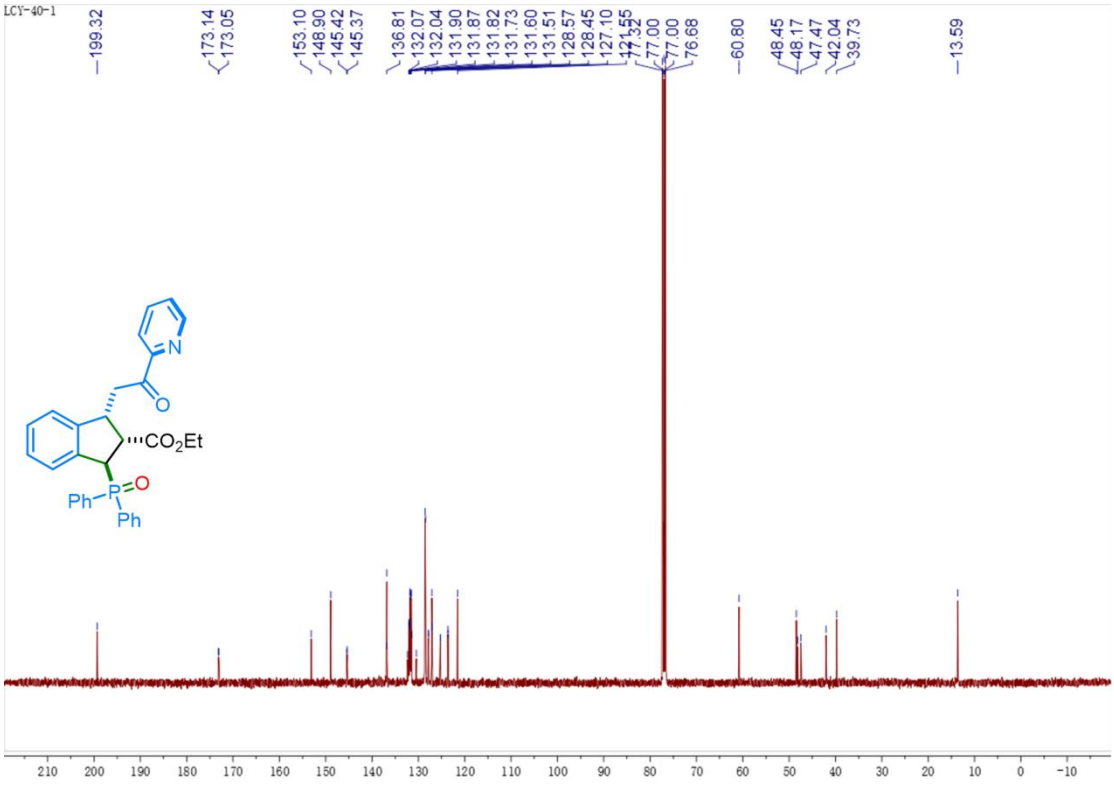
^{31}P NMR spectrum of **3o** (202 MHz, $CDCl_3$)



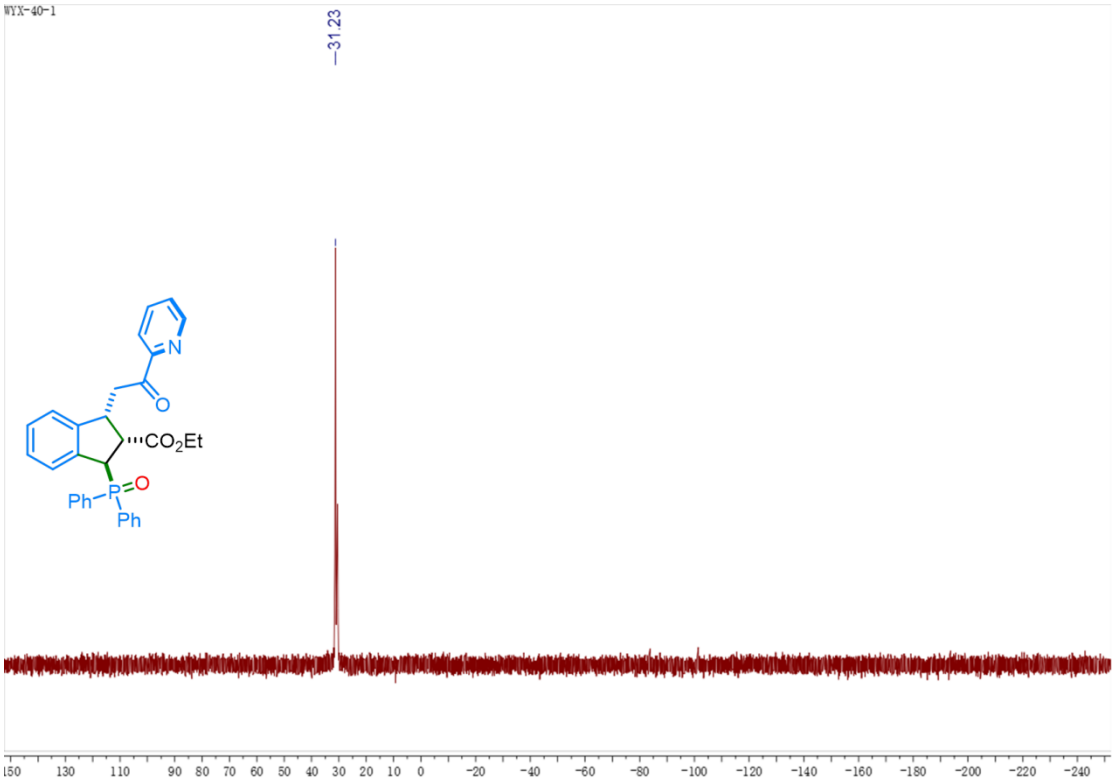
^{1}H NMR spectrum of **3p** (500 MHz, $CDCl_3$)



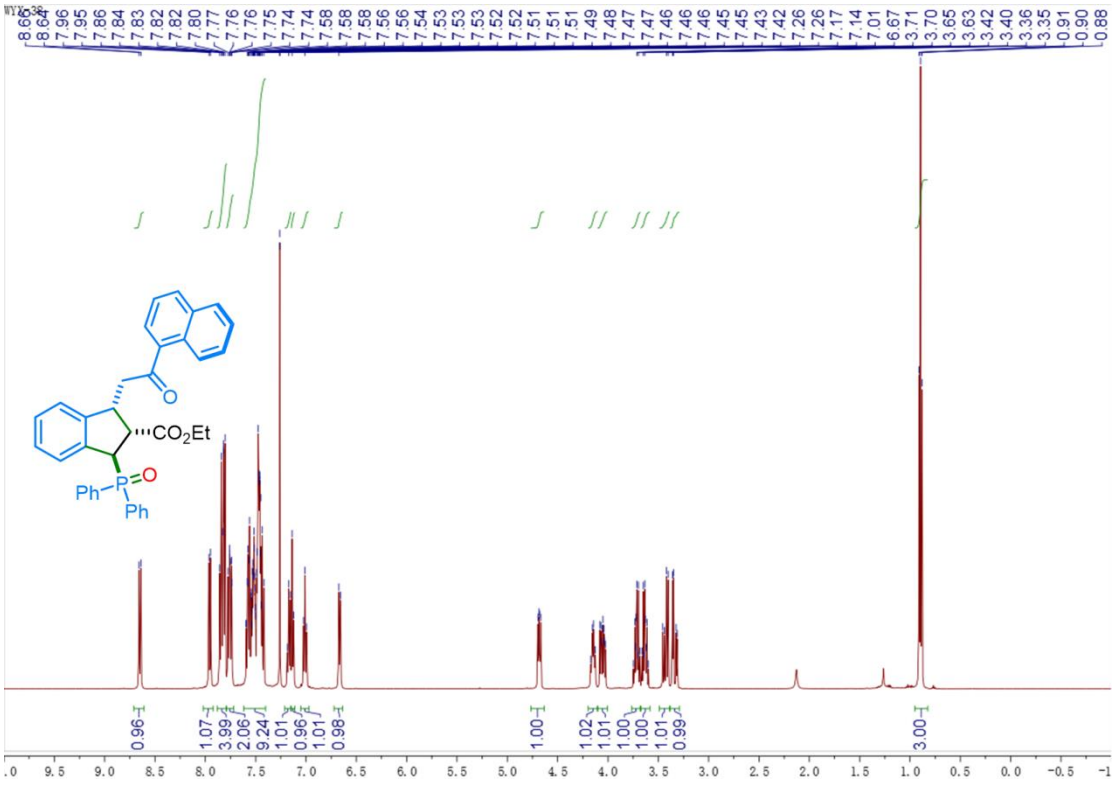
^{13}C NMR spectrum of **3p** (125 MHz, $CDCl_3$)



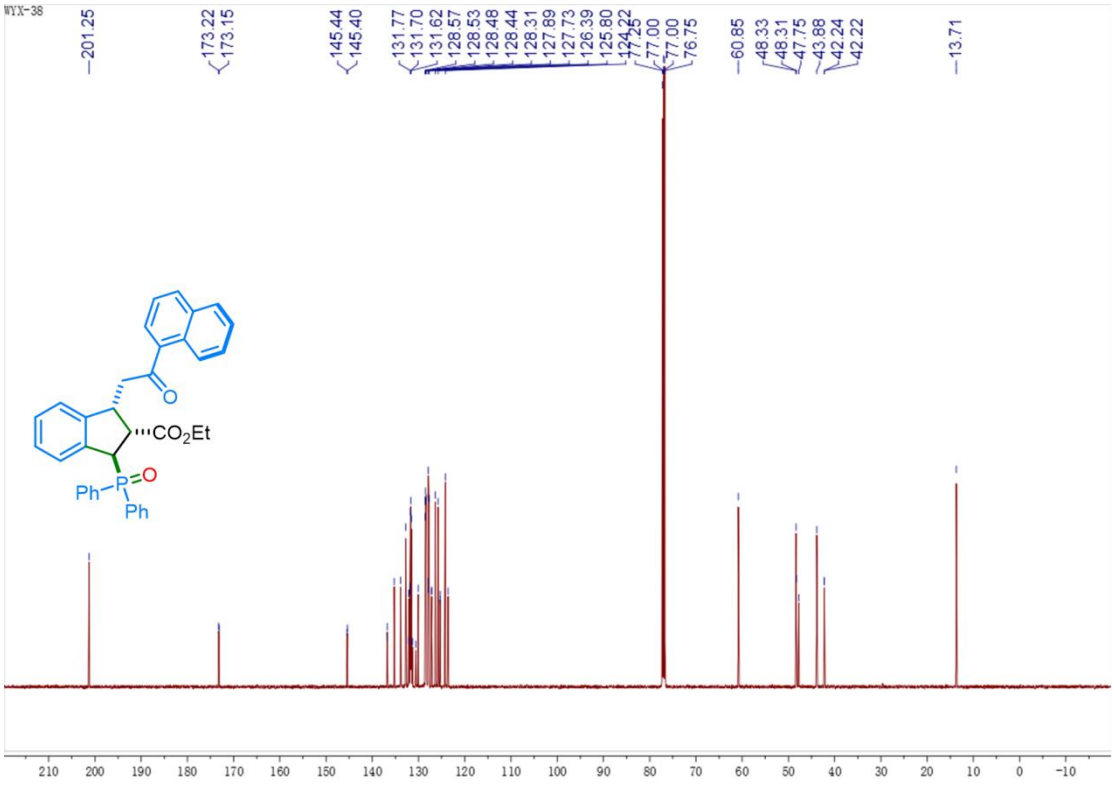
^{31}P NMR spectrum of **3p** (202 MHz, $CDCl_3$)



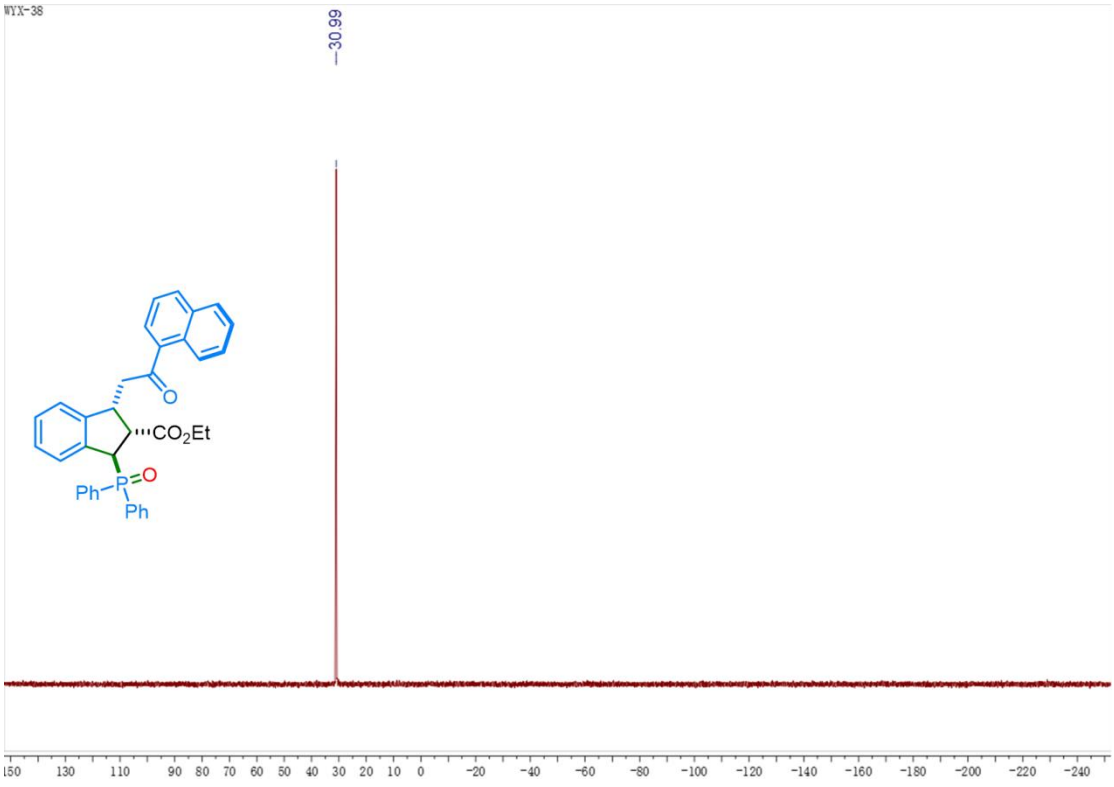
^{1}H NMR spectrum of **3q** (500 MHz, $CDCl_3$)



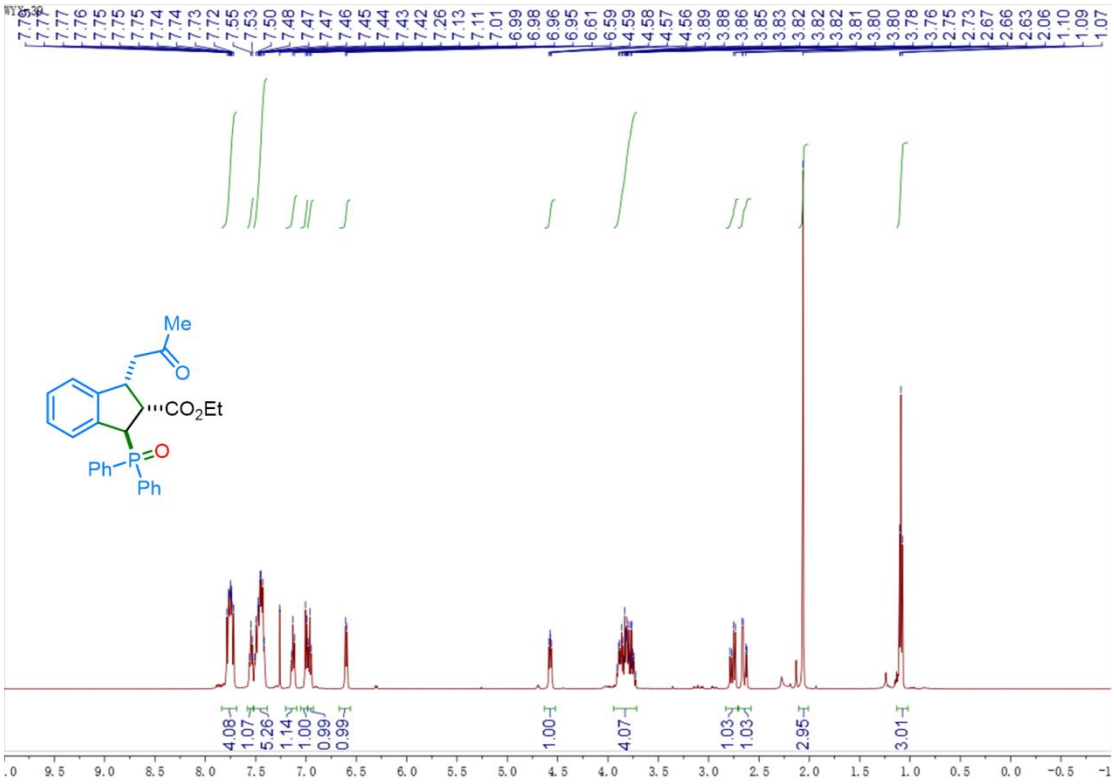
^{13}C NMR spectrum of **3q** (125 MHz, $CDCl_3$)



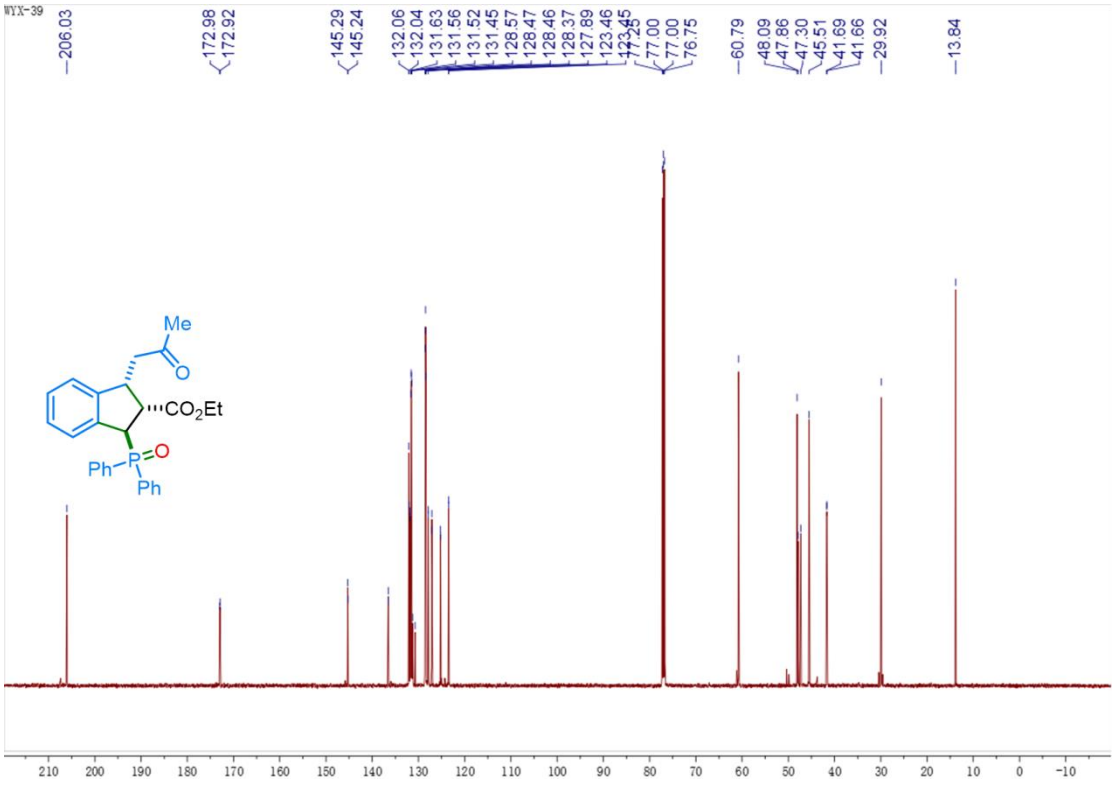
^{31}P NMR spectrum of **3q** (202 MHz, $CDCl_3$)



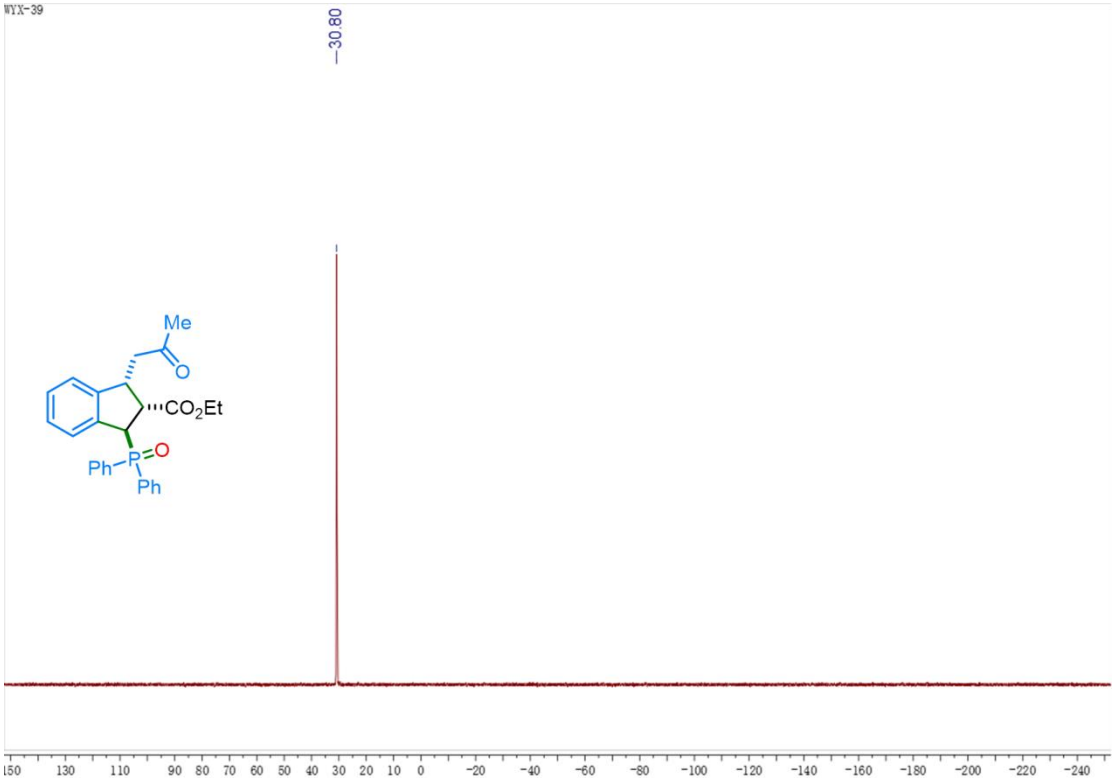
^{1}H NMR spectrum of **3r** (500 MHz, $CDCl_3$)



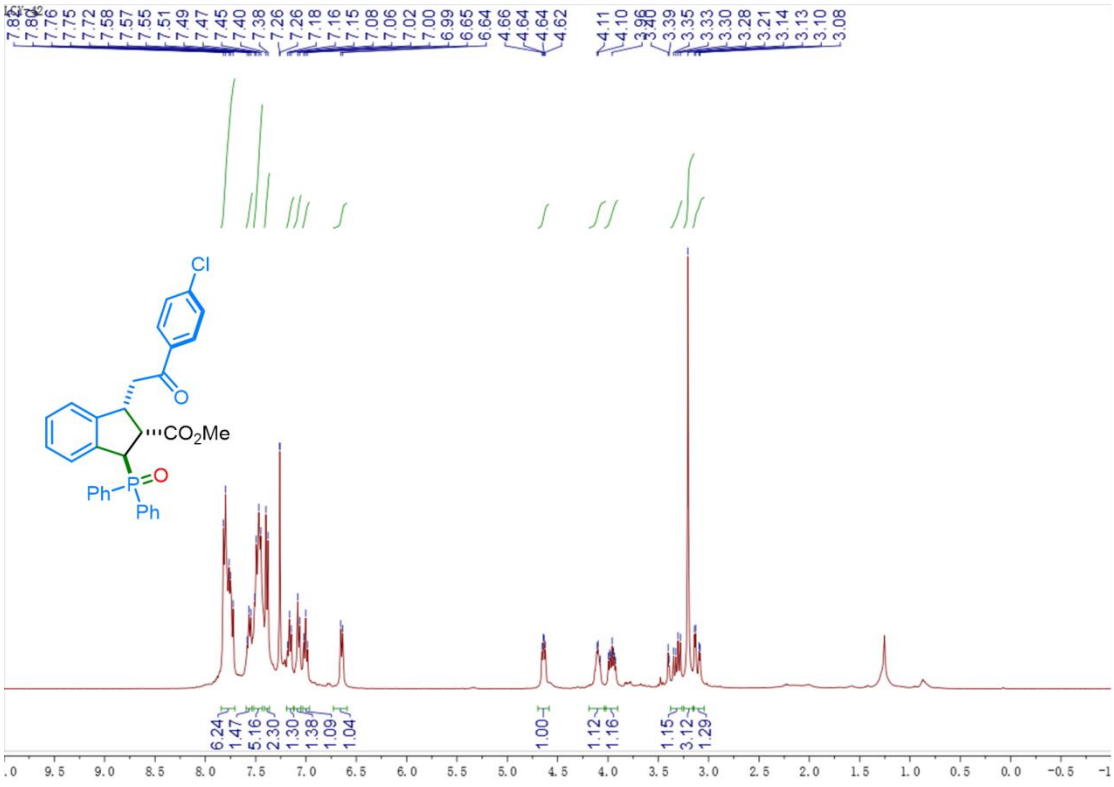
^{13}C NMR spectrum of **3r** (125 MHz, $CDCl_3$)



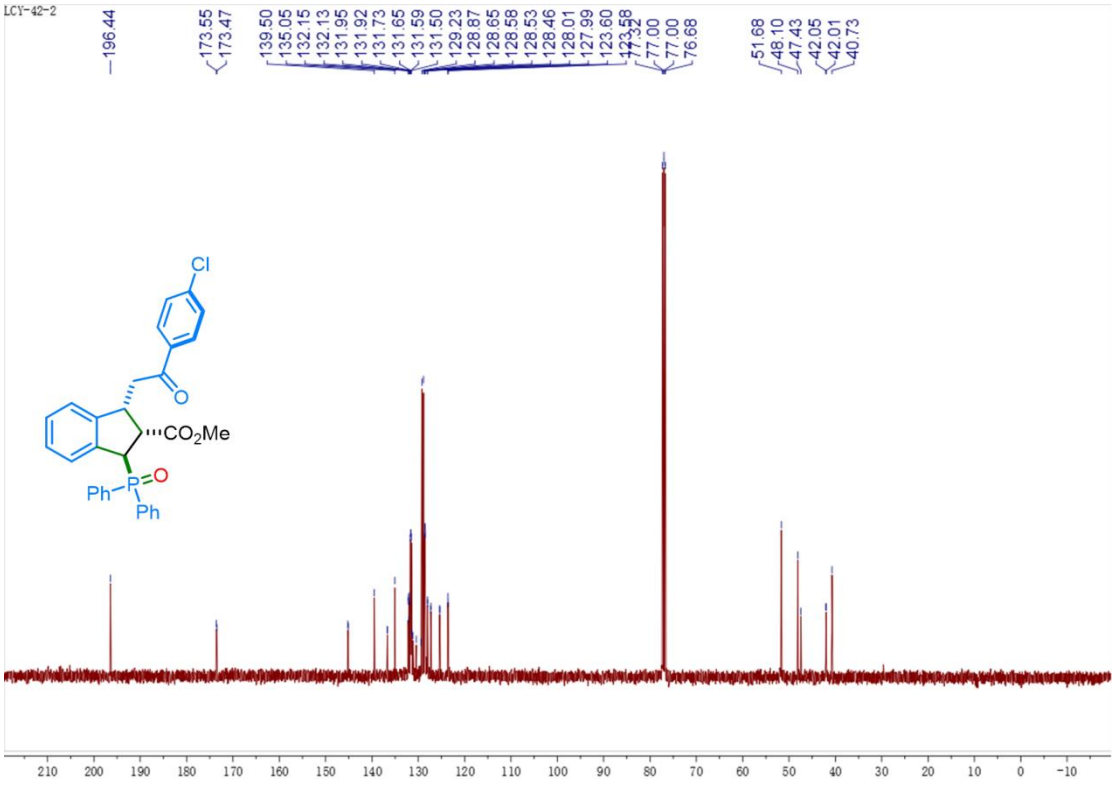
^{31}P NMR spectrum of **3r** (202 MHz, $CDCl_3$)



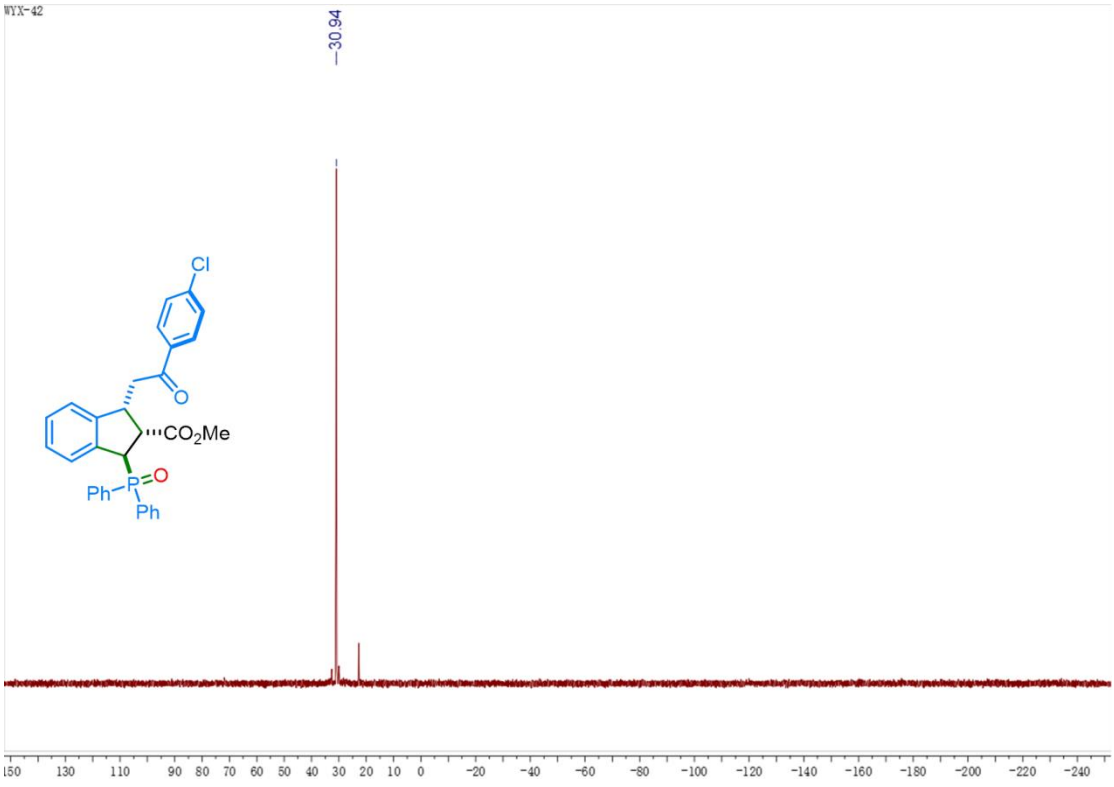
^{1}H NMR spectrum of **3s** (400 MHz, $CDCl_3$)



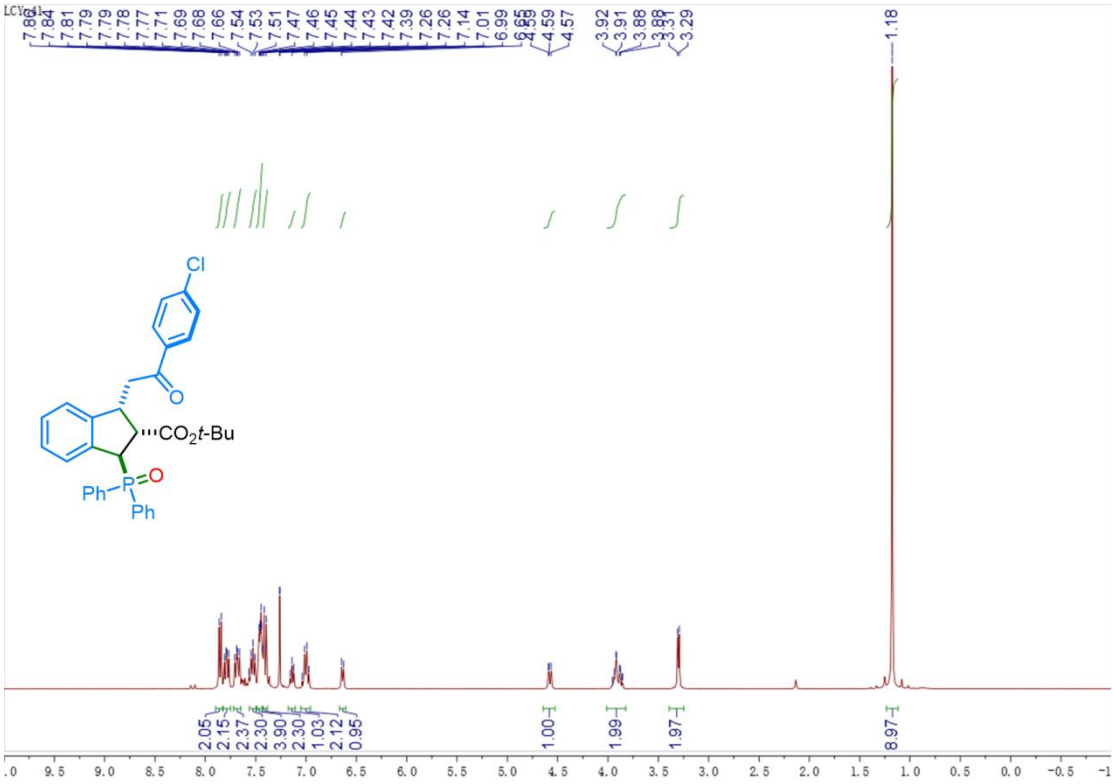
^{13}C NMR spectrum of **3s** (100 MHz, $CDCl_3$)



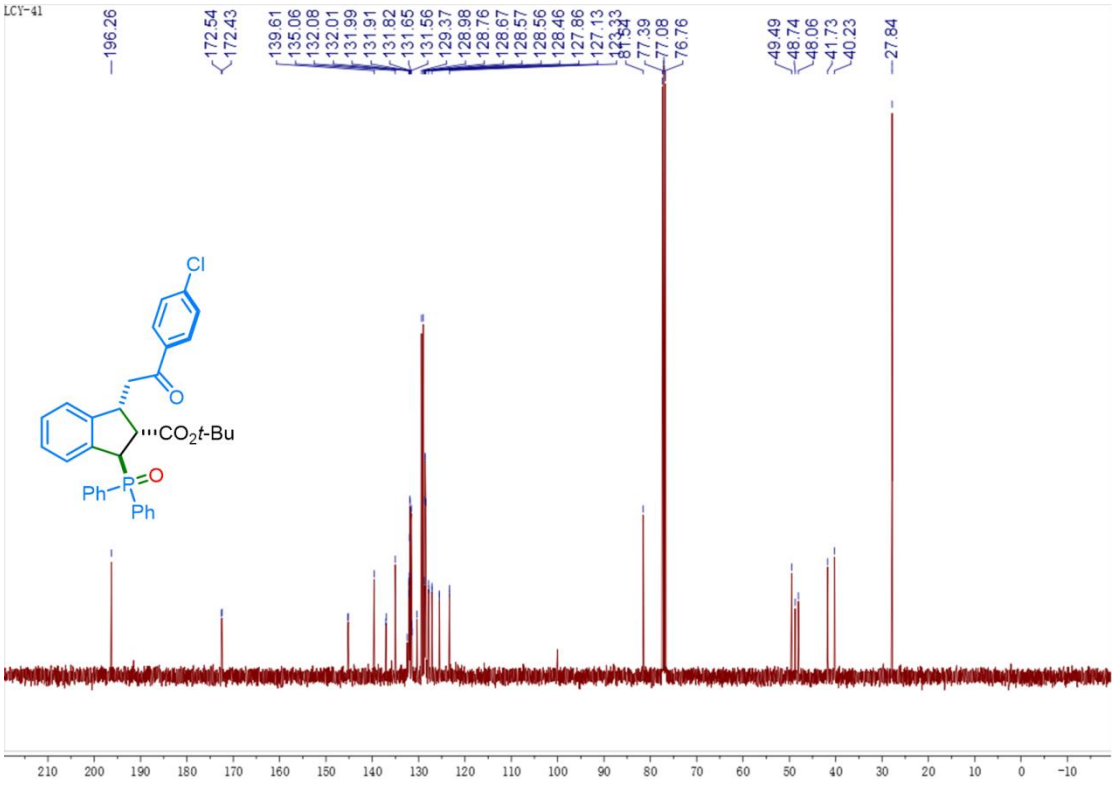
^{31}P NMR spectrum of **3s** (202 MHz, $CDCl_3$)



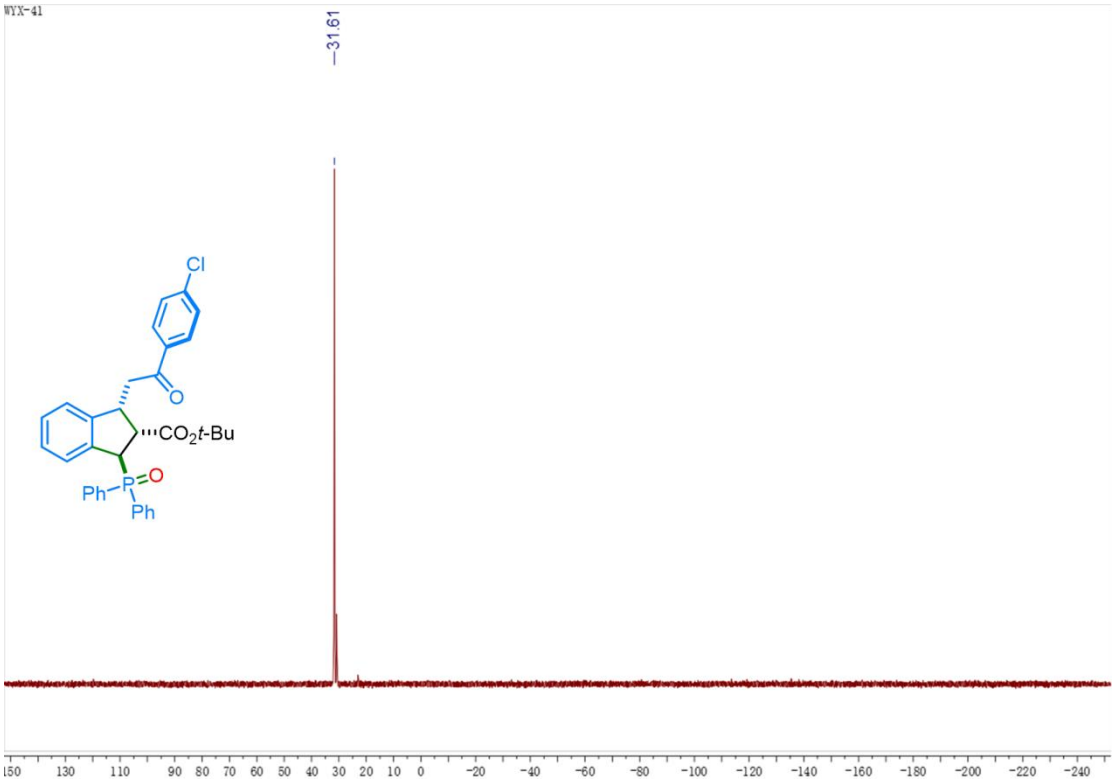
^{1}H NMR spectrum of **3t** (400 MHz, $CDCl_3$)



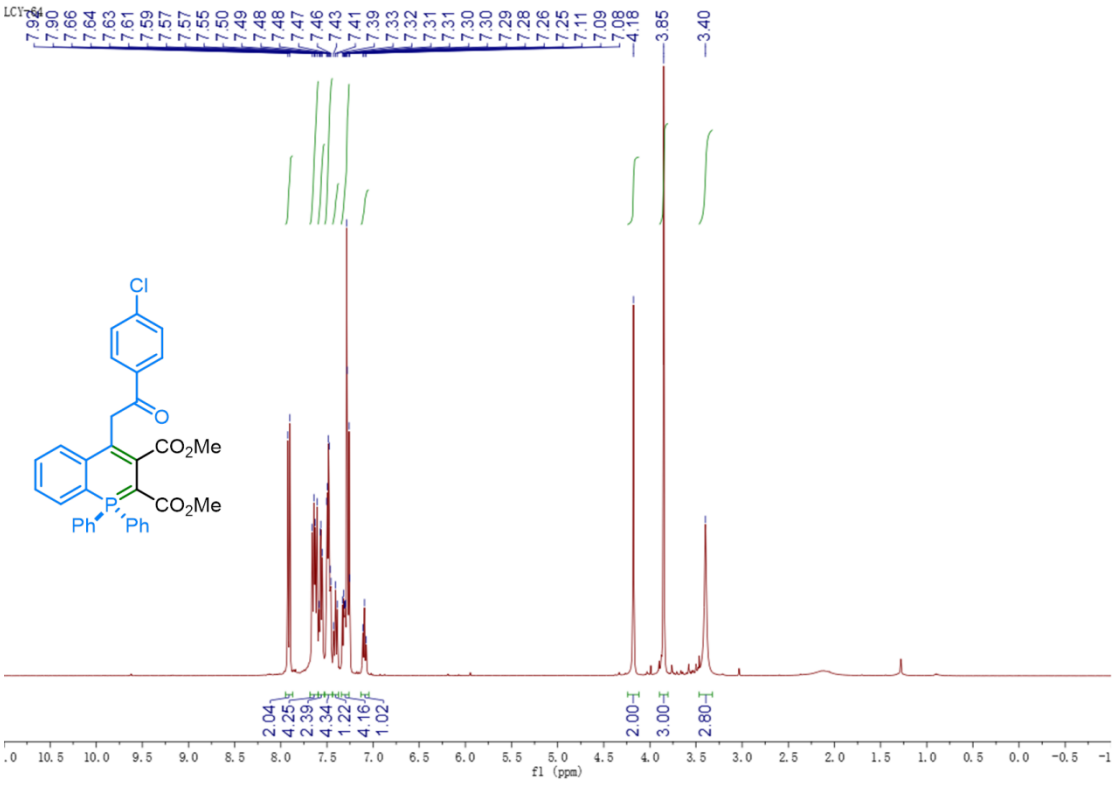
^{13}C NMR spectrum of **3t** (100 MHz, $CDCl_3$)



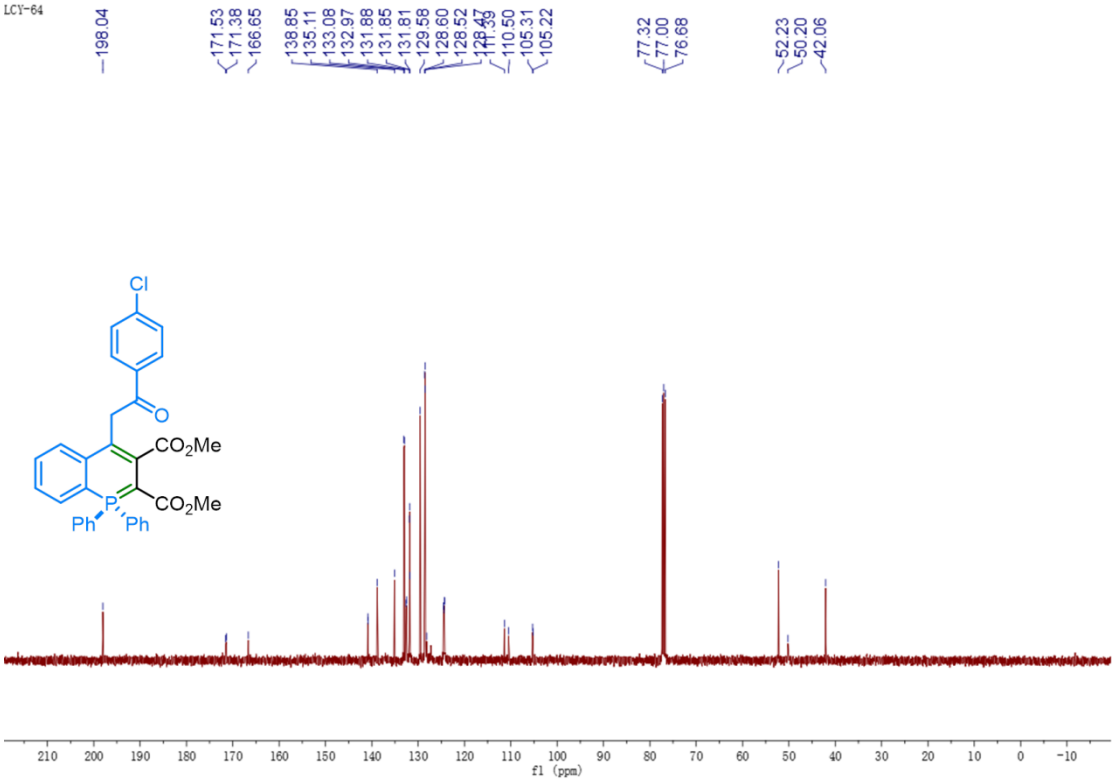
^{31}P NMR spectrum of **3t** (202 MHz, $CDCl_3$)



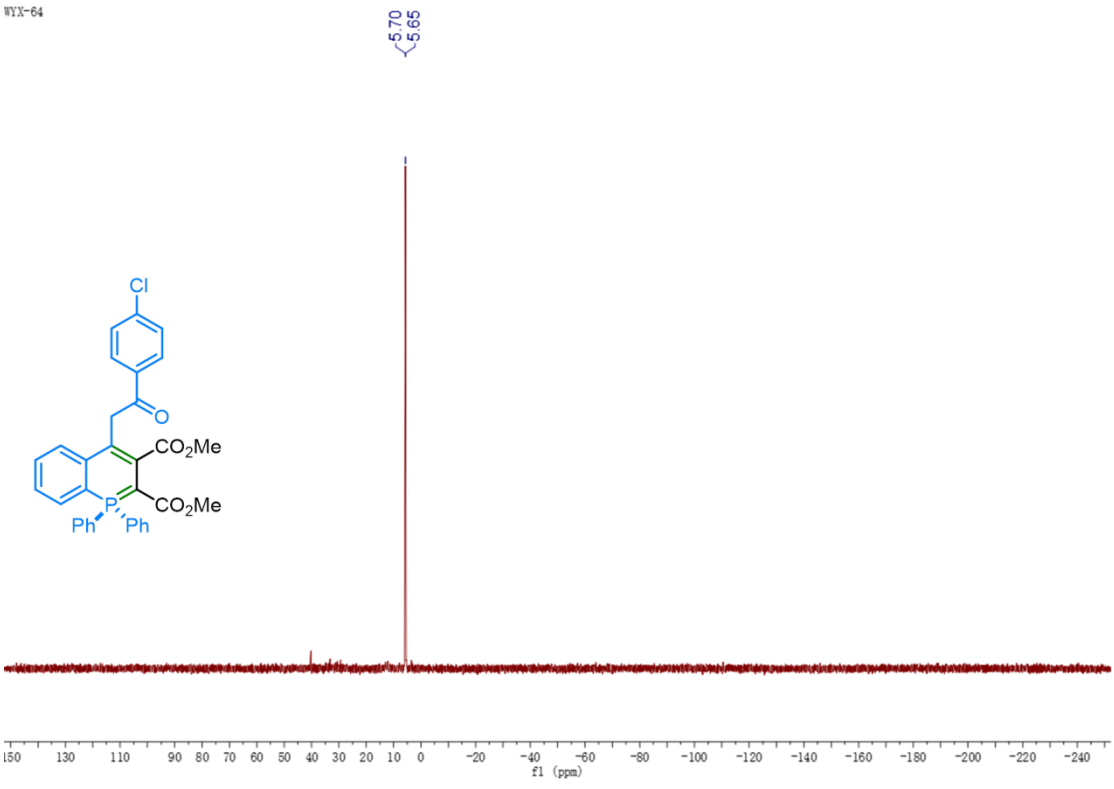
^{1}H NMR spectrum of **5a** (400 MHz, $CDCl_3$)



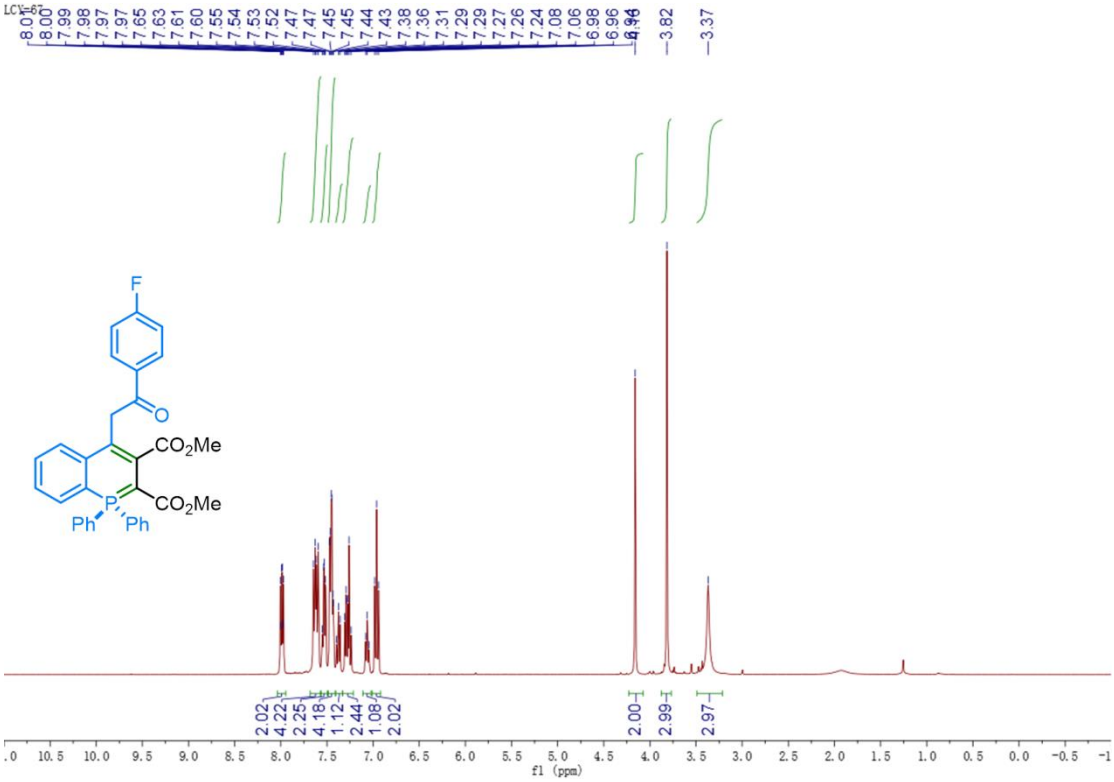
^{13}C NMR spectrum of **5a** (100 MHz, $CDCl_3$)



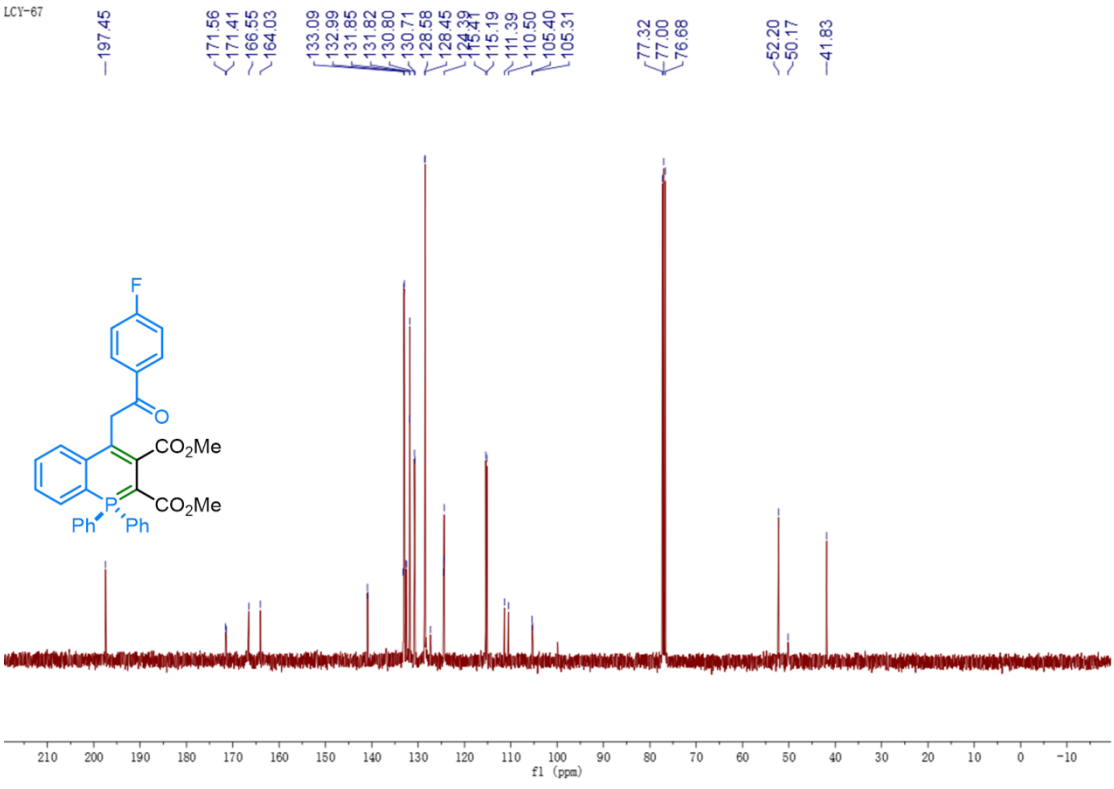
^{31}P NMR spectrum of **5a** (202 MHz, $CDCl_3$)



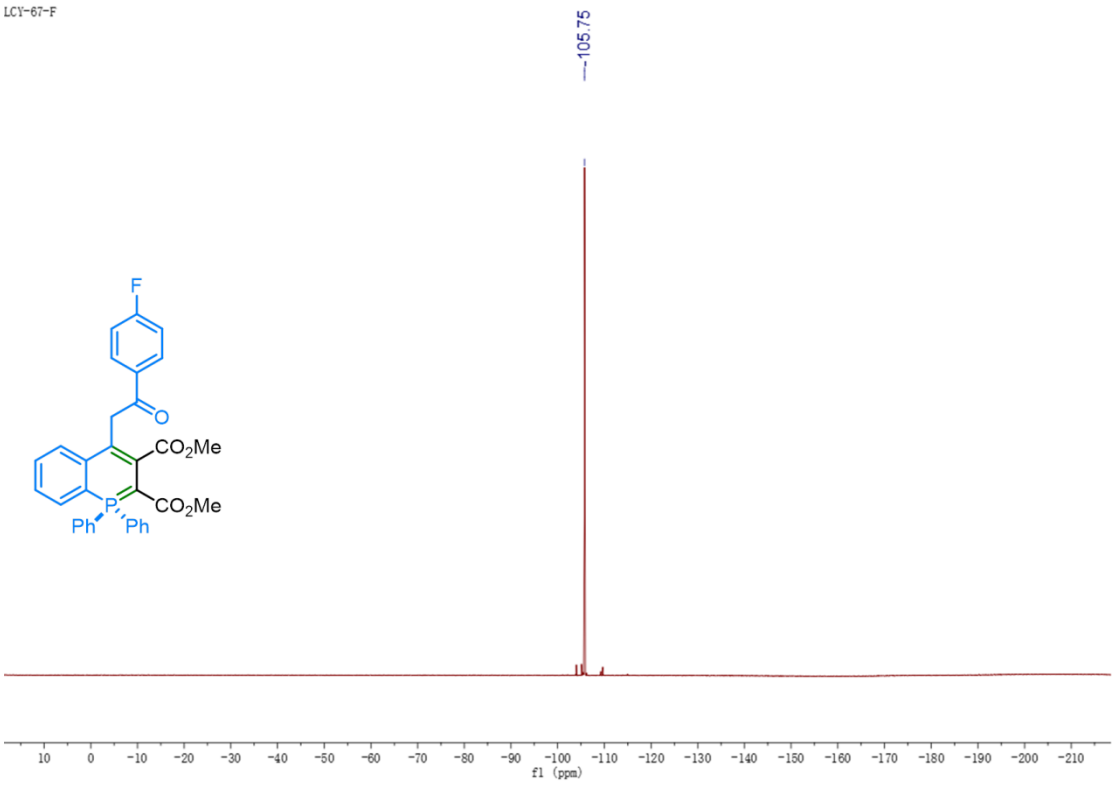
^{1}H NMR spectrum of **5b** (400 MHz, $CDCl_3$)



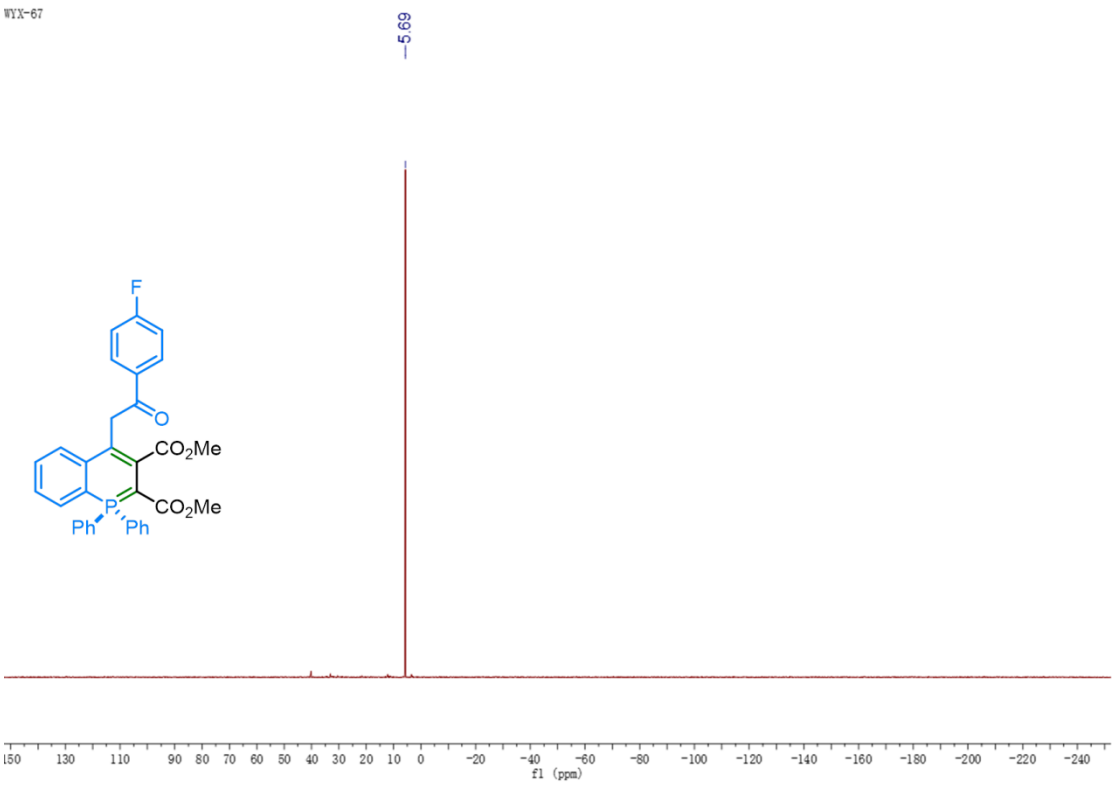
^{13}C NMR spectrum of **5b** (100 MHz, $CDCl_3$)



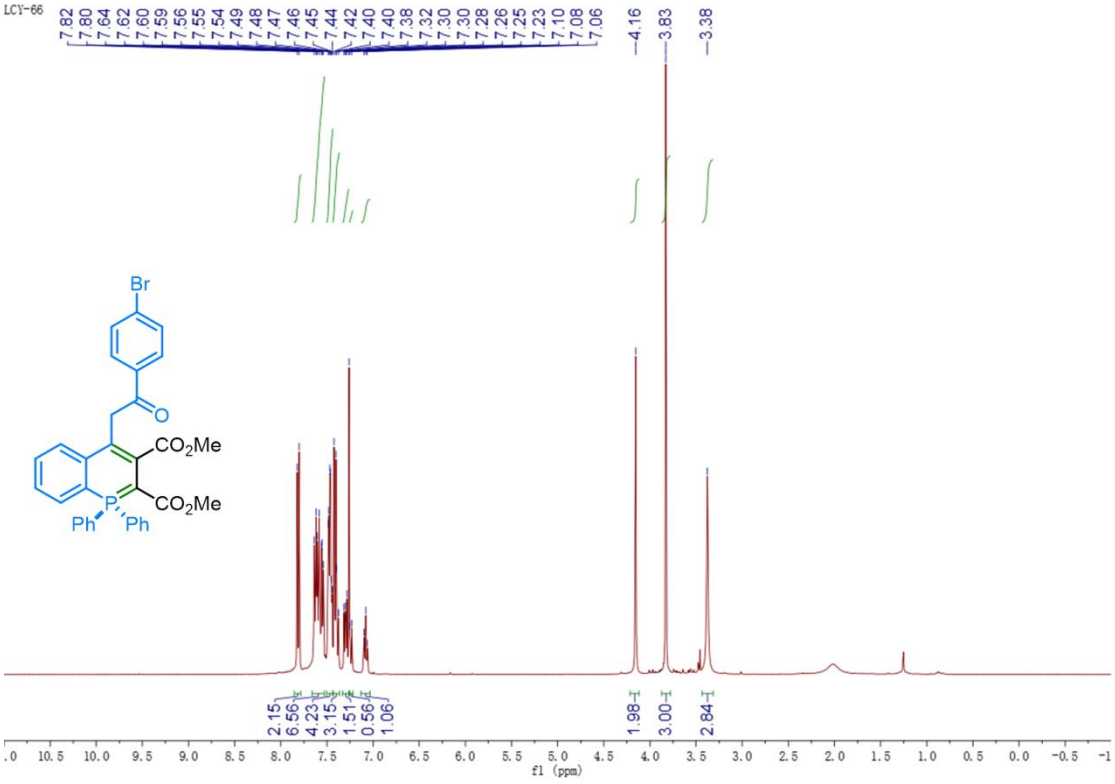
^{19}F NMR spectrum of **5b** (375 MHz, $CDCl_3$)



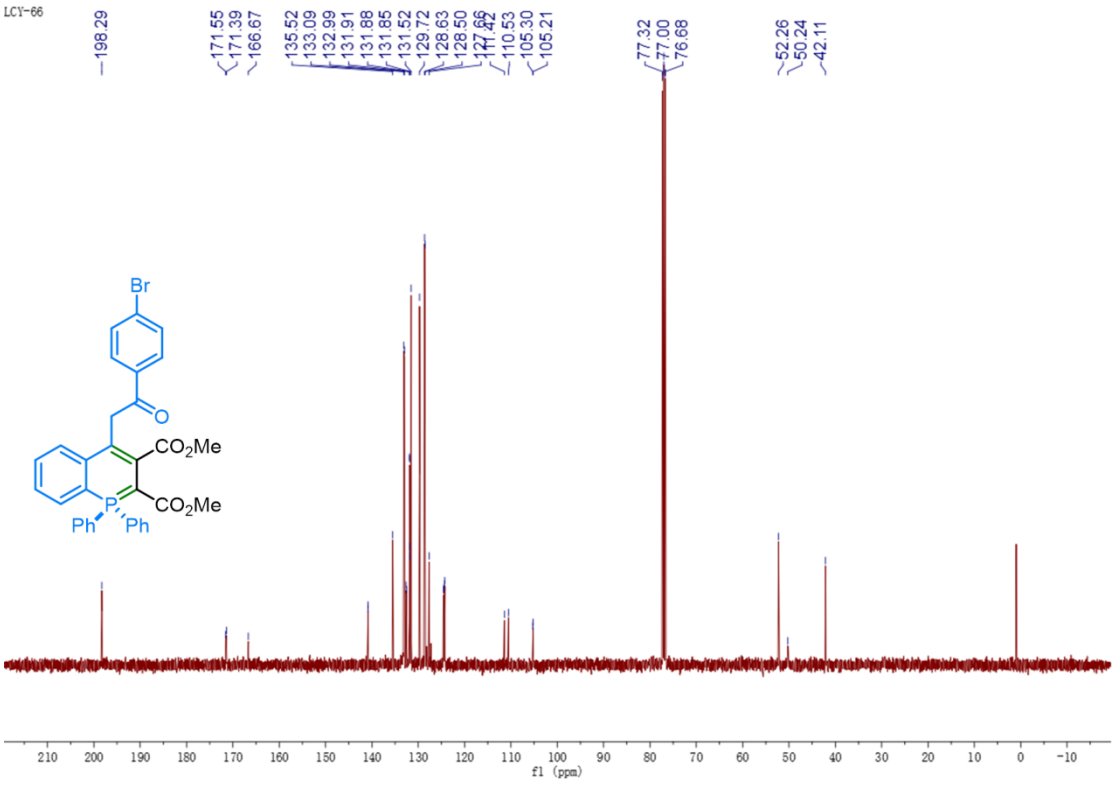
^{31}P NMR spectrum of **5b** (202 MHz, $CDCl_3$)



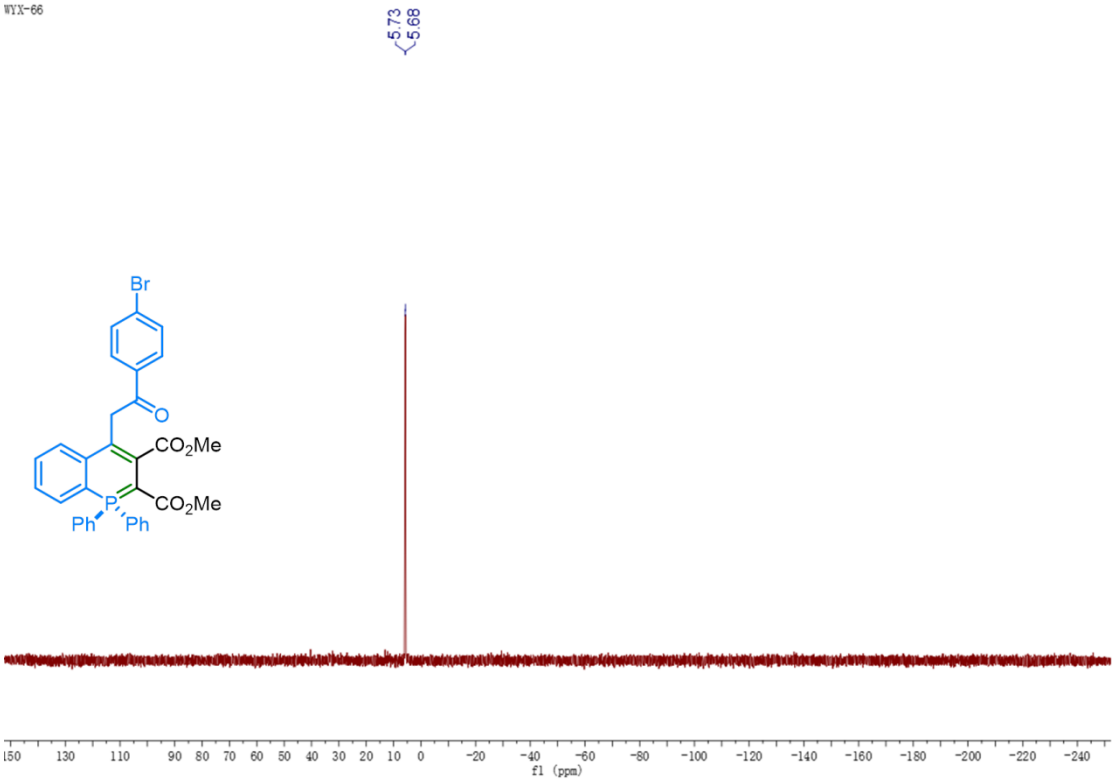
^{1}H NMR spectrum of **5c** (400 MHz, $CDCl_3$)



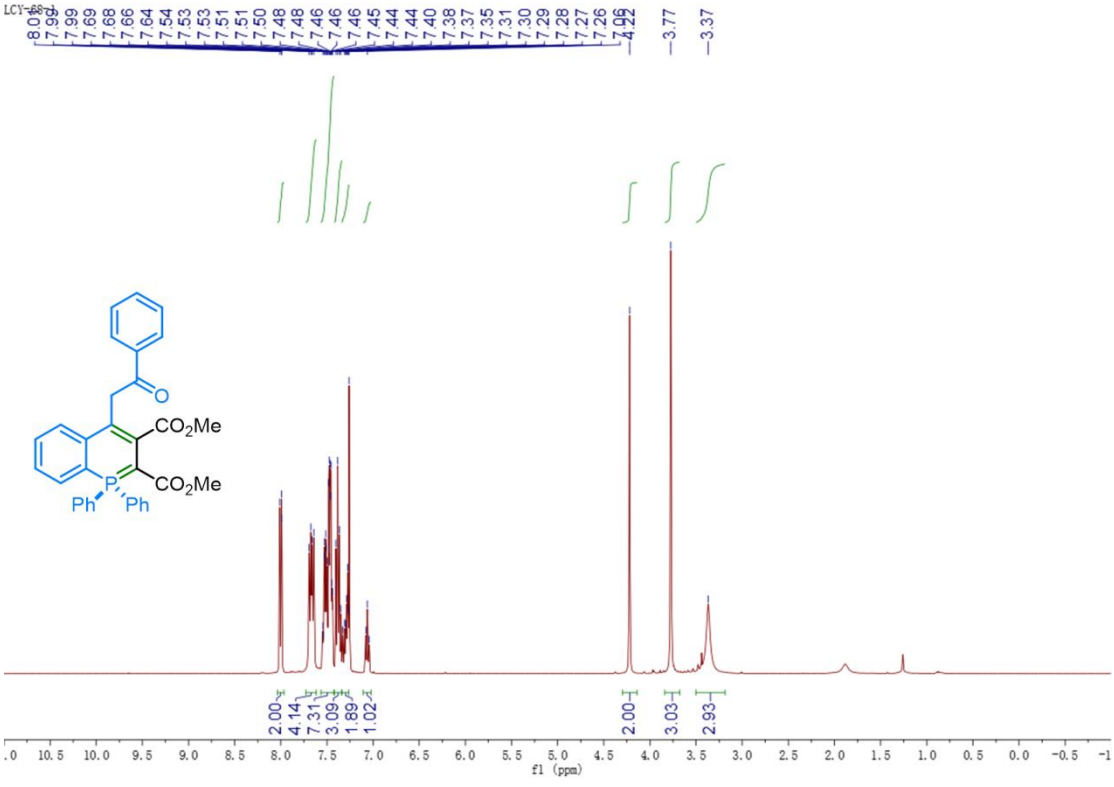
^{13}C NMR spectrum of **5c** (100 MHz, $CDCl_3$)



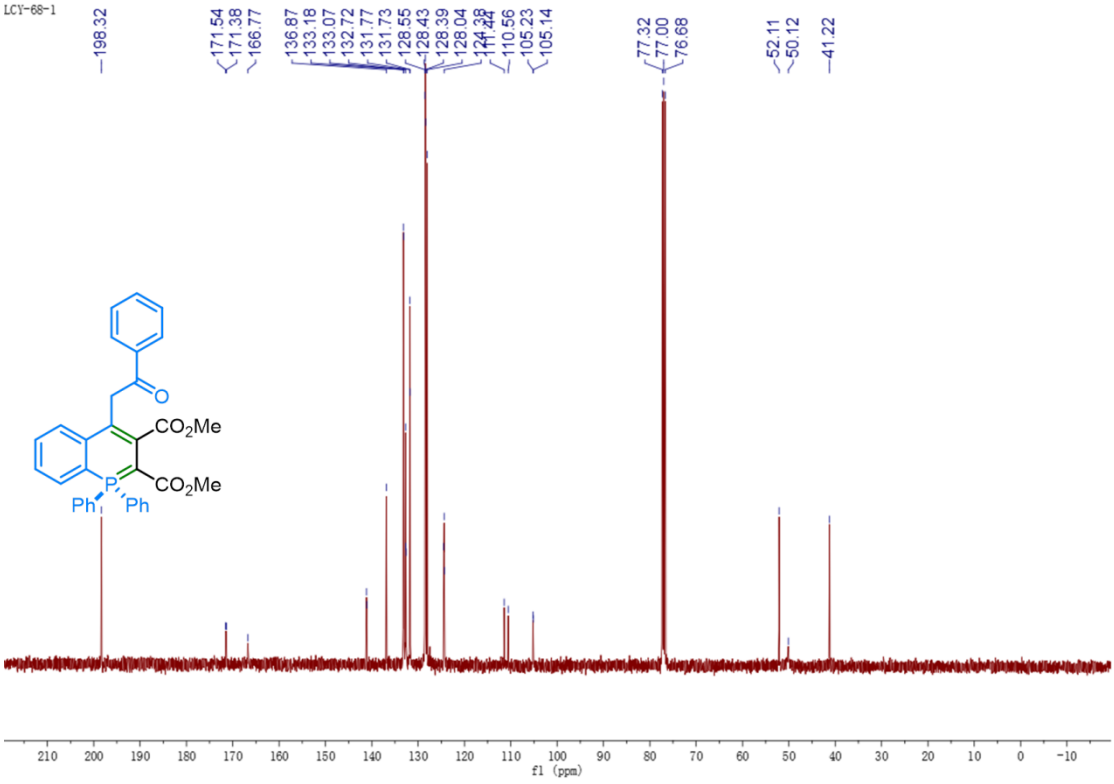
^{31}P NMR spectrum of **5c** (202 MHz, $CDCl_3$)



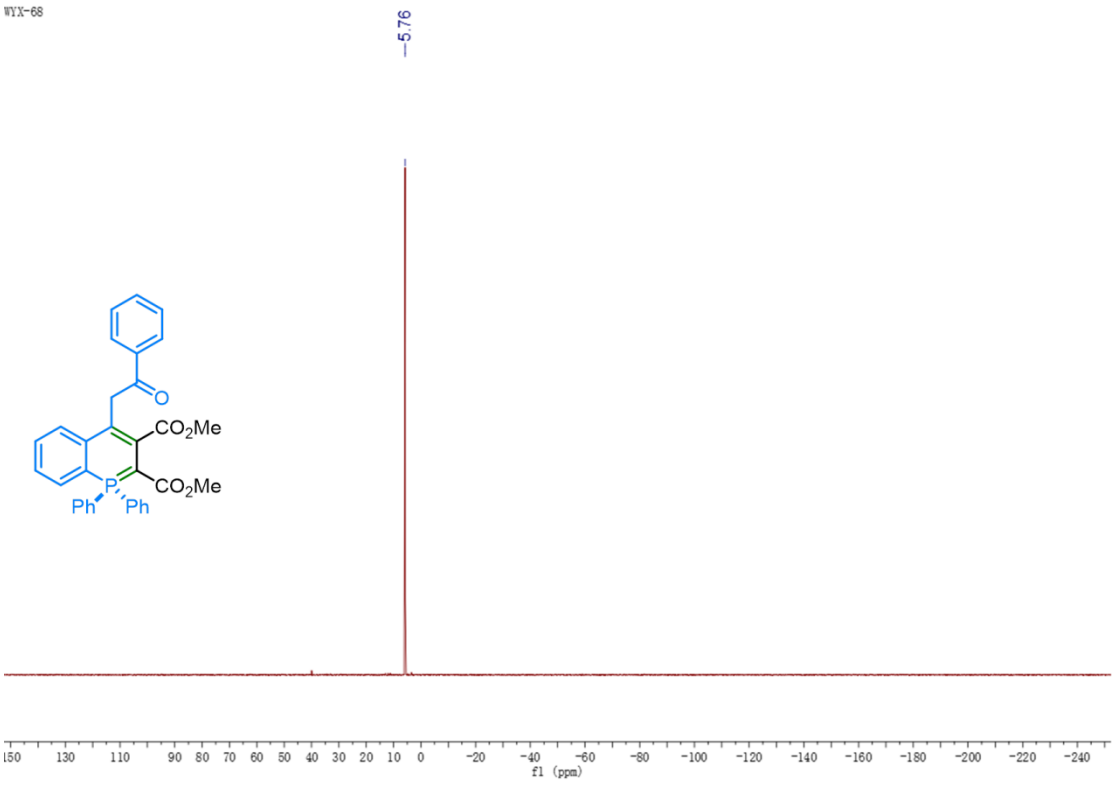
^{1}H NMR spectrum of **5d** (400 MHz, $CDCl_3$)



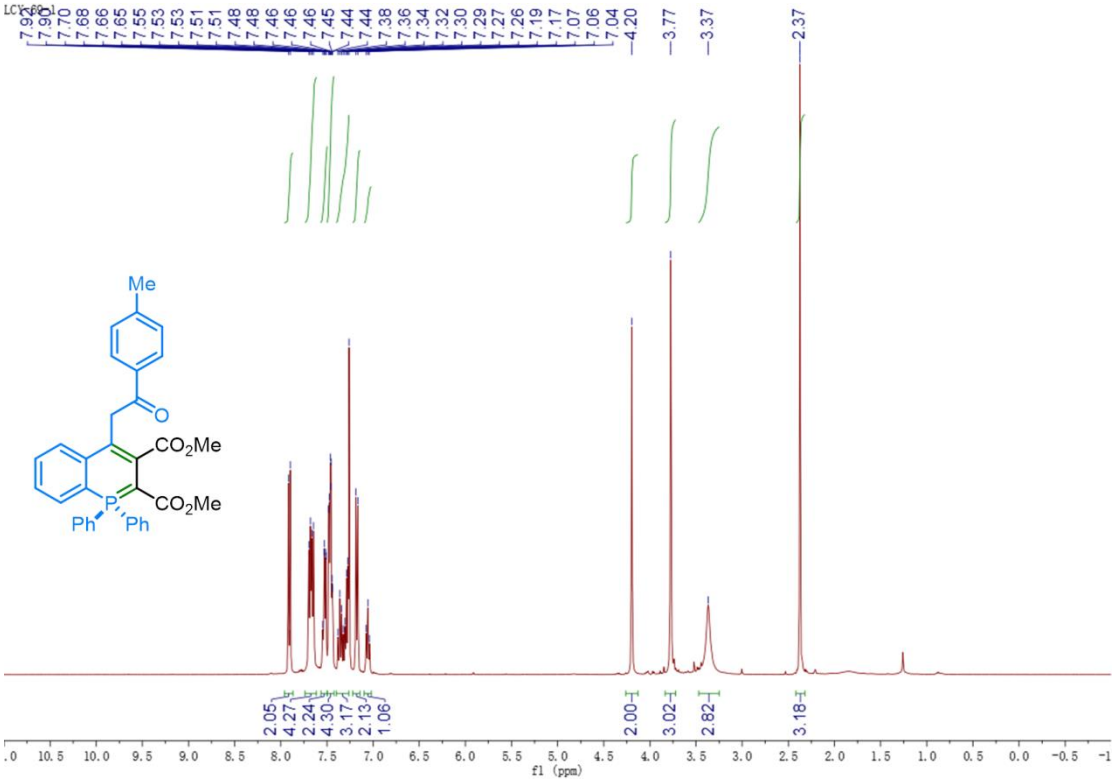
^{13}C NMR spectrum of **5d** (100 MHz, $CDCl_3$)



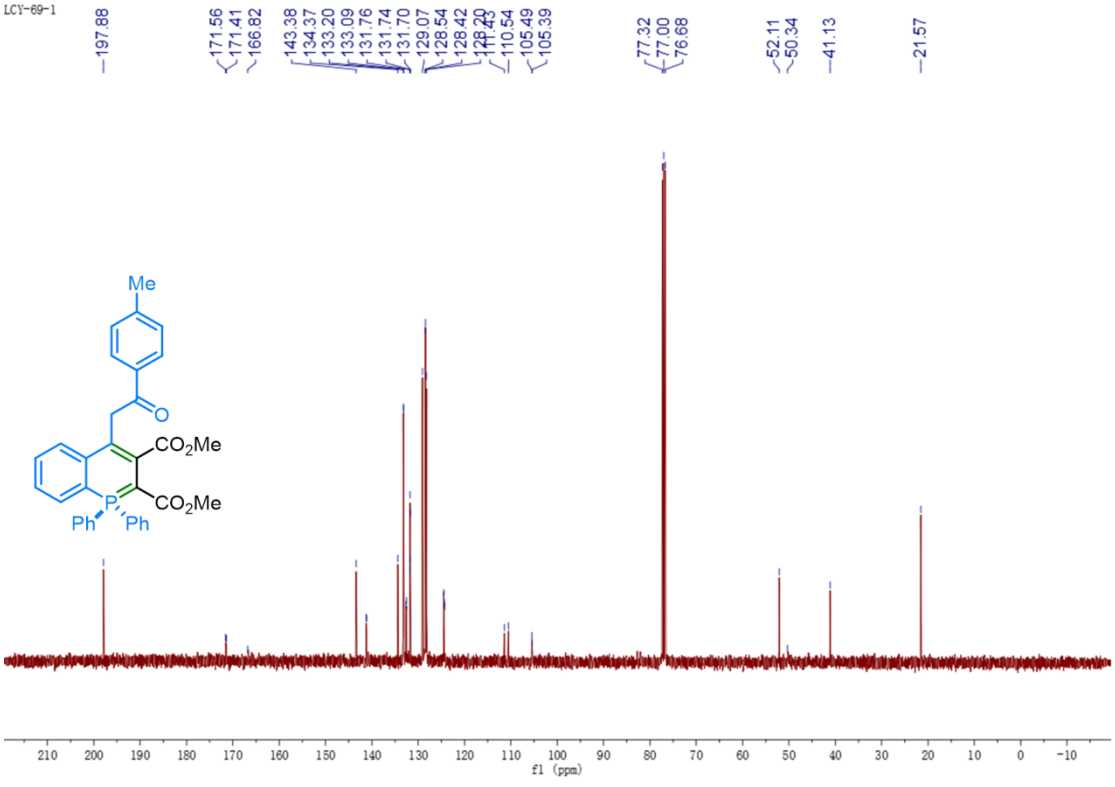
^{31}P NMR spectrum of **5d** (202 MHz, $CDCl_3$)



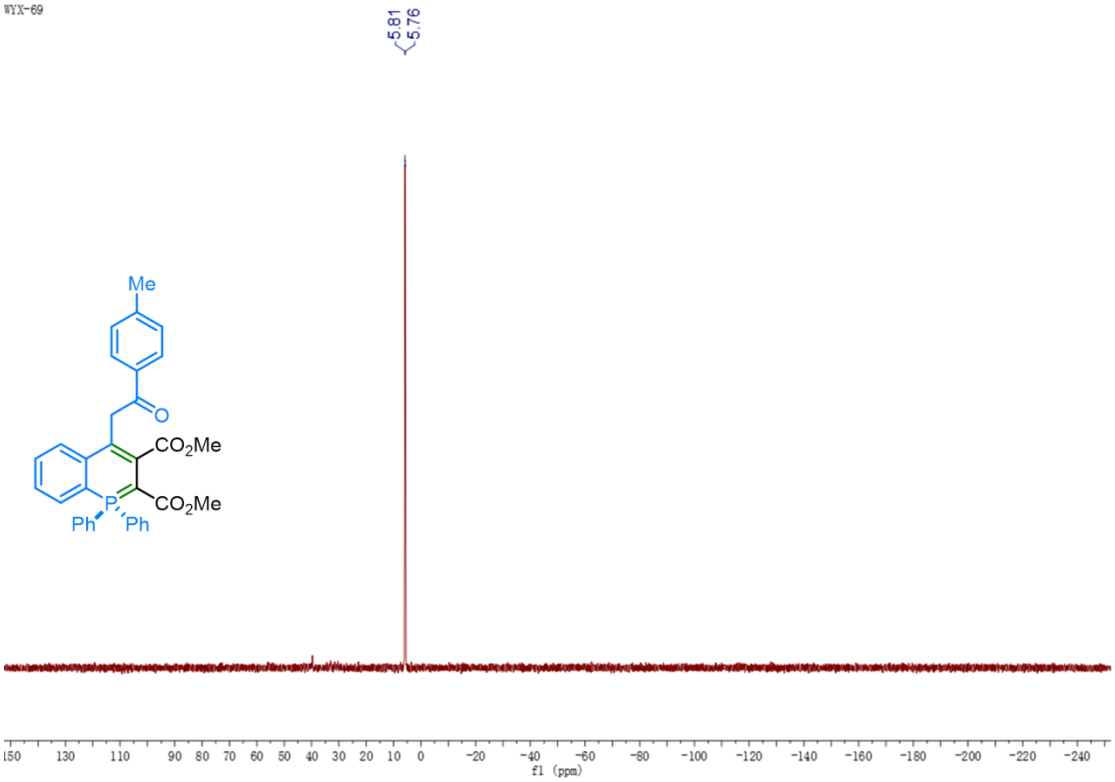
^{1}H NMR spectrum of **5e** (400 MHz, $CDCl_3$)



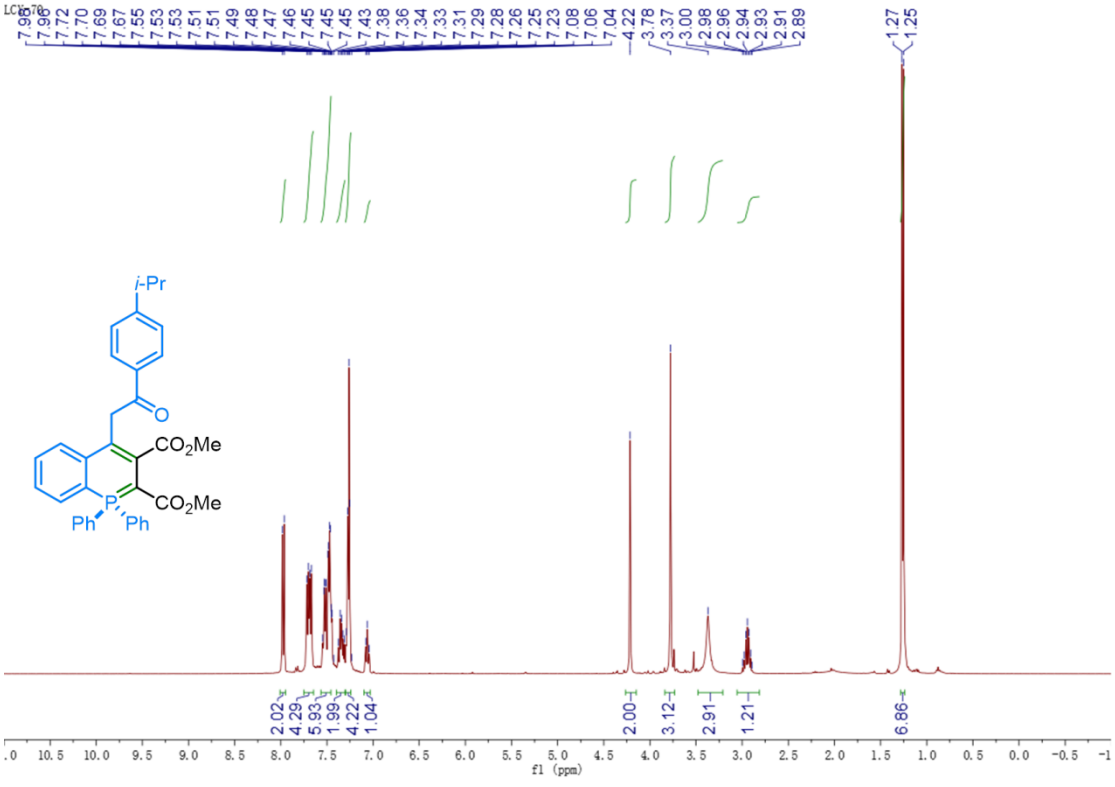
^{13}C NMR spectrum of **5e** (100 MHz, $CDCl_3$)



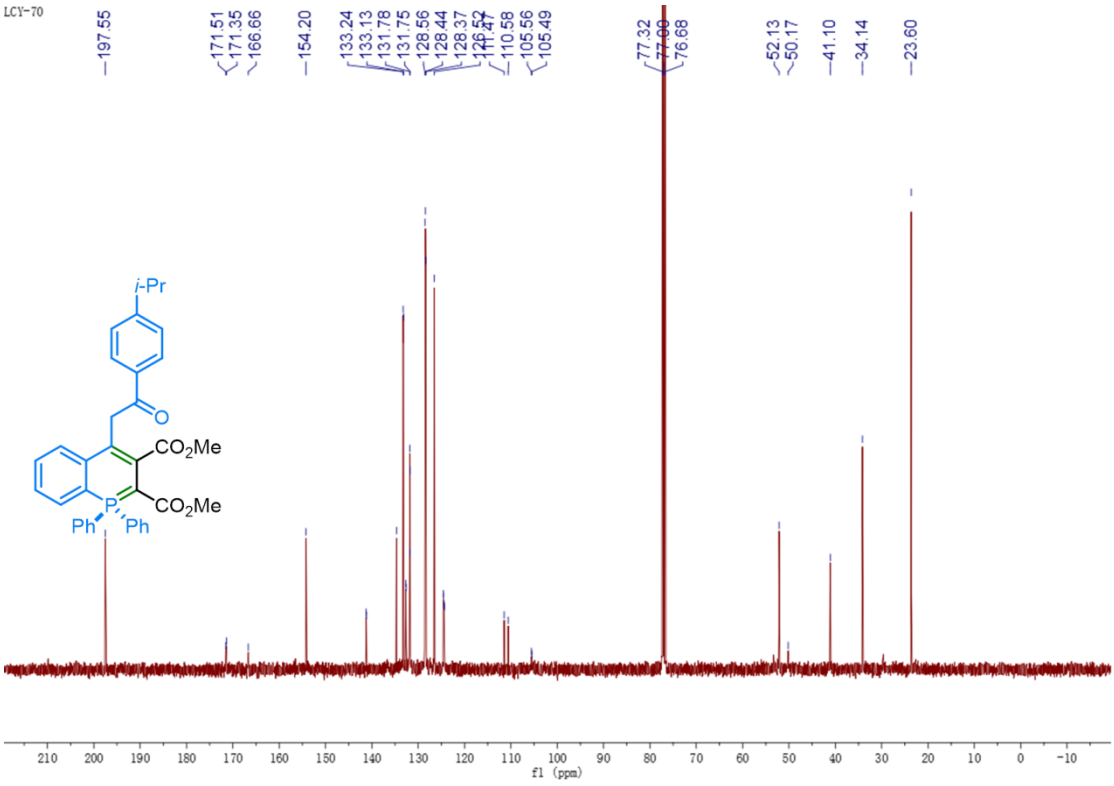
^{31}P NMR spectrum of **5e** (202 MHz, $CDCl_3$)



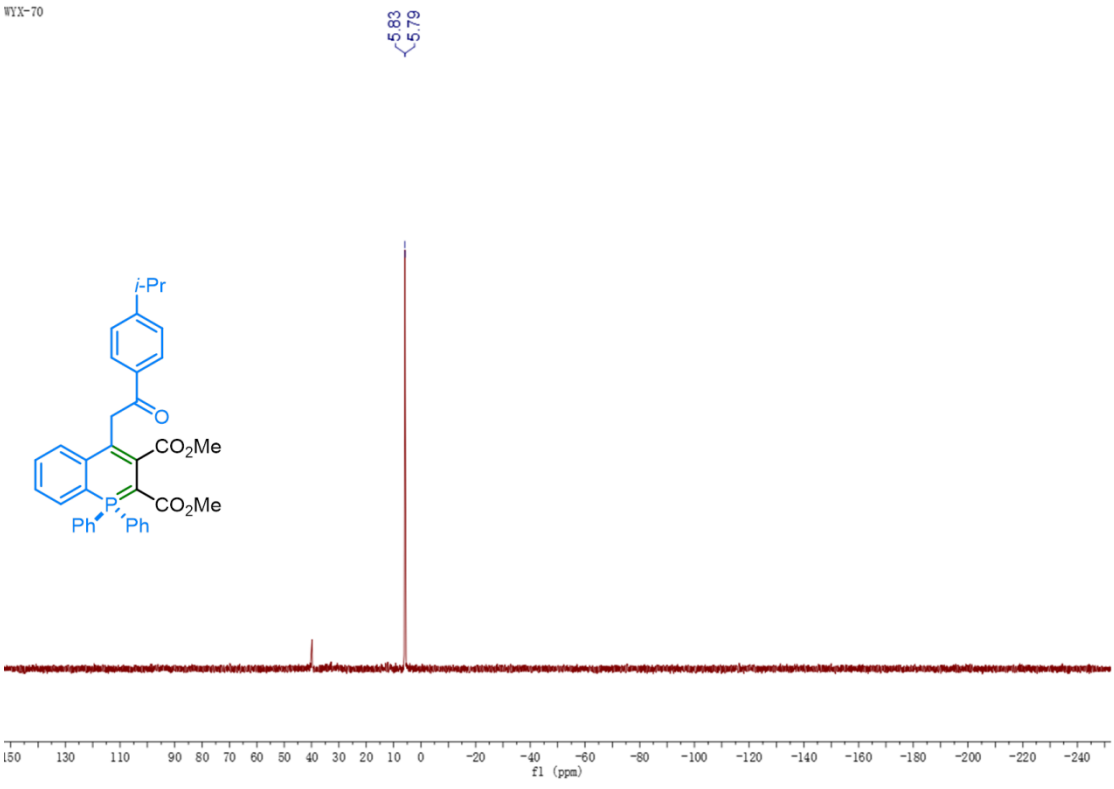
^{1}H NMR spectrum of **5f** (400 MHz, $CDCl_3$)



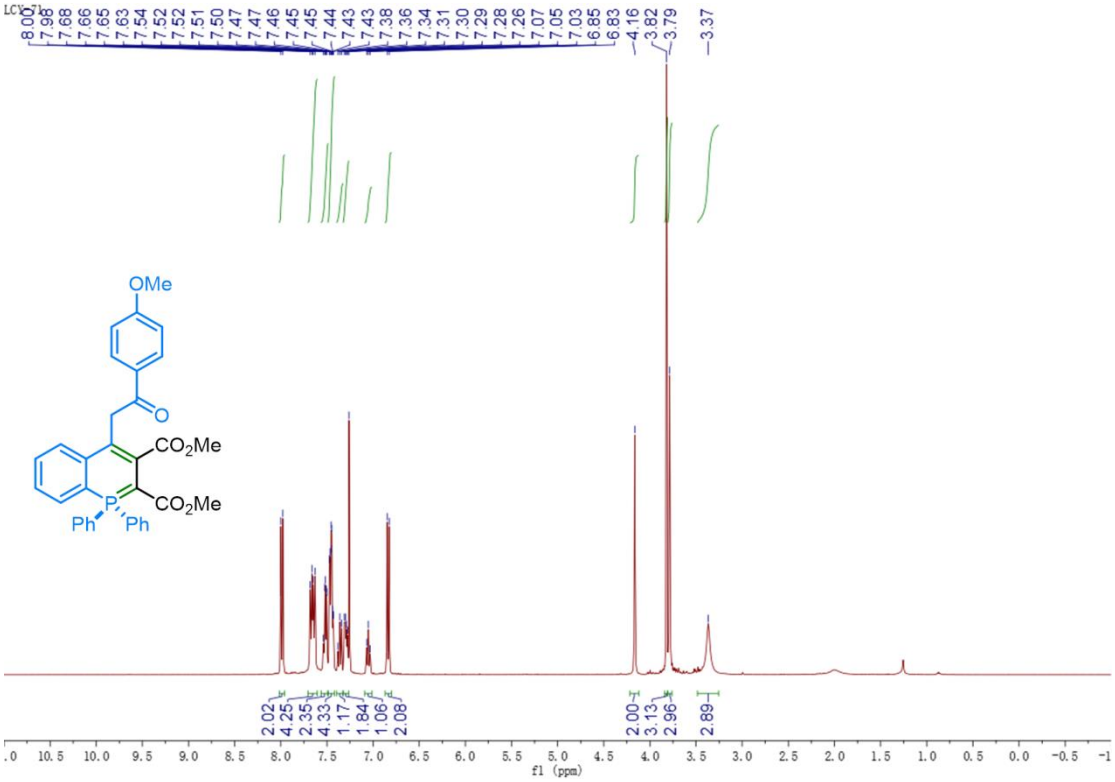
^{13}C NMR spectrum of **5f** (100 MHz, $CDCl_3$)



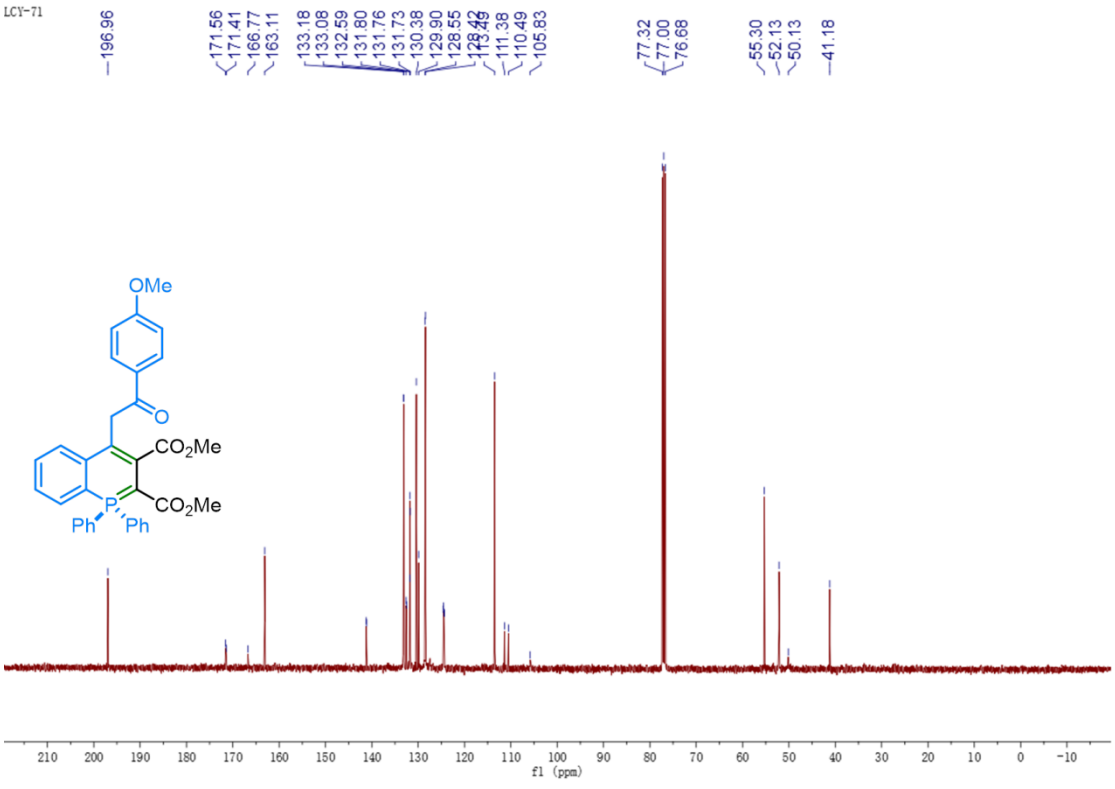
^{31}P NMR spectrum of **5f** (202 MHz, $CDCl_3$)



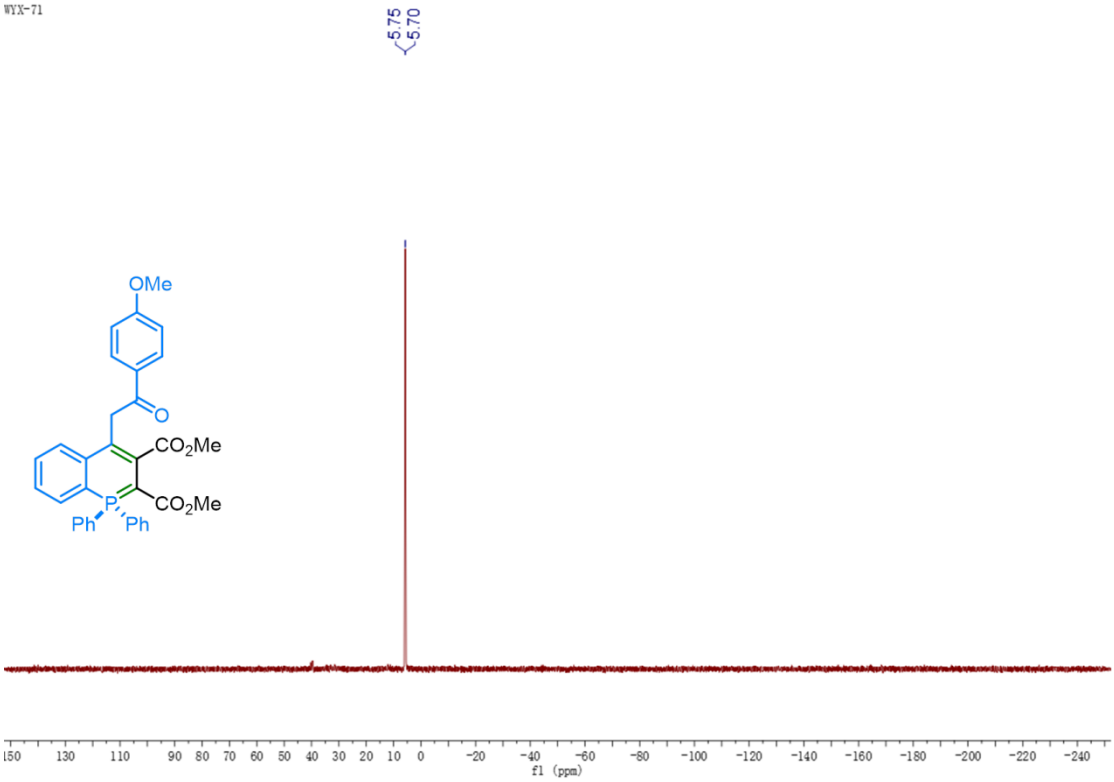
^{1}H NMR spectrum of **5g** (400 MHz, $CDCl_3$)



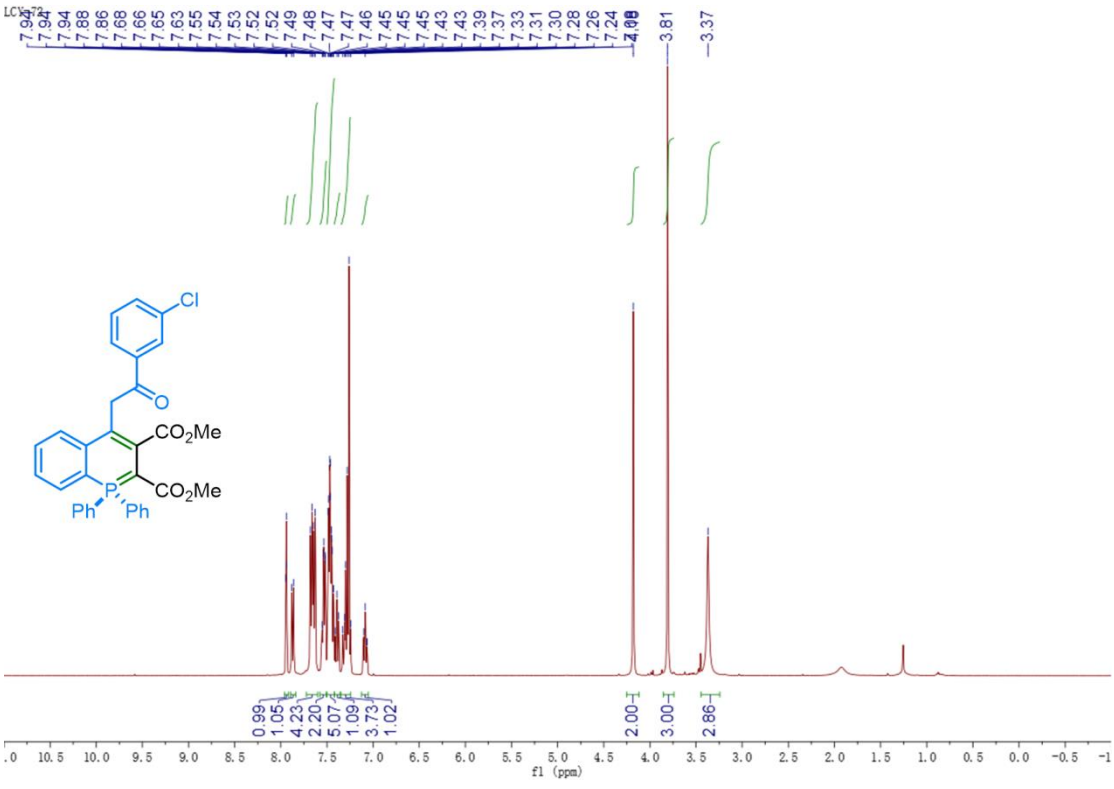
^{13}C NMR spectrum of **5g** (100 MHz, $CDCl_3$)



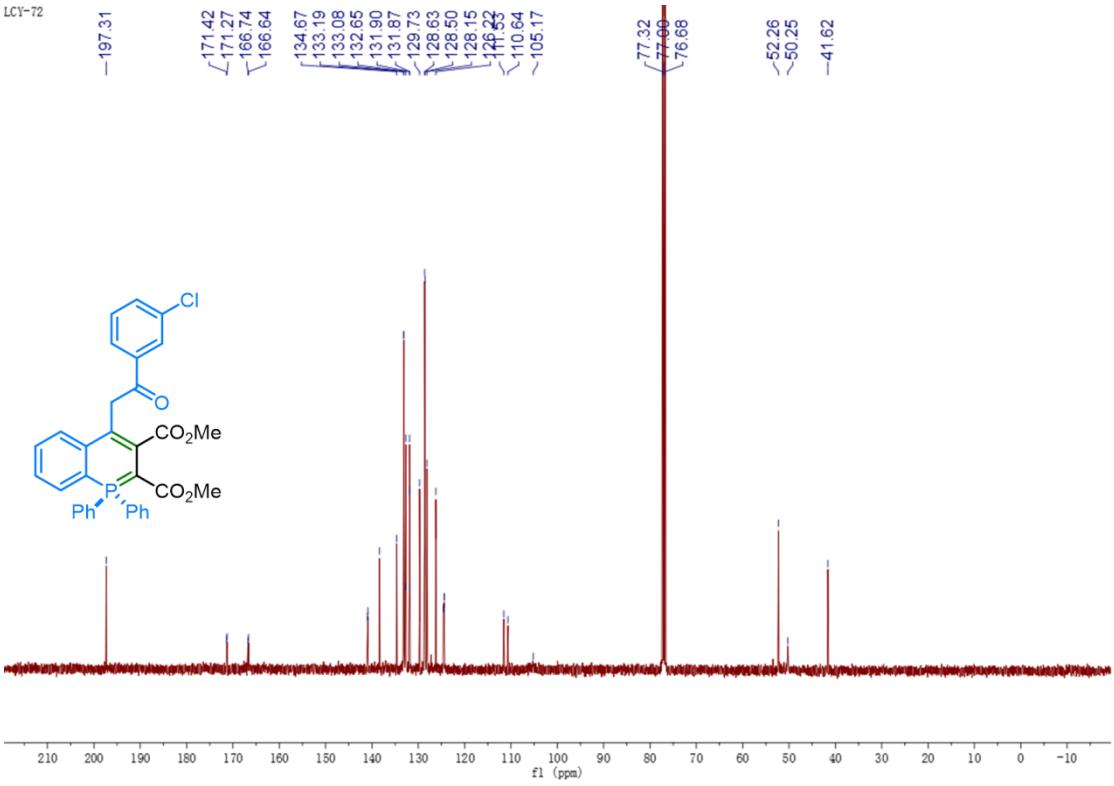
^{31}P NMR spectrum of **5g** (202 MHz, $CDCl_3$)



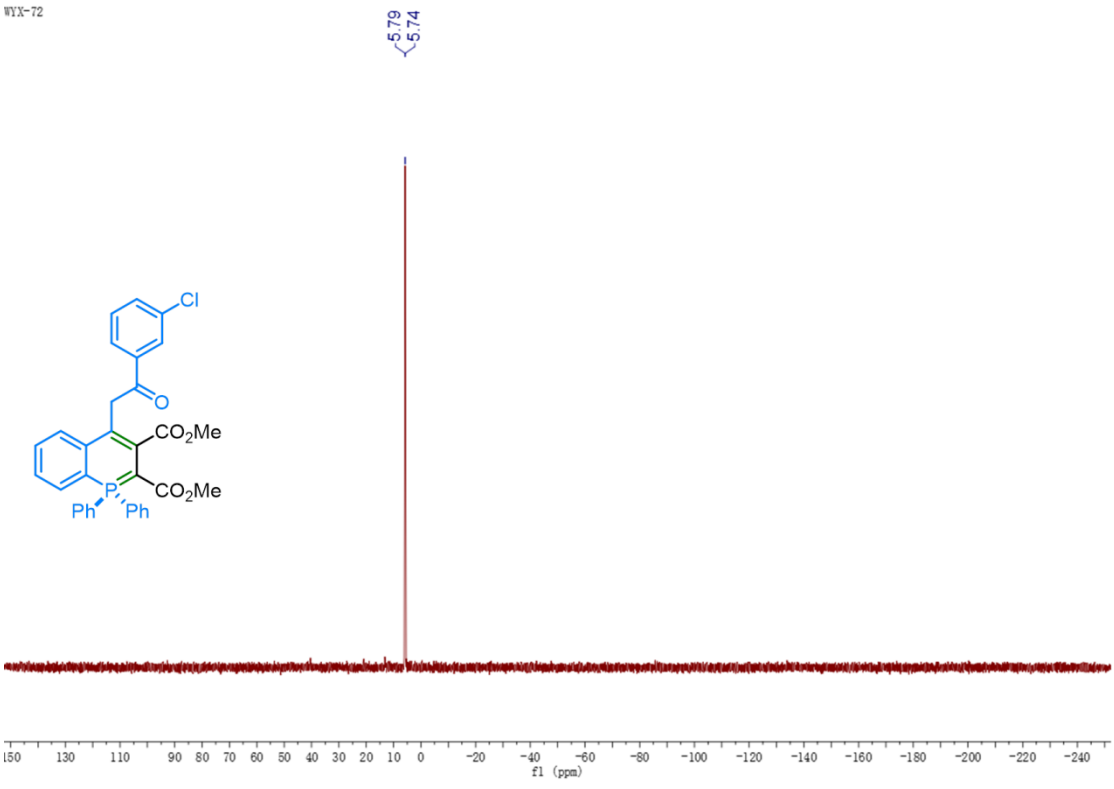
^{1}H NMR spectrum of **5h** (400 MHz, $CDCl_3$)



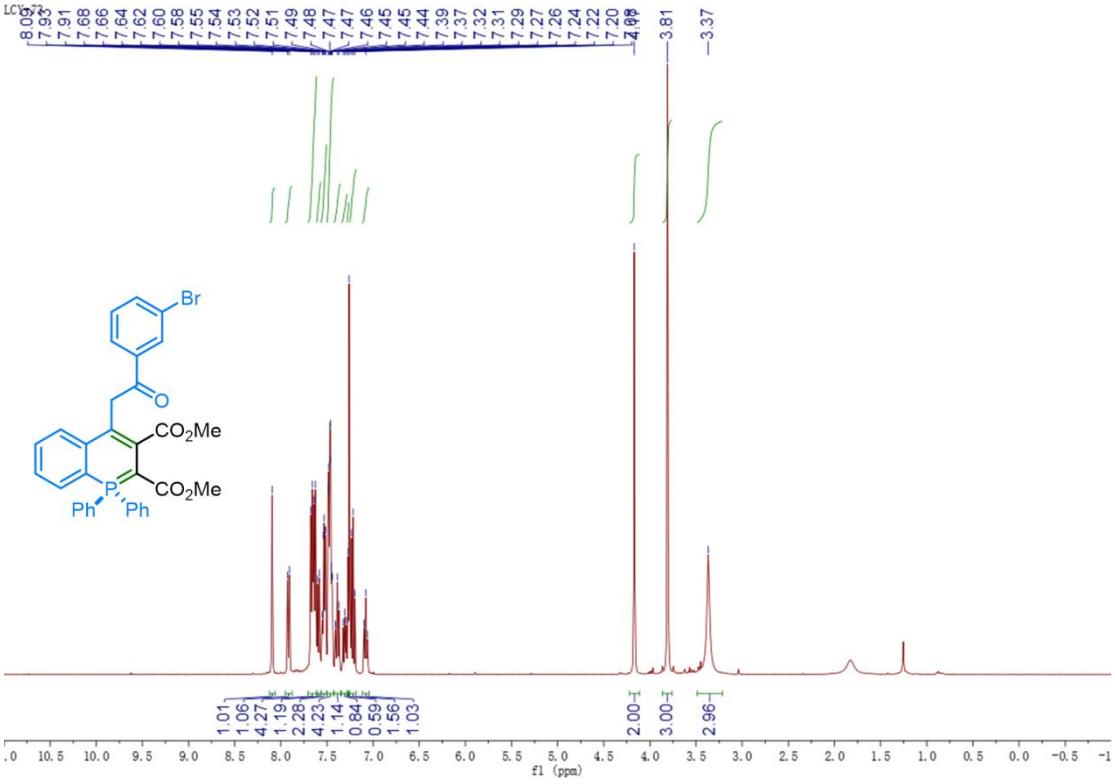
^{13}C NMR spectrum of **5h** (100 MHz, $CDCl_3$)



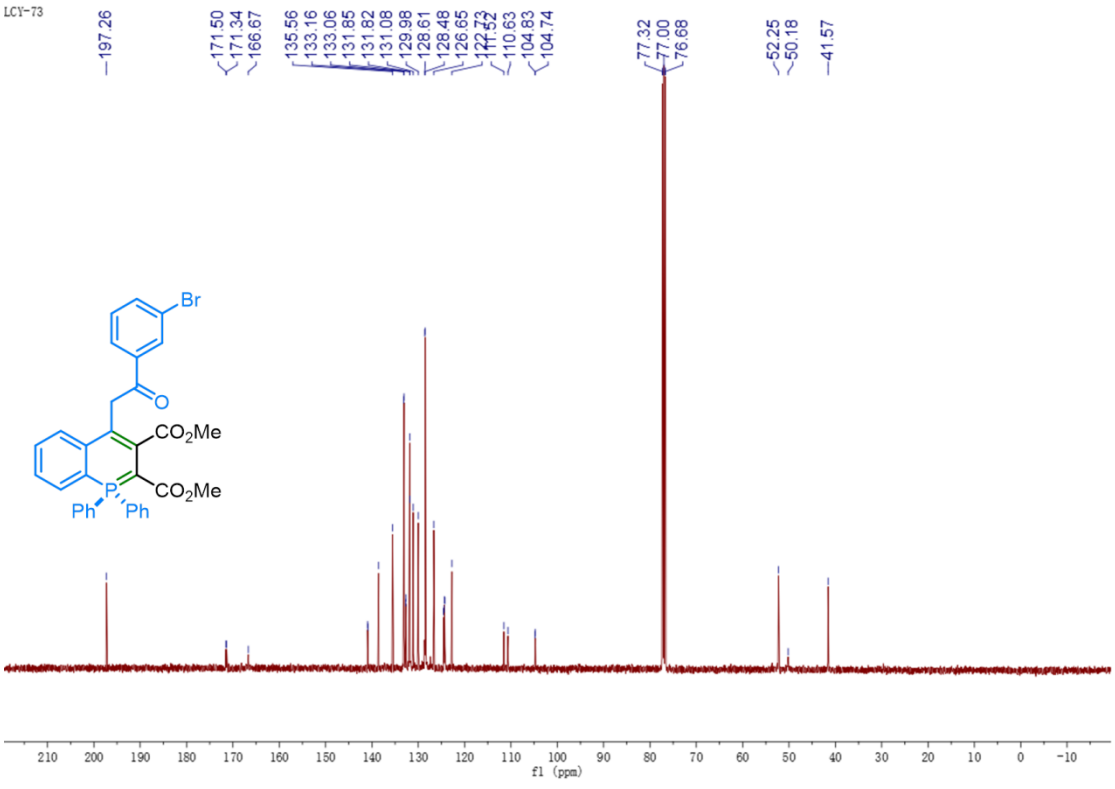
^{31}P NMR spectrum of **5h** (202 MHz, $CDCl_3$)



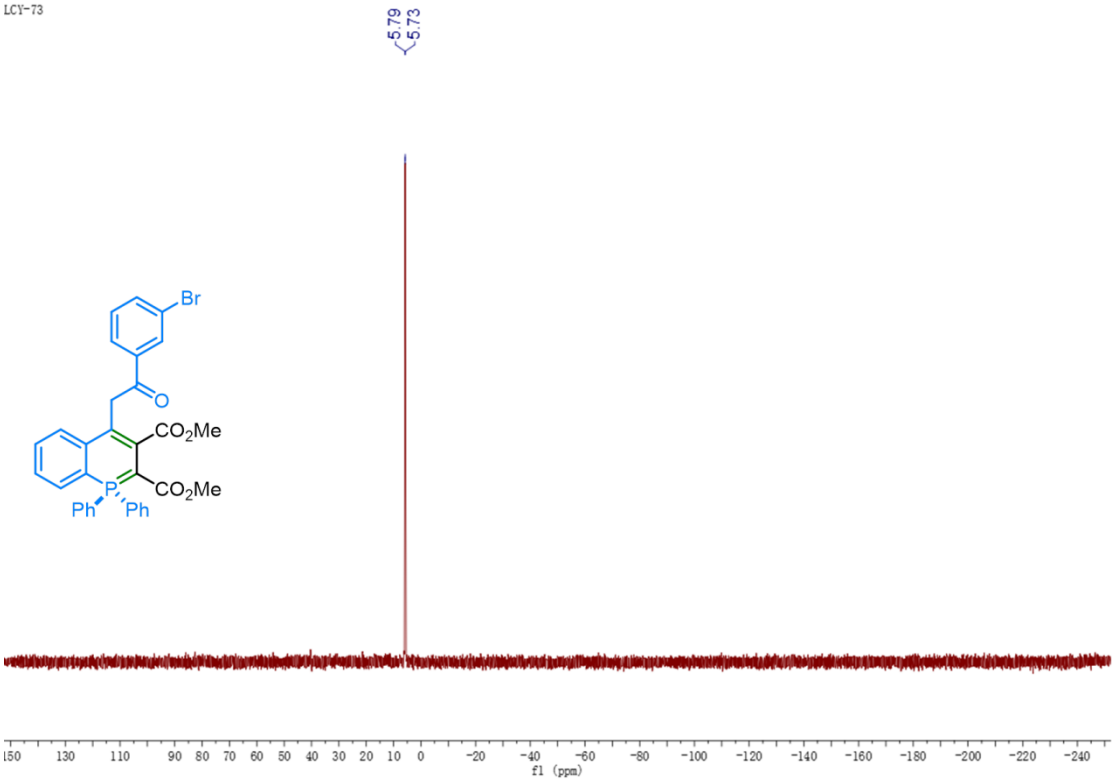
^{1}H NMR spectrum of **5i** (400 MHz, $CDCl_3$)



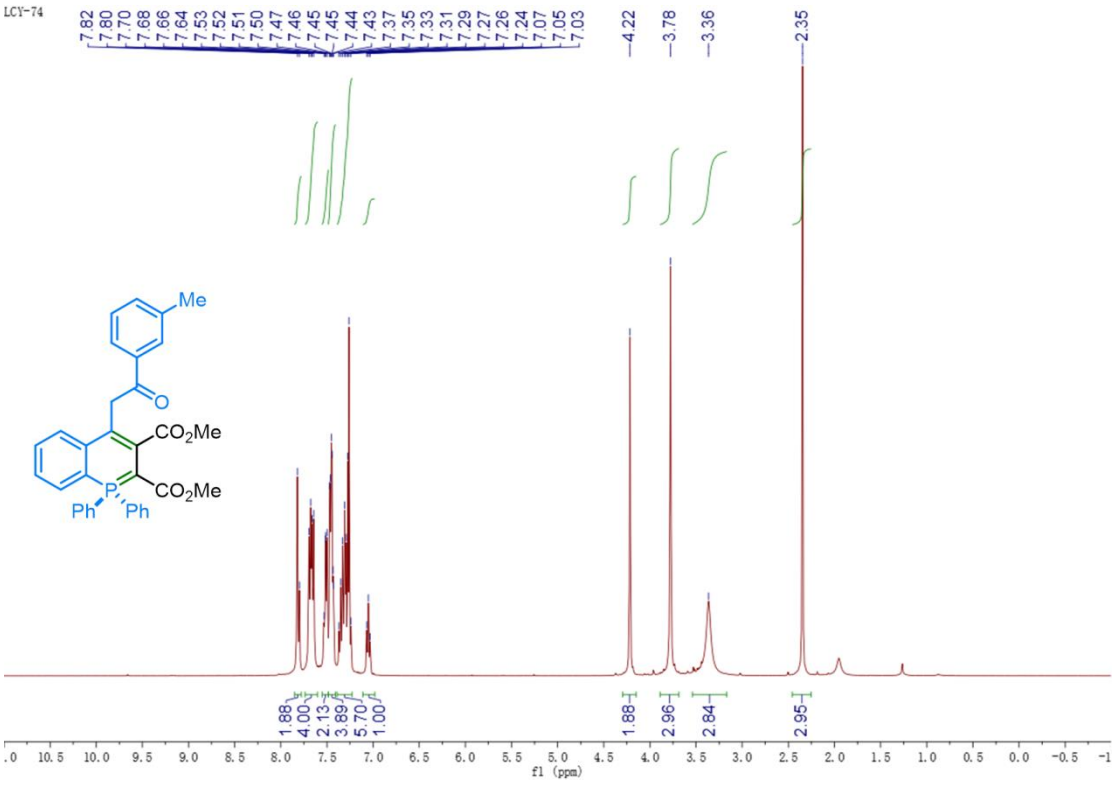
^{13}C NMR spectrum of **5i** (100 MHz, $CDCl_3$)



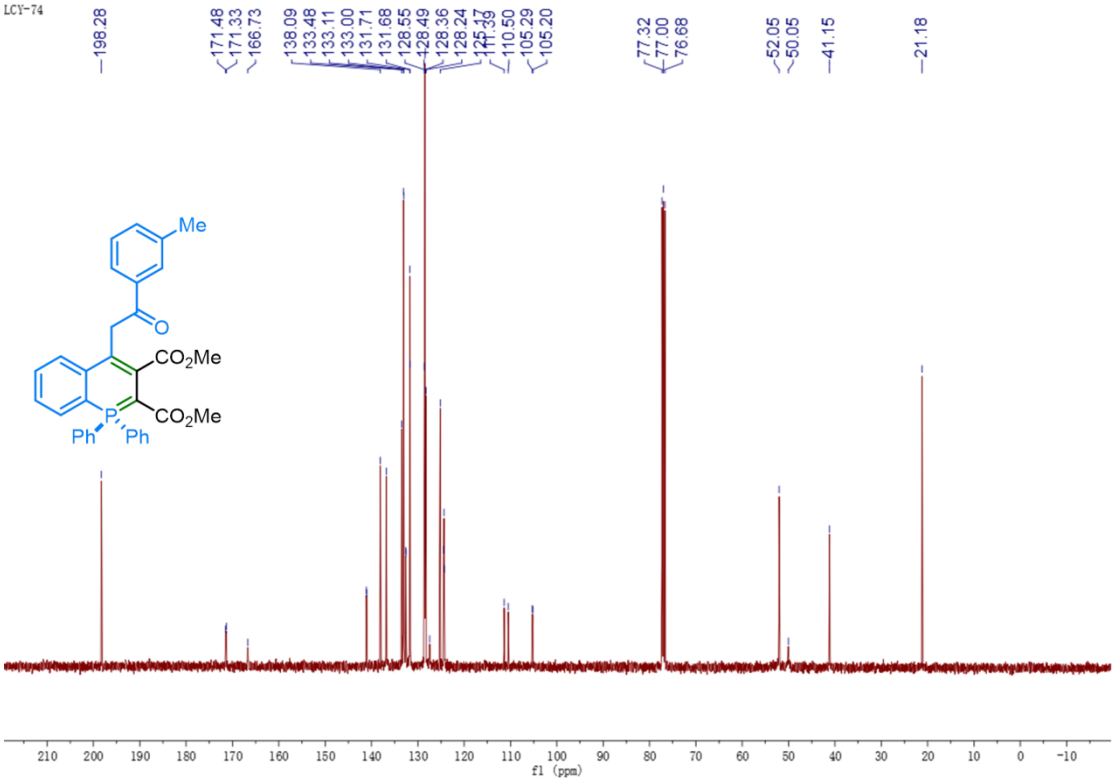
^{31}P NMR spectrum of **5i** (202 MHz, $CDCl_3$)



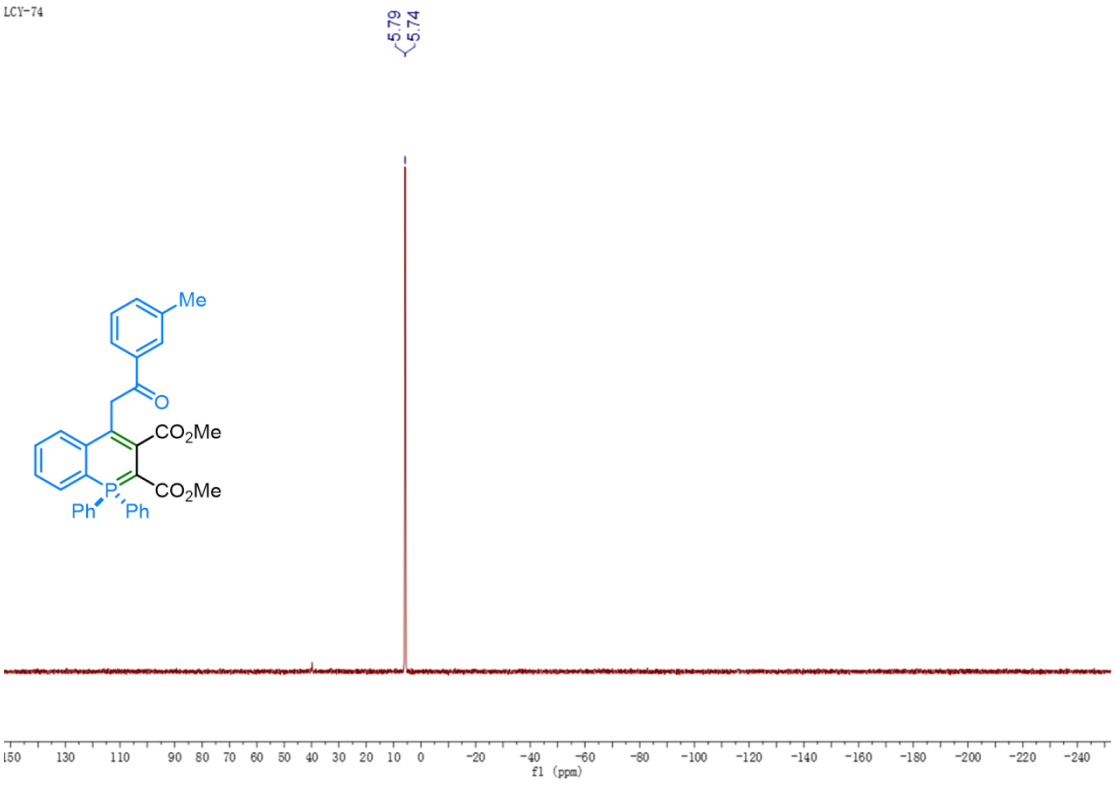
^{1}H NMR spectrum of **5j** (400 MHz, $CDCl_3$)



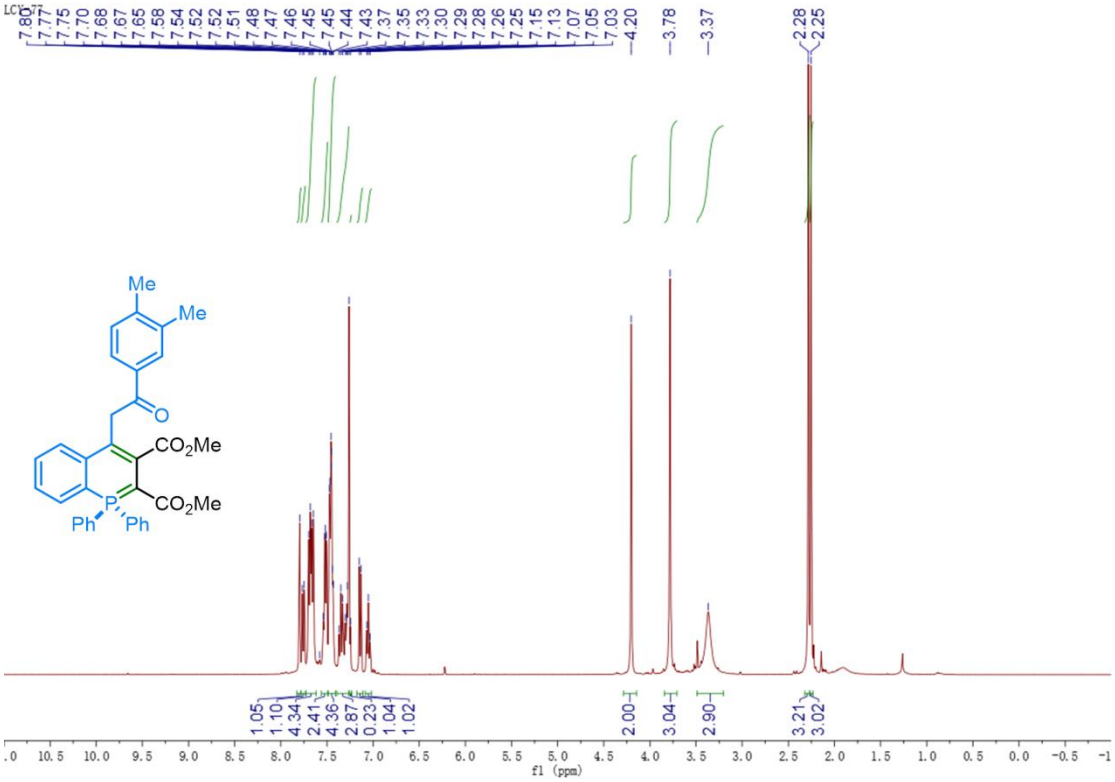
^{13}C NMR spectrum of **5j** (100 MHz, $CDCl_3$)



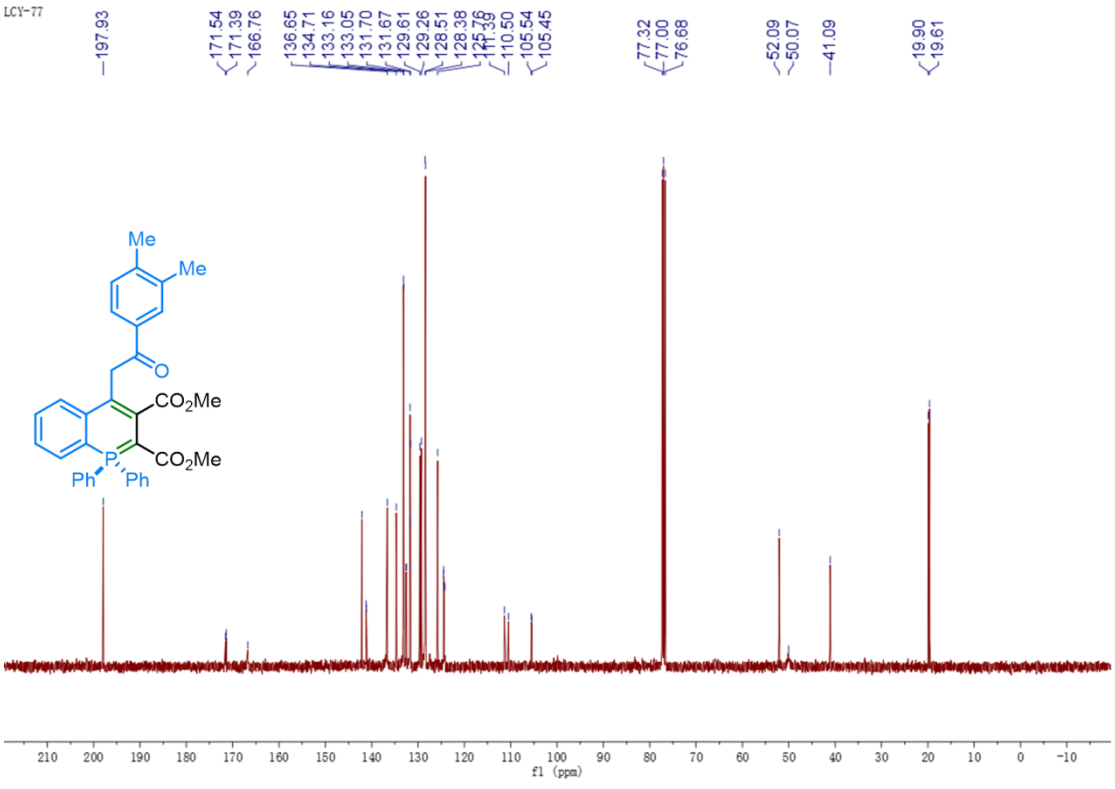
^{31}P NMR spectrum of **5j** (202 MHz, $CDCl_3$)



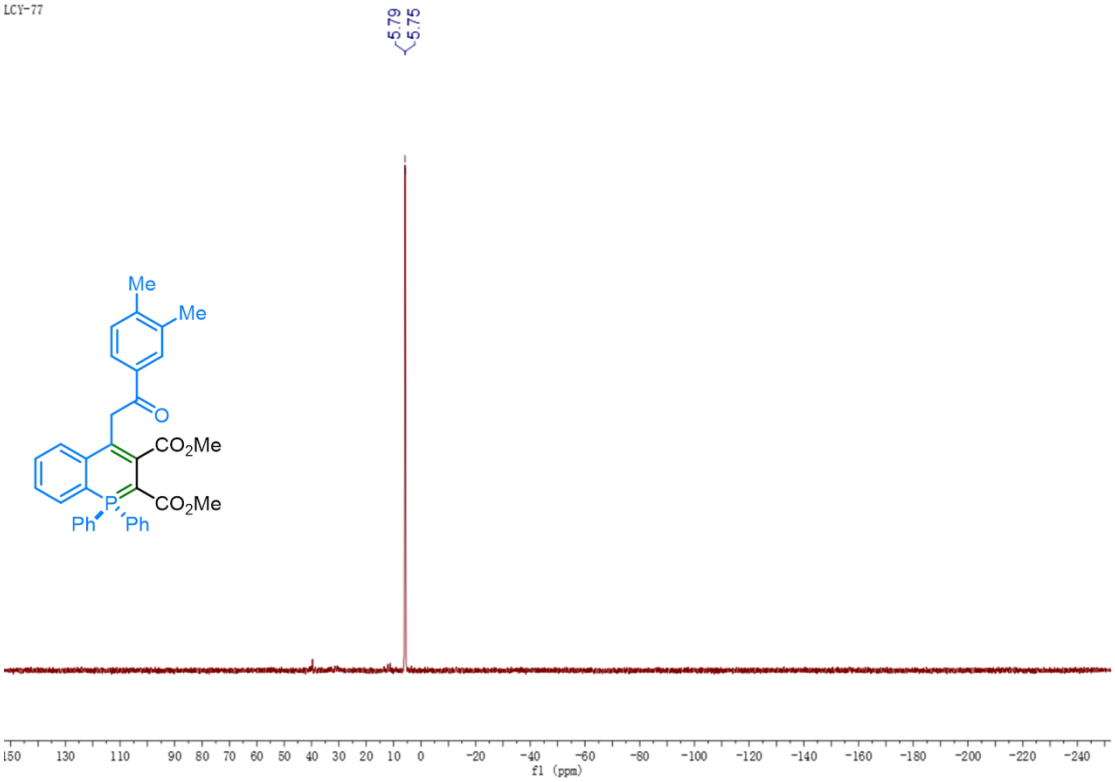
^{1}H NMR spectrum of **5k** (400 MHz, $CDCl_3$)



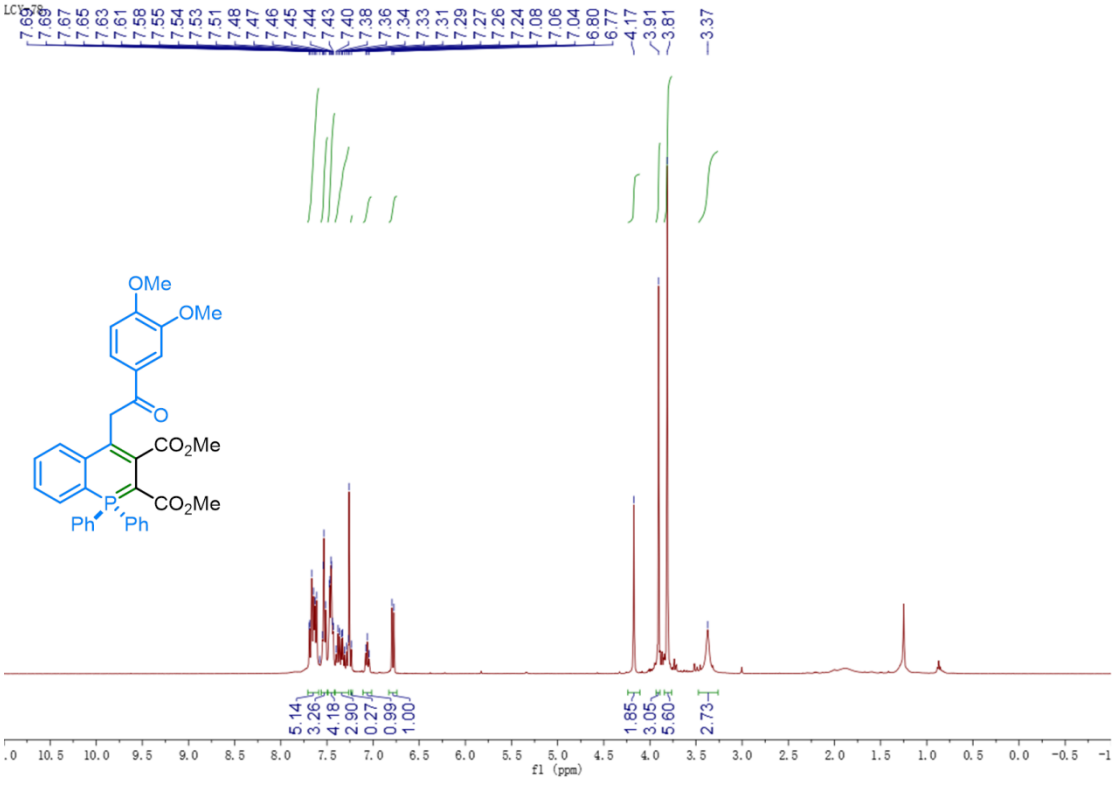
^{13}C NMR spectrum of **5k** (100 MHz, $CDCl_3$)



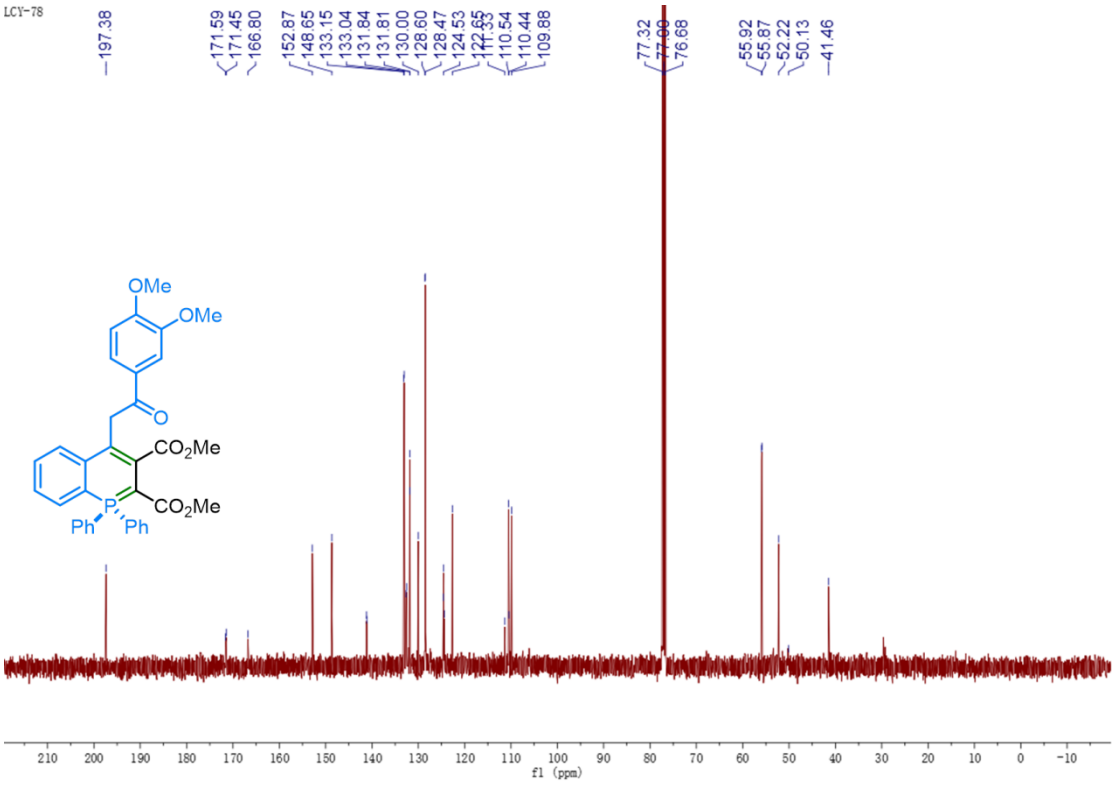
^{31}P NMR spectrum of **5k** (202 MHz, $CDCl_3$)



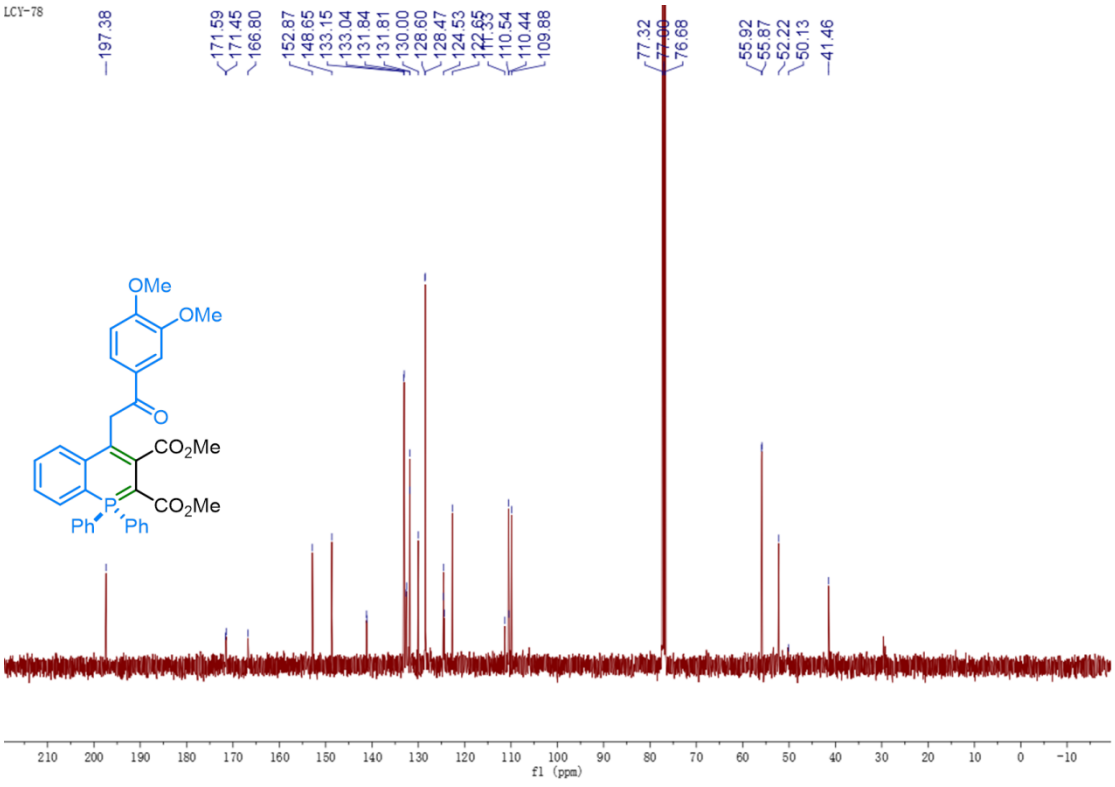
^{1}H NMR spectrum of **5l** (400 MHz, $CDCl_3$)



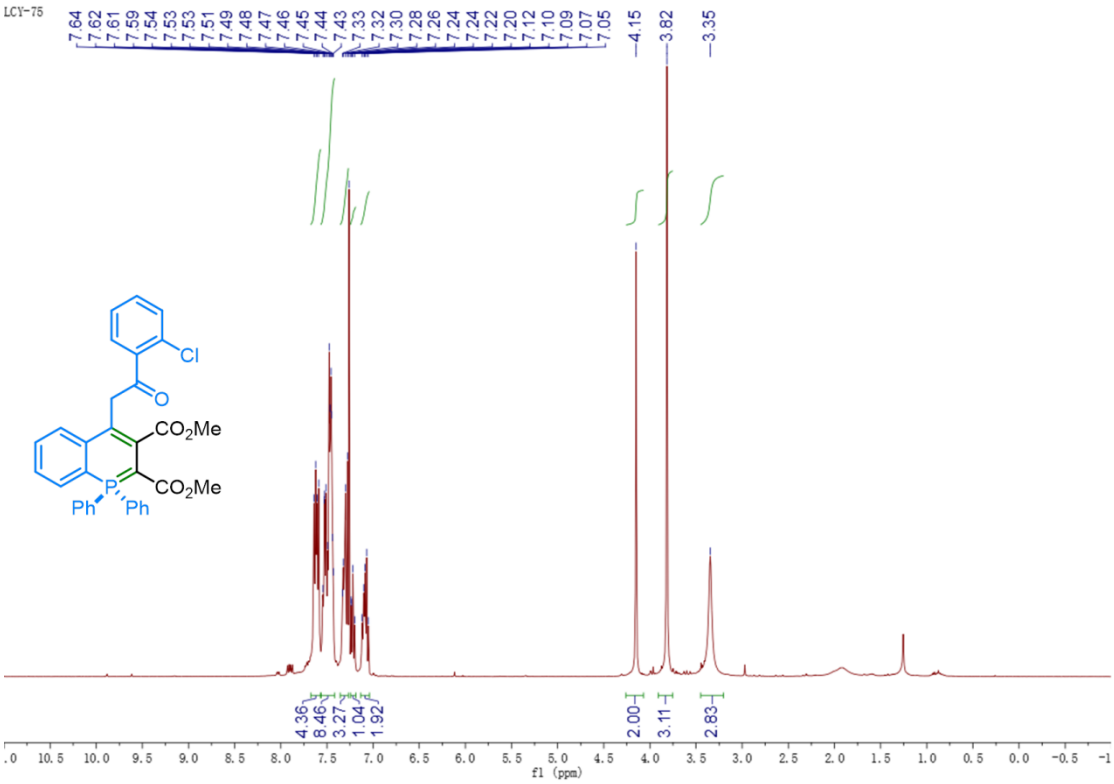
^{13}C NMR spectrum of **5l** (100 MHz, $CDCl_3$)



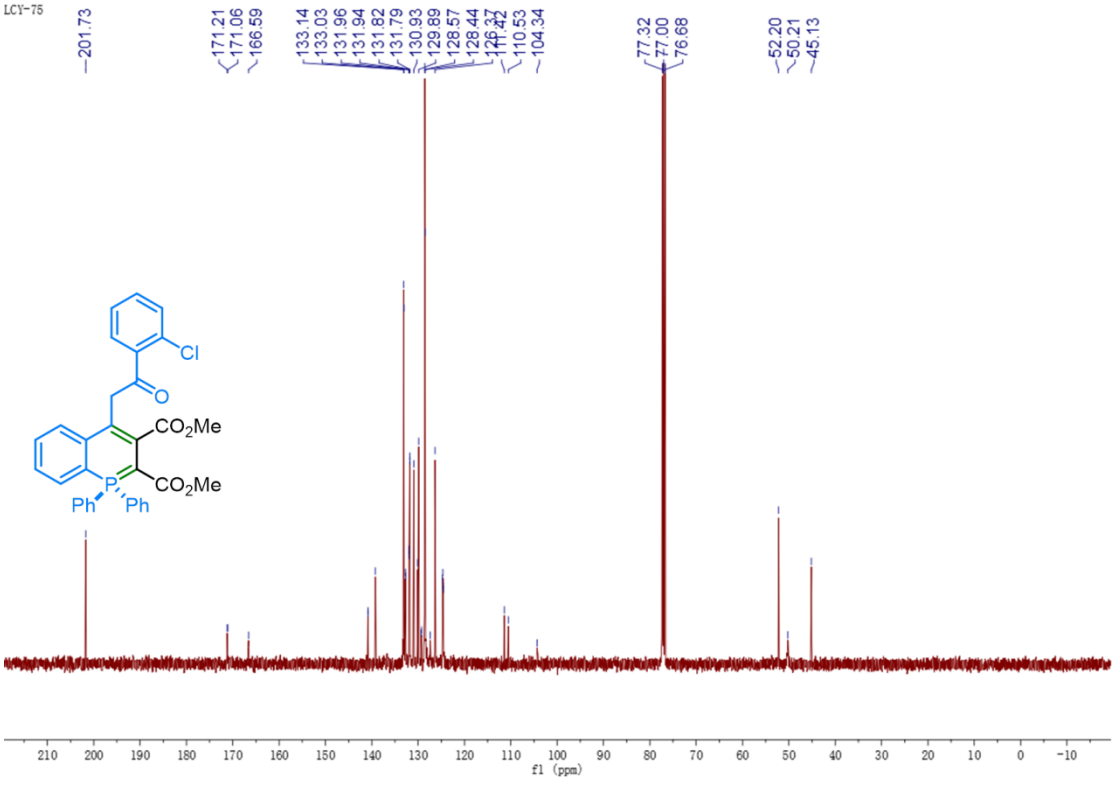
^{31}P NMR spectrum of **5l** (202 MHz, $CDCl_3$)



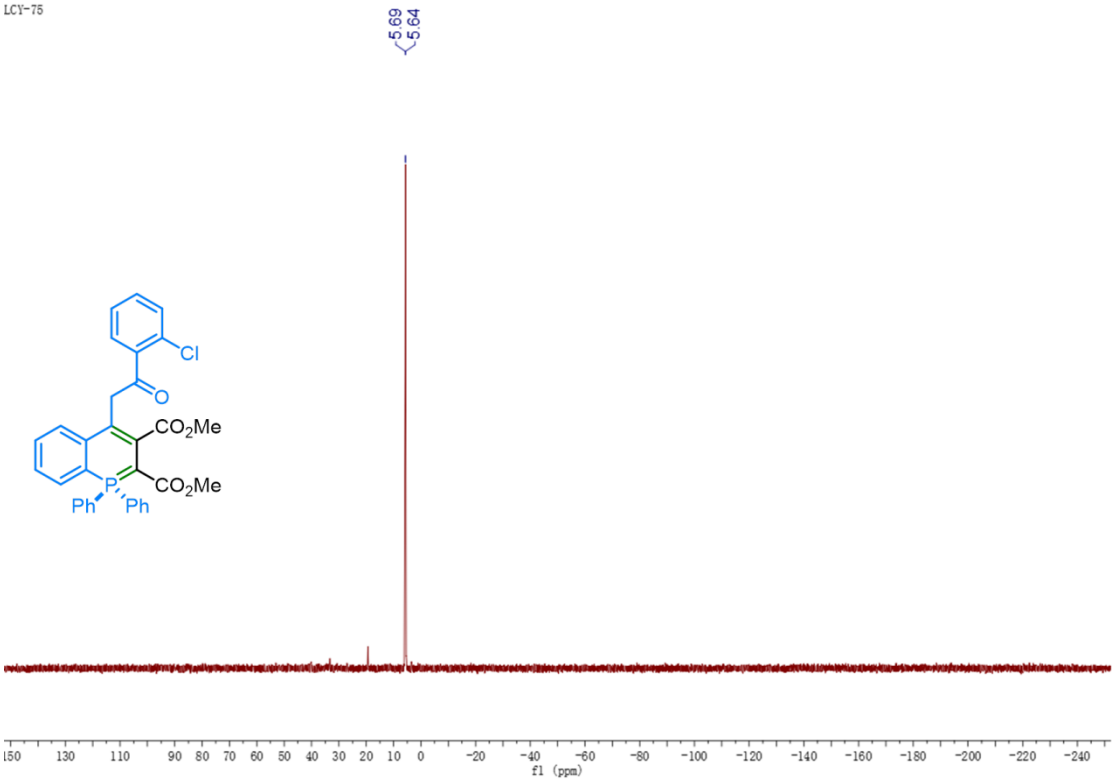
^{1}H NMR spectrum of **5m** (400 MHz, $CDCl_3$)



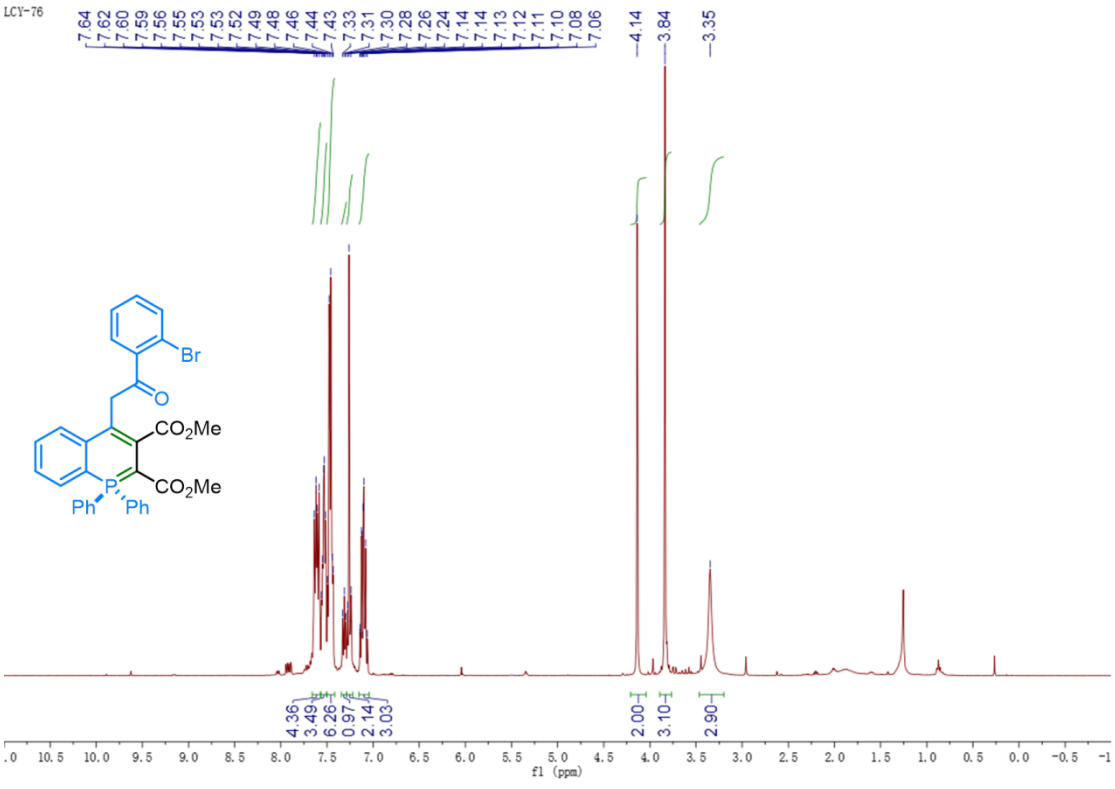
^{13}C NMR spectrum of **5m** (100 MHz, $CDCl_3$)



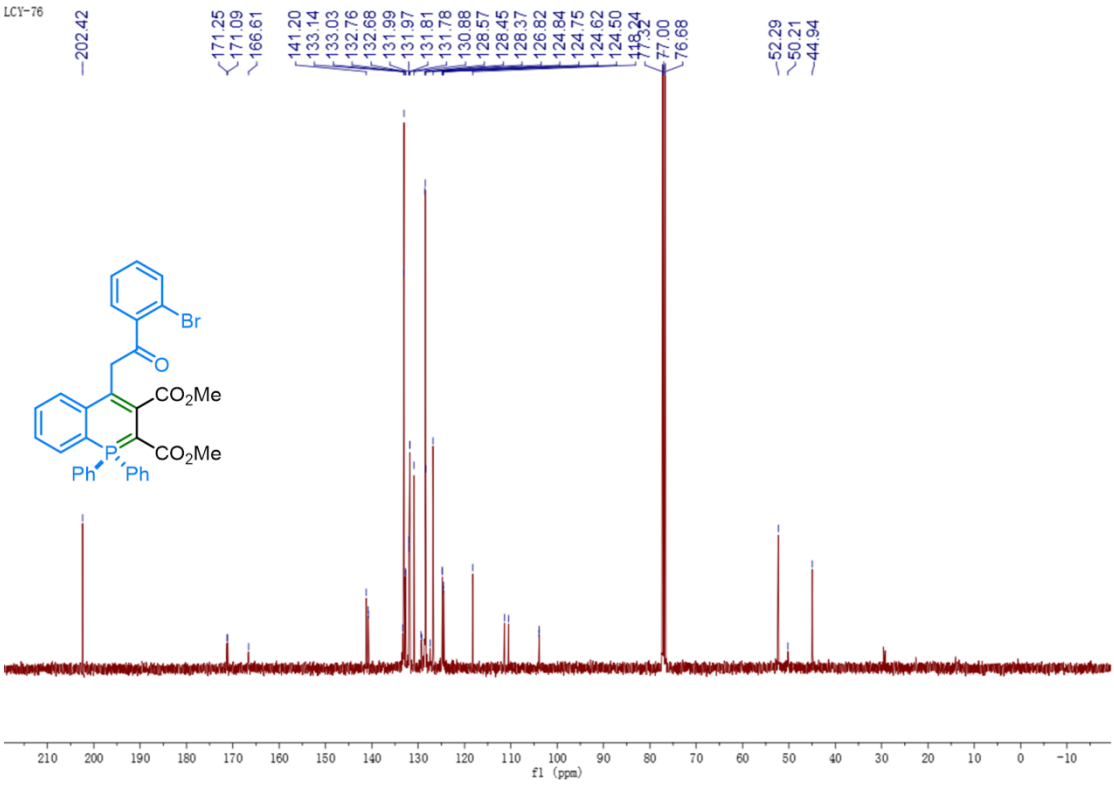
^{31}P NMR spectrum of **5m** (202 MHz, $CDCl_3$)



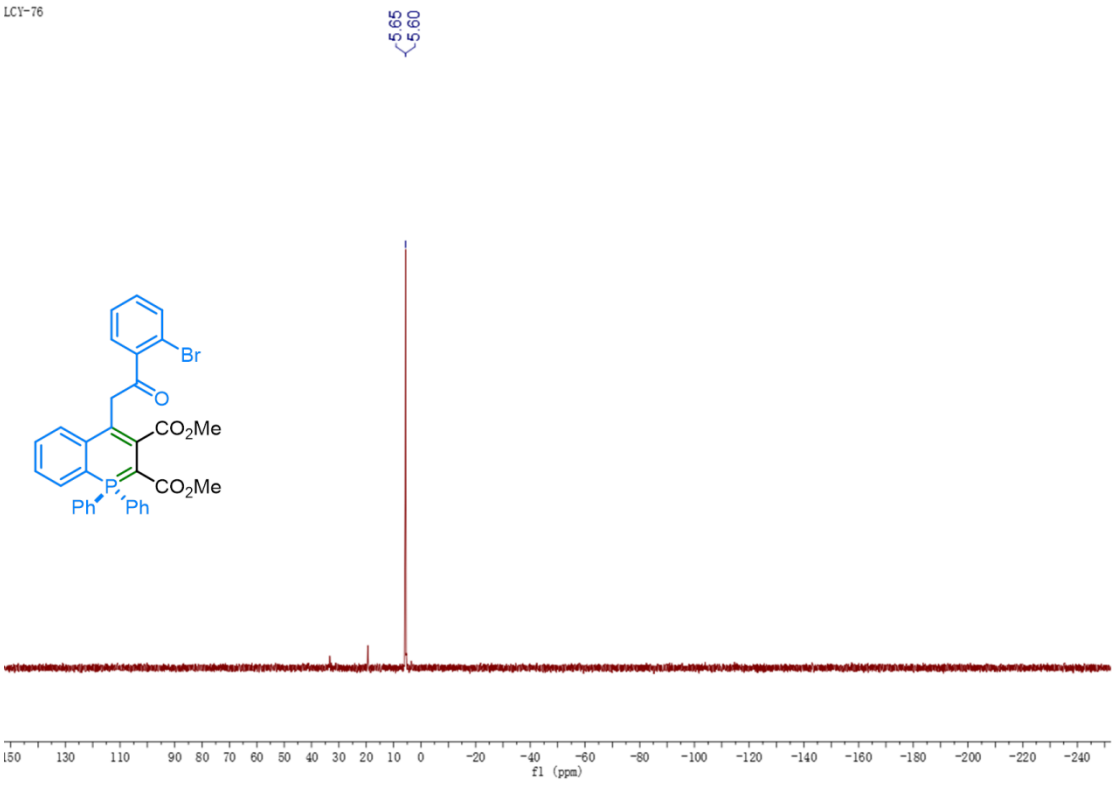
^{1}H NMR spectrum of **5n** (400 MHz, $CDCl_3$)



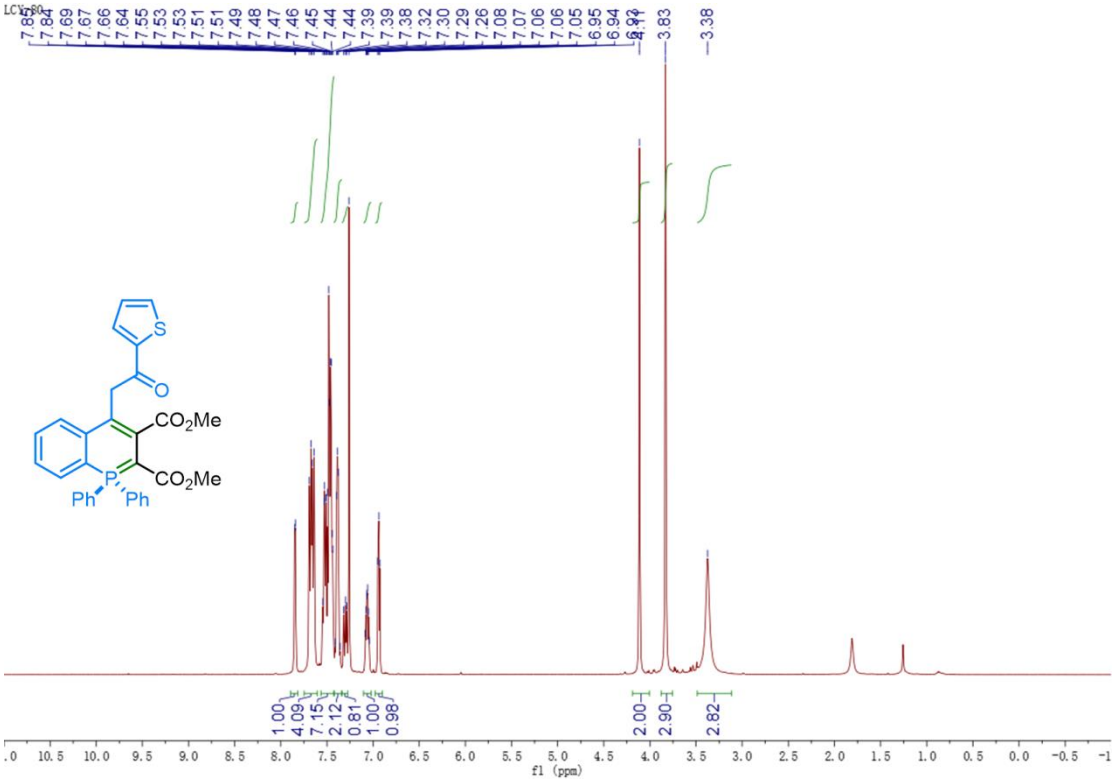
^{13}C NMR spectrum of **5n** (100 MHz, $CDCl_3$)



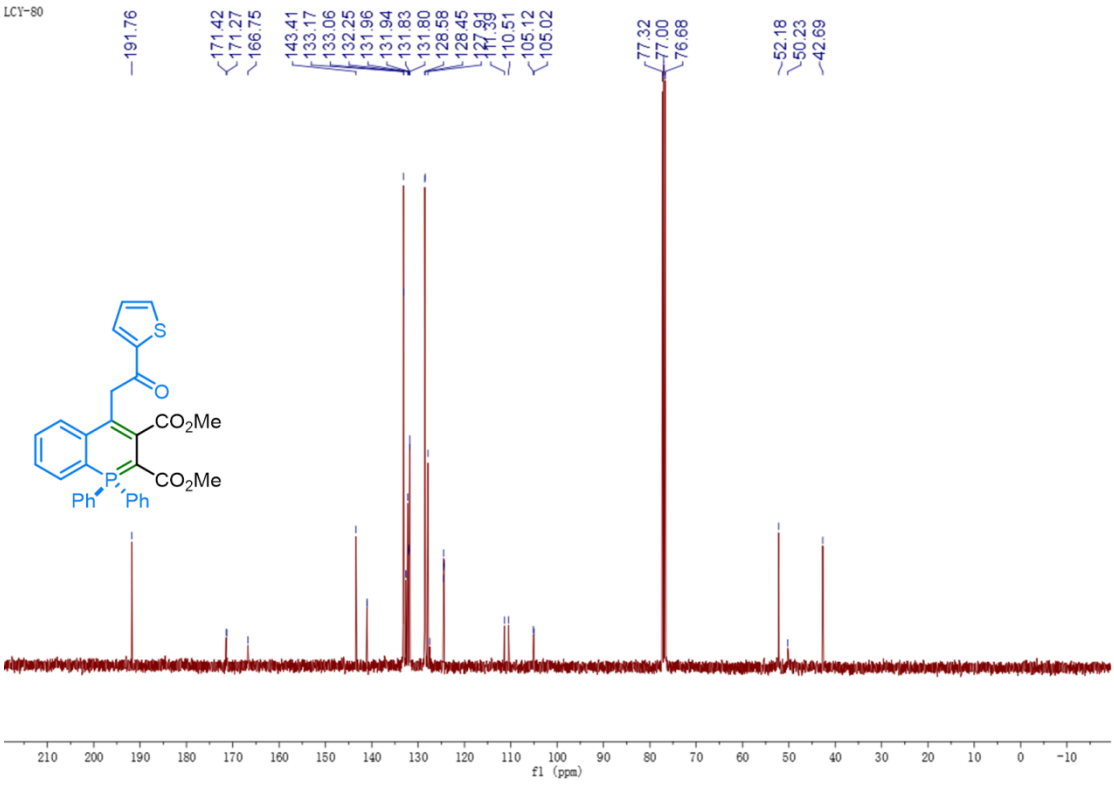
^{31}P NMR spectrum of **5n** (202 MHz, $CDCl_3$)



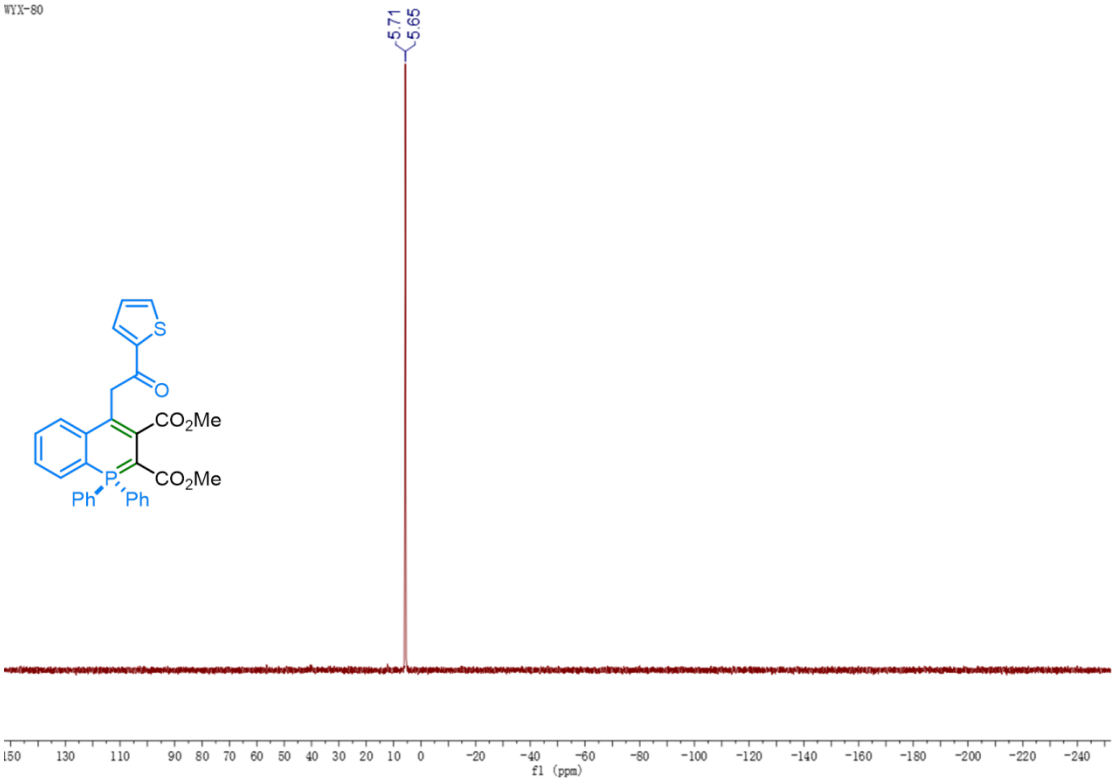
^{1}H NMR spectrum of **5o** (400 MHz, $CDCl_3$)



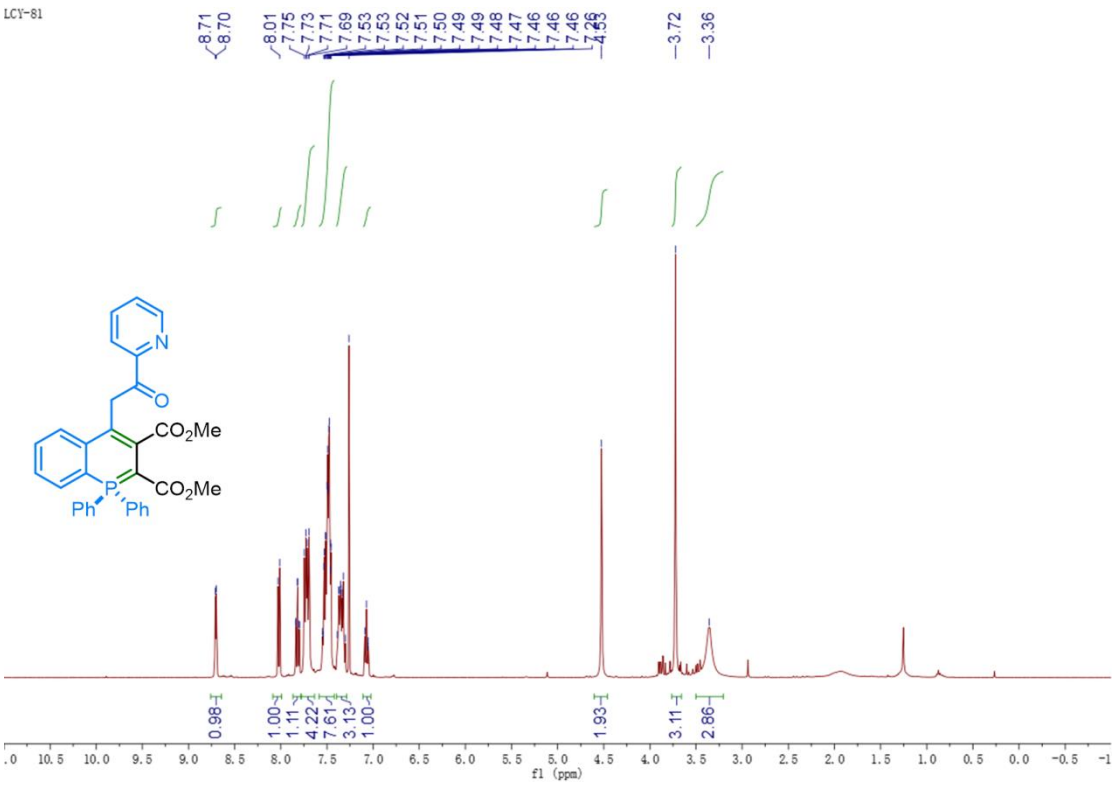
^{13}C NMR spectrum of **5o** (100 MHz, $CDCl_3$)



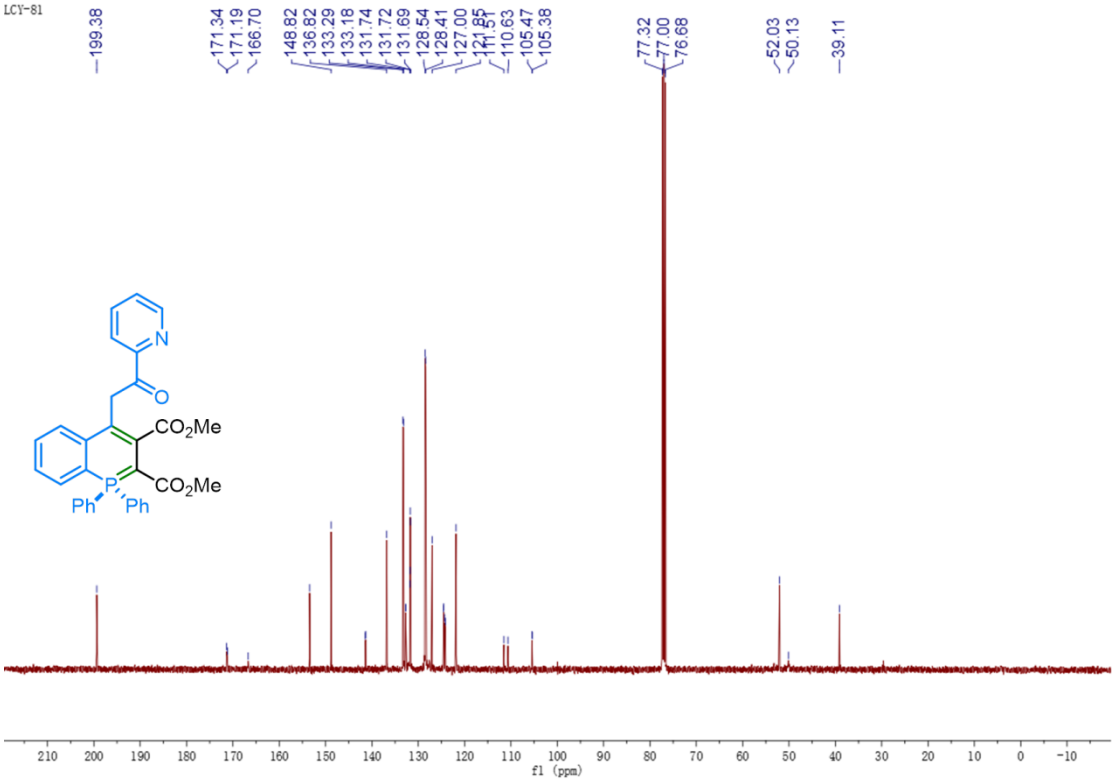
^{31}P NMR spectrum of **5o** (202 MHz, $CDCl_3$)



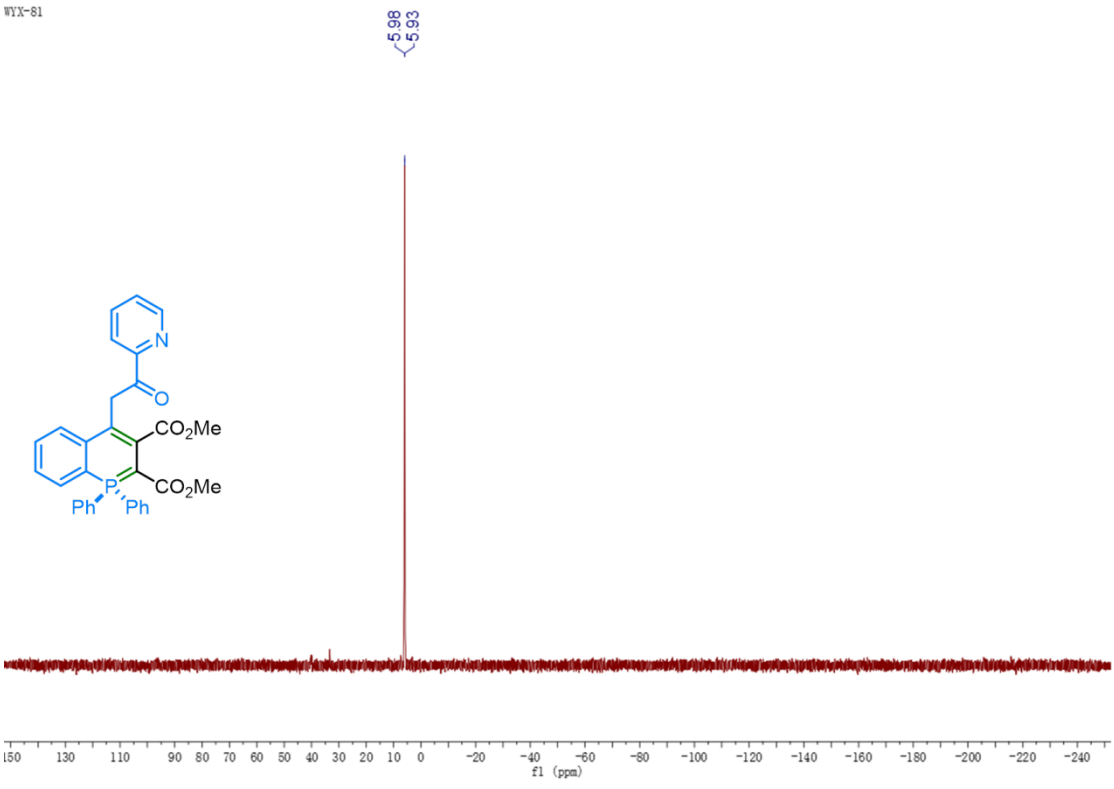
^{1}H NMR spectrum of **5p** (400 MHz, $CDCl_3$)



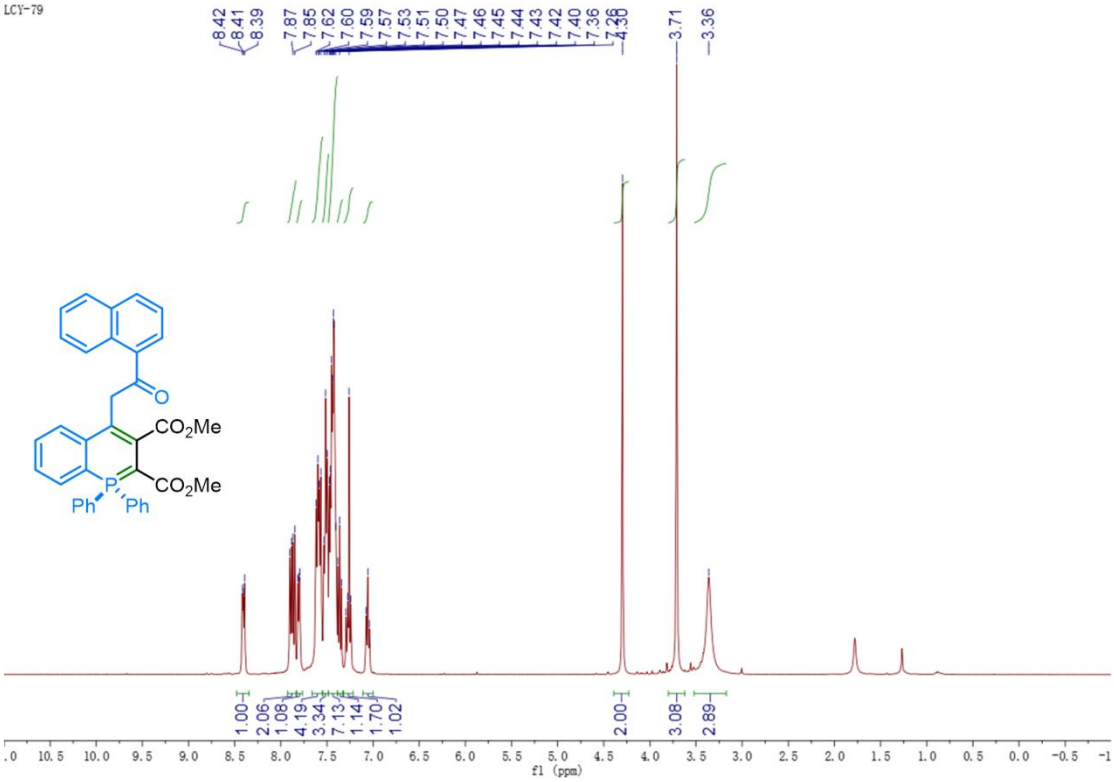
^{13}C NMR spectrum of **5p** (100 MHz, $CDCl_3$)



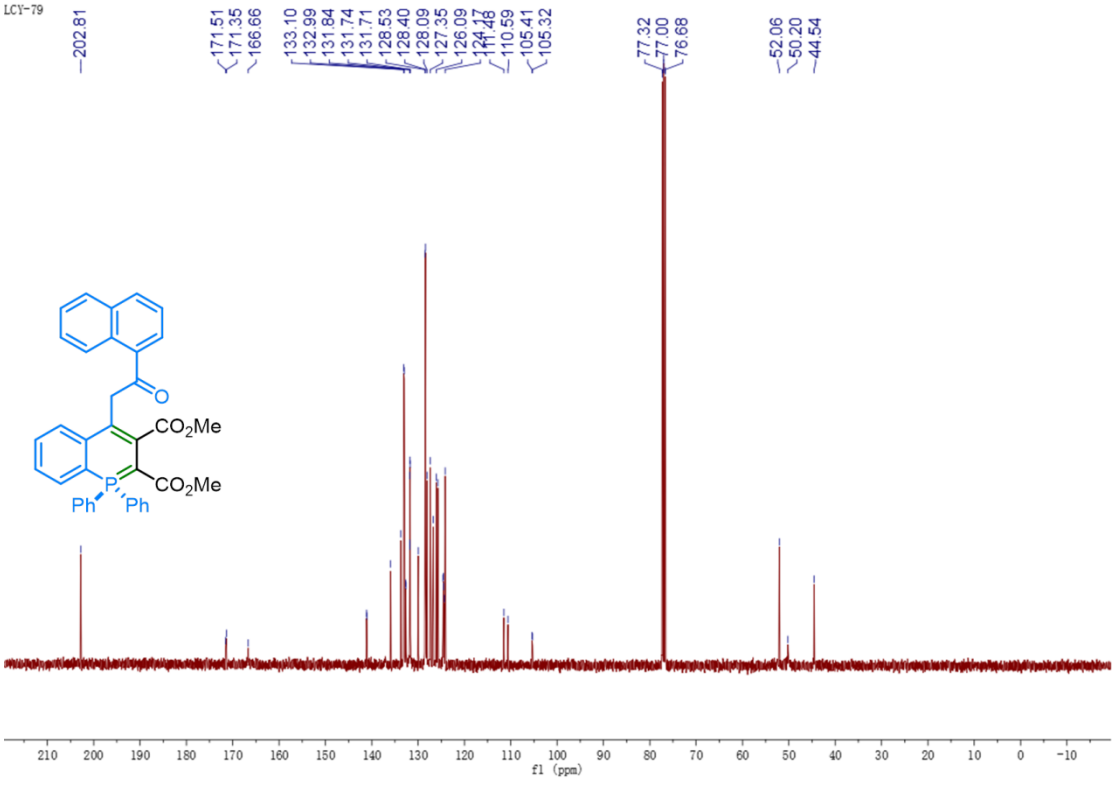
^{31}P NMR spectrum of **5p** (202 MHz, $CDCl_3$)



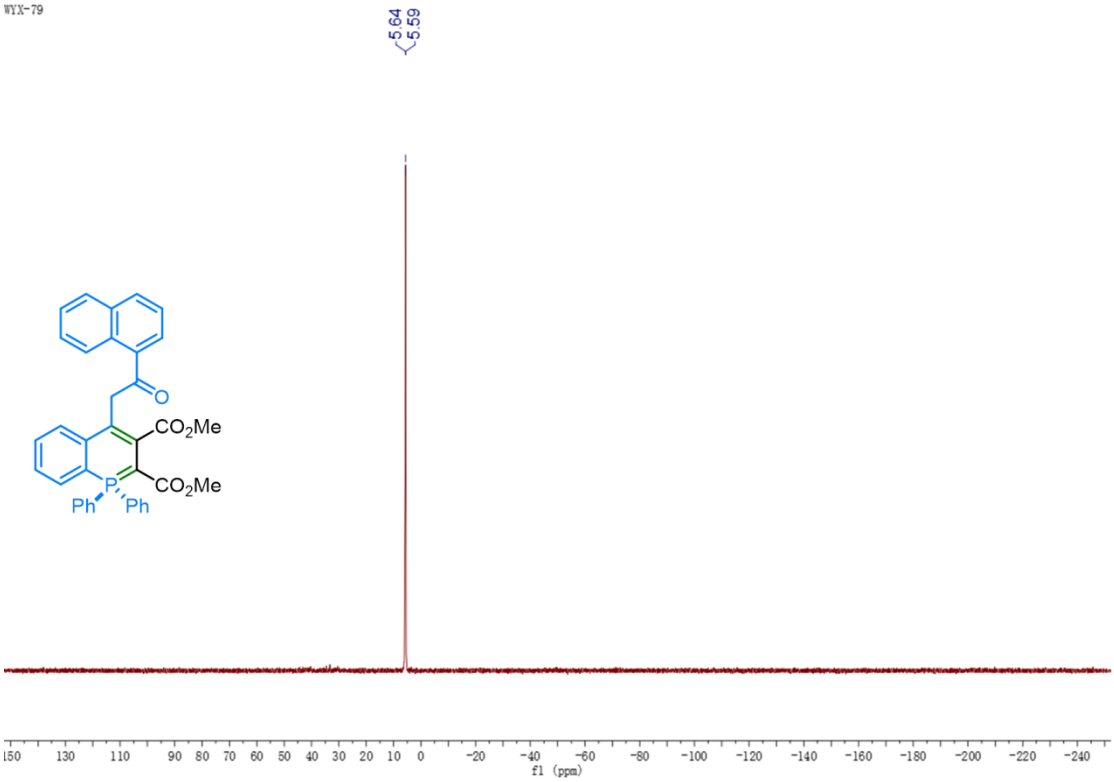
^{1}H NMR spectrum of **5q** (400 MHz, $CDCl_3$)



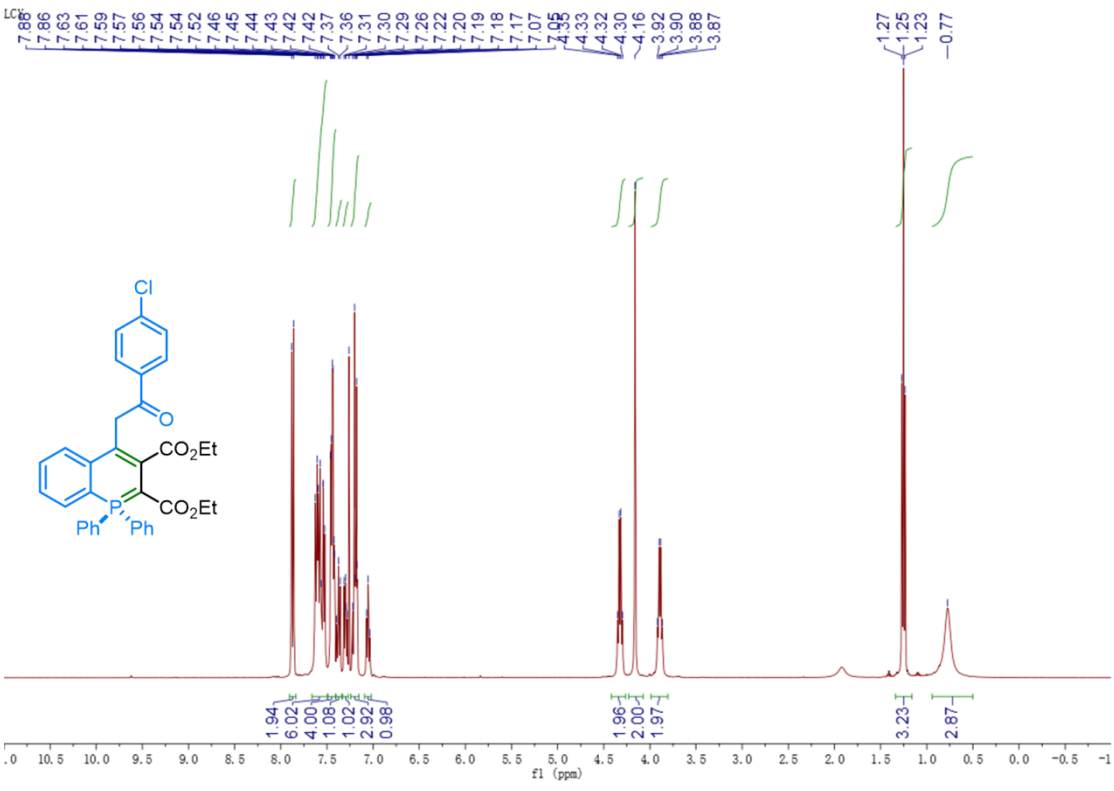
^{13}C NMR spectrum of **5q** (100 MHz, $CDCl_3$)



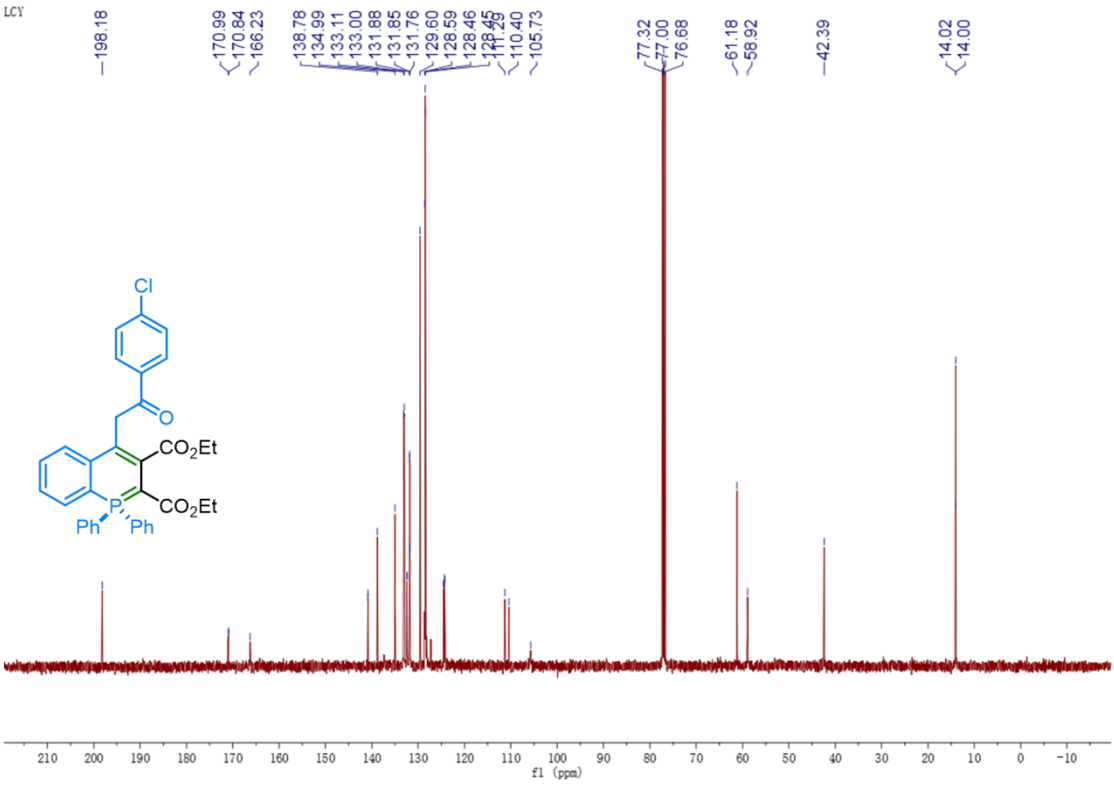
^{31}P NMR spectrum of **5q** (202 MHz, $CDCl_3$)



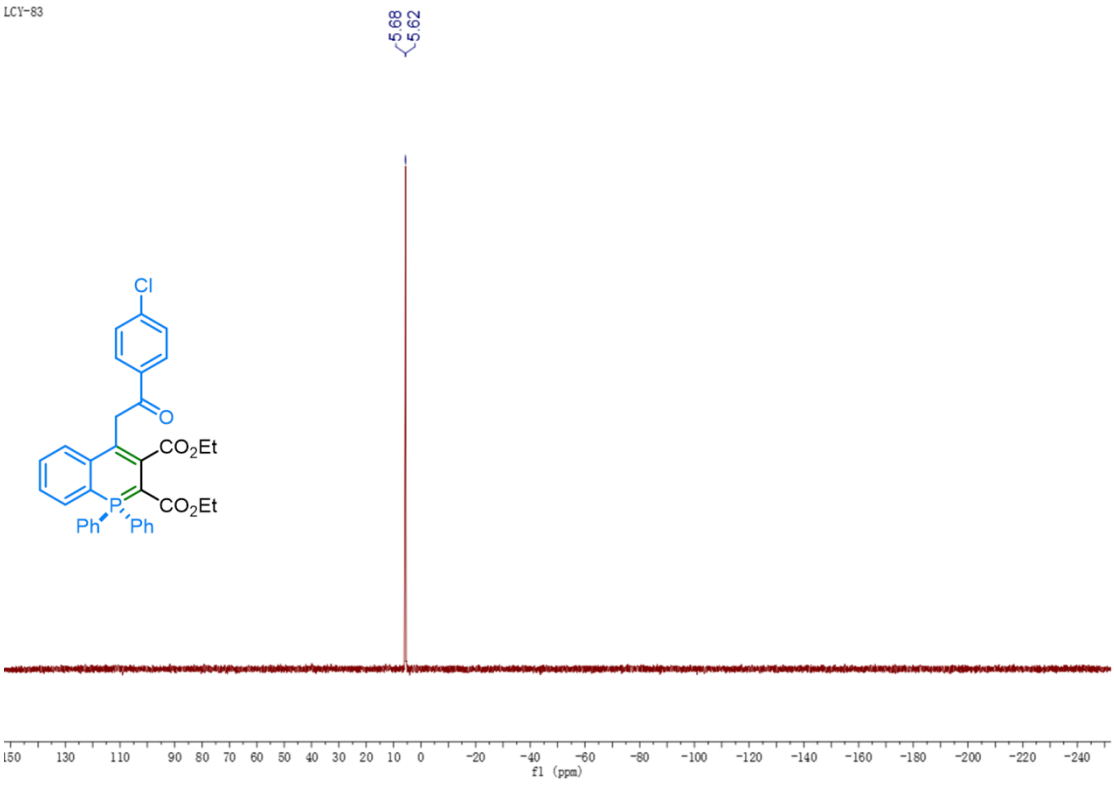
^{1}H NMR spectrum of **5r** (400 MHz, $CDCl_3$)



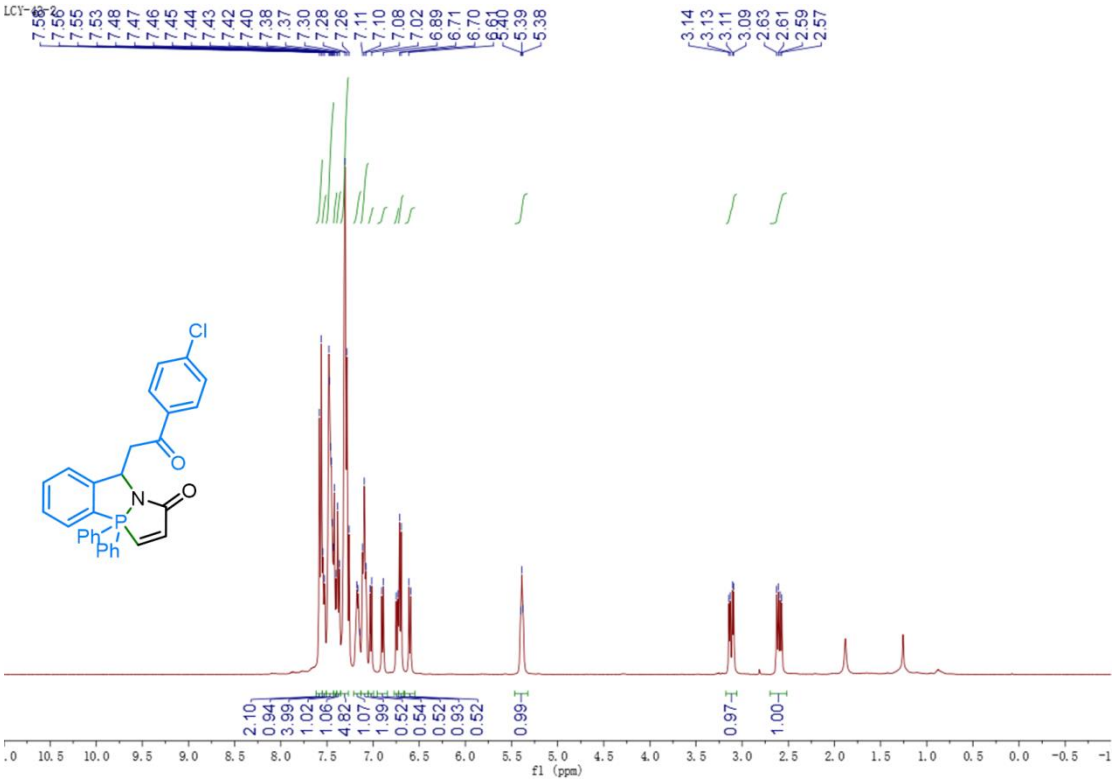
^{13}C NMR spectrum of **5r** (100 MHz, $CDCl_3$)



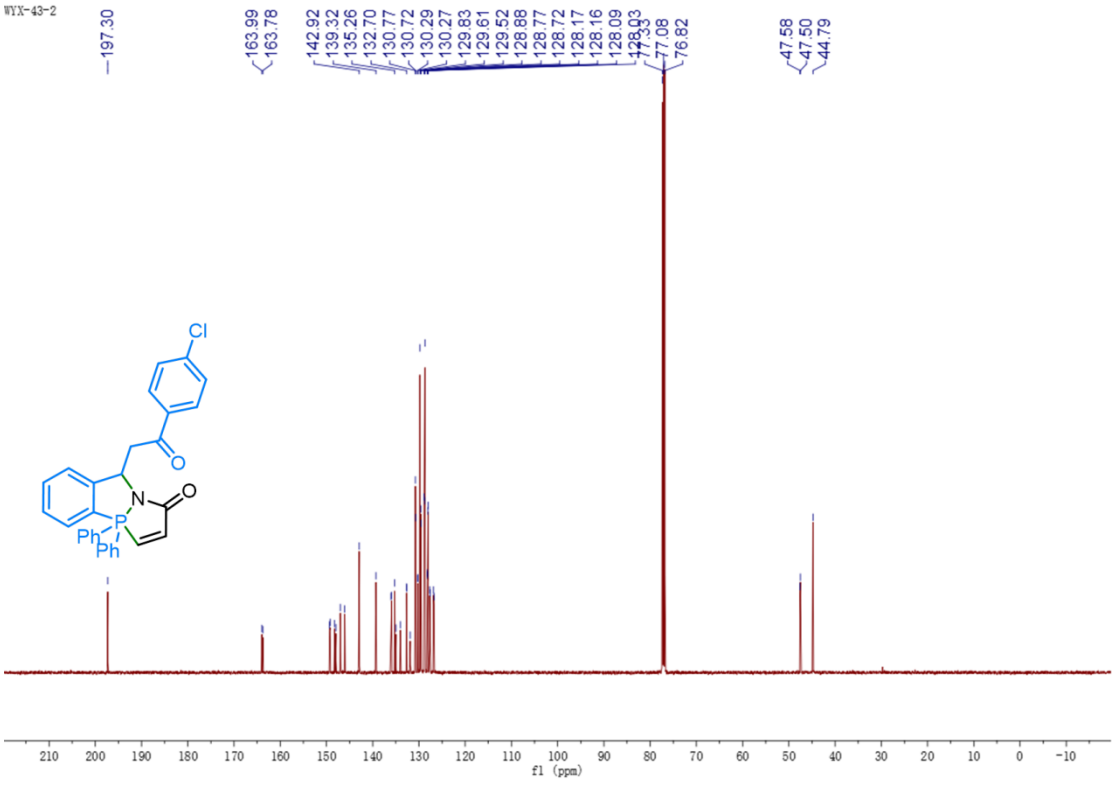
^{31}P NMR spectrum of **5r** (202 MHz, $CDCl_3$)



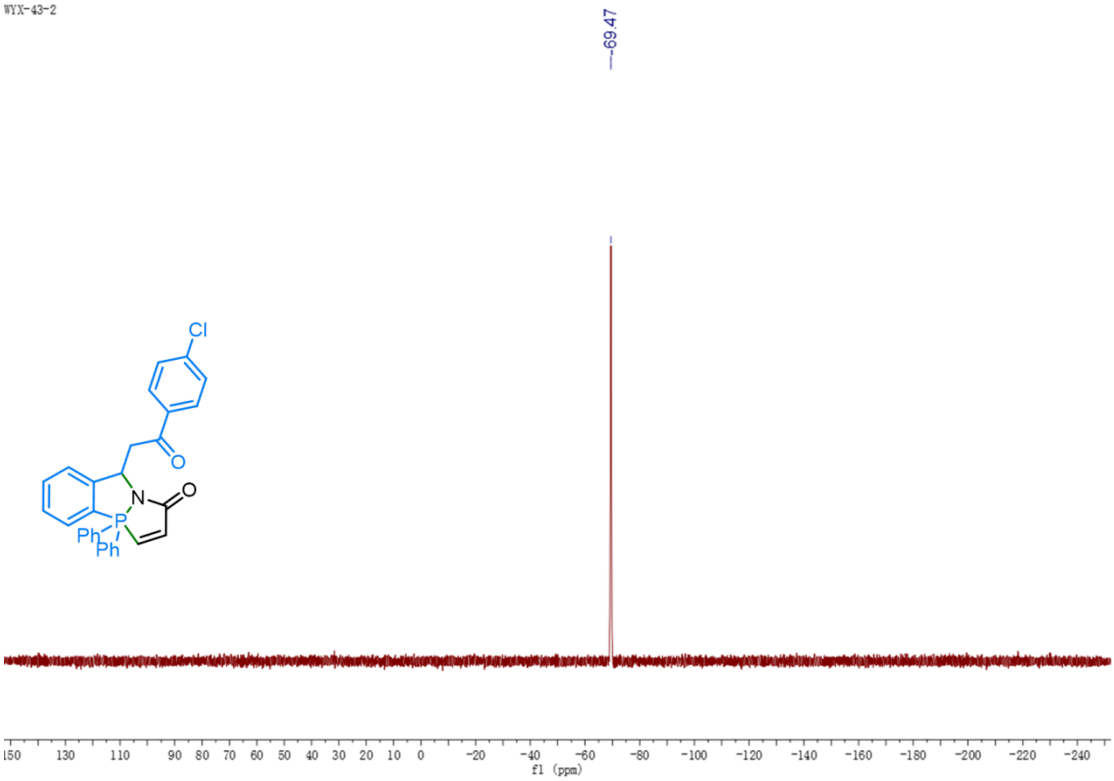
^{1}H NMR spectrum of **7** (400 MHz, $CDCl_3$)



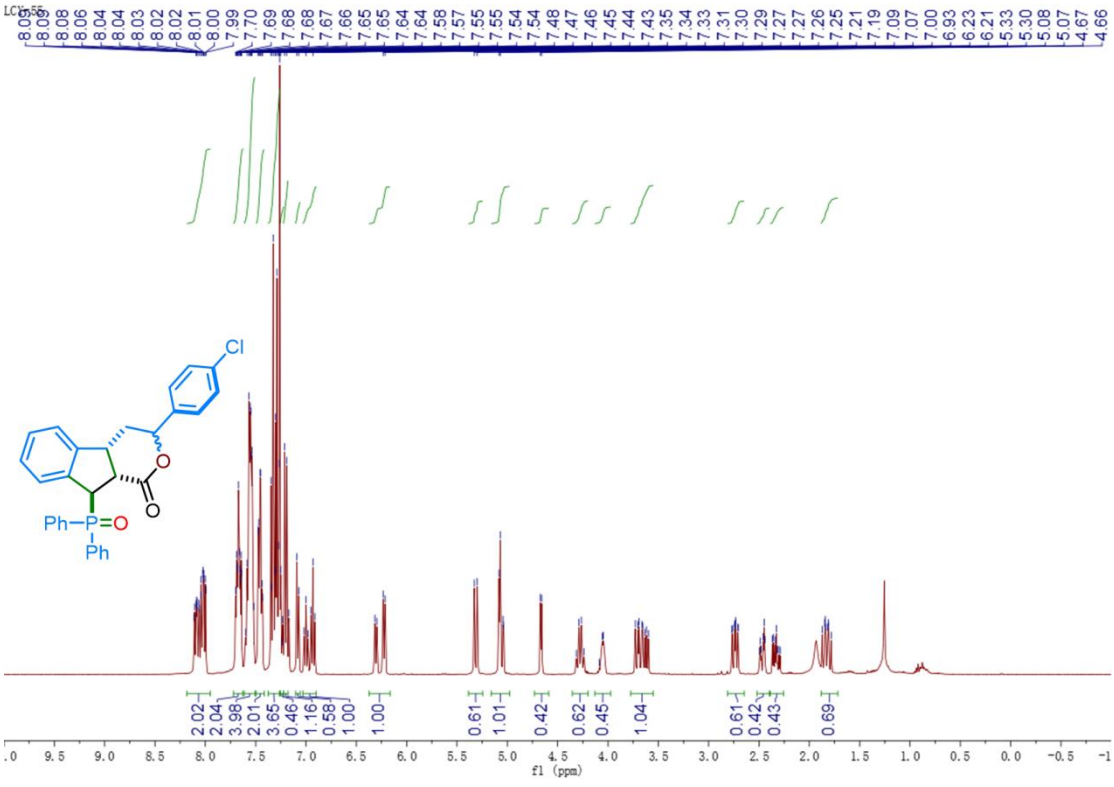
^{13}C NMR spectrum of **7** (500 MHz, $CDCl_3$)



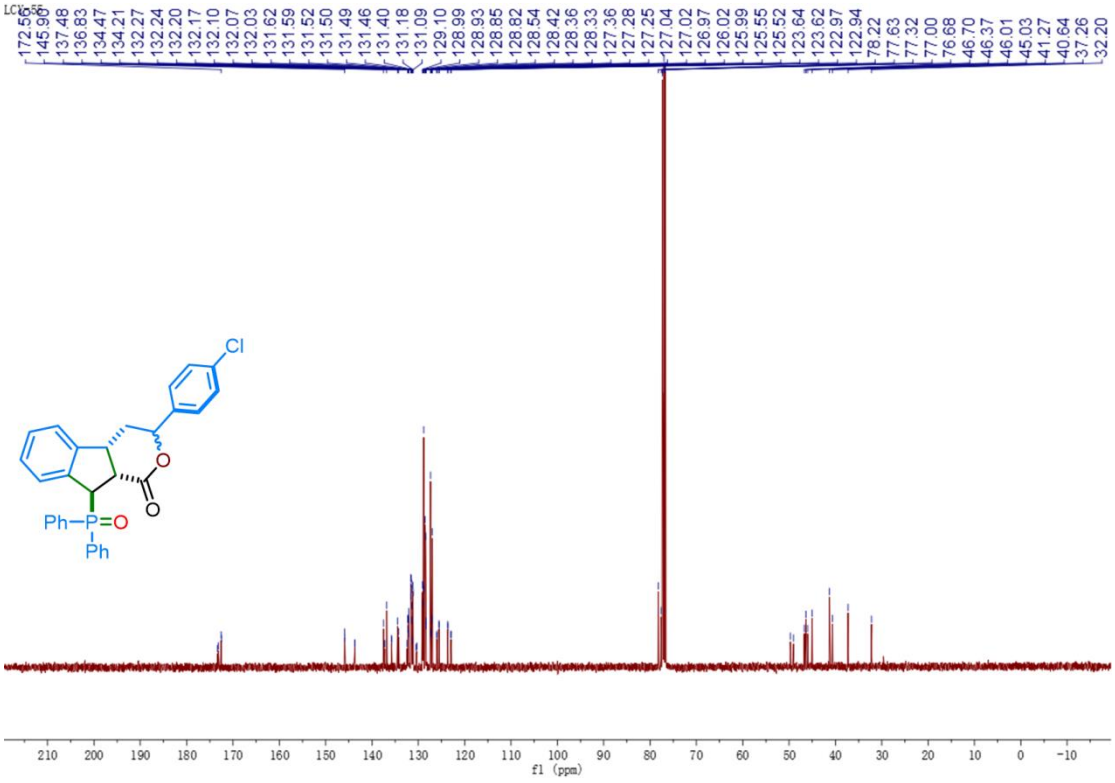
^{31}P NMR spectrum of **7** (202 MHz, $CDCl_3$)



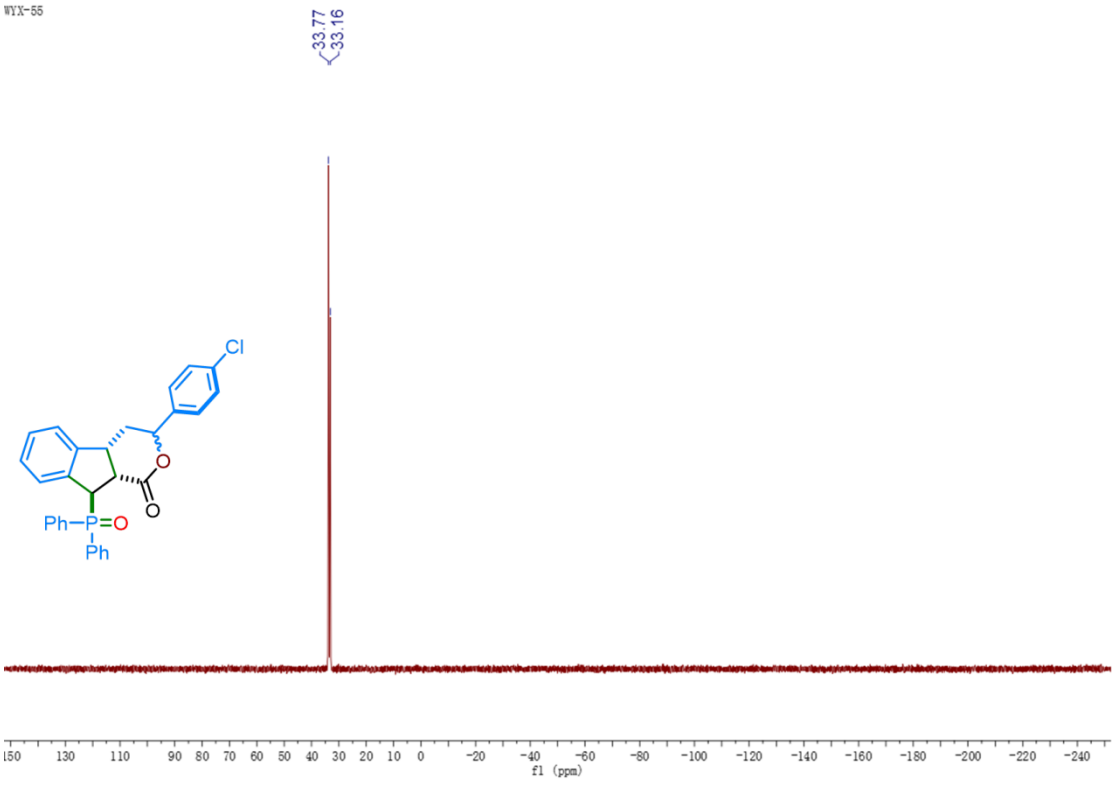
^{1}H NMR spectrum of **8** (400 MHz, $CDCl_3$)



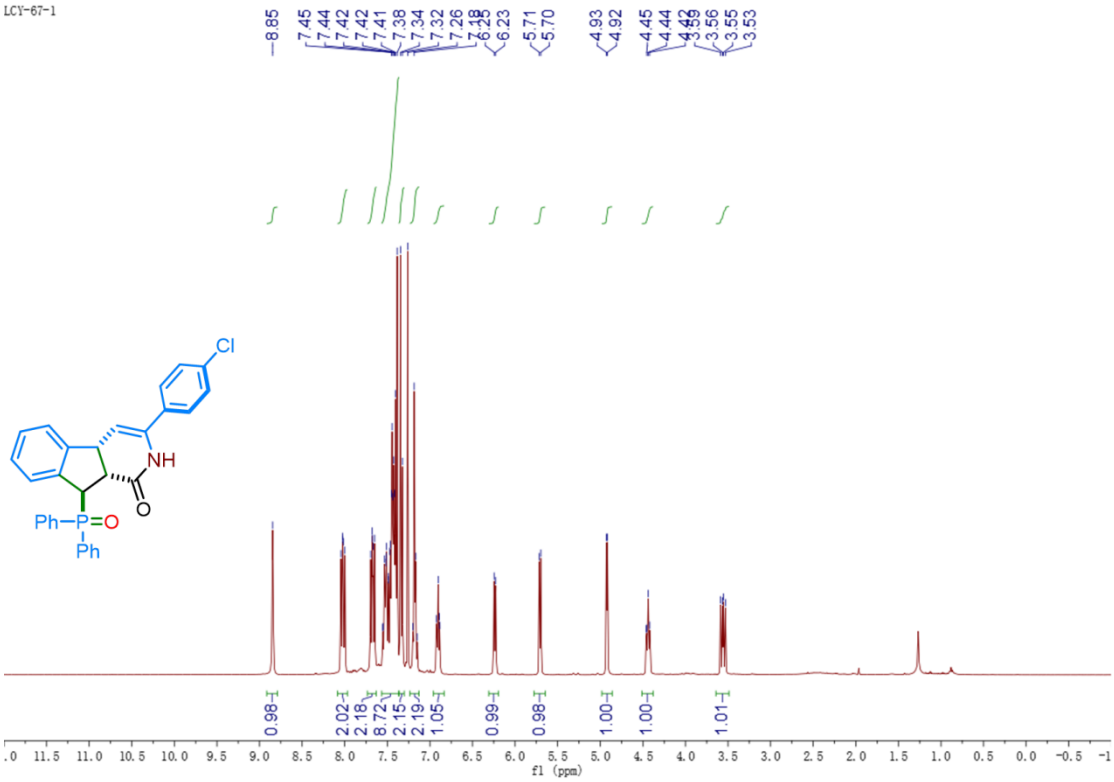
^{13}C NMR spectrum of **8** (100 MHz, $CDCl_3$)



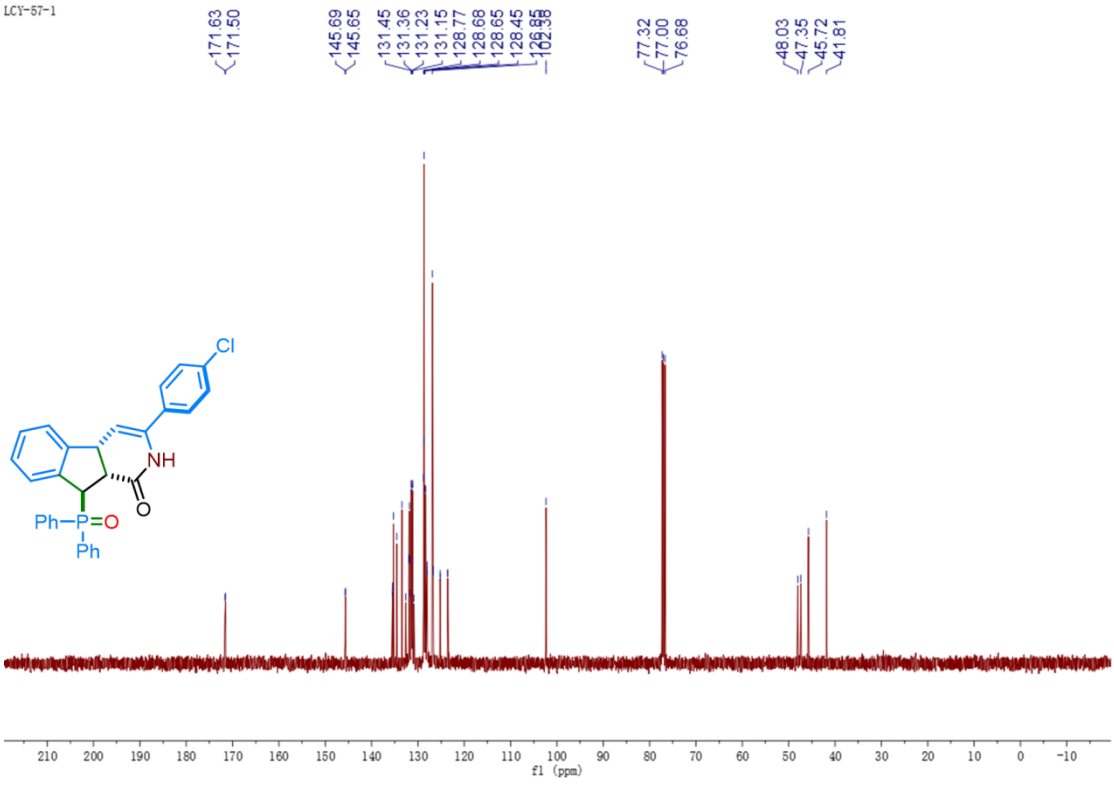
^{31}P NMR spectrum of **8** (202 MHz, $CDCl_3$)



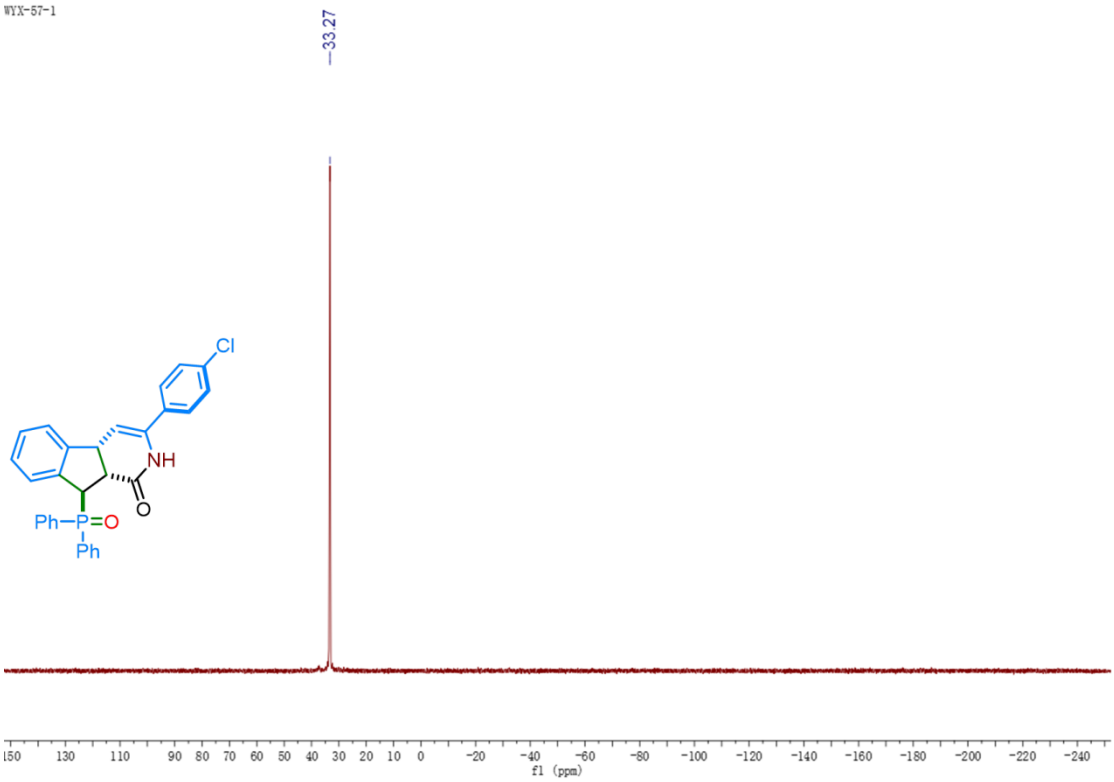
^{1}H NMR spectrum of **9** (400 MHz, $CDCl_3$)



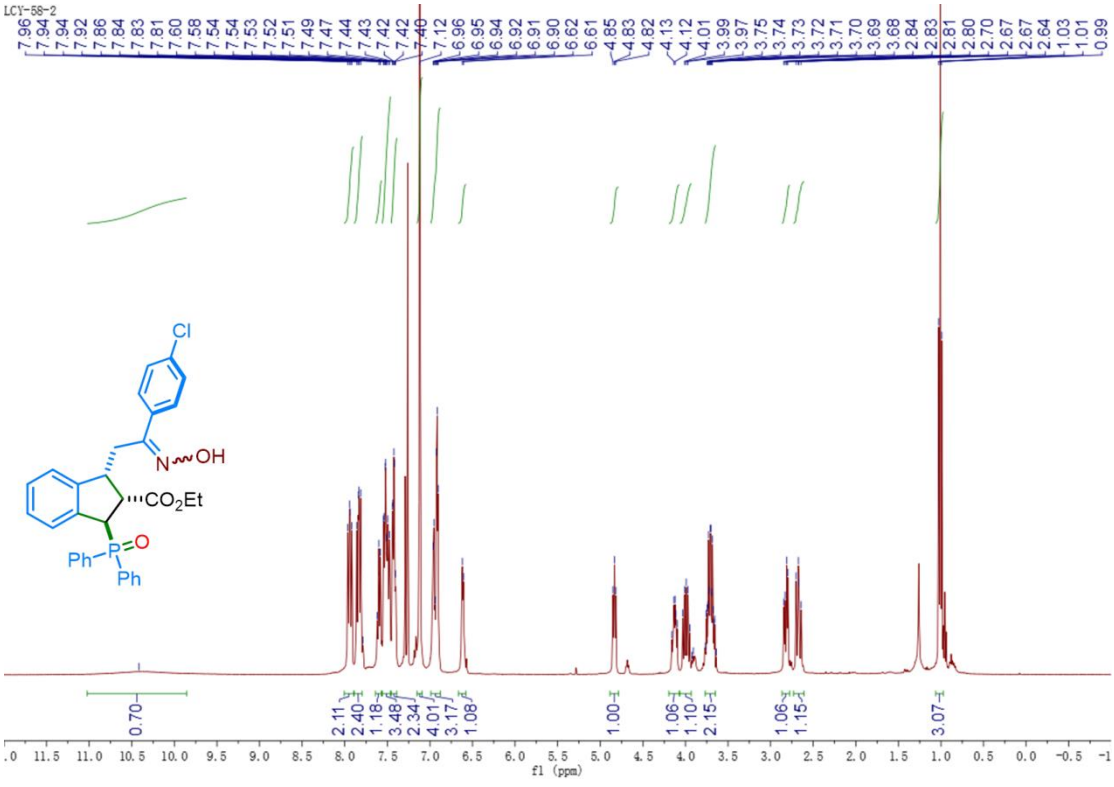
^{13}C NMR spectrum of **9** (100 MHz, $CDCl_3$)



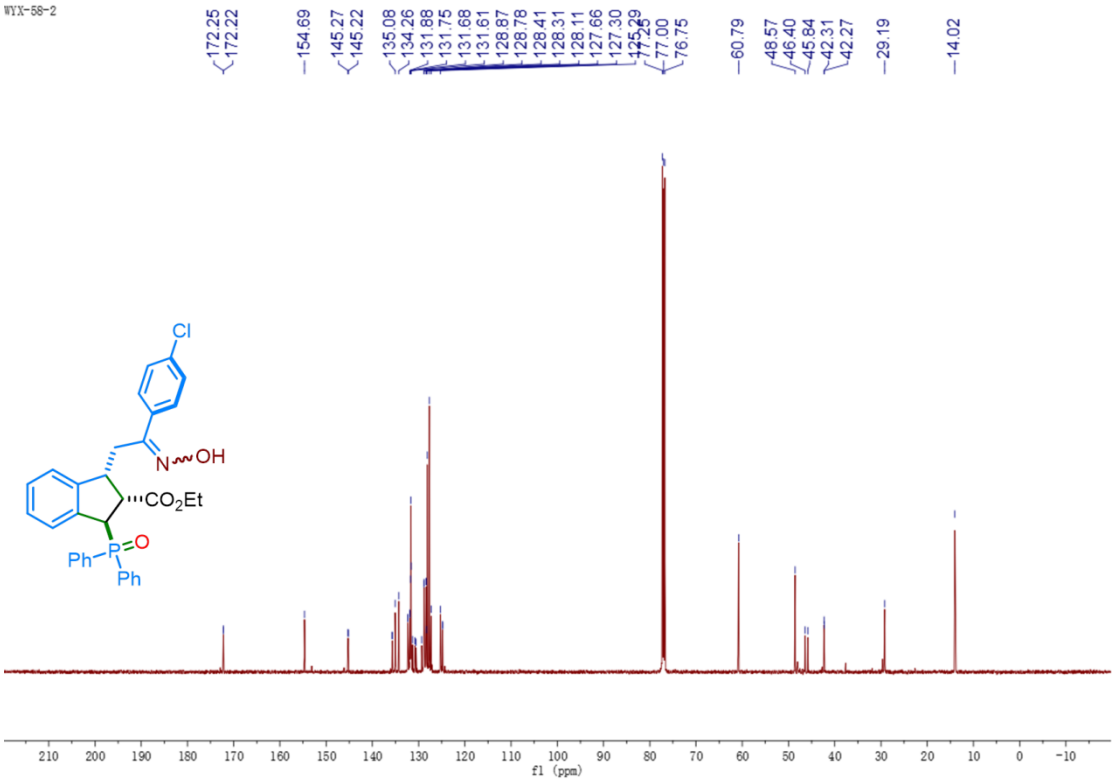
^{31}P NMR spectrum of **9** (202 MHz, $CDCl_3$)



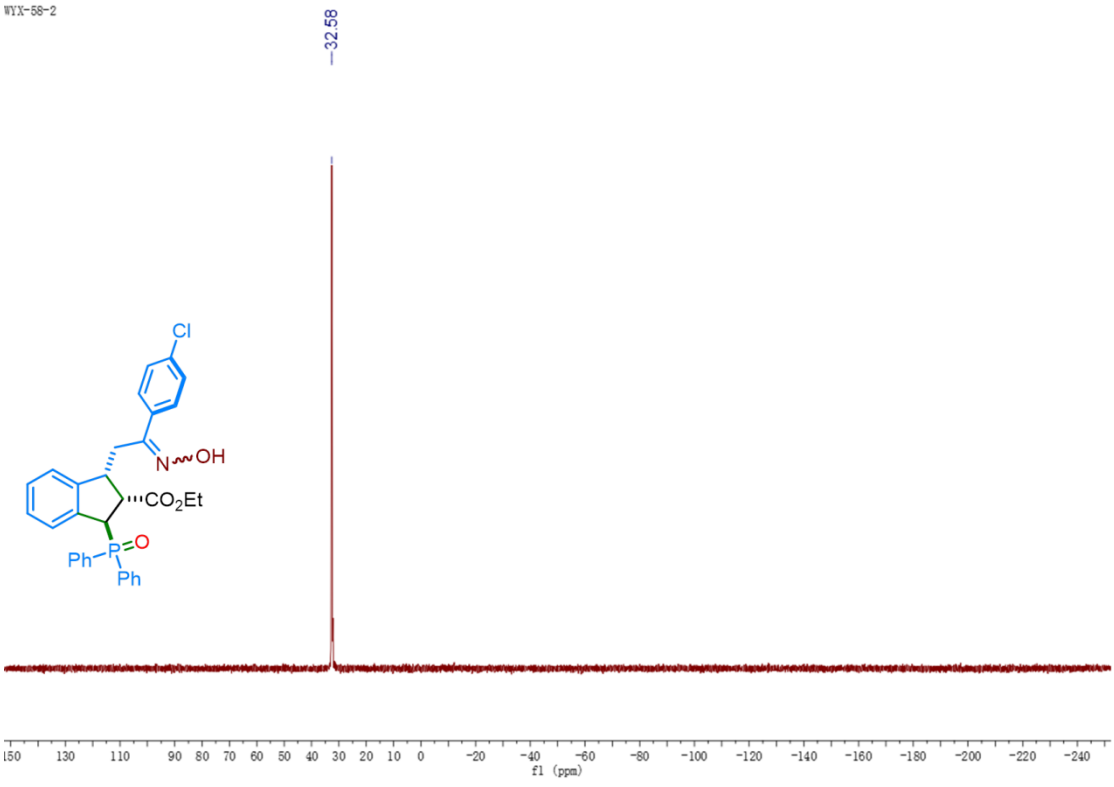
^{1}H NMR spectrum of **10** (400 MHz, $CDCl_3$)



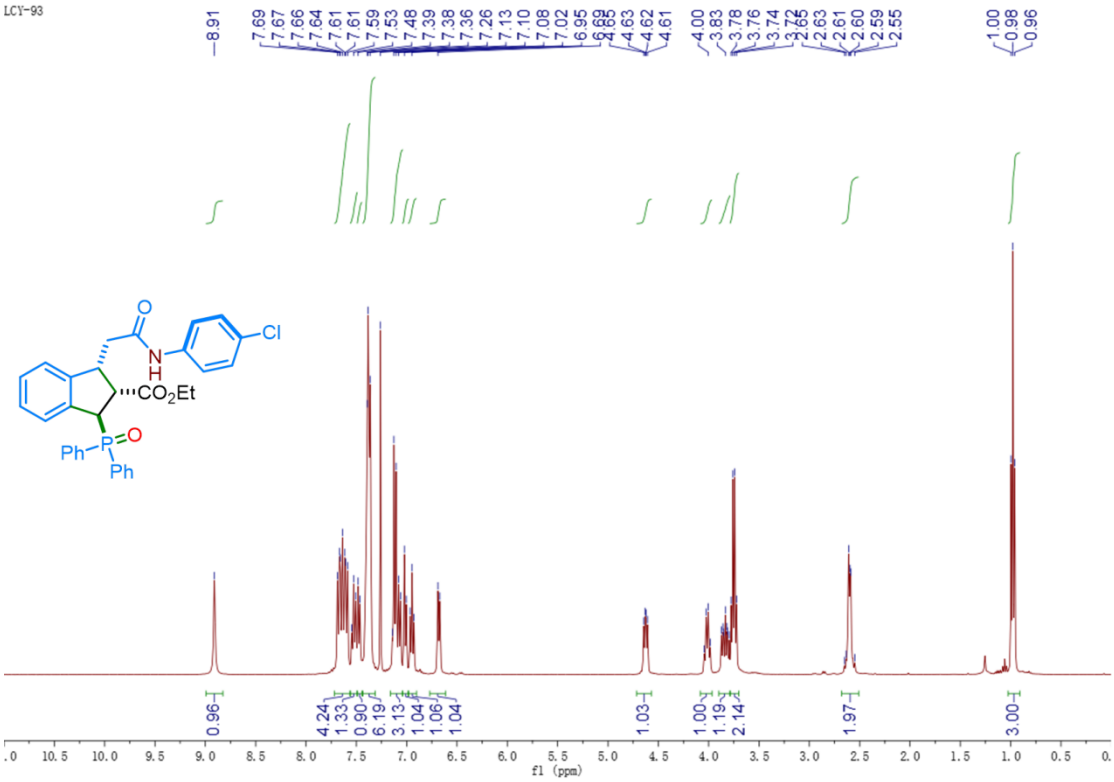
^{13}C NMR spectrum of **10** (125 MHz, $CDCl_3$)



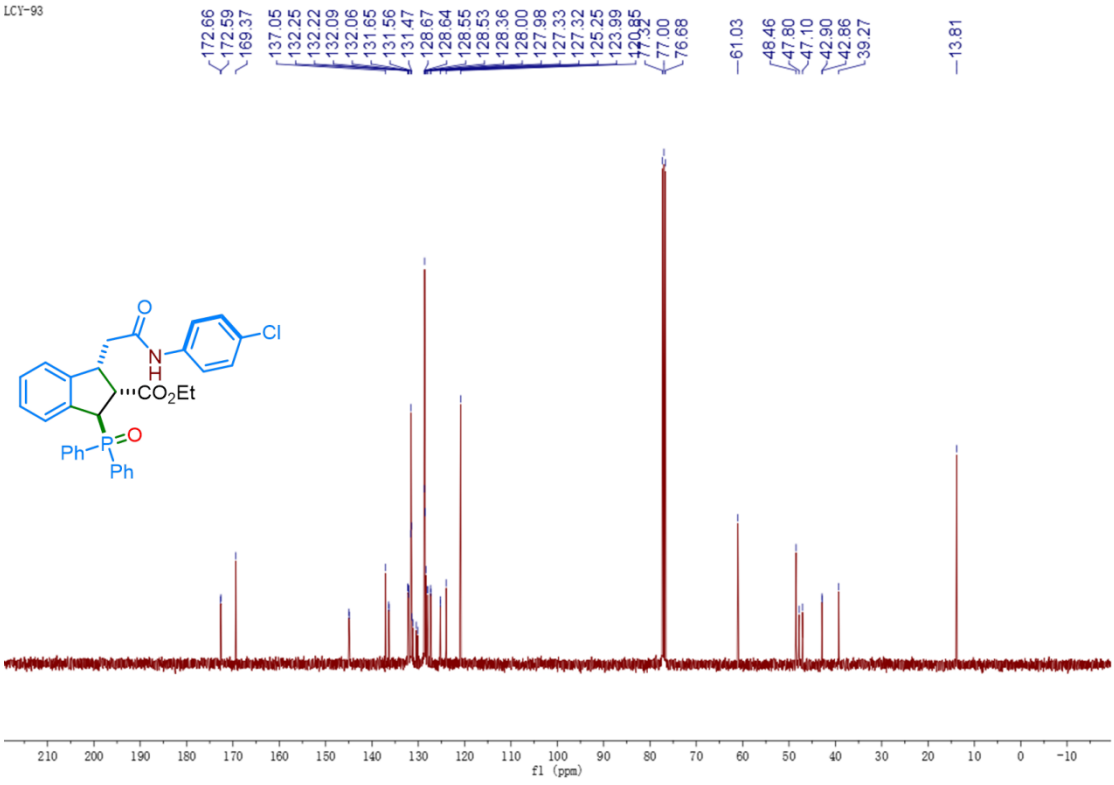
^{31}P NMR spectrum of **10** (202 MHz, $CDCl_3$)



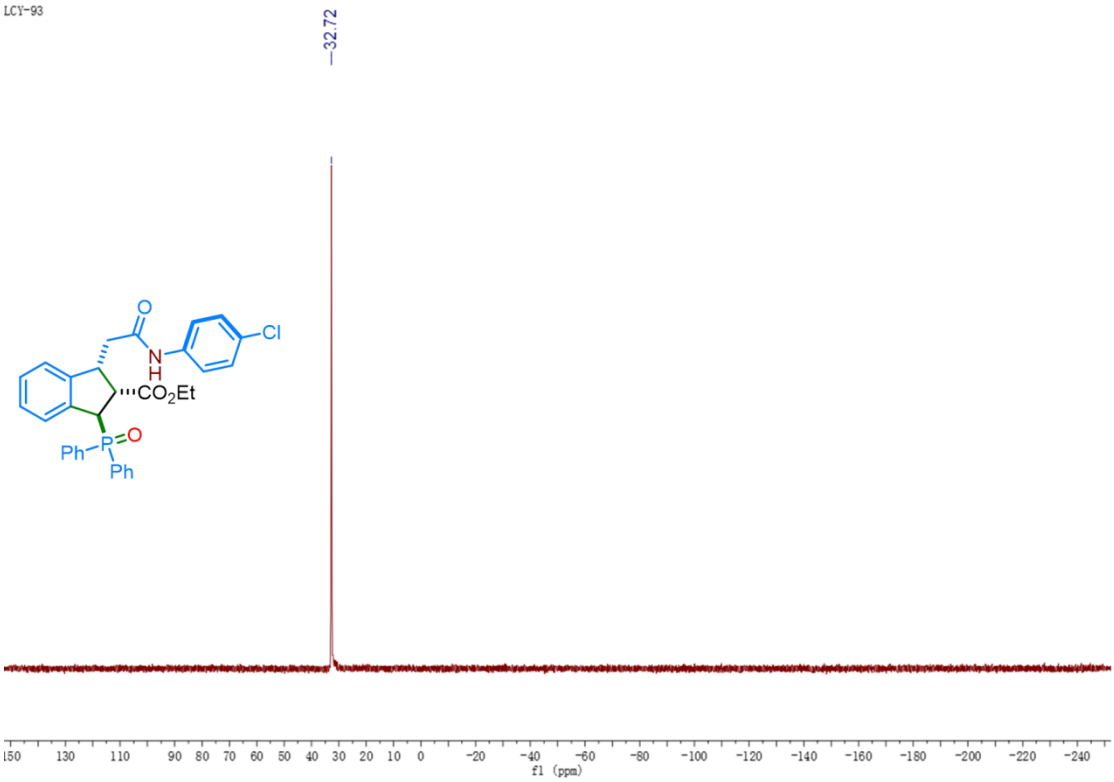
^{1}H NMR spectrum of **11** (400 MHz, $CDCl_3$)



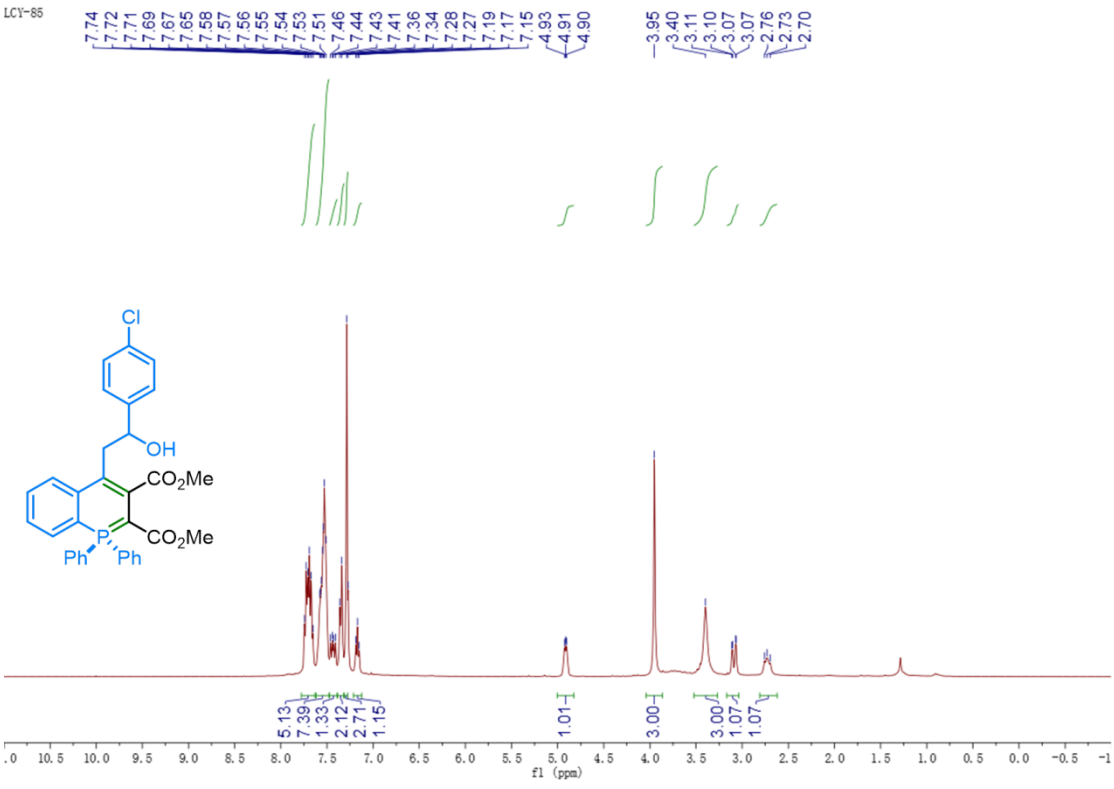
^{13}C NMR spectrum of **11** (100 MHz, $CDCl_3$)



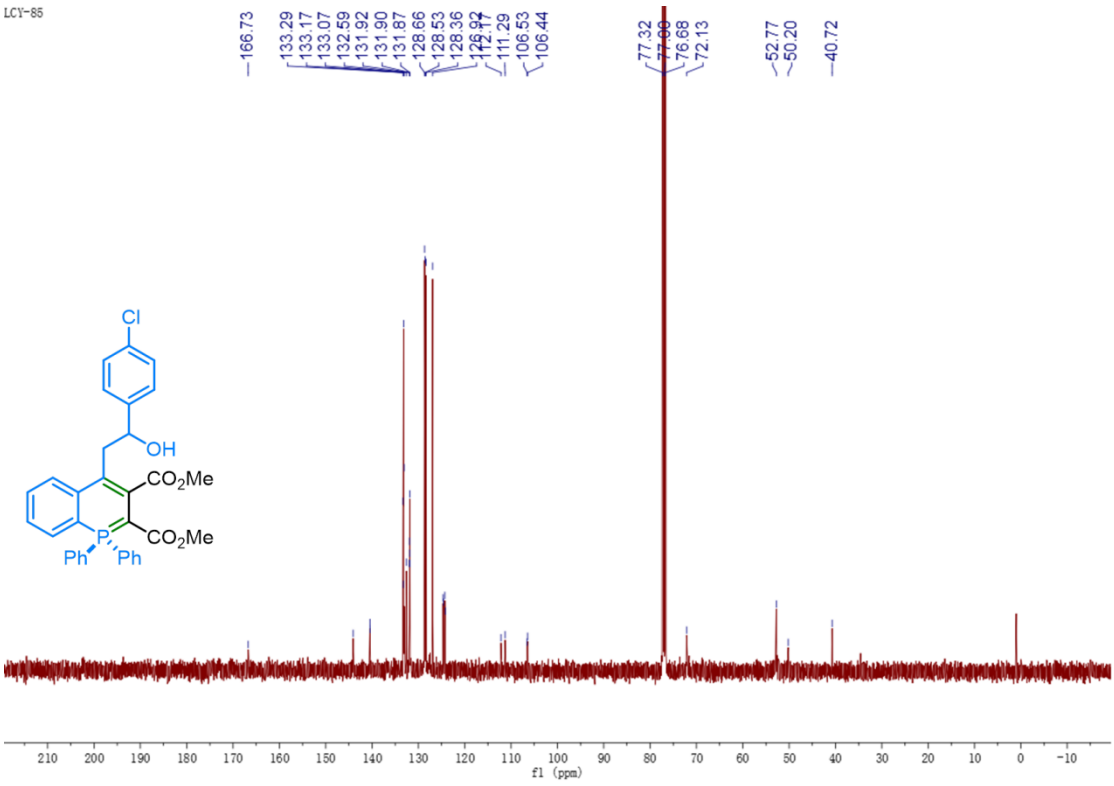
^{31}P NMR spectrum of **11** (202 MHz, $CDCl_3$)



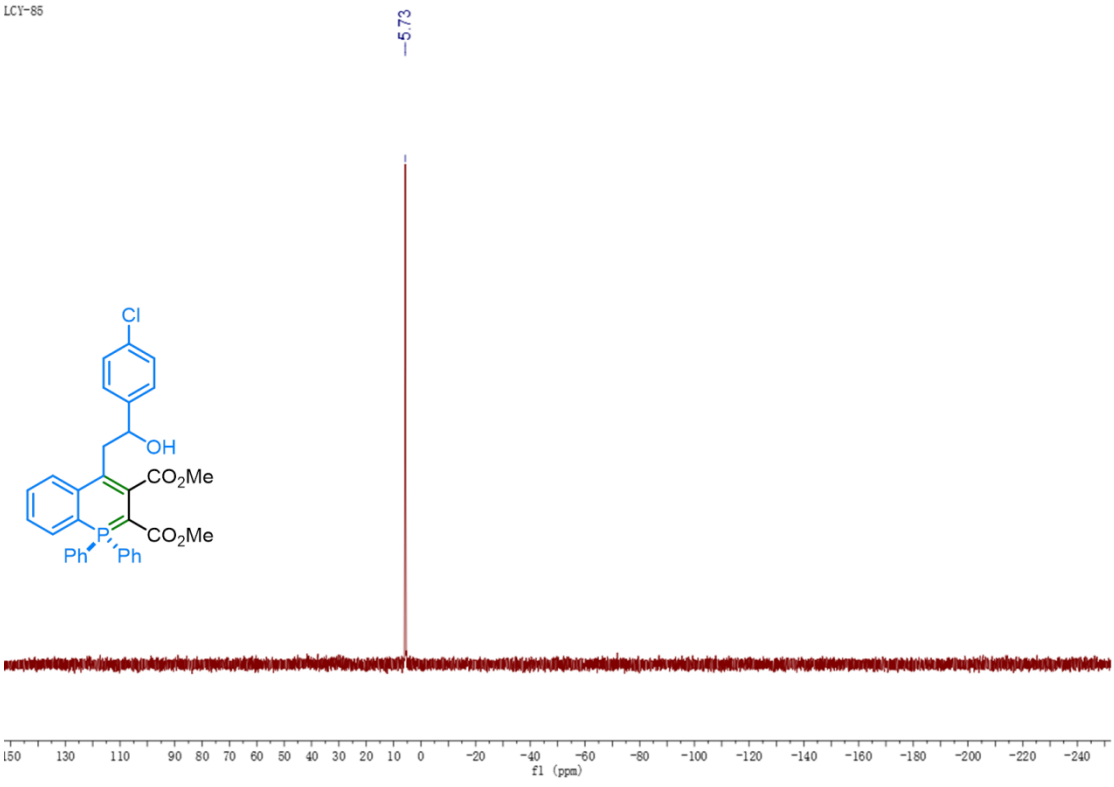
^{1}H NMR spectrum of **12** (400 MHz, $CDCl_3$)



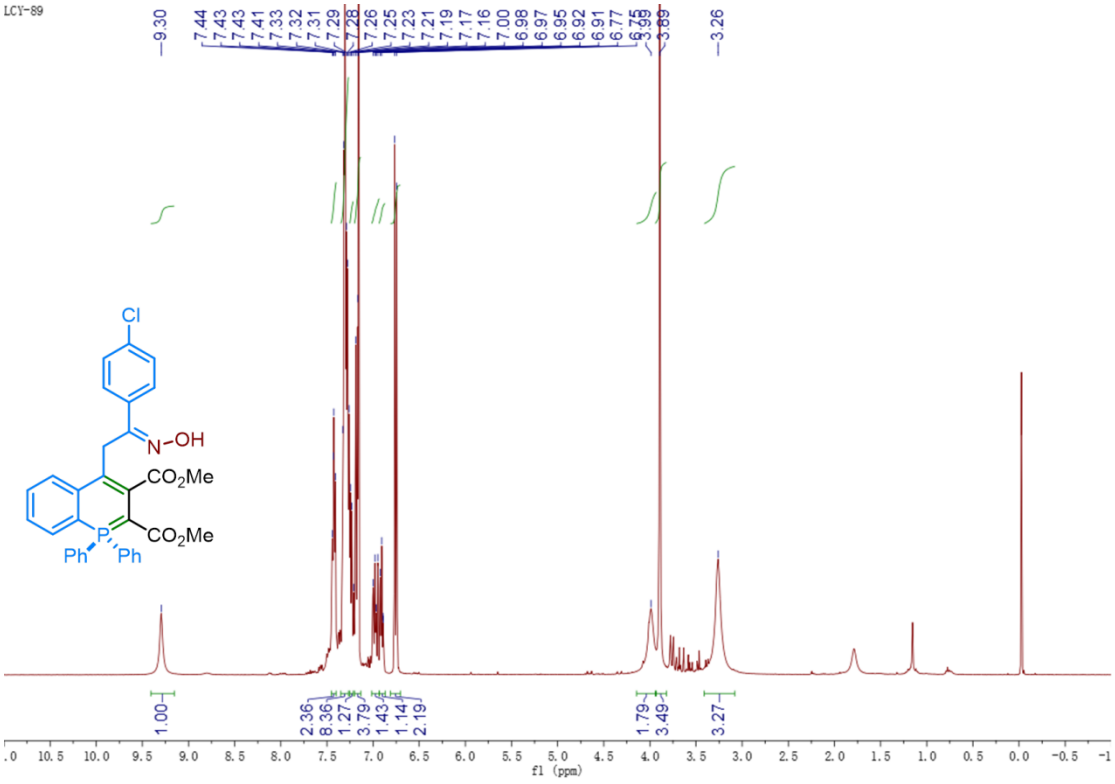
^{13}C NMR spectrum of **12** (100 MHz, $CDCl_3$)



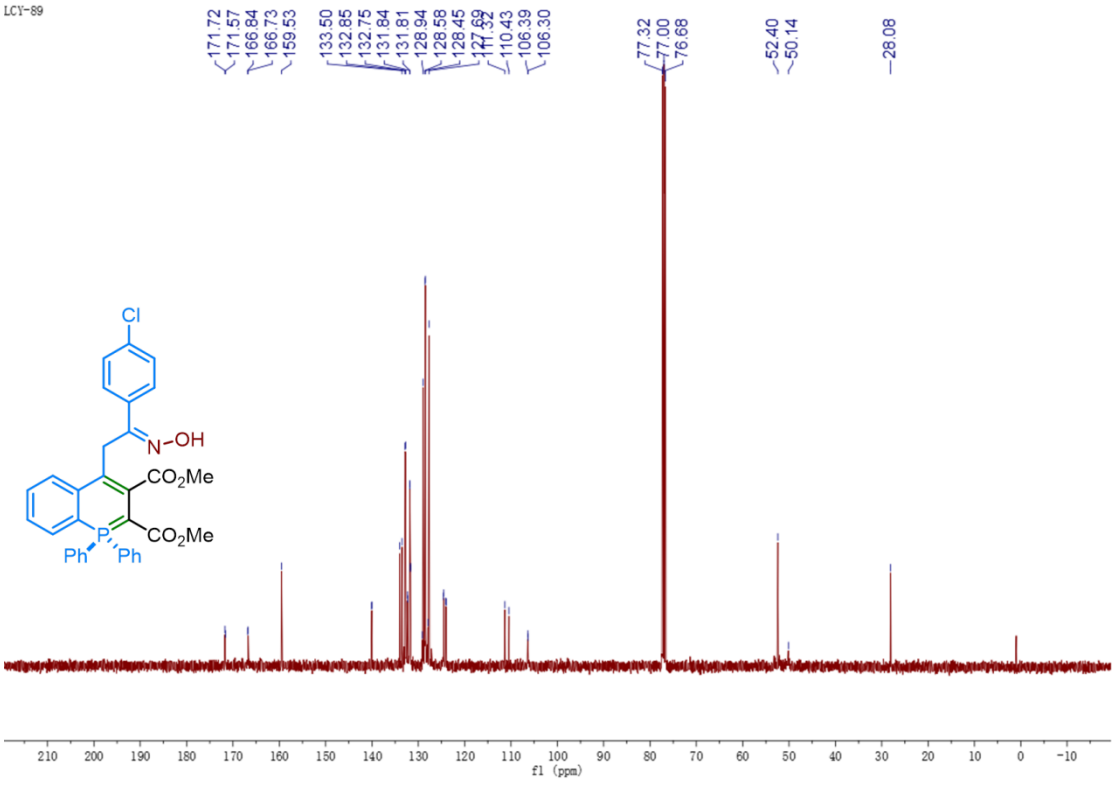
^{31}P NMR spectrum of **12** (202 MHz, $CDCl_3$)



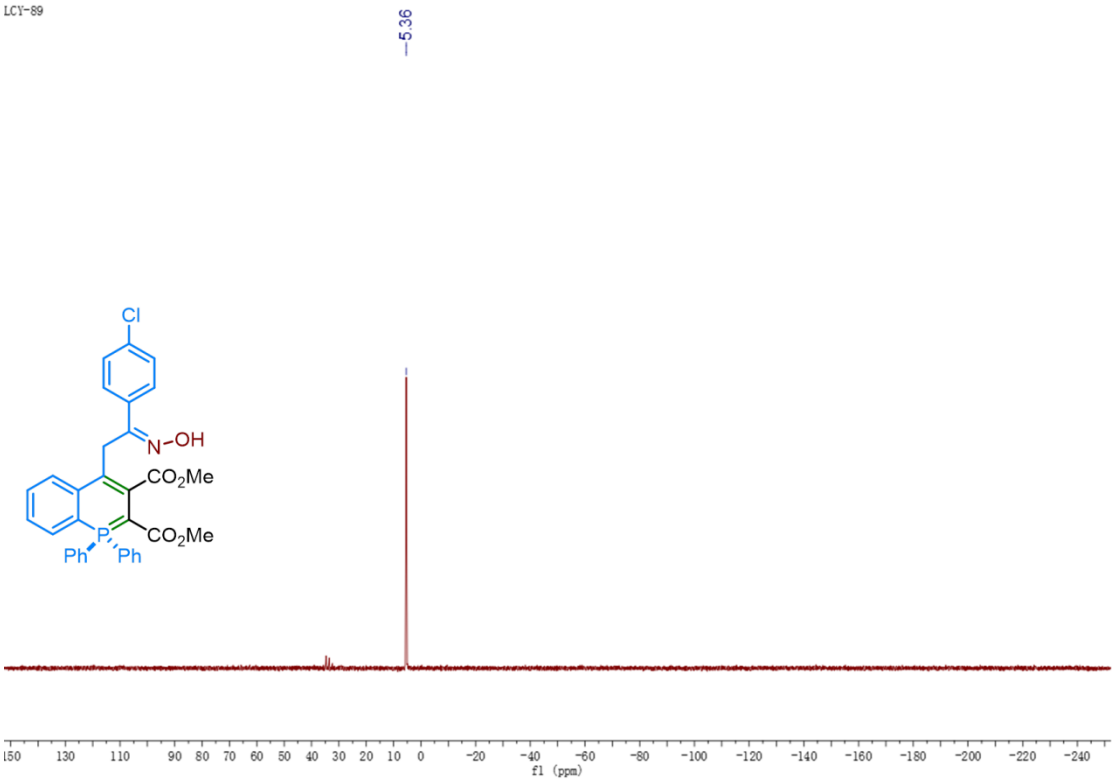
^{1}H NMR spectrum of **13** (400 MHz, $CDCl_3$)



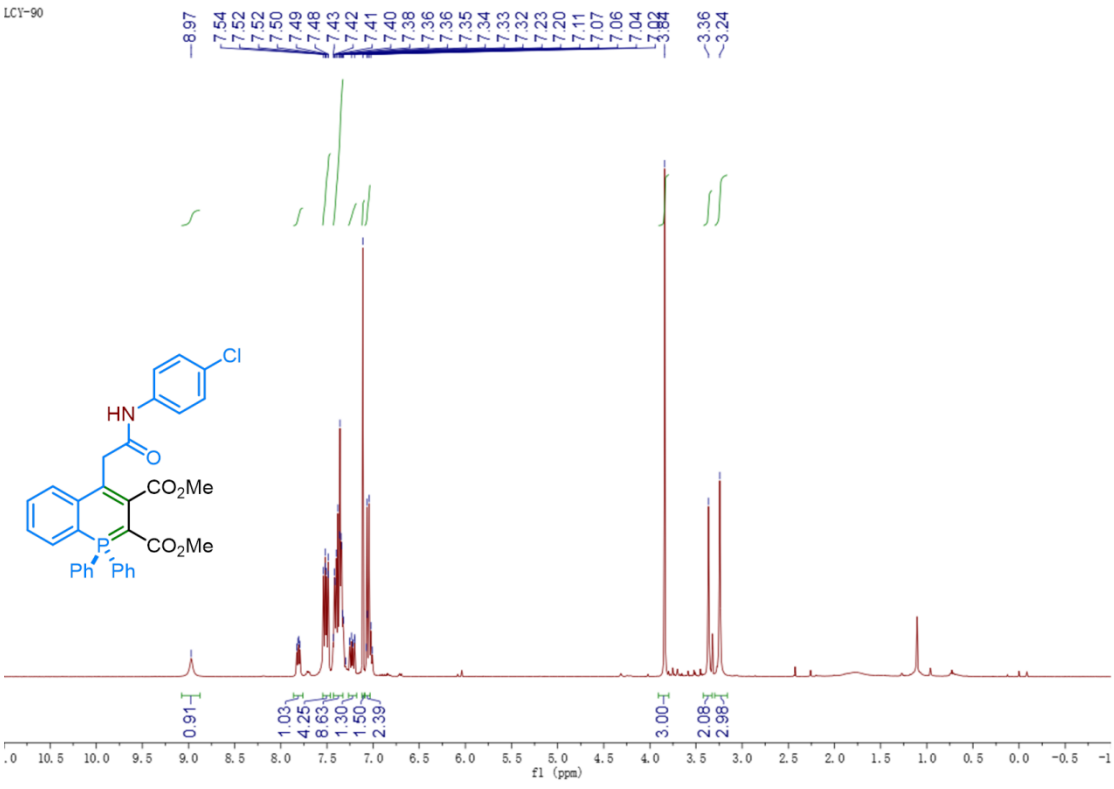
^{13}C NMR spectrum of **13** (100 MHz, $CDCl_3$)



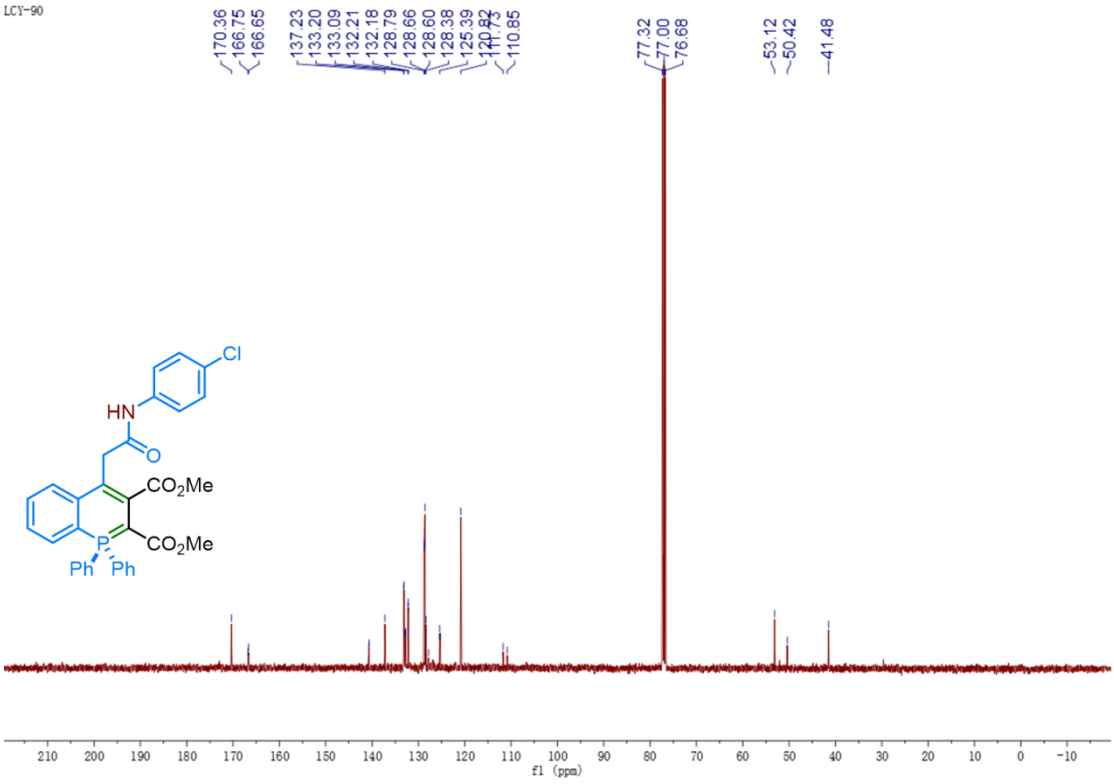
^{31}P NMR spectrum of **13** (202 MHz, $CDCl_3$)



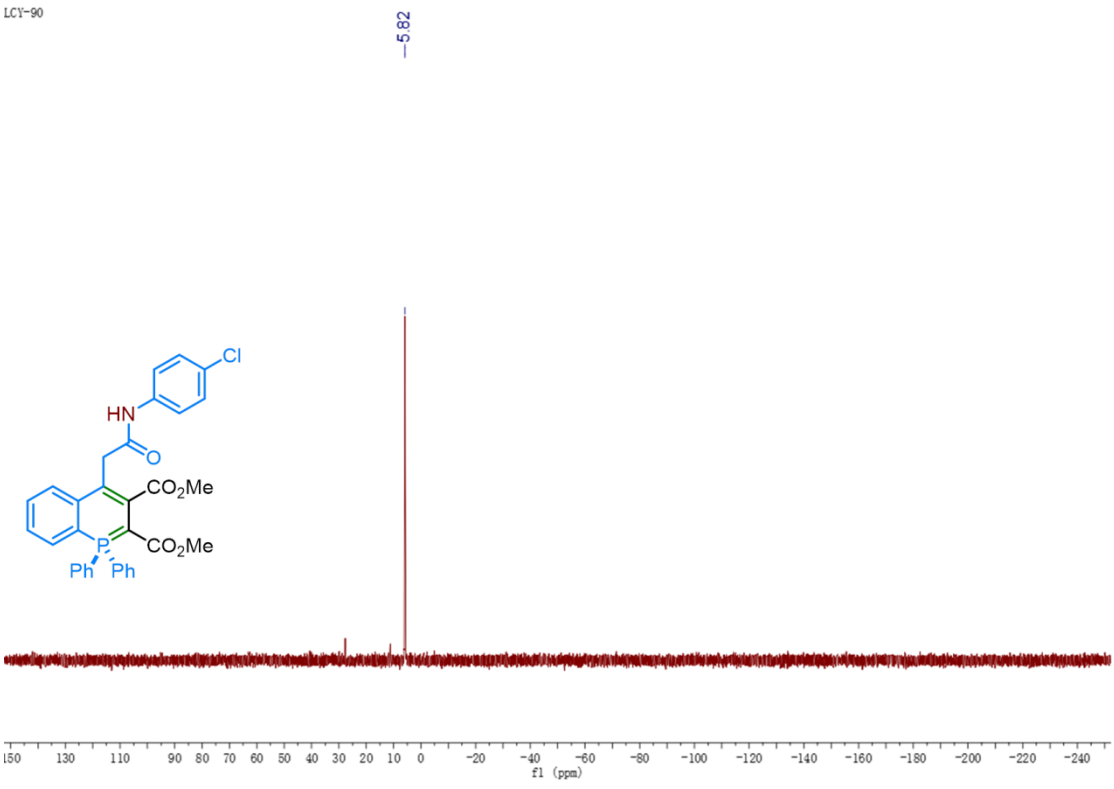
^{1}H NMR spectrum of **14** (400 MHz, $CDCl_3$)



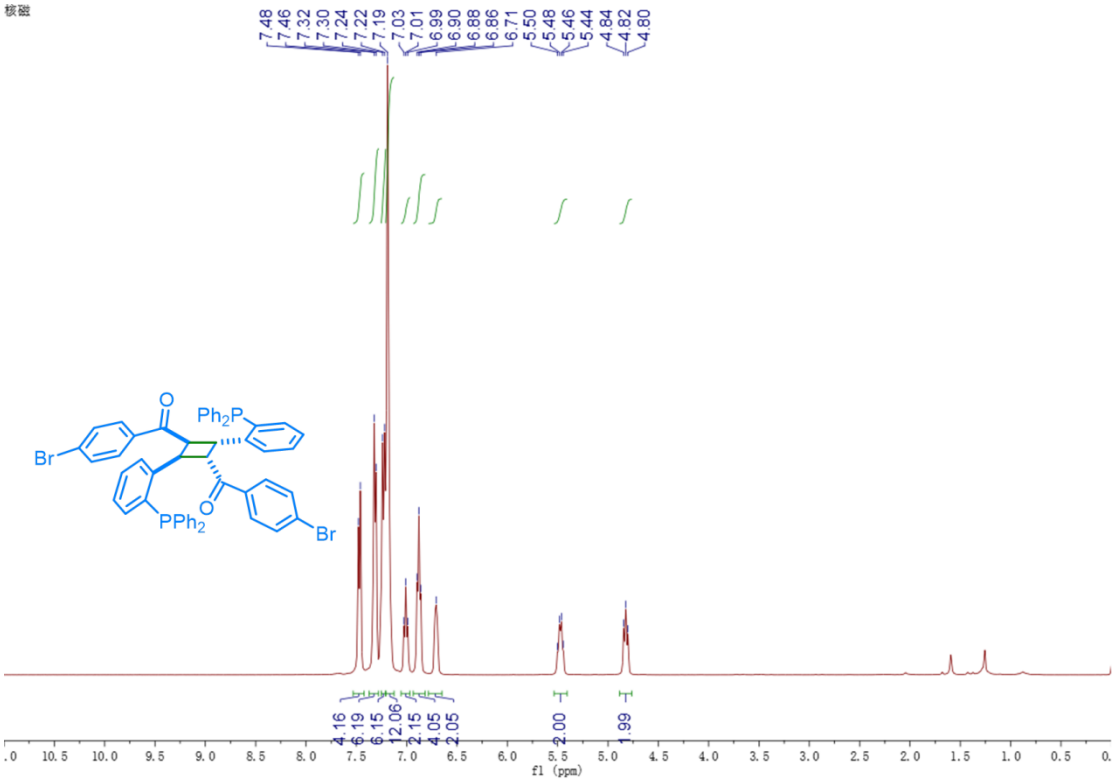
^{13}C NMR spectrum of **14** (100 MHz, $CDCl_3$)



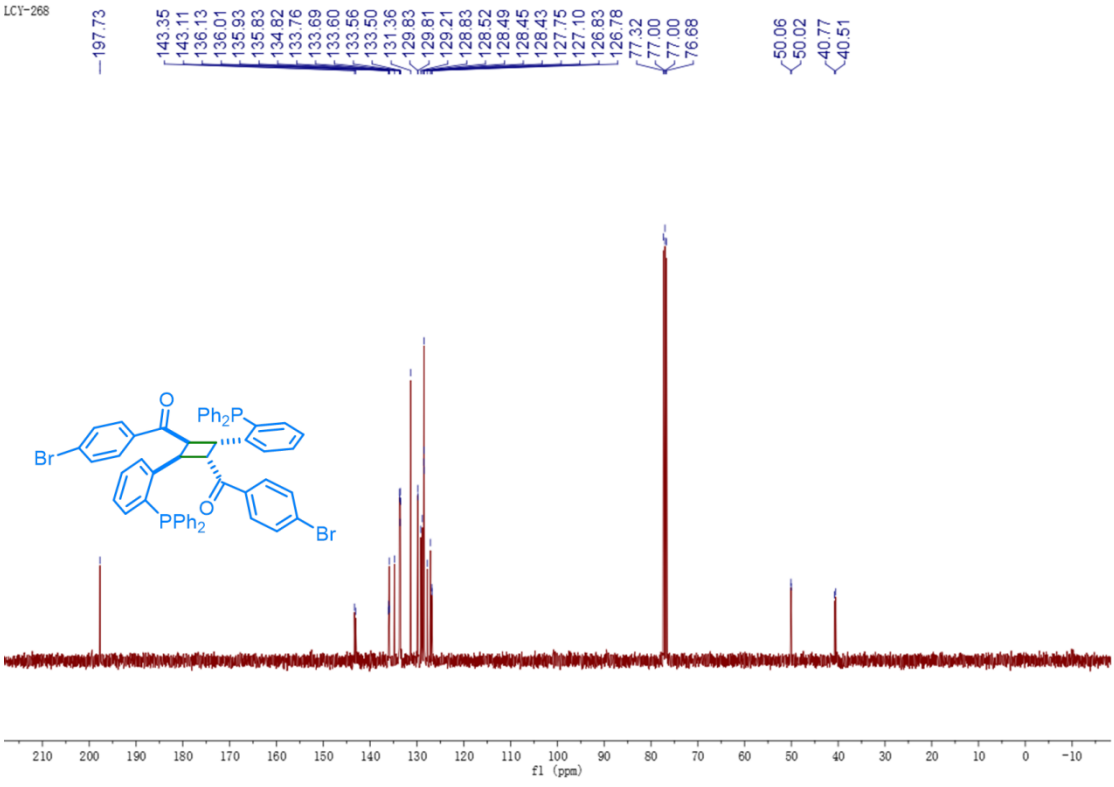
^{31}P NMR spectrum of **14** (202 MHz, $CDCl_3$)



^{1}H NMR spectrum of **15** (400 MHz, $CDCl_3$)



^{13}C NMR spectrum of **15** (100 MHz, $CDCl_3$)



^{31}P NMR spectrum of **15** (162 MHz, $CDCl_3$)