Supplementary materials

Synthesis of Alpha Olefins: Catalytic Decarbonylation of Carboxylic Acids and Vegetable Oil Deodorizer Distillate (VODD)

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1. General Considerations

Unless otherwise noted, all reagents were purchased from commercial suppliers and used without purification [1]. Toluene and THF were freshly distilled from sodium and sodium benzophenone ketyl under nitrogen. All decarbonylation reactions were performed in resealable screw cap Schlenk tube (approx. 15 mL volume) in the presence of Teflon-coated magnetic stirrer bar (4 mm × 10 mm).2-(2-Bromophenyl)naphthalene and Ligands **L3 – L9** were purchased from commercial suppliers. New bottle of *n*-butyllithium was used (*Note*: since the concentration of *n*-BuLi may vary, we recommend performing a titration prior to use). Thin layer chromatography was performed on pre-coated silica gel 60 F_{254} plates. Silica gel (Merck, 70-230 and 230-400 mesh) was used for column chromatography. Melting points were recorded on an uncorrected Büchi Melting Point B-545 instrument. NMR spectra were recorded on a Brüker spectrometer (400 MHz for ^{1}H, 100 MHz for ^{13}C and 162 MHz for ^{31}P). Spectra were referenced internally to the residual proton resonance in $CDCl_3$ (δ 7.26 ppm) as the internal standard. Chemical shifts (δ) were reported as part per million (ppm) in δ scale downfield from TMS. ^{13}C NMR spectra were referenced to $CDCl_3$ (δ 77.0 ppm, the middle peak). ^{31}P NMR spectra were referenced to 85% H_3PO_4 externally. Coupling constants (*J*) were reported in Hertz (Hz). Mass spectra (EI-MS and ES-MS) were recorded on a HP 5989B Mass Spectrometer. High-resolution mass spectra (HRMS) were obtained on a Bruker APEX 47e FTICR mass spectrometer (ESI-MS). GC-MS analysis was conducted on a HP 5973 GCD system using a HP5MS column (30 m × 0.25 mm). The products described in GC yield were accorded to the authentic samples/dodecane calibration standard from Agilent 6890A GC-FID system. X-ray crystal structure was determined by Bruker D8 Venture. All yields reported refer to isolated yield of compounds estimated to be greater than 95% purity as determined by capillary gas chromatography (GC) or ^{1}H NMR. Compounds described in the literature were characterized by comparison of their ^{1}H and/or ^{13}CNMR spectra to the previously reported data. The procedures in this section are representative, and thus the yields may differ from those reported in tables.

2. Determination of free fatty acid % (FFA%) in canola oil deodorizer distillate by titrimetric method

0.5–2.0 g of samples (based on the expected acidity) were weighed into Erlenmeyer flasks. Neutralized 2-propanol (50 mL) was added. The flask was placed on a hot plate and the temperature was regulated to about 40 °C. The sample was shaken gently while being titrated against standard KOH (0.1 M) to the first permanent pink colour using phenolphthalein as indicator. The colour must persist for 30 s.

FFA% (in terms of oleic acid) = $\frac{(V-B)x\ N\ x\ 28.2}{m}$

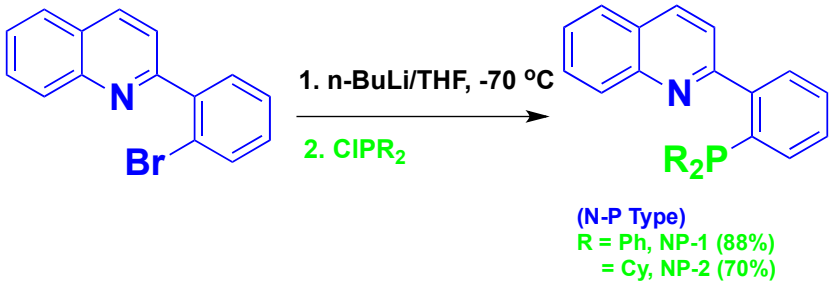
V = volume of potassium hydroxide used in sample.
B = volume of potassium hydroxide used in blank sample.
N = Normality of potassium hydroxide
m = weight of sample, in g.

3. Determination of the composition of fatty acids in canola oil deodorizer distillate by GC method

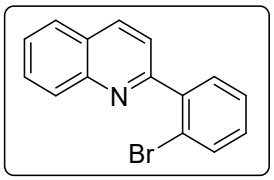
0.1 mL canola oil deodorizer distillate was placed into 10 mL centrifugal tubes to which 2 mL of H_2SO_4–MeOH solution (1 v/v%) was added. The mixture was heated at 70 °C for 1 h. After cooling to room temperature, 3 mL of n-hexane and 2 mL of distilled water were added and mixed thoroughly. The extracts were removed and injected for GC analysis. Peaks are identified against fatty acid methyl esters (FAMEs) standard purchased from sigma Aldrich (Supelco® 37 Component FAME Mix). Analysis of FAME products by GC–FID analysis was carried out using an Agilent 6890A. Operating conditions: temperature (°C): injector, 225; detector, 285;
initial temp, 100 (hold 4 min); ramp, 3°C/min; final temp 240; hold 15 min;
carrier gas, helium; flow rate, 0.75 mL/min; linear velocity,18 cm/s; split ratio, 200:1.
Capillary column.—SP2560 100 m x 0.25 mm with 0.20 μm.

4. Preparation of quinoline-scaffold monophosphine (NP-1, NP-2) and naphthalene-scaffold monophosphine (CP-1, CP-2) ligands

Synthetic pathway for NP ligands

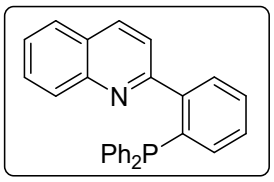


2-(2-Bromophenyl)quinoline



Synthesis of 2-(2-Bromophenyl)quinoline was according to literature procedure.[2] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (td, *J*= 1.6Hz, 7.6Hz, 1H), 7.45 (t, *J*= 7.5Hz, 1H), 7.58 (t, *J*= 7.5Hz, 1H), 7.65 (dd, *J*= 1.5Hz, 7.6Hz, 1H), 7.71 (d, *J*= 8.8Hz, 2H), 7.75 (t, *J*= 7.6Hz, 1H), 7.87 (d, *J*= 8.2Hz, 1H) 8.21 (t, *J*= 8.3Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 121.8, 126.4, 126.8, 127.1, 127.5, 127.7, 129.5, 129.7, 130.0, 131.6, 133.2, 135.7, 141.5, 147.8, 158.6; MS (EI): *m*/*z* (relative intensity) 283.1 (M^+, 50), 204.2 (100), 176.2 (25), 102.1 (32)

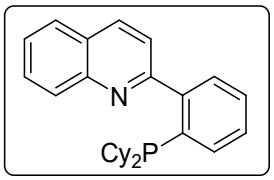
(2-(Quinoline-2-yl)phenyl)diphenylphosphine, **NP-1**



2-(2-Bromophenyl)quinoline (0.849 g, 3.0 mmol) was dissolved in freshly distilled THF (20 mL) at room temperature under a nitrogen atmosphere. The solution was cooled to -78 °C in dry ice/acetone bath. Titrated *n*-BuLi (3.3 mmol) was added dropwise by syringe. After the reaction mixture was stirred for 30 min at -78 °C, chlorodiphenylphosphine (0.66 mL, 3.3 mmol) in THF (5 mL) was added. The reaction was allowed to warm to room temperature and stirred overnight. Solvent was removed under reduced pressure. After

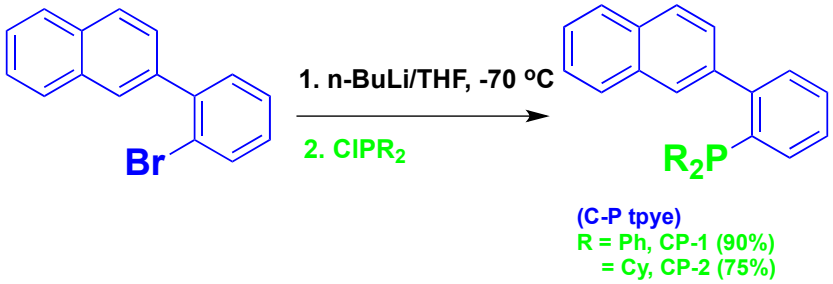
the solvent was removed under vacuum, the product was successively washed with cold MeOH/EtOH mixture. The product was then dried under vacuum. Pale yellow solid of (2-(Quinoline-2-yl)phenyl)diphenylphosphine **NP-1** (1.03 g, 88 %) were obtained. Melting point. 162.6-163.3 °C; ^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.21 (dd, *J*= 3.4Hz, 7.9Hz, 1H), 7.31-7.42 (m, 11H), 7.55 (t, *J*= 8.0Hz, 2H), 7.59-7.67 (m, 2H), 7.76 (d, *J*= 8.3Hz, 1H), 7.83-7.88 (m, 2H), 8.21 (d, *J*= 8.3Hz, 1H); ^{13}C NMR (100 MHz, CD_2Cl_2) δ121.3, 126.4, 126.6, 127.4, 128.1 (d, *J*= 4.0Hz), 128.2, 128.5, 128.6, 128.9, 129.3 (d, *J*= 4.0Hz), 129.4, 133.8 (d, *J*= 19.8Hz), 135.4, 135.9, 137.1 (d, *J*= 18.8Hz), 139.4 (d, *J*= 11.1Hz), 145.7 (d, *J*= 23.3Hz), 146.9, 158.3; ^{31}P NMR (162 MHz, CD_2Cl_2) δ -10.86; MS (EI): *m*/*z* (relative intensity) 389.3 (M^+, 23), 312.2 (100), 235.2 (35), 194.7 (7); HRMS: calcd. for C27H21NP+: 390.1412, found 390.1403.

(2-(Quinoline-2-yl)phenyl)dicyclohexylphosphine, **NP-2**

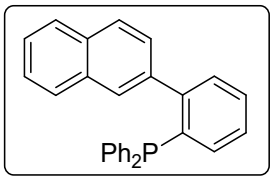


2-(2-Bromophenyl)quinoline (0.849 g, 3.0 mmol) was dissolved in freshly distilled THF (20 mL) at room temperature under a nitrogen atmosphere. The solution was cooled to -78 °C in dry ice/acetone bath. Titrated *n*-BuLi (3.3 mmol) was added dropwise by syringe. After the reaction mixture was stirred for 30 min at -78 °C, chlorodicyclohexylphosphine (0.72 mL, 3.3 mmol) in THF (5 mL) was added. The reaction was allowed to warm to room temperature and stirred overnight. Solvent was removed under reduced pressure. After the solvent was removed under vacuum, the product was successively washed with cold MeOH/EtOH mixture. The product was then dried under vacuum. White solid of (2-(Quinoline-2-yl)phenyl)dicyclohexylphosphine **NP-2** (0.84 g, 70 %) were obtained. Melting point. 136.6-137.2 °C; ^{1}H NMR (400 MHz, CD_2Cl_2) δ 1.09-1.32 (m, 10H), 1.63-1.76 (m, 10H), 1.99 (td, *J*= 3.0Hz, 12.0Hz, 2H), 7.48-7.52 (m, 2H), 7.56-7.62 (m, 3H), 7.70-7.73 (m, 1H), 7.76 (td, *J*= 1.3Hz, 7.2Hz, 1H), 7.91 (d, *J*= 8.2Hz, 1H), 8.12 (d, *J*= 8.2Hz, 1H), 8.18 (d, *J*= 8.2Hz, 1H); ^{13}C NMR (100 MHz, CD_2Cl_2) δ 26.4, 27.1 (d, *J*= 7.0Hz), 27.2 (d, *J*= 4.3Hz), 29.7 (d, *J*= 10.5Hz), 30.3 (d, *J*= 17.5Hz), 34.5 (d, *J*= 13.4Hz), 124.3 (d, *J*= 6.6Hz), 126.2, 126.7, 127.5 (d, *J*= 2.7Hz), 128.3, 129.3 (d, *J*= 16.6Hz), 129.8 (d, *J*= 5.0Hz), 132.9 (d, *J*= 2.0Hz), 134.2, 134.7 (d, *J*= 23.6Hz), 147.6, 149.3 (d, *J*= 27.3Hz), 161.0 (d, *J*= 4.9Hz); ^{31}P NMR (162 MHz, CD_2Cl_2) δ -11.01; MS (EI): *m*/*z* (relative intensity) 401.4 (M^+, 2), 318.3 (100), 235.2 (43). HRMS: calcd. for C27H33NP+: 402.2351, found 402.2342.

Synthetic pathway for CP ligands

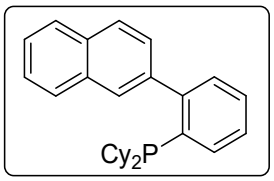


(2-(Naphthalene-2-yl)phenyl)diphenylphosphine, **CP-1**[3]



2-(2-Bromophenyl)naphthalene (0.849 g, 3.0 mmol) was dissolved in freshly distilled THF (20 mL) at room temperature under a nitrogen atmosphere. The solution was cooled to -78 °C in dry ice/acetone bath. Titrated *n*-BuLi (3.3 mmol) was added dropwise by syringe. After the reaction mixture was stirred for 30 min at -78 °C, chlorodiphenylphosphine (0.66 mL, 3.3 mmol) in THF (5 mL) was added. The reaction was allowed to warm to room temperature and stirred overnight. Solvent was removed under reduced pressure. After the solvent was removed under vacuum, the product was successively washed with cold MeOH/EtOH mixture. The product was then dried under vacuum. White solid of (2-(Naphthalene-2-yl)phenyl)diphenylphosphine **CP-1** (1.05 g, 90 %) were obtained. ^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.14 (dd, *J*= 3.8Hz, 7.6Hz, 1H), 7.22-7.26 (m, 4H), 7.32-7.34 (m, 7H), 7.4-7.51 (m, 5H), 7.57 (s, 1H), 7.63 (d, *J*= 7.6Hz, 1H), 7.78 (d, *J*= 8.2Hz, 1H), 7.86 (d, *J*= 8.2Hz, 1H); ^{13}C NMR (100 MHz, CD_2Cl_2) δ 125.8 (d, *J*= 10.0Hz), 126.8, 127.3, 127.4, 127.8, 127.9 (d, *J*= 2.3Hz), 128.2, 128.3, 128.4, 128.6, 130 (d, *J*= 5.0Hz), 132.5 (d, *J*= 29.0Hz), 133.6, 133.8, 134.1, 137.6, 137.7, 139.2, 148.1 (d, *J*= 27.0Hz); ^{31}P NMR (162 MHz, CD_2Cl_2) δ -13.70; MS (EI): *m*/*z* (relative intensity) 387.3 (M^+, 100), 309.2 (5), 233.2 (16).

(2-(Naphthalene-2-yl)phenyl)dicyclohexylphosphine, **CP-2**



2-(2-Bromophenyl)naphthalene (0.849 g, 3.0 mmol) was dissolved in freshly distilled THF (20 mL) at room temperature under a nitrogen atmosphere. The solution was cooled to -78 °C in dry ice/acetone bath. Titrated *n*-BuLi (3.3 mmol) was added dropwise by syringe. After the reaction mixture was stirred for 30 min at -78 °C, chlorodicyclohexylphosphine (0.72 mL, 3.3 mmol) in THF (5 mL) was added. The reaction was allowed to warm to room temperature and stirred overnight. Solvent was removed under reduced pressure. After the solvent was removed under vacuum, the product was successively washed with cold MeOH/EtOH mixture. The product was then dried under vacuum. White solid of (2-(Naphthalene-2-yl)phenyl)dicyclohexylphosphine **CP-2** (0.90 g, 75 %) were obtained. Melting point. 128.6-129.8 °C;^{1}H NMR (400 MHz, CD_2Cl_2) δ 1.07-1.34 (m, 10H), 1.56-1.72 (m, 10H), 1.90 (t, *J*= 11.4Hz, 2H), 7.39-7.46 (m, 3H), 7,49-7.55 (m, 3H), 7.69-7.71 (m, 1H), 7.76 (s, 1H), 7.86-7.93 (m, 3H); ^{13}C NMR (100 MHz, CD_2Cl_2) δ 26.4, 27.1 (d, *J*= 4.0Hz), 27.2, 29.4 (d, *J*= 9.3Hz), 30.6 (d, *J*= 17.5Hz), 34.9 (d, *J*= 17.4Hz), 125.8 (d, *J*= 21.9Hz), 126.2, 126.6, 127.7 (d, *J*= 33.0Hz), 128.2, 129.0 (d, *J*= 3.0Hz), 129.6 (d, *J*= 4.9Hz), 130.2 (d, *J*= 4.9Hz), 132.1, 132.9, 133.0 (d, *J*= 4.0Hz), 134.5 (d, *J*= 22.9Hz), 140.8 (d, *J*= 7.1Hz), 150.4 (d, *J*= 30.3Hz); ^{31}P NMR (162 MHz, CD_2Cl_2) δ -10.19; MS (EI): *m*/*z* (relative intensity) 399.4 (M^+, 100), 317.3 (60), 233.2 (87), 202.2 (16). HRMS: calcd. for C28H34P+: 401.2398, found 401.2395.

5. Determination of fatty acid profile of canola oil deodorizer distillate by GC-FID

Figure S1: Determination of fatty acid profile of canola oil deodorizer by H_2SO_4 catalyzed transesterification

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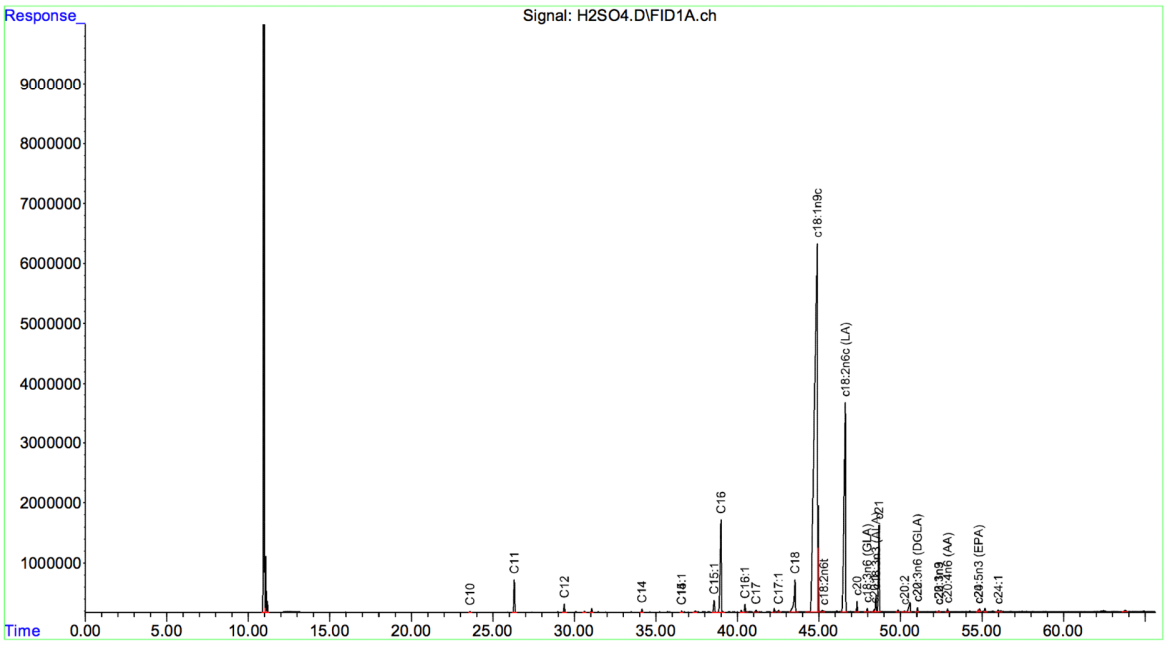

Table S1: Fatty acids composition of canola oil deodorizer distillate determined by GC-FID

	H_2SO_4 catalyzed transesterification		
Fatty acid	Weight of individual fatty acids, mg)	Weight of fatty acids in terms of carbon chain number, mg	Wt% of fatty acids, %
C11	9.36	C11: 9.36	1.05
C12	2.22	C12: 2.22	0.25
C14	0.66	C14: 0.66	0.07
C15	0.23	C15: 3.34	0.38
C15:1	3.11		
C16	**25.37**	**C16**: 26.9	3.02
C16:1	1.53		
C17	0.44	C17: 0.73	0.08
C17:1	0.29		
C18	10.25	**C18**: 372.52	**41.86**
C18:1 oleic acid	**261.94**		
C18:2	77.03		
C18:3	3.04		
C18:3	20.26		
C20	1.74	C20: 6.22	0.7
C20:1	2.78		
C20:2	0.20		
C20:3n6	0.82		
C20:3n3	0.24		
C20:4n6	0.44		
Total weight of fatty acid, mg	424.94		
Weight of sample, mg	890.00		
wt% of fatty acid, %	**47.75**		

Figure S2: Olefin product determined by GC-FID

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                                                  Inj Volume : 1 µl
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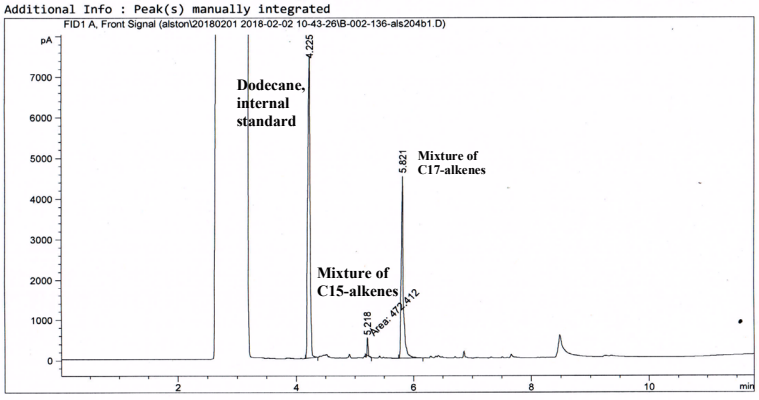


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======================================================================
                        Area Percent Report
======================================================================

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Multiplier            :      1.0000
Dilution              :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs


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Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [pA*s]      [pA]        %
----|-------|----|-------|----------|----------|--------|
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   2   5.218 MM    0.0183  472.41168  430.00131  1.45893
   3   5.821 BV R  0.0348 1.11615e4  4508.83350 34.46980

Totals :                  3.23806e4  1.24260e4
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Figure S3: Olefin product determined by GC-MS

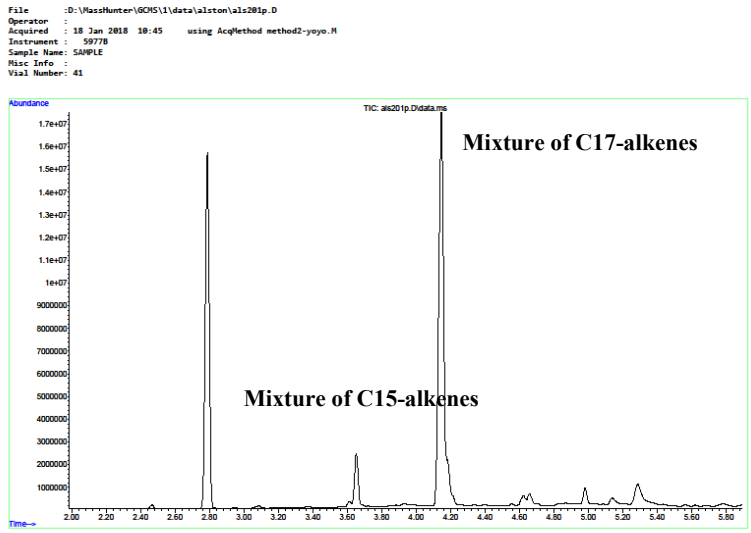

Figure S4: GCMS spectrum of mixture of C15-alkenes at retention time 3.6 min.

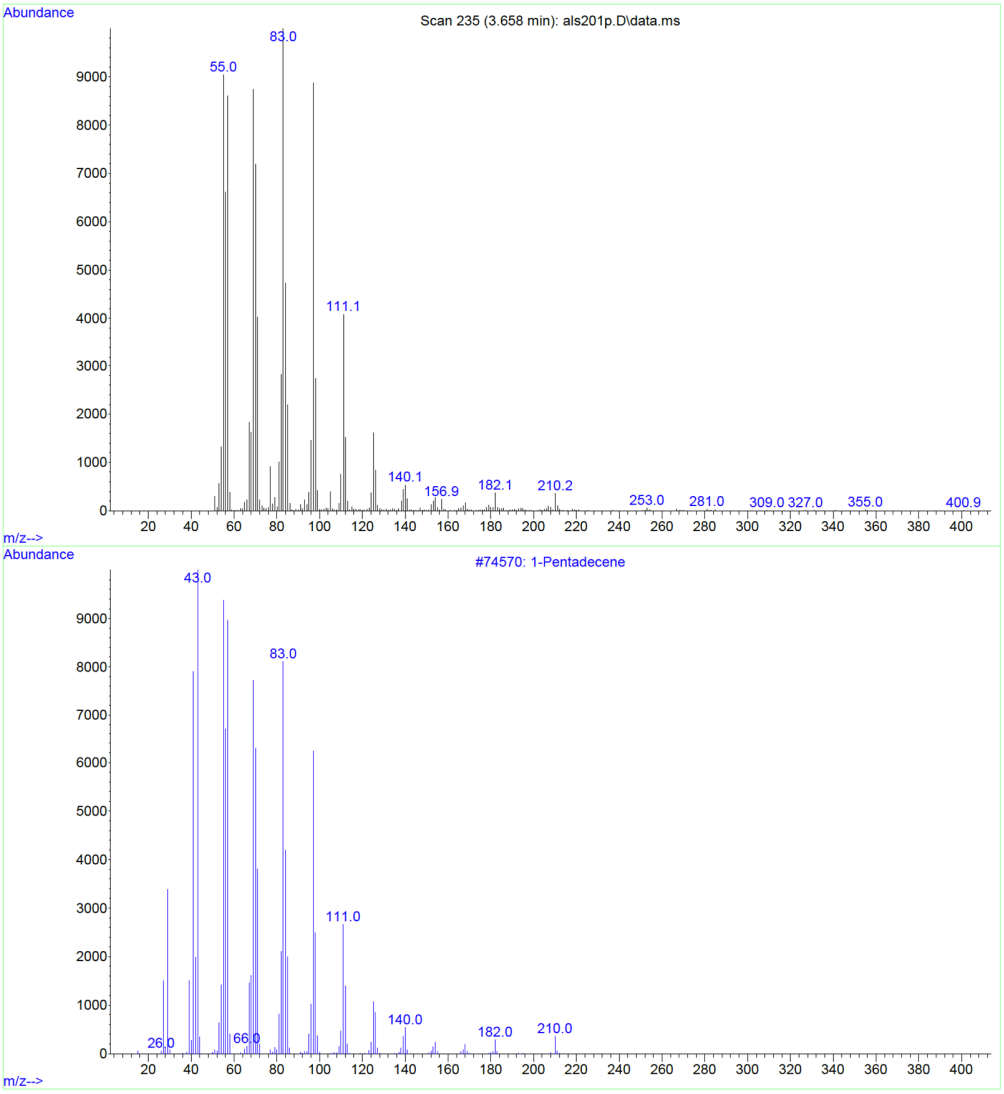

Figure S5: GCMS spectrum of mixture of C17-alkenes at retention time 4.5 min

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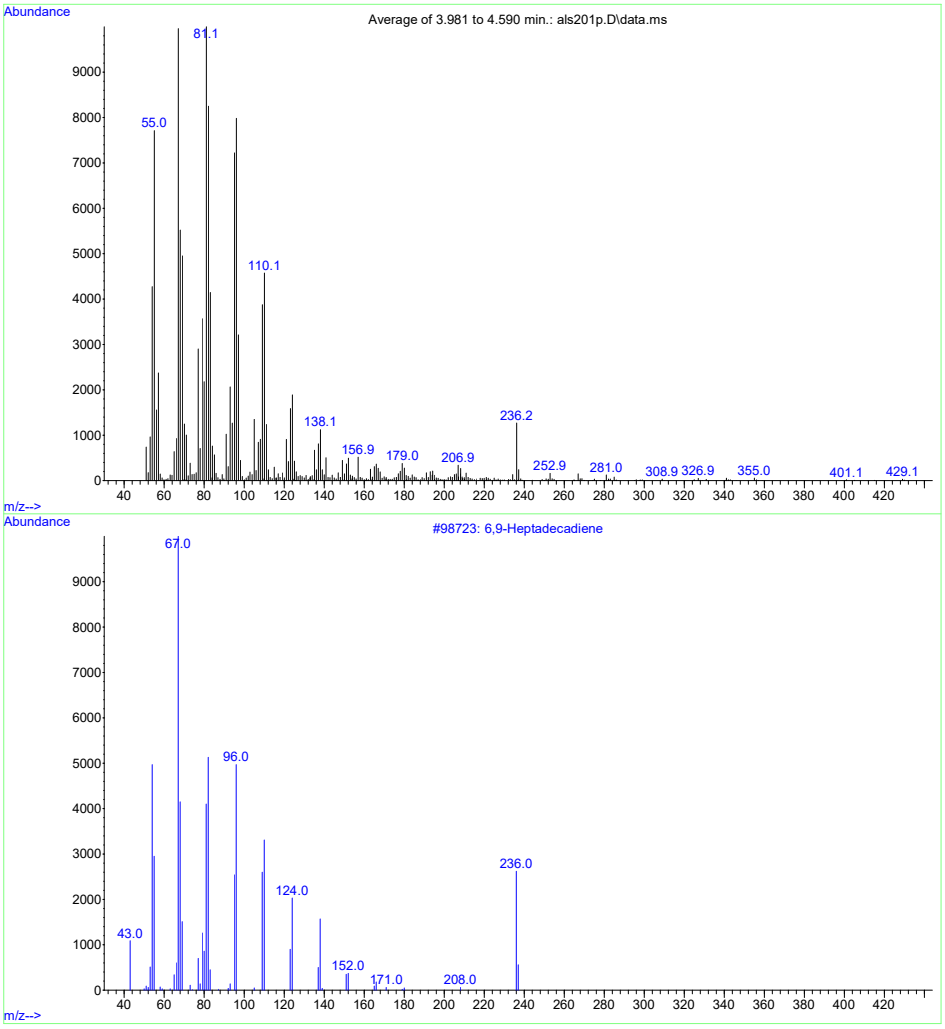
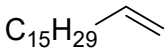


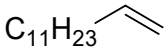
6. Characterization data for alkene products

(*Z*)-Heptadeca-1,8-diene (Table 2, **2a**) [4]



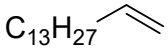
Eluents (Hexane, R_f= 0.7) was used for flash column chromatography. ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.76-5.86 (m, 1H), 5.34-5.37 (m, 2H), 4.92-5.02 (m, 2H), 2.03-2.06 (m, 6H), 1.28-1.39 (m, 18H), 0.89 (t, *J*= 7.9Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.0, 129.9, 129.7, 114.1, 33.7, 32.4, 31.9, 29.7, 29.6, 29.5, 29.3, 28.8, 28.7, 27.2, 27.1, 22.6,14.0; MS (EI): *m*/*z* (relative intensity) 236.4 (M^+, 20), 138.2 (11), 124.2 (22), 109.2 (36), 96.2 (96), 81.2 (100), 67.2 (97), 55.2 (98).

1-Tridecene (Table 2, **2b**) [5]



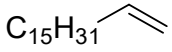
Eluents (Hexane, R_f= 0.7) was used for flash column chromatography. ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.77-5.87 (m, 1H), 5.00 (dd, *J*= 1.8Hz, 17.6Hz, 1H), 4.93 (d, *J*= 10.7Hz, 1H), 2.05 (q, *J*= 7.9Hz, 2H), 1.27 (s, 18H), 0.89 (t, *J*= 7.9Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.2, 114.0, 33.8, 31.9, 29.7, 29.68, 29.66, 29.5, 29.3, 29.2, 28.9, 22.7, 14.1; MS (EI): *m*/*z* (relative intensity) 182.4 (M^+, 9), 125.3 (10), 111.3 (35), 97.2 (80), 83.2 (96), 69.2 (95), 55.2 (100).

1-Pentadecene (Table 2, **2c**) [5]



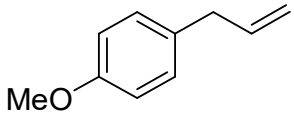
Eluents (Hexane, R_f= 0.7) was used for flash column chromatography. ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.78-5.85 (m, 1H), 5.01 (dd, *J*= 1.9Hz, 17.7Hz, 1H), 4.92 (d, *J*= 10.0Hz, 1H), 2.05 (q, *J*= 7.4Hz, 2H), 1.27 (s, 22H), 0.89 (t, *J*= 7.0Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.2, 114.0, 33.8, 31.9, 29.7, 29.6, 29.5, 29.4, 29.2, 29.0, 22.7, 14.1; MS (EI): *m*/*z* (relative intensity) 210.4 (M^+, 7), 182.4 (5), 140.3 (7), 125.3 (17), 111.3 (46), 97.2 (95), 83.2 (100), 69.2 (87), 55.2 (93).

1-Heptadecene (Table 2, **2d**) [5]



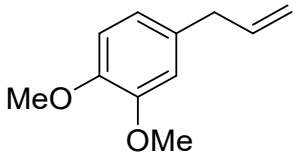
Eluents (Hexane, R_f= 0.7) was used for flash column chromatography. ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.77-5.87 (m, 1H), 5.01 (dd, *J*= 1.9Hz, 17.1Hz, 1H), 4.93 (d, *J*= 10.0Hz, 1H), 2.05 (q, *J*= 7.0Hz, 2H), 1.27 (s, 26H), 0.89 (t, *J*= 7.2Hz, 3H);
^{13}C NMR (100 MHz, $CDCl_3$) δ 139.2, 114.0, 33.8, 31.9, 29.7, 29.6, 29.5, 29.4, 29.2, 29.0, 22.7, 14.1; MS (EI): *m*/*z* (relative intensity) 238.5 (M^+, 7), 210.4 (5), 125.3 (28), 111.3 (57), 97.2 (100), 83.2 (98), 69.2 (78), 55.2 (85).

1-Allyl-4-methoxybenzene (Table 2, **2e**) [6]



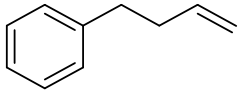
Eluents (Hexane: ethyl acetate 10:1, R_f= 0.6) was used for flash column chromatography. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.11 (d, *J*= 8.5Hz, 2H), 6.85 (d, *J*= 8.6Hz, 2H), 5.91-6.01 (m, 1H), 5.04-5.0 (m, 2H), 3.79 (s, 3H), 3.34 (d, *J*= 6.6Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.9, 137.8, 132.0, 129.4, 115.3, 113.8, 55.2, 39.3; MS (EI): *m*/*z* (relative intensity) 148.2 (M^+, 100), 133.1 (23), 121.1 (38), 105.1 (21), 91.1 (21), 77.1 (23).

1-Allyl-3,4-dimethoxybenzene (Table 2, **2f**) [7]



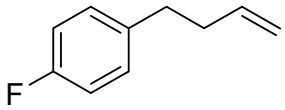
Eluents (Hexane: ethyl acetate 10:1, R_f= 0.3) was used for flash column chromatography. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.78-6.81 (m, 1H), 6.72 (d, *J*= 7.6Hz, 2H), 5.91-5.99 (m, 1H), 5.05-5.10 (m, 2H), 3.86 (s, 3H), 3.85 (s, 3H), 3.33 (d, *J*= 6.6Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.8, 147.3, 137.6, 134.4, 120.3, 115.5, 111.8, 111.2, 55.8, 55.7, 39.7; MS (EI): *m*/*z* (relative intensity) 178.2 (M^+, 100), 163.1 (30), 147.1 (30), 103.1 (25), 91.1 (25), 77.1 (20).

4-Phenyl-1-butene (Table 2, **2g**) [8]



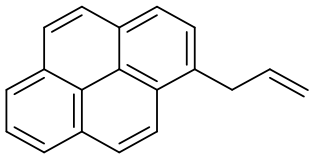
Eluents (Hexane, R_f= 0.6) was used for flash column chromatography. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28-7.32 (m, 2H), 7.20-7.22 (m, 3H), 5.83-5.93 (m, 1H), 5.06 (dd, *J*= 1.8Hz, 17.3Hz, 1H), 4.99 (d, *J*= 10.2Hz, 1H), 2.73 (t, *J*= 7.6Hz, 2H), 2.40 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.8, 138.0, 128.4, 128.2, 125.7, 114.8, 35.4, 35.3; MS (EI): *m*/*z* (relative intensity) 132.1 (M^+, 20), 91.1 (100).

4-(4-Fluorophenyl)-1-butene (Table 2, **2h**) [9]



Eluents (Hexane, R_f= 0.5) was used for flash column chromatography. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.11-7.14 (m, 2H), 6.96 (t, *J*= 8.6Hz, 2H), 5.78-5.88 (m, 1H), 4.97-5.05 (m, 2H), 2.68 (t, *J*= 7.7Hz, 2H), 2.34 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.2 (d, *J*= 243.0Hz), 137.7, 137.3 (d, *J*= 3.0Hz), 129.6 (d, *J*= 7.9Hz), 115.0 (d, J= 4.3Hz), 114.8, 35.5, 34.5; MS (EI): *m*/*z* (relative intensity) 150.2 (M^+, 14), 109.2 (100), 83.2 (7).

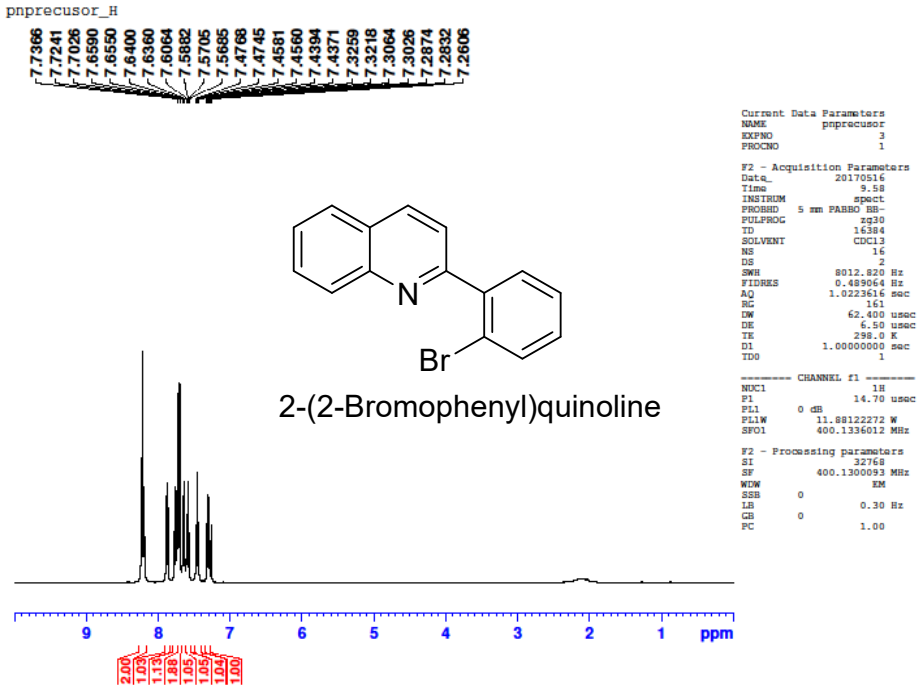
1-Allyl-pyrene (Table 2, **2i**) [10]



Eluents (Hexane, R_f= 0.5) was used for flash column chromatography. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03-8.30 (m, 8H), 7.92 (d, *J*= 7.5Hz, 1H), 6.26-6.36 (m, 1H), 5.17-5.27 (m, 2H), 4.15 (d, *J*= 6.6Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.2, 133.7, 131.2, 130.7, 129.9, 128.8,

127.38, 127.35, 127.2, 127.1, 126.6, 125.6, 124.9, 124.8, 124.7, 123.4, 116.0, 37.5; MS (EI): *m*/*z* (relative intensity) 242.2 (M^+, 100), 227.2(29), 215.2 (33), 119.9 (20).

7. ^{1}H, ^{13}C, ^{31}P NMR, MS and HRMS spectra

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TD                16384
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES         0.489064 Hz
AQ             1.0223616 sec
RG                 161
DW              62.400 usec
DE               6.50 usec
TE              298.0 K
D1           1.00000000 sec
TD0                    1

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P1                14.70 usec
PL1       0 dB
PL1W        11.88122272 W
SFO1        400.1336012 MHz

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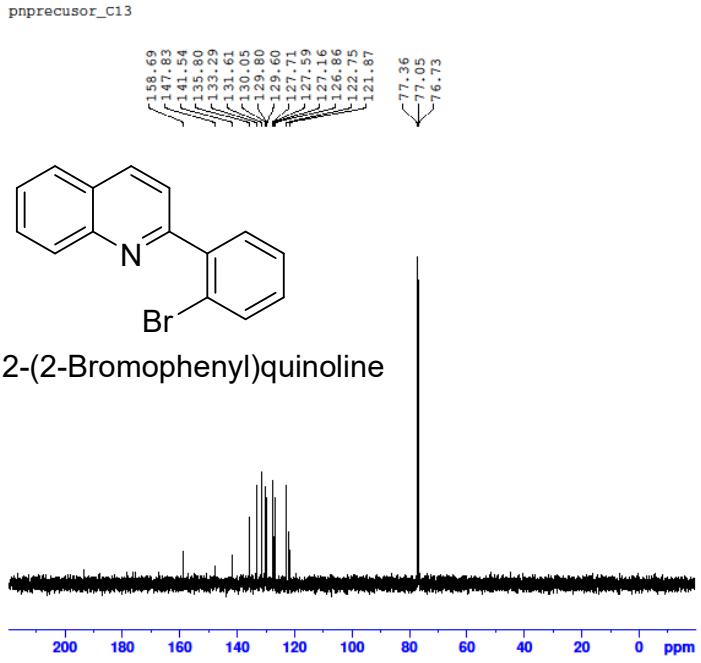


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TD                65536
SOLVENT           CDCl3
NS                   29
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                 181
DW              20.800 usec
DE               6.50 usec
TE              298.5 K
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D11          0.03000000 sec
TD0                    1

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NUC1                 13C
P1                 9.50 usec
PL1               -2.00 dB
PL1W        58.52175522 W
SFO1        100.6228298 MHz

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NUC2                  1H
PCPD2              80.00 usec
PL2       0 dB
PL12              15.00 dB
PL13              15.00 dB
PL2W        11.88122272 W
PL12W        0.37571725 W
PL13W        0.37571725 W
SFO2        400.1316005 MHz

F2 - Processing parameters
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WDW                   EM
SSB       0
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PC                1.40
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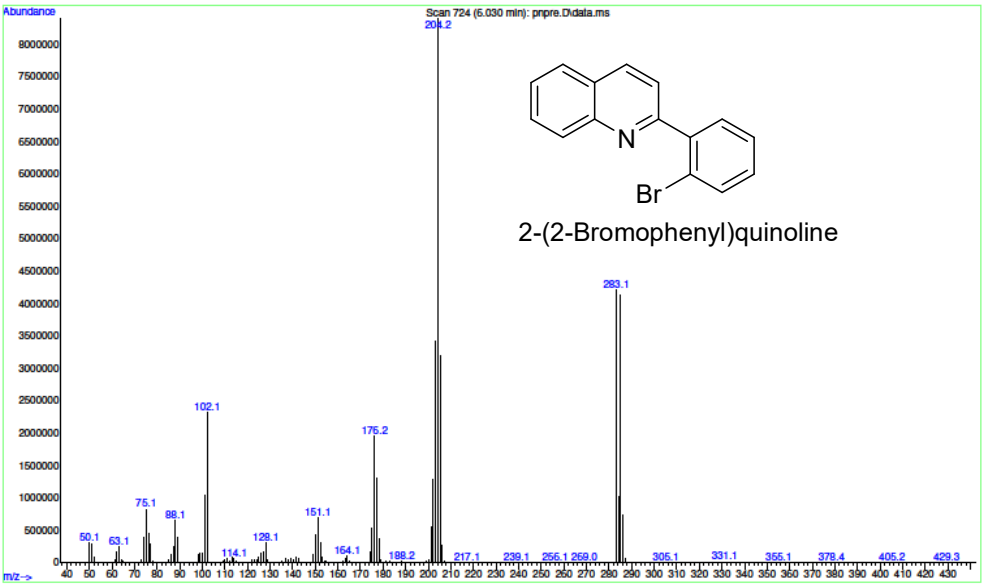
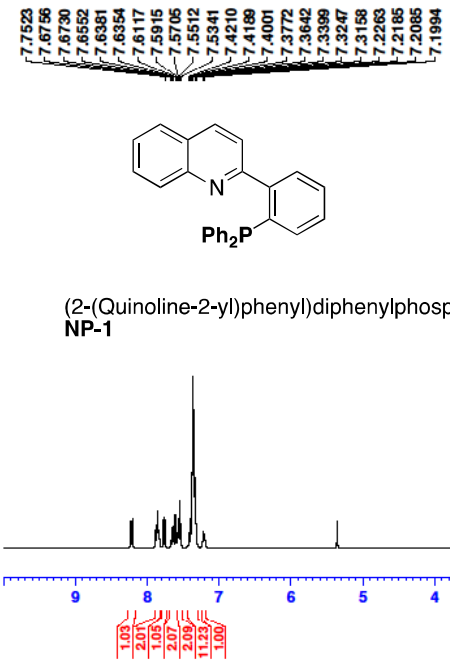


2-(2-Bromophenyl)quinoline

FSyn14H



(2-(Quinoline-2-yl)phenyl)diphenylphosphine,
NP-1

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EXPNO                      4
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SOLVENT            CD2Cl2
NS                        16
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DW                    62.400 usec
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D1                 1.00000000 sec
TD0                        1

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SFO1           400.1324008 MHz

F2 - Processing parameters
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PC                     1.00
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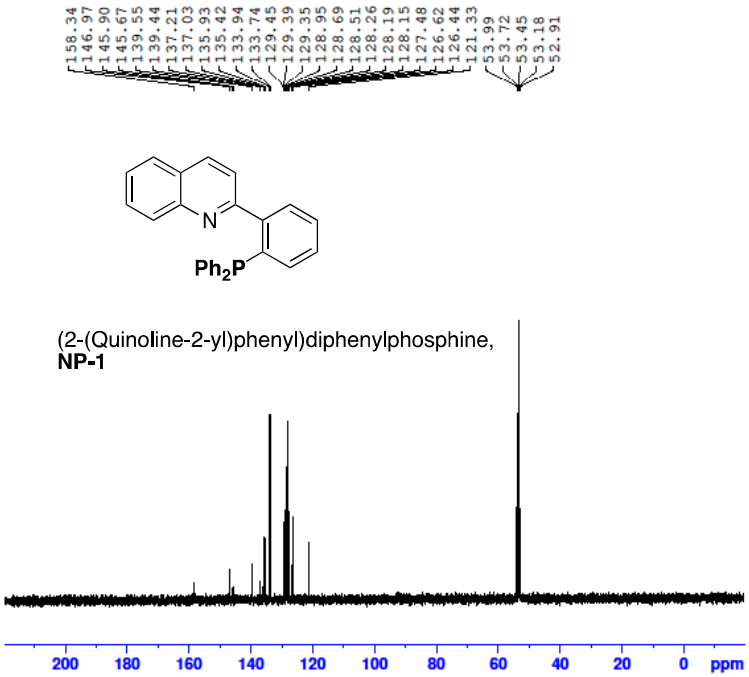
FSyn14C



(2-(Quinoline-2-yl)phenyl)diphenylphosphine,
NP-1

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PROCNO                     1

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TD                    65536
SOLVENT            CD2Cl2
NS                        53
DS                         2
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631488 sec
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DW                    20.800 usec
DE                     6.50 usec
TE                    296.3 K
D1                 1.00000000 sec
D11                0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      13C
P1                     9.50 usec
PL1                   -2.00 dB
PL1W           58.52175522 W
SFO1           100.6228298 MHz

======== CHANNEL f2 ========
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NUC2                       1H
PCPD2                 80.00 usec
PL2          0 dB
PL12                  15.00 dB
PL13                  15.00 dB
PL2W           11.88122272 W
PL12W           0.37571725 W
PL13W           0.37571725 W
SFO2           400.1316005 MHz

F2 - Processing parameters
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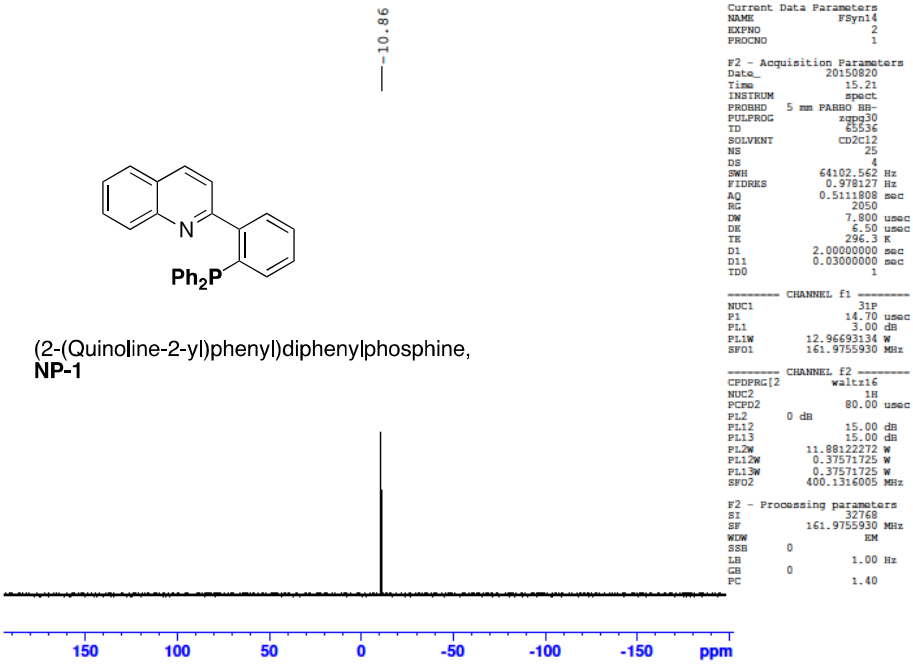
FSyn14P



(2-(Quinoline-2-yl)phenyl)diphenylphosphine,
NP-1

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EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
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Time                   15.21
INSTRUM                spect
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PULPROG              zgpg30
TD                    65536
SOLVENT              CD2Cl2
NS                        25
DS                         4
SWH                64102.562 Hz
FIDRES             0.978127 Hz
AQ                 0.5111808 sec
RG                      2050
DW                    7.800 usec
DE                    6.50 usec
TE                    296.3 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     31P
P1                     14.70 usec
PL1                     3.00 dB
PL1W              12.96693134 W
SFO1             161.9755930 MHz

======== CHANNEL f2 ========
CPDPRG[2              waltz16
NUC2                     1H
PCPD2                 80.00 usec
PL2          0 dB
PL12                   15.00 dB
PL13                   15.00 dB
PL2W              11.88122272 W
PL12W              0.37571725 W
PL13W              0.37571725 W
SFO2             400.1316005 MHz

F2 - Processing parameters
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SF               161.9755930 MHz
WDW                          EM
SSB          0
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PC                     1.40
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Operator   : duan
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Vial Number: 7
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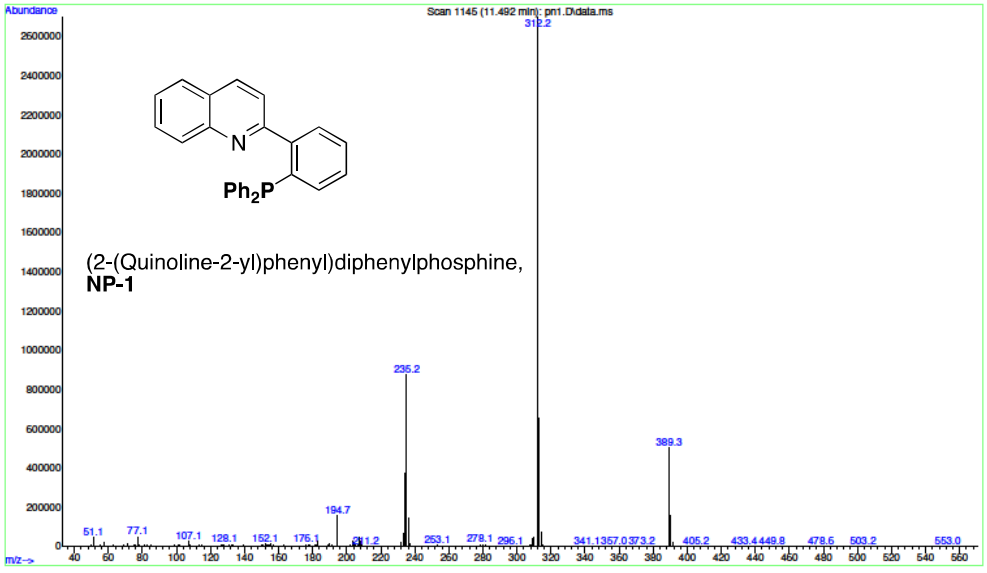
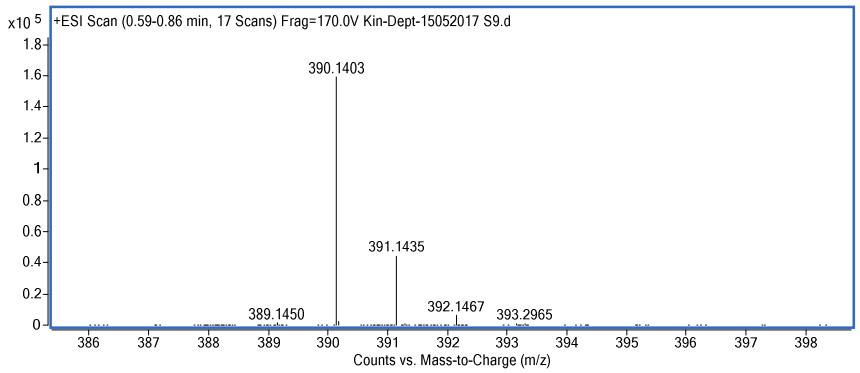
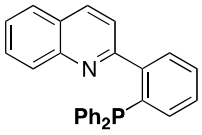


(2-(Quinoline-2-yl)phenyl)diphenylphosphine,
NP-1





(2-(Quinoline-2-yl)phenyl)diphenylphosphine,
NP-1

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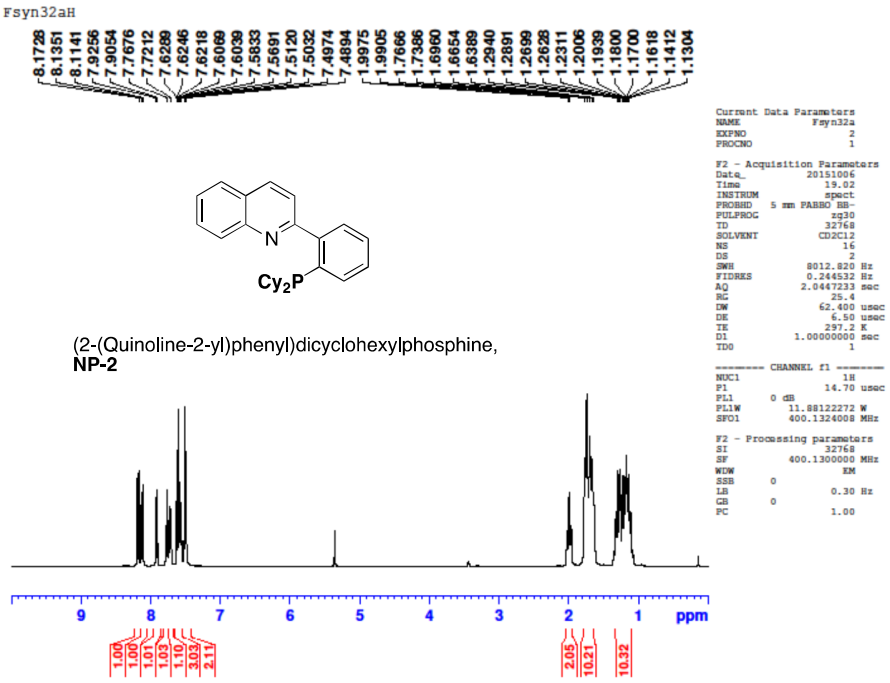
Fsyn32aH



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PROCNO 1

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TD 32768
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FIDRES 0.244532 Hz
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RG 25.4
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DE 6.50 usec
TE 297.2 K
D1 1.00000000 sec
TD0 1

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P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
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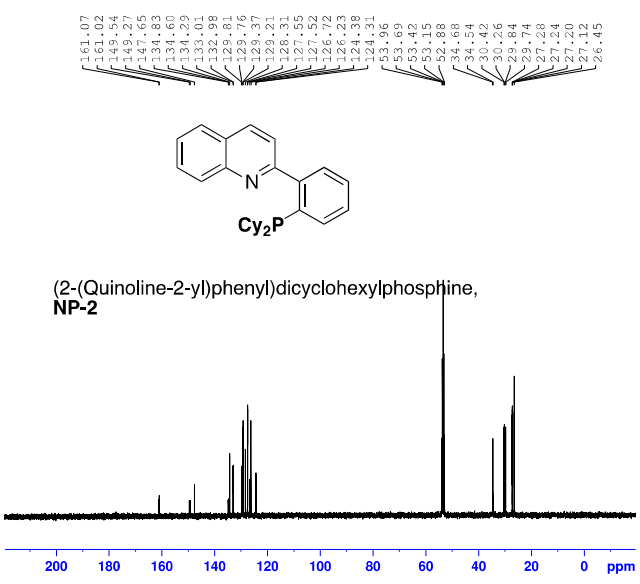
PC 1.00

(2-(Quinoline-2-yl)phenyl)dicyclohexylphosphine,
NP-2

Fsyn32aC



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PROCNO 1

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PULPROG zgpg30
TD 65536
SOLVENT CD2Cl2
NS 220
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 297.9 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
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NUC2 1H
PCPD2 80.00 usec
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PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz

F2 - Processing parameters
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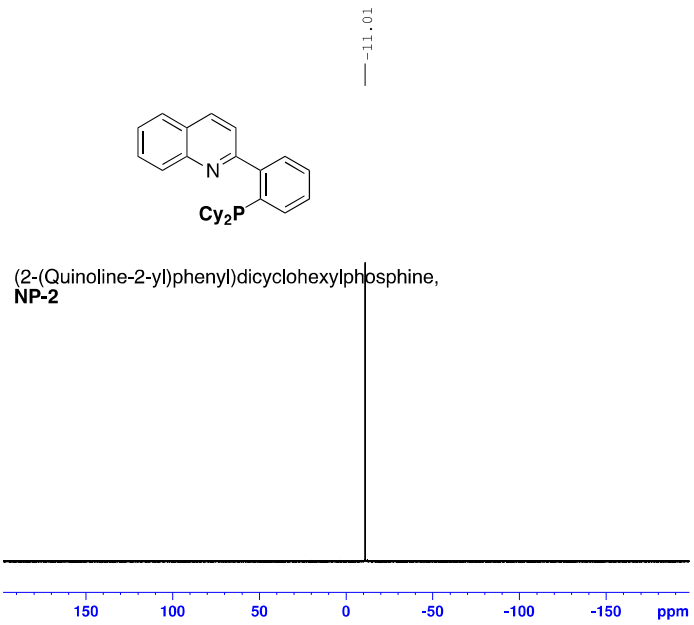
GB 0
PC 1.40

(2-(Quinoline-2-yl)phenyl)dicyclohexylphosphine,
NP-2

Fsyn32aP

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TE                     297.0 K
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D11               0.03000000 sec
TD0                         1

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PL1                     3.00 dB
PL1W              12.96693134 W
SFO1              161.9755930 MHz

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NUC2                      1H
PCPD2                  80.00 usec
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PL12                   15.00 dB
PL13                   15.00 dB
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PL12W              0.37571725 W
PL13W              0.37571725 W
SFO2              400.1316005 MHz

F2 - Processing parameters
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Vial Number: 8
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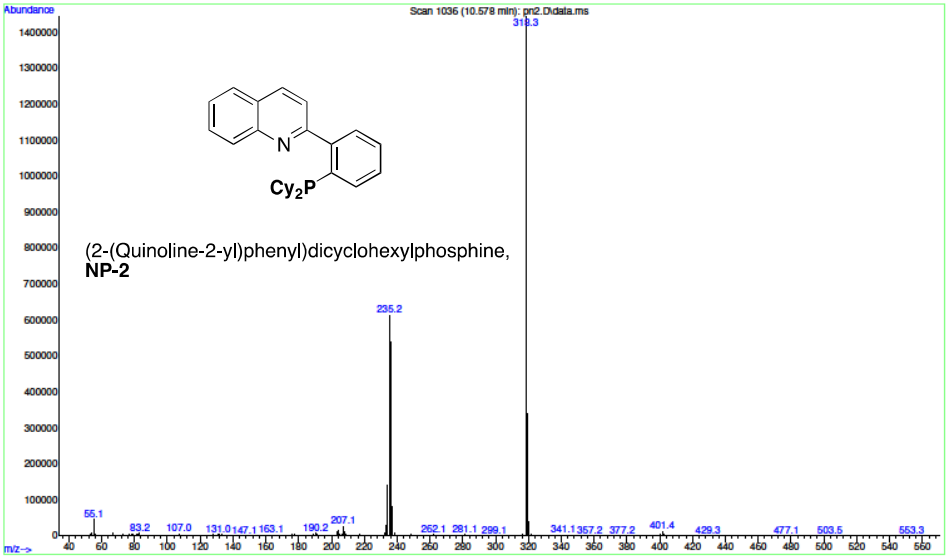
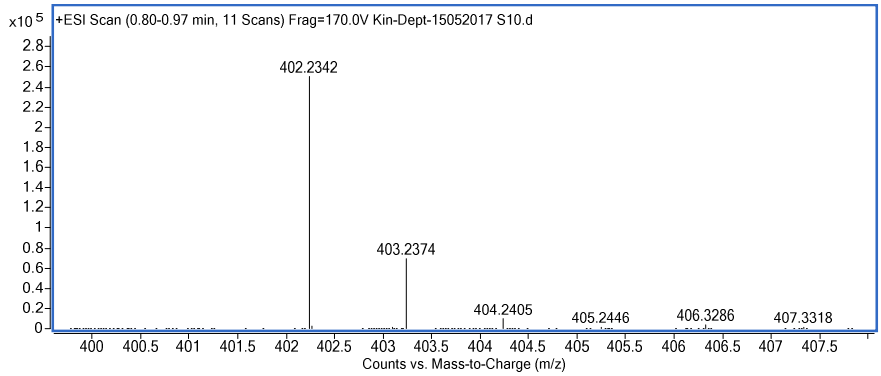
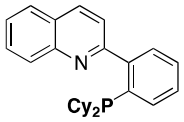


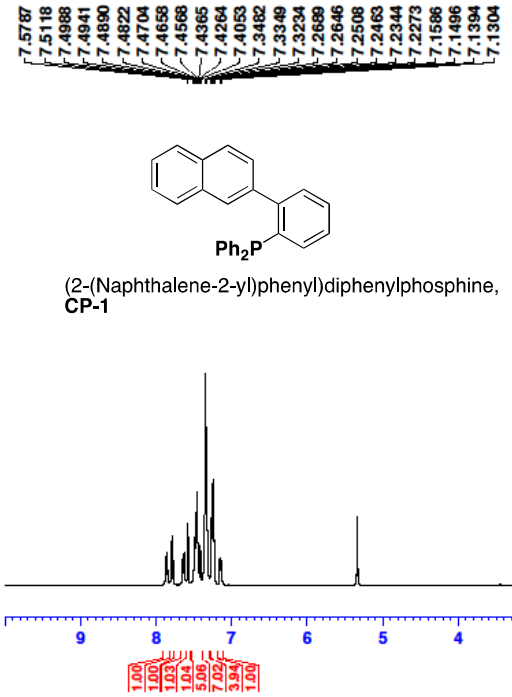




(2-(Quinoline-2-yl)phenyl)dicyclohexylphosphine,
NP-2

Mass	Calc. Mass	mDa	PPM	Formula
402.2342	402.2351	-0.9	-2.1	C27 H33 N P

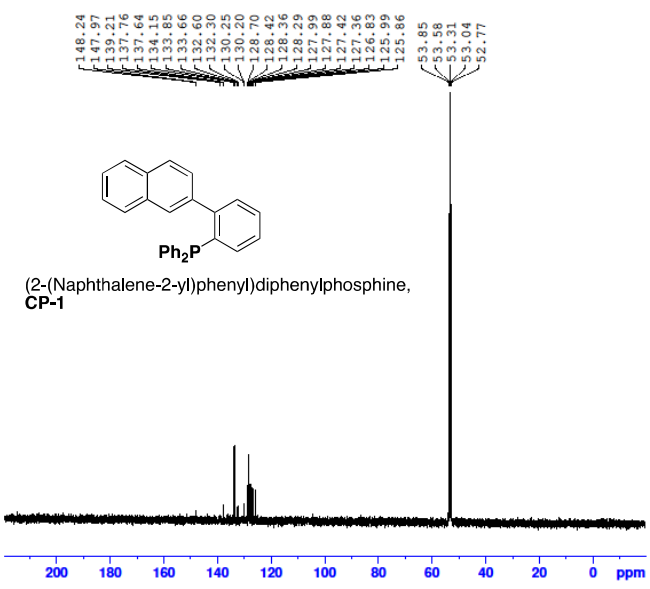
Fsyn92H



(2-(Naphthalene-2-yl)phenyl)diphenylphosphine,
CP-1

```
Current Data Parameters
NAME                 Fsyn92
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_               20160519
Time                   18.24
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    32768
SOLVENT              CD2Cl2
NS                        16
DS                         2
SWH                8012.820 Hz
FIDRES             0.244532 Hz
AQ                 2.0447233 sec
RG                      181
DW                   62.400 usec
DE                    6.50 usec
TE                  298.6 K
D1                  1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                    14.70 usec
PL1          0 dB
PL1W             11.88122272 W
SFO1            400.1324008 MHz

F2 - Processing parameters
SI                        32768
SF                 400.1300094 MHz
WDW                        EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

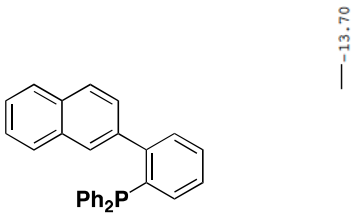
Fsyn92C



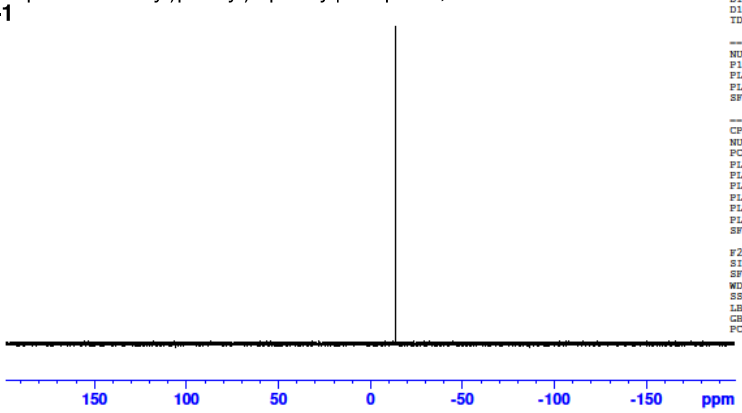
(2-(Naphthalene-2-yl)phenyl)diphenylphosphine,
CP-1

```
Current Data Parameters
NAME                 Fsyn92
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_               20160519
Time                   18.26
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT              CD2Cl2
NS                       201
DS                         2
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631488 sec
RG                      144
DW                   20.800 usec
DE                    6.50 usec
TE                  299.4 K
D1                  1.00000000 sec
D11                 0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      13C
P1                     9.50 usec
PL1                   -2.00 dB
PL1W             58.52175522 W
SFO1            100.6229298 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                      1H
PCPD2                 80.00 usec
PL2          0 dB
PL12                  15.00 dB
PL13                  15.00 dB
PL2W             11.88122272 W
PL12W             0.37571725 W
PL13W             0.37571725 W
SFO2            400.1316005 MHz

F2 - Processing parameters
SI                        32768
SF                 100.6127769 MHz
WDW                        EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

Fsyn92P

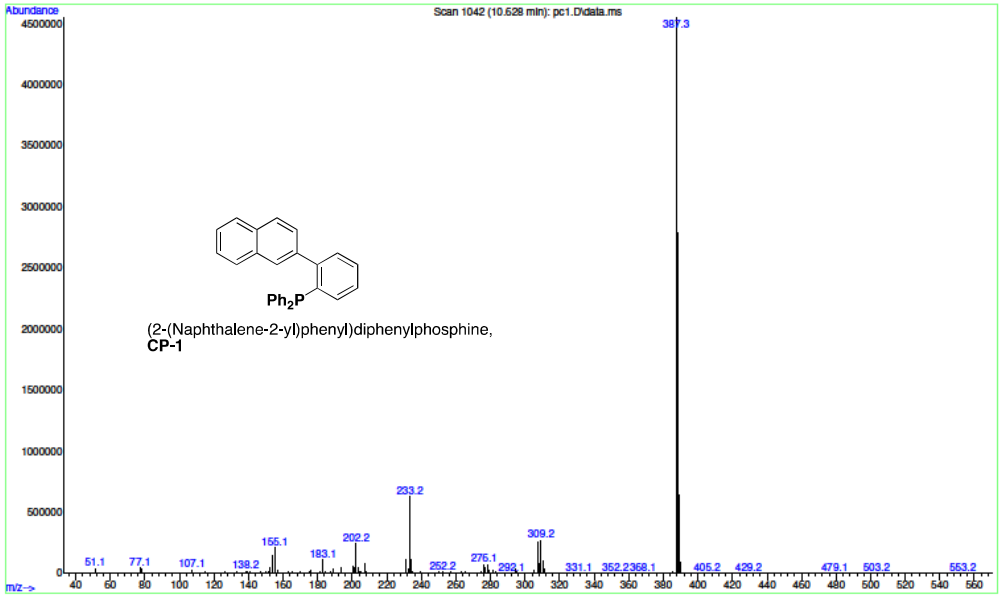


(2-(Naphthalene-2-yl)phenyl)diphenylphosphine,
CP-1

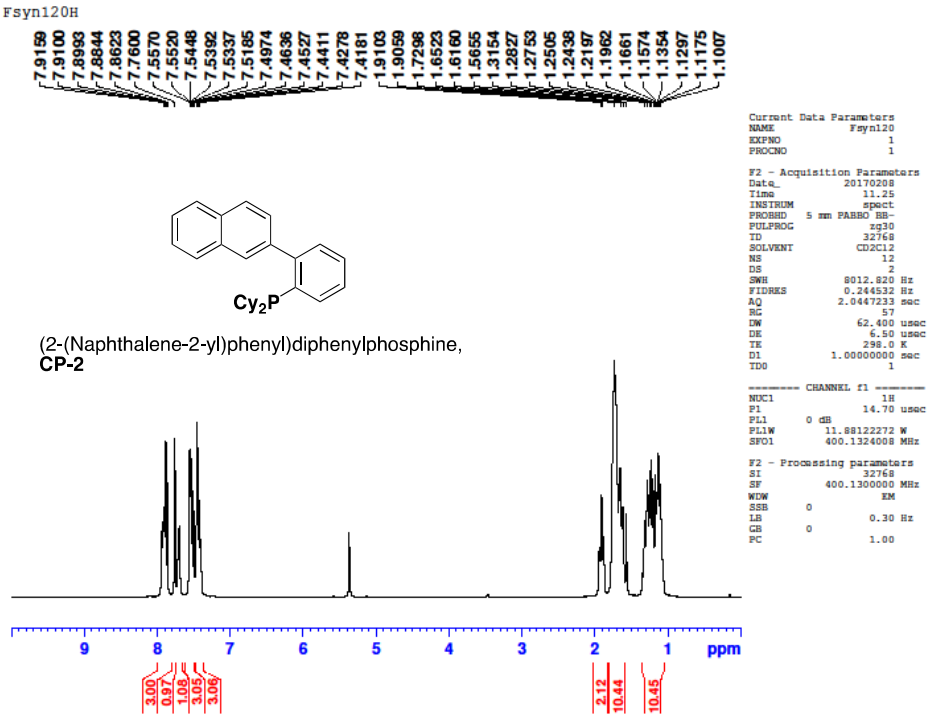



```
Current Data Parameters
NAME                 Fsyn92
EXPNO                     3
PROCNO                    1

F2 - Acquisition Parameters
Date_               20160519
Time                   18.36
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT              CD2Cl2
NS                        23
DS                         4
SWH                64102.562 Hz
FIDRES             0.978127 Hz
AQ                 0.5111808 sec
RG                       203
DW                    7.800 usec
DE                    6.50 usec
TE                   299.7 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     31P
P1                    14.70 usec
PL1                    3.00 dB
PL1W              12.96693134 W
SFO1             161.9755930 MHz

======== CHANNEL f2 ========
CPDPRG[2              waltz16
NUC2                     1H
PCPD2                 80.00 usec
PL2          0 dB
PL12                  15.00 dB
PL13                  15.00 dB
PL2W              11.88122272 W
PL12W              0.37571725 W
PL13W              0.37571725 W
SFO2             400.1316005 MHz

F2 - Processing parameters
SI                       32768
SF               161.9755930 MHz
WDW                         EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

```
File       :D:\MassHunter\GCMS\1\data\alston\pc1.D
Operator   : duan
Acquired   : 12 May 2017  11:55     using AcqMethod M3.M
Instrument :   5977
Sample Name: pc1
Misc Info  :
Vial Number: 9
```



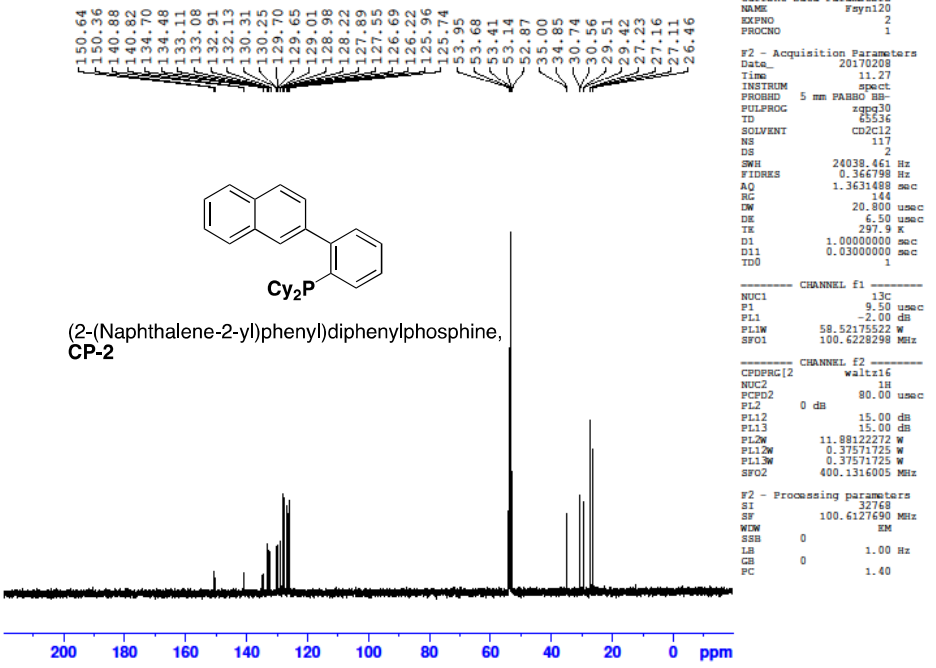
Fsyn120H



(2-(Naphthalene-2-yl)phenyl)diphenylphosphine,
CP-2

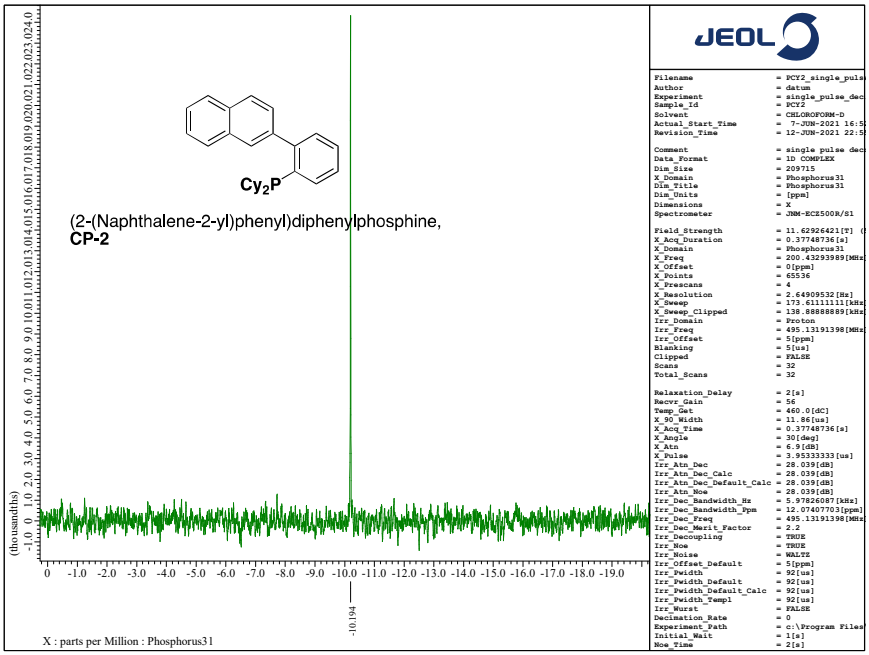
```
Current Data Parameters
NAME                  Fsyn120
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_               20170208
Time                   11.25
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG                zg30
TD                    32768
SOLVENT             CD2Cl2
NS                         12
DS                          2
SWH                 8012.820 Hz
FIDRES              0.244532 Hz
AQ                  2.0447233 sec
RG                         57
DW                    62.400 usec
DE                     6.50 usec
TE                    298.0 K
D1                  1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                      14.70 usec
PL1            0 dB
PL1W           11.88122272 W
SFO1          400.1324008 MHz

F2 - Processing parameters
SI                         32768
SF                400.1300000 MHz
WDW                           EM
SSB            0
LB                      0.30 Hz
GB             0
PC                         1.00
```

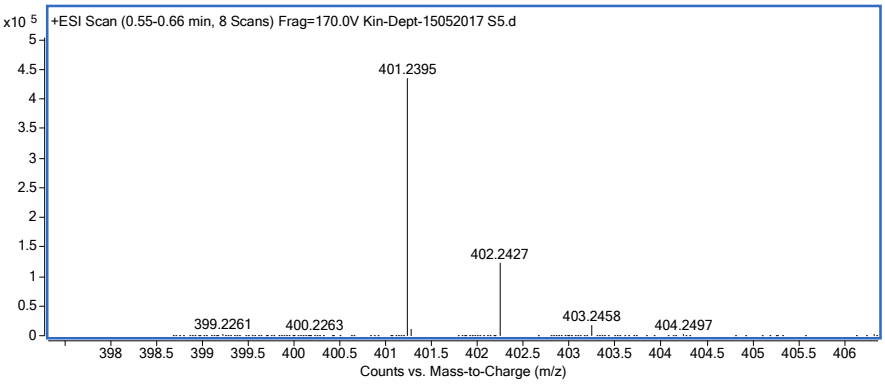
Fsyn120C

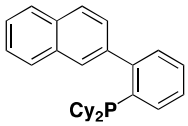


(2-(Naphthalene-2-yl)phenyl)diphenylphosphine,
CP-2

```
Current Data Parameters
NAME                  Fsyn120
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_               20170208
Time                   11.27
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT             CD2Cl2
NS                        117
DS                          2
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631488 sec
RG                        144
DW                    20.800 usec
DE                     6.50 usec
TE                    297.9 K
D1                  1.00000000 sec
D11                 0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       13C
P1                      9.50 usec
PL1                    -2.00 dB
PL1W           58.52175522 W
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG[2                waltz16
NUC2                       1H
PCPD2                  80.00 usec
PL2            0 dB
PL12                   15.00 dB
PL13                   15.00 dB
PL2W           11.88122272 W
PL12W           0.37571725 W
PL13W           0.37571725 W
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                         32768
SF                100.6127690 MHz
WDW                           EM
SSB            0
LB                      1.00 Hz
GB             0
PC                         1.40
```



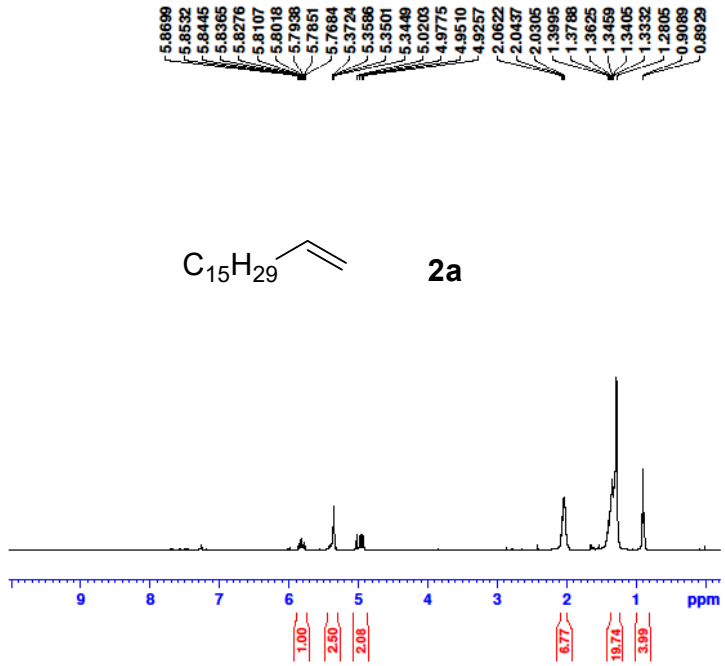




(2-(Naphthalene-2-yl)phenyl)diphenylphosphine,
CP-2

Mass	Calc. Mass	mDa	PPM	Formula
401.2395	401.2398	-0.3	-0.7	C28 H34 P

als175a_H



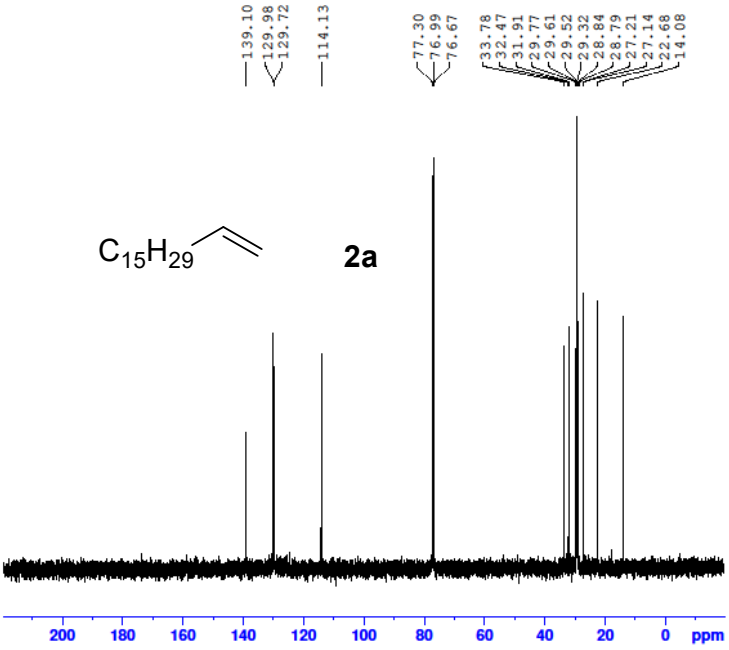
Current Data Parameters
NAME als175a
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170210
Time 9.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.489064 Hz
AQ 1.0223616 sec
RG 20.2
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1336012 MHz

F2 - Processing parameters
SI 32768
SF 400.1300110 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

als175a_C13



Current Data Parameters
NAME als175a
EXPNO 2
PROCNO 1

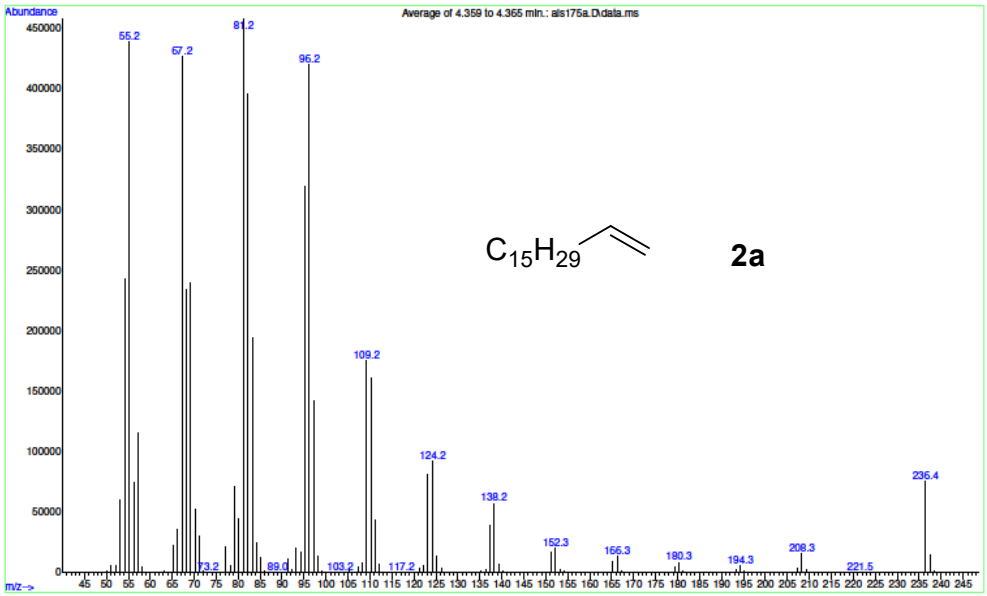
F2 - Acquisition Parameters
Date_ 20170210
Time 9.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 40
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 181
DW 20.800 usec
DE 6.50 usec
TE 298.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz

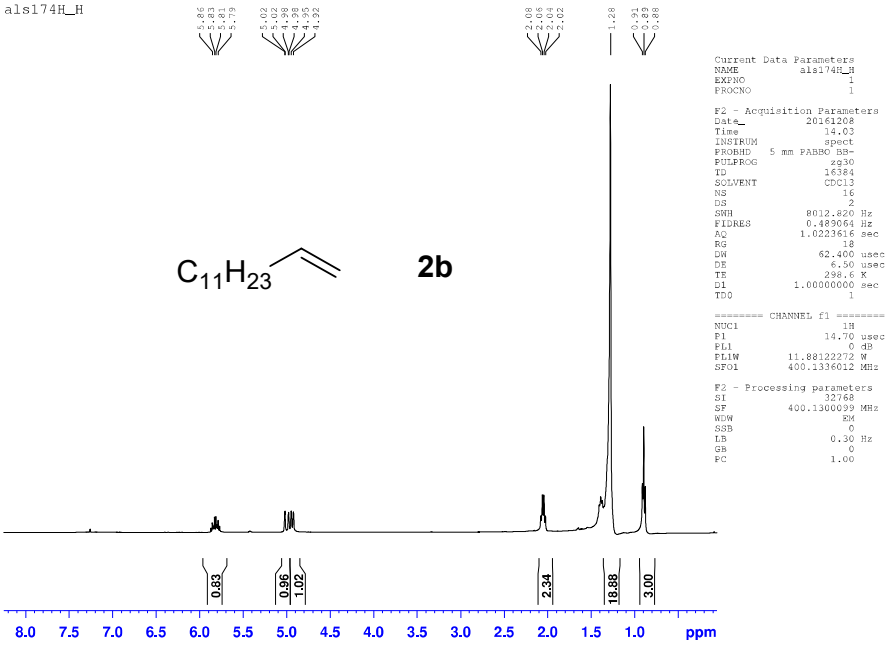
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz

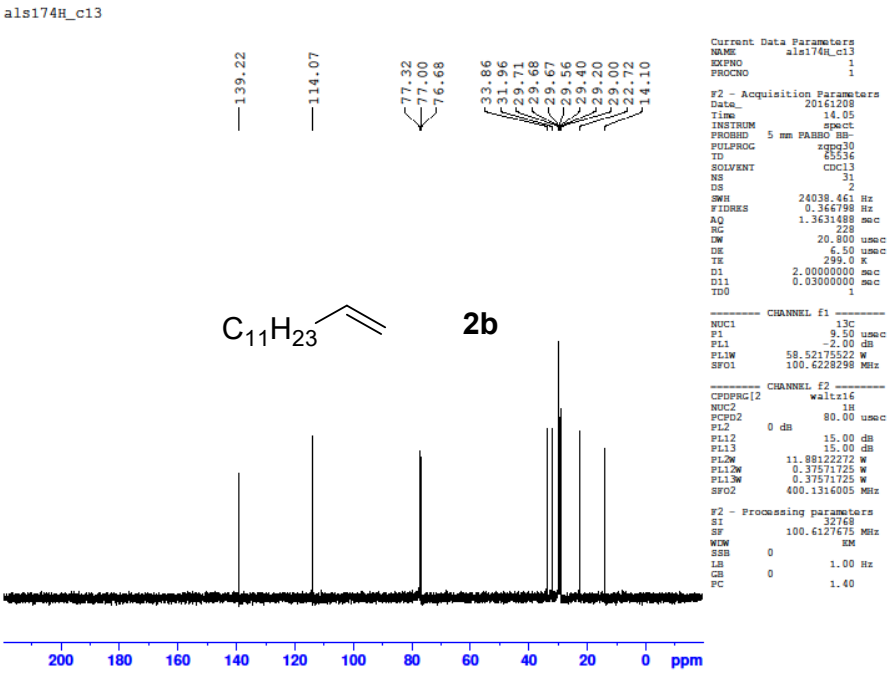
F2 - Processing parameters
SI 32768
SF 100.6127712 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

```
File       :D:\MassHunter\GCMS\1\data\alston\als175a.D
Operator   : duan
Acquired   : 07 Feb 2017  14:50     using AcqMethod M1.M
Instrument :   5977
Sample Name: als175a
Misc Info  :
Vial Number: 146
```

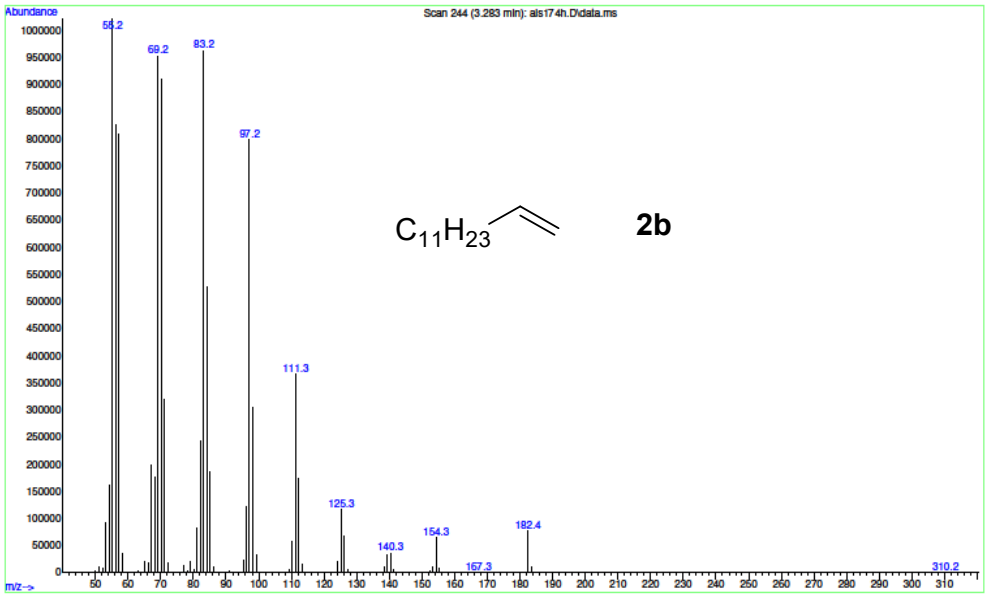


$C_{15}H_{29}$ **2a**


als174H_H
5.85
5.83
5.81
5.79
5.02
5.02
4.98
4.98
4.95
4.92
2.08
2.06
2.04
2.02
1.28
0.91
0.89
0.88
$C_{11}H_{23}$
2b
0.83
0.96
1.02
2.34
18.88
3.00
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
Current Data Parameters
NAME als174H_H
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161208
Time 14.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.489064 Hz
AQ 1.0223616 sec
RG 18
DW 62.400 usec
DE 6.50 usec
TE 298.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1336012 MHz
F2 - Processing parameters
SI 32768
SF 400.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

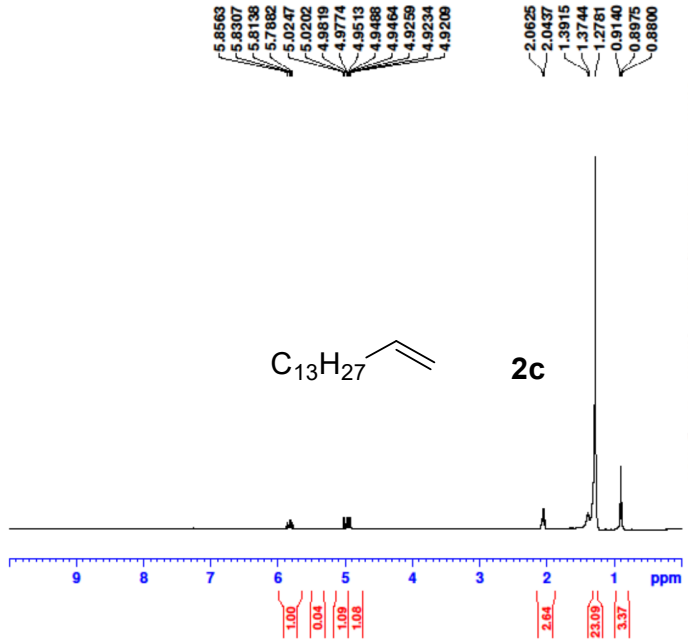

als174H_c13
139.22
114.07
77.32
77.00
76.68
33.86
31.96
29.71
29.68
29.67
29.56
29.40
29.20
29.00
22.72
14.10
$C_{11}H_{23}$
2b
200 180 160 140 120 100 80 60 40 20 0 ppm
Current Data Parameters
NAME als174H_c13
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161208
Time 14.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 31
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 228
DW 20.800 usec
DE 6.50 usec
TE 299.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127675 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

```
File       :D:\MassHunter\GCMS\1\data\alston\als174h.D
Operator   : duan
Acquired   : 02 Dec 2016  11:31     using AcqMethod M1.M
Instrument :   5977
Sample Name: als174h
Misc Info  :
Vial Number: 8
```



$C_{11}H_{23}$ **2b**

als174e_H



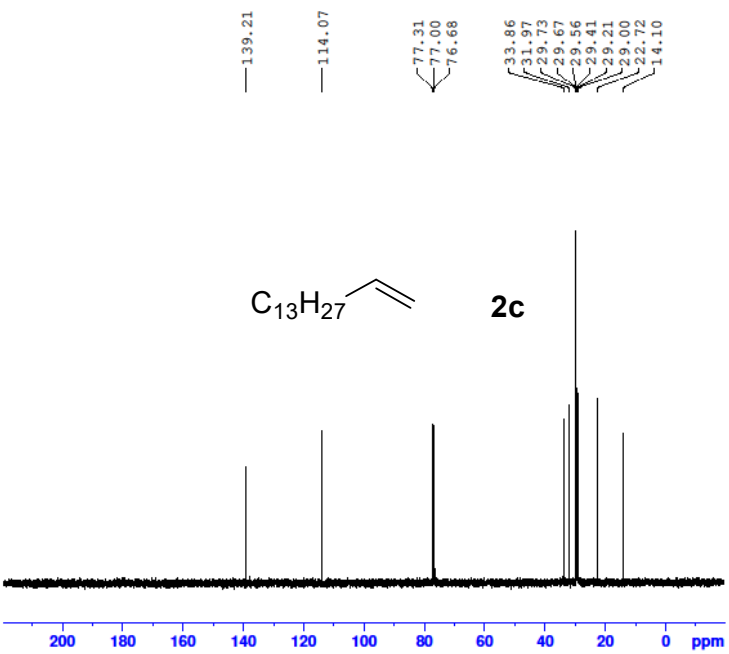
Current Data Parameters
NAME als174e_H
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161208
Time 14.23
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.489064 Hz
AQ 1.0223616 sec
RG 18
DW 62.400 usec
DE 6.50 usec
TE 298.8 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1336012 MHz

F2 - Processing parameters
SI 32768
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

als174e_c13



Current Data Parameters
NAME als174e_c13
EXPNO 1
PROCNO 1

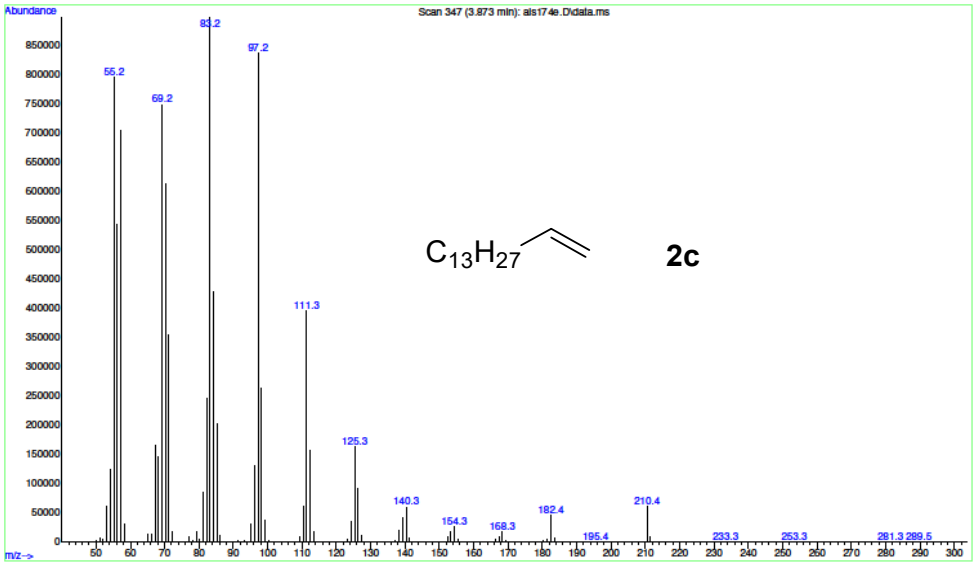
F2 - Acquisition Parameters
Date_ 20161208
Time 14.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 35
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 228
DW 20.800 usec
DE 6.50 usec
TE 298.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz

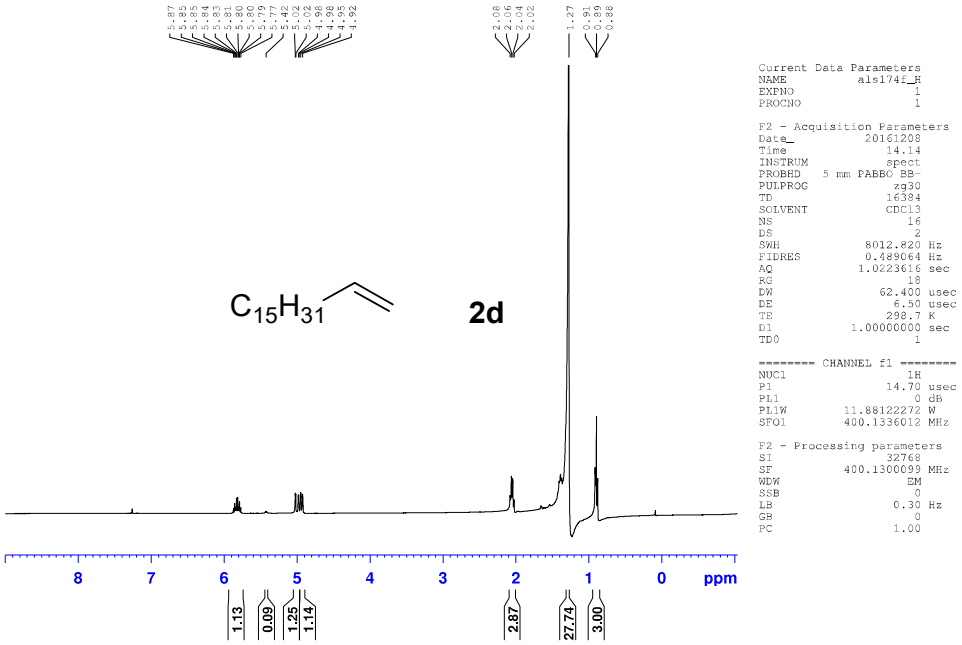
F2 - Processing parameters
SI 32768
SF 100.6127670 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

```
File       :D:\MassHunter\GCMS\1\data\alston\als174e.D
Operator   : duan
Acquired   : 02 Dec 2016  11:06     using AcqMethod M1.M
Instrument :   5977
Sample Name: als174e
Misc Info  :
Vial Number: 6
```



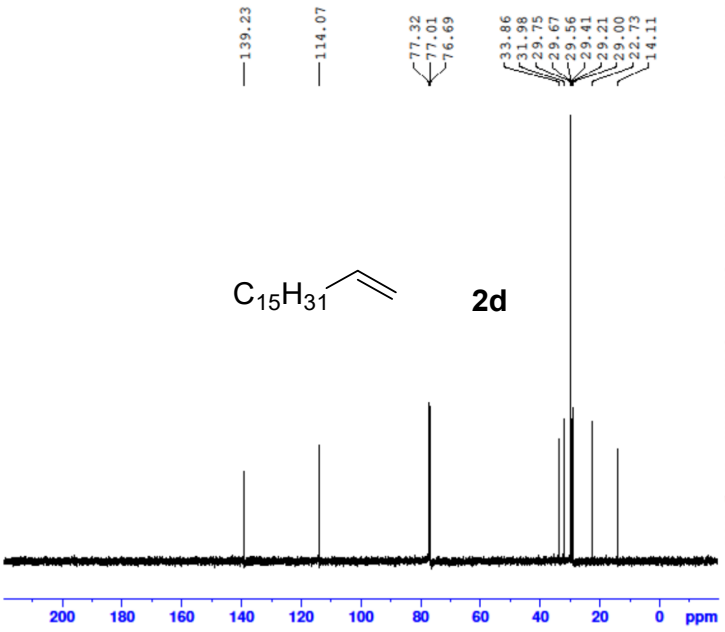
$C_{13}H_{27}$ **2c**

als174f_H



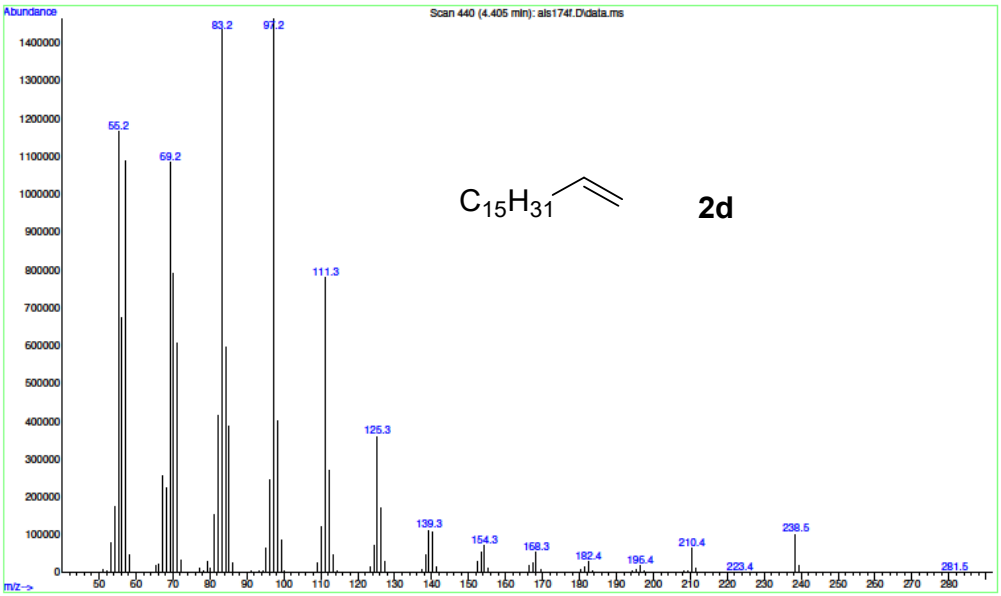

```
Current Data Parameters
NAME            als174f_H
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20161208
Time                14.14
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 16384
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8012.820 Hz
FIDRES           0.489064 Hz
AQ               1.0223616 sec
RG                     18
DW                62.400 usec
DE                 6.50 usec
TE                298.7 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  14.70 usec
PL1                    0 dB
PL1W           11.88122272 W
SFO1          400.1336012 MHz

F2 - Processing parameters
SI                  32768
SF            400.1300099 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

als174f_c13



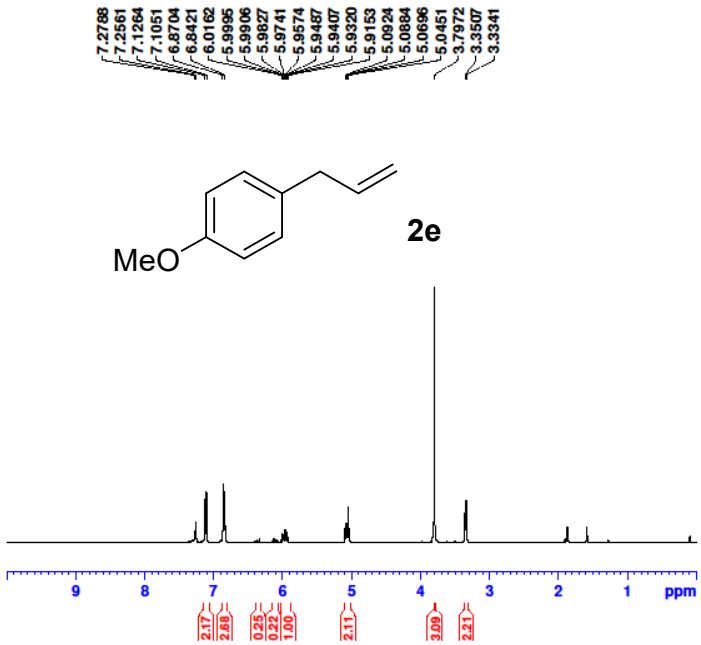

```
Current Data Parameters
NAME          als174f_c13
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20161208
Time                14.16
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 65536
SOLVENT             CDCl3
NS                     47
DS                      2
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631488 sec
RG                    228
DW                20.800 usec
DE                 6.50 usec
TE                299.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   13C
P1                   9.50 usec
PL1                 -2.00 dB
PL1W           58.52175522 W
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2            0 dB
PL12                15.00 dB
PL13                15.00 dB
PL2W           11.88122272 W
PL12W           0.37571725 W
PL13W           0.37571725 W
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                  32768
SF            100.6127671 MHz
WDW                    EM
SSB             0
LB                   1.00 Hz
GB              0
PC                   1.40
```

```
File       :D:\MassHunter\GCMS\1\data\alston\als174f.D
Operator   : duan
Acquired   : 02 Dec 2016  11:19     using AcqMethod M1.M
Instrument :   5977
Sample Name: als174f
Misc Info  :
Vial Number: 7
```



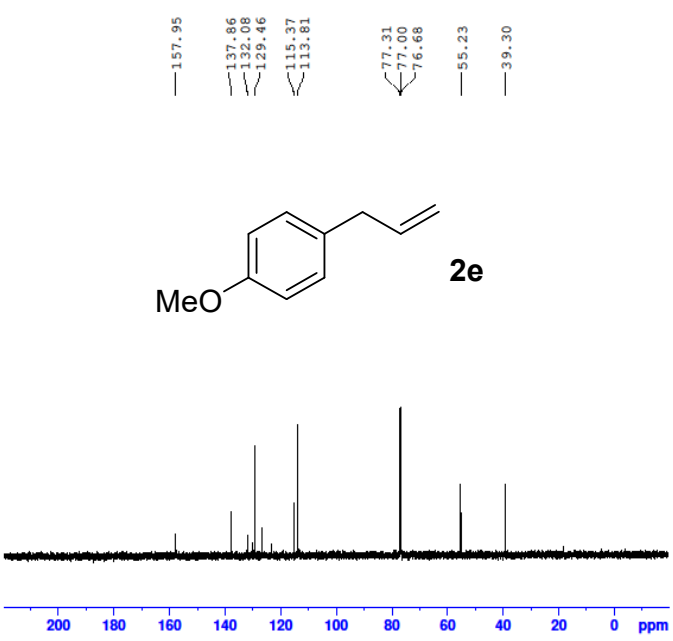
$C_{15}H_{31}$ **2d**

als184e_H



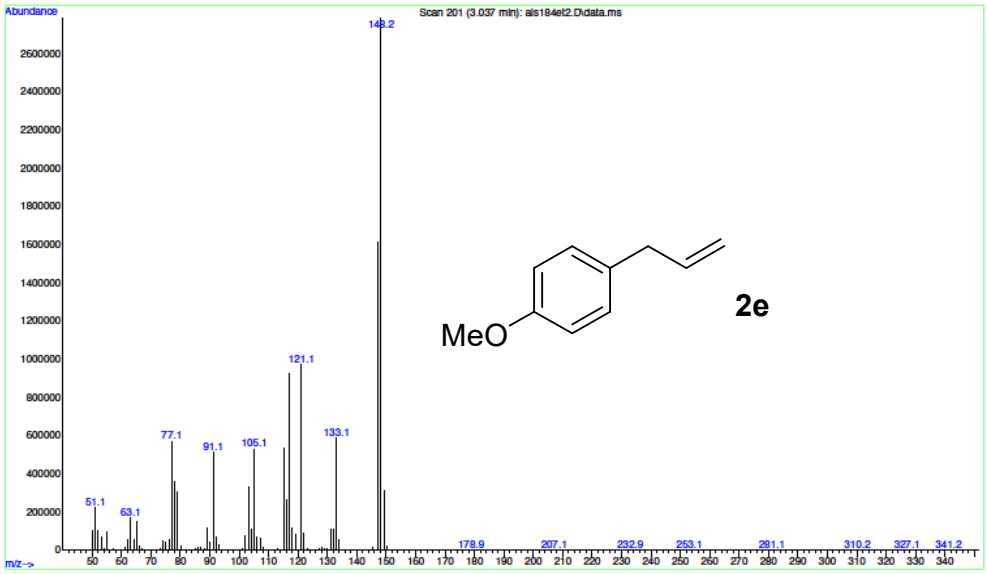

```
Current Data Parameters
NAME                  als184e
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_                20170427
Time                     9.54
INSTRUM                 spect
PROBHD    5 mm PABBO BB-
PULPROG                 zg30
TD                     16384
SOLVENT                CDCl3
NS                         16
DS                          2
SWH                 8012.820 Hz
FIDRES              0.489064 Hz
AQ                  1.0223616 sec
RG                       80.6
DW                     62.400 usec
DE                      6.50 usec
TE                     297.9 K
D1                  1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                      14.70 usec
PL1             0 dB
PL1W               11.88122272 W
SFO1              400.1336012 MHz

F2 - Processing parameters
SI                      32768
SF                400.1300113 MHz
WDW                        EM
SSB             0
LB                      0.30 Hz
GB              0
PC                      1.00
```

als184e_13C

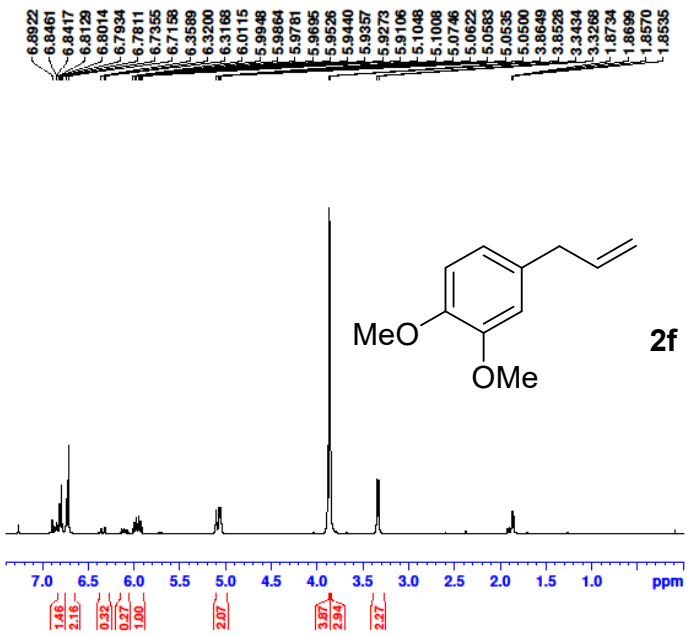



```
Current Data Parameters
NAME                  als184e
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_                20170427
Time                    10.00
INSTRUM                 spect
PROBHD    5 mm PABBO BB-
PULPROG              zgpg30
TD                     65536
SOLVENT                CDCl3
NS                         29
DS                          2
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631488 sec
RG                        203
DW                     20.800 usec
DE                      6.50 usec
TE                     298.7 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       13C
P1                       9.50 usec
PL1                     -2.00 dB
PL1W               58.52175522 W
SFO1              100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG[2                waltz16
NUC2                       1H
PCPD2                   80.00 usec
PL2             0 dB
PL12                    15.00 dB
PL13                    15.00 dB
PL2W               11.88122272 W
PL12W               0.37571725 W
PL13W               0.37571725 W
SFO2              400.1316005 MHz

F2 - Processing parameters
SI                      32768
SF                100.6127736 MHz
WDW                        EM
SSB             0
LB                      1.00 Hz
GB              0
PC                      1.40
```

```
File       :D:\MassHunter\GCMS\1\data\alston\als184et2.D
Operator   : duan
Acquired   : 26 Apr 2017  15:37     using AcqMethod M1.M
Instrument :    5977
Sample Name: als184et2
Misc Info  :
Vial Number: 2
```

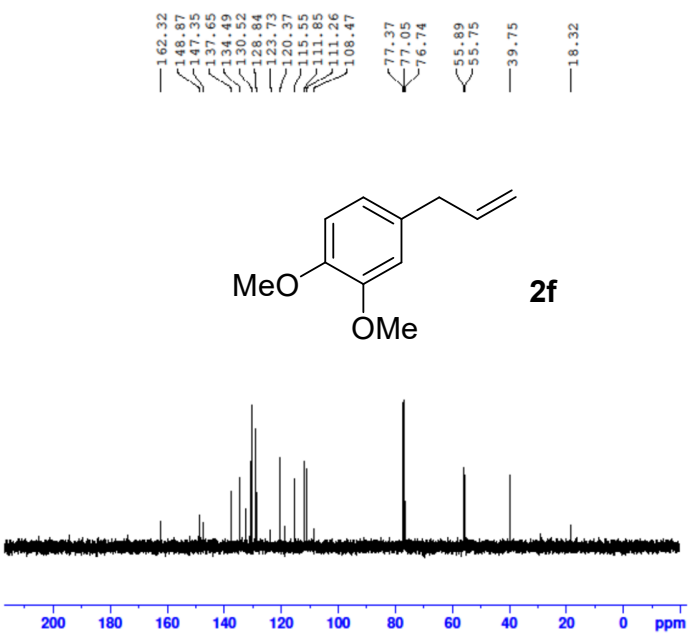


als184g_H



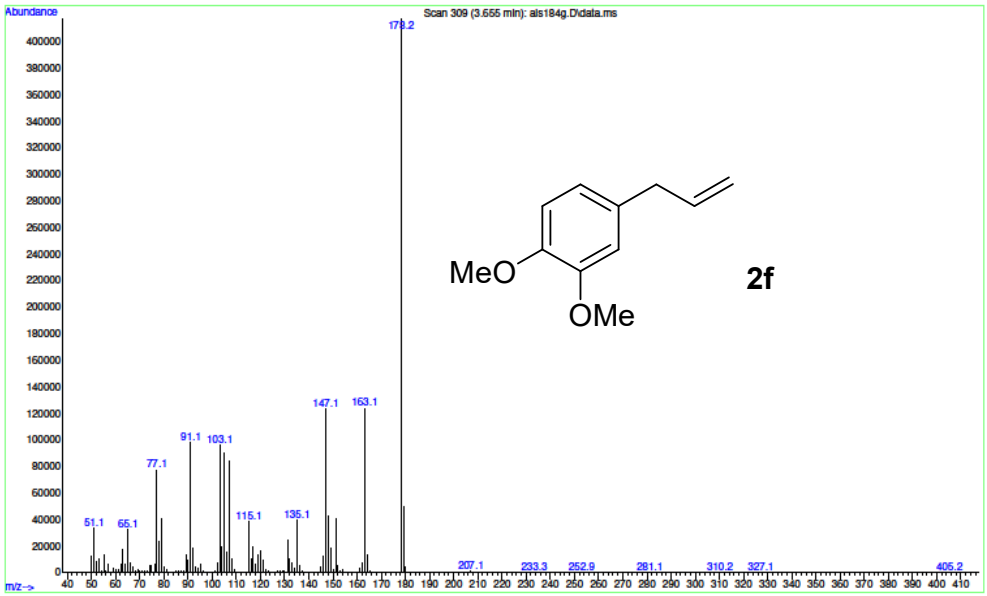

```
Current Data Parameters
NAME                  als184g
EXPNO                       3
PROCNO                      1

F2 - Acquisition Parameters
Date_               20170427
Time                   13.00
INSTRUM                spect
PROBHD     5 mm PABBO BB-
PULPROG                zg30
TD                    16384
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8012.820 Hz
FIDRES             0.489064 Hz
AQ                 1.0223616 sec
RG                       32
DW                    62.400 usec
DE                     6.50 usec
TE                   298.1 K
D1                 1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                     14.70 usec
PL1          0 dB
PL1W           11.88122272 W
SFO1          400.1336012 MHz

F2 - Processing parameters
SI                    32768
SF                400.1300095 MHz
WDW                      EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

als184gc13



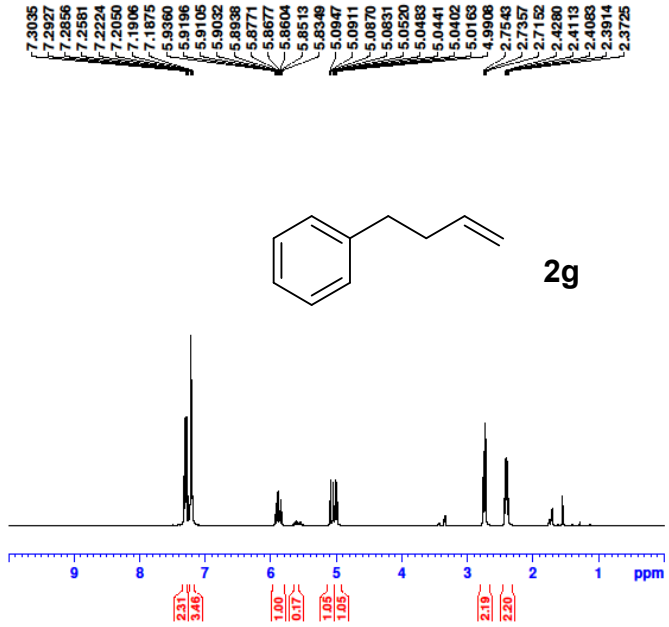

```
Current Data Parameters
NAME                  als184g
EXPNO                       4
PROCNO                      1

F2 - Acquisition Parameters
Date_               20170427
Time                   13.06
INSTRUM                spect
PROBHD     5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                       8
DS                       2
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631488 sec
RG                     228
DW                   20.800 usec
DE                     6.50 usec
TE                   298.2 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     13C
P1                     9.50 usec
PL1                   -2.00 dB
PL1W           58.52175522 W
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG[2            waltz16
NUC2                     1H
PCPD2                 80.00 usec
PL2          0 dB
PL12                  15.00 dB
PL13                  15.00 dB
PL2W           11.88122272 W
PL12W           0.37571725 W
PL13W           0.37571725 W
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF                100.6127741 MHz
WDW                      EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

```
File       :D:\MassHunter\GCMS\1\data\alston\als184g.D
Operator   : duan
Acquired   : 26 Apr 2017  12:17     using AcqMethod M1.M
Instrument :   5977
Sample Name: als184g
Misc Info  :
Vial Number: 4
```



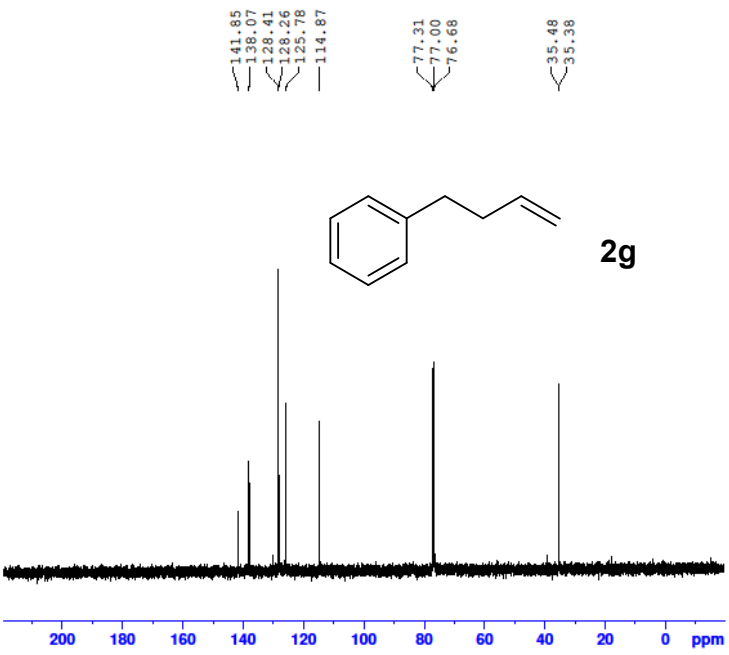
2f

als169H_H



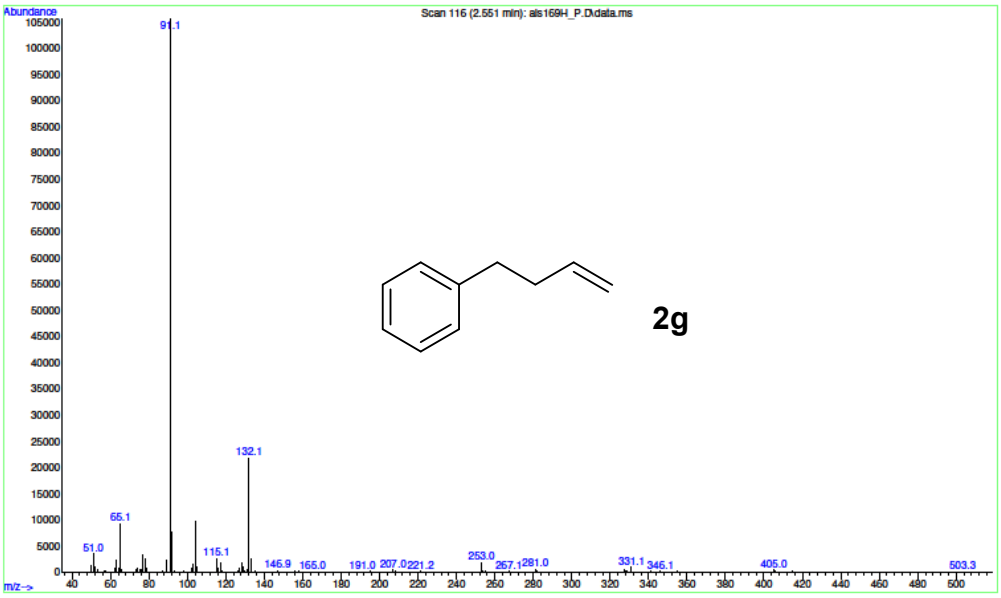

```
Current Data Parameters
NAME                  als169H_H
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_               20160915
Time                    15.38
INSTRUM                 spect
PROBHD    5 mm PABBO BB-
PULPROG                 zg30
TD                     16384
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                8012.820 Hz
FIDRES             0.489064 Hz
AQ                 1.0223616 sec
RG                      80.6
DW                    62.400 usec
DE                     6.50 usec
TE                    297.7 K
D1                 1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                         1H
P1                        14.70 usec
PL1            0 dB
PL1W              11.88122272 W
SFO1              400.1336012 MHz

F2 - Processing parameters
SI                        32768
SF                400.1300104 MHz
WDW                          EM
SSB            0
LB                         0.30 Hz
GB             0
PC                         1.00
```

als169H_13C



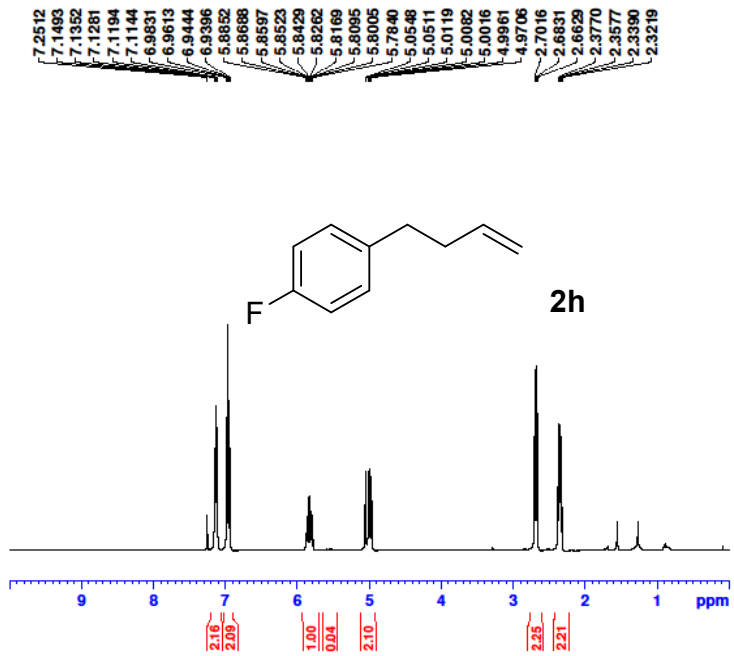

```
Current Data Parameters
NAME                 als169H_13C
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_               20160919
Time                    10.35
INSTRUM                 spect
PROBHD    5 mm PABBO BB-
PULPROG              zgpg30
TD                     65536
SOLVENT                CDCl3
NS                       108
DS                         2
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631488 sec
RG                       203
DW                    20.800 usec
DE                     6.50 usec
TE                    299.8 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                        13C
P1                         9.50 usec
PL1                       -2.00 dB
PL1W              58.52175522 W
SFO1              100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG[2                waltz16
NUC2                         1H
PCPD2                     80.00 usec
PL2            0 dB
PL12                      15.00 dB
PL13                      15.00 dB
PL2W              11.88122272 W
PL12W              0.37571725 W
PL13W              0.37571725 W
SFO2              400.1316005 MHz

F2 - Processing parameters
SI                        32768
SF                100.6127741 MHz
WDW                          EM
SSB            0
LB                         1.00 Hz
GB             0
PC                         1.40
```

```
File       :D:\MassHunter\GCMS\1\data\alston\als169H_P.D
Operator   : duan
Acquired   : 14 Sep 2016  15:28     using AcqMethod M1.M
Instrument :   5977
Sample Name: als169H_P
Misc Info  :
Vial Number: 20
```



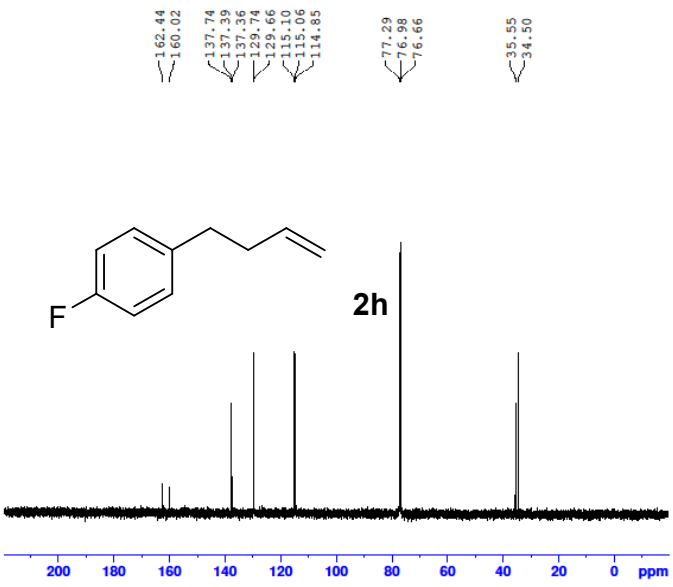
2g

als173b_H



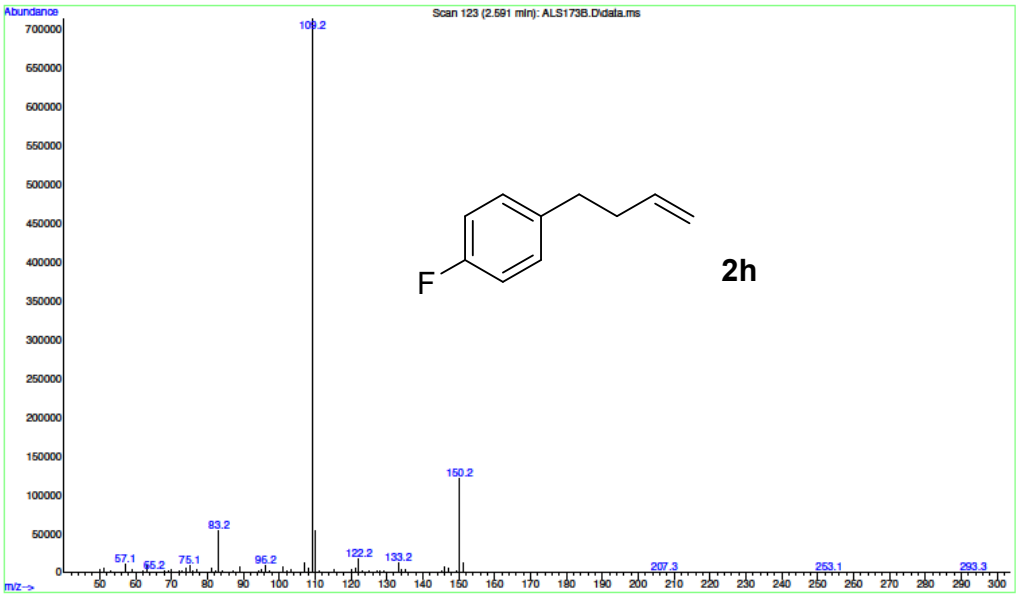

```
Current Data Parameters
NAME                  als173b_H
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20161124
Time                      14.40
INSTRUM                   spect
PROBHD     5 mm PABBO BB-
PULPROG                   zg30
TD                       16384
SOLVENT                  CDCl3
NS                          16
DS                           2
SWH                   8012.820 Hz
FIDRES                0.489064 Hz
AQ                    1.0223616 sec
RG                         90.5
DW                       62.400 usec
DE                        6.50 usec
TE                       298.1 K
D1                    1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                         1H
P1                       14.70 usec
PL1             0 dB
PL1W             11.88122272 W
SFO1             400.1336012 MHz

F2 - Processing parameters
SI                           32768
SF                    400.1300131 MHz
WDW                             EM
SSB             0
LB                            0.30 Hz
GB              0
PC                            1.00
```

als173b_C13

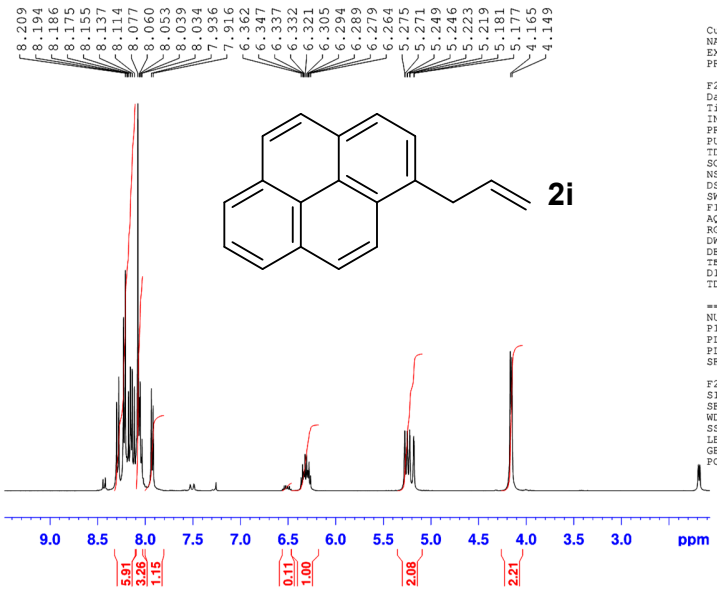



```
Current Data Parameters
NAME                  als173b_C13
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20161124
Time                      14.44
INSTRUM                   spect
PROBHD     5 mm PABBO BB-
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                         139
DS                           2
SWH                  24038.461 Hz
FIDRES                0.366798 Hz
AQ                    1.3631488 sec
RG                         228
DW                       20.800 usec
DE                        6.50 usec
TE                       298.8 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                        13C
P1                        9.50 usec
PL1                      -2.00 dB
PL1W             58.52175522 W
SFO1             100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG[2                waltz16
NUC2                        1H
PCPD2                    80.00 usec
PL2             0 dB
PL12                     15.00 dB
PL13                     15.00 dB
PL2W             11.88122272 W
PL12W             0.37571725 W
PL13W             0.37571725 W
SFO2             400.1316005 MHz

F2 - Processing parameters
SI                           32768
SF                    100.6127730 MHz
WDW                             EM
SSB             0
LB                            1.00 Hz
GB              0
PC                            1.40
```

```
File       :D:\MassHunter\GCMS\1\data\alston\ALS173B.D
Operator   : duan
Acquired   : 11 Nov 2016  14:58     using AcqMethod M1.M
Instrument :
  5977
Sample Name: ALS173B
Misc Info  :
Vial Number: 2
```

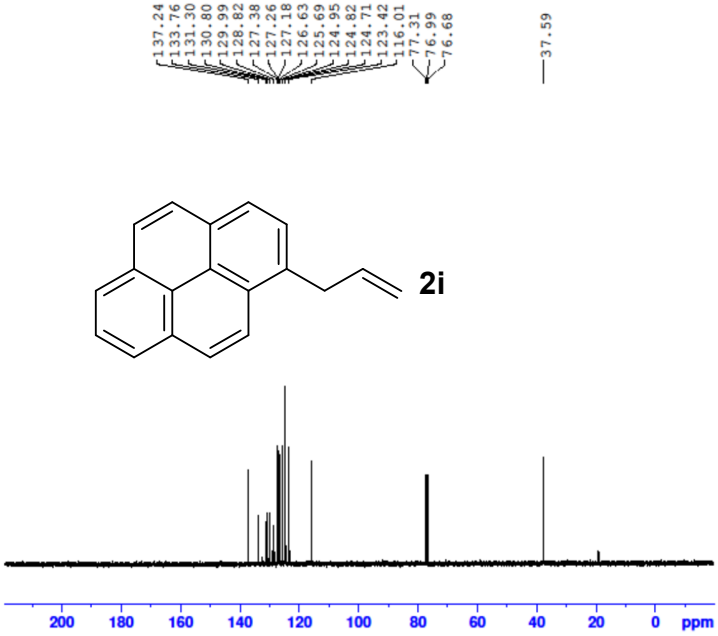


als175e_H



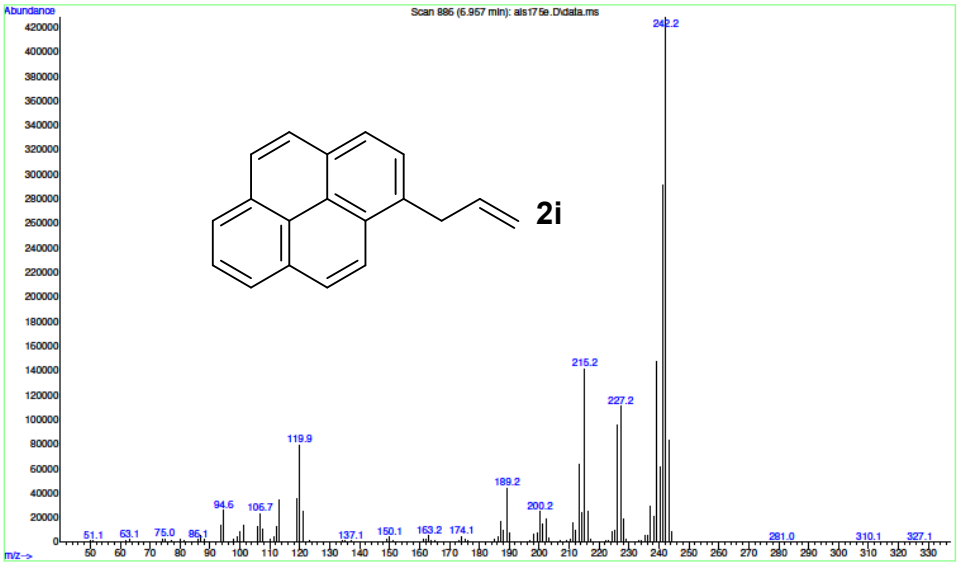

```
Current Data Parameters
NAME                  als175e
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_               20170210
Time                    9.22
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                 zg30
TD                     16384
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                8012.820 Hz
FIDRES             0.489064 Hz
AQ                 1.0223616 sec
RG                      22.6
DW                    62.400 usec
DE                     6.50 usec
TE                    297.9 K
D1                 1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                      14.70 usec
PL1                        0 dB
PL1W              11.88122272 W
SFO1              400.1336012 MHz

F2 - Processing parameters
SI                         32768
SF                400.1300103 MHz
WDW                           EM
SSB                            0
LB                          0.30 Hz
GB                             0
PC                          1.00
```

als175e_C13




```
Current Data Parameters
NAME                  als175e
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_               20170210
Time                    9.28
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                     65536
SOLVENT                CDCl3
NS                        43
DS                         2
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631488 sec
RG                       144
DW                   20.800 usec
DE                     6.50 usec
TE                    298.2 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                      13C
P1                      9.50 usec
PL1                    -2.00 dB
PL1W              58.52175522 W
SFO1              100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG[2             waltz16
NUC2                       1H
PCPD2                  80.00 usec
PL2            0 dB
PL12                   15.00 dB
PL13                   15.00 dB
PL2W              11.88122272 W
PL12W              0.37571725 W
PL13W              0.37571725 W
SFO2              400.1316005 MHz

F2 - Processing parameters
SI                         32768
SF                100.6127909 MHz
WDW                           EM
SSB            0
LB                          1.00 Hz
GB             0
PC                          1.40
```

```
File       :D:\MassHunter\GCMS\1\data\alston\als175e.D
Operator   : duan
Acquired   : 07 Feb 2017  15:39     using AcqMethod M1.M
Instrument :   5977
Sample Name: als175e
Misc Info  :
Vial Number: 150
```



8. X-ray crystalline structure for Pd-complexes

Figure S6: Crystalline structure of $[PdCl_2(C_{28}H_{21}P)]_2$, Pd-CP-1 complex

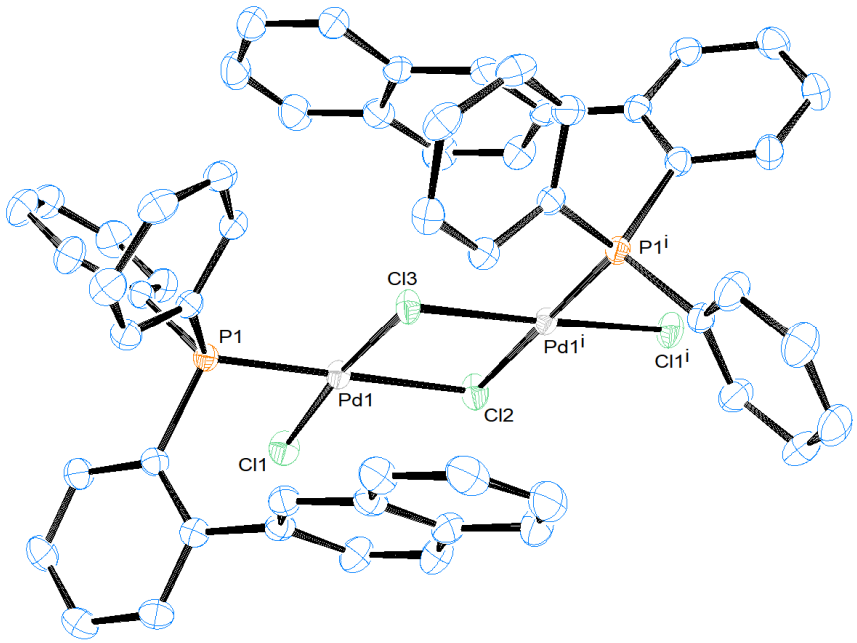


Table S2. Crystal data and structure refinement for $[PdCl_2(C_{28}H_{21}P)]_2$, Pd-CP-1.

Identification code	ALS1702
Empirical formula	C58 H46 Cl8 P2 Pd2
Formula weight	1301.29
Temperature	298(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, C 2/c
Unit cell dimensions	a = 26.9421(86) A alpha = 90 deg. b = 11.1527(33) A beta = 114.7781(86) deg. c = 19.7203(59) A gamma = 90 deg.
Volume	5380(3) A^3
Z, Calculated density	4, 1.607 Mg/m^3
Absorption coefficient	1.164 mm^-1
F(000)	2608
Crystal size	0.16 x 0.10 x 0.08 mm
Theta range for data collection	2.76 to 27.51 deg.
Limiting indices	-34<=h<=34, -14<=k<=14, -25<=l<=25
Reflections collected / unique	60625 / 6168 [R(int) = 0.0426]
Completeness to theta = 27.51	99.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9126 and 0.8356
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6168 / 0 / 317

Goodness-of-fit on F^2 1.029

Final R indices [I>2sigma(I)] R1 = 0.0342, wR2 = 0.0774

R indices (all data) R1 = 0.0515, wR2 = 0.0850

Largest diff. peak and hole 0.675 and -0.910 e.A^-3

Table S3. Bond lengths [A] and angles [deg] for [PdCl2(C28H21P)]2, Pd-CP-1.

Pd(1)-P(1)	2.2563(8)
Pd(1)-Cl(1)	2.2937(9)
Pd(1)-Cl(3)	2.3181(8)
Pd(1)-Cl(2)	2.4293(9)
Cl(2)-Pd(1)#1	2.4293(9)
Cl(3)-Pd(1)#1	2.3181(8)
P(1)-C(1)	1.820(3)
P(1)-C(13)	1.824(3)
P(1)-C(7)	1.830(3)
C(1)-C(6)	1.389(4)
C(1)-C(2)	1.392(4)
C(2)-C(3)	1.378(4)
C(2)-H(2A)	0.9300
C(3)-C(4)	1.375(5)
C(3)-H(3A)	0.9300
C(4)-C(5)	1.374(5)
C(4)-H(4A)	0.9300
C(5)-C(6)	1.381(4)
C(5)-H(5A)	0.9300
C(6)-H(6A)	0.9300
C(7)-C(8)	1.383(4)
C(7)-C(12)	1.386(4)
C(8)-C(9)	1.395(5)
C(8)-H(8A)	0.9300
C(9)-C(10)	1.364(6)
C(9)-H(9A)	0.9300
C(10)-C(11)	1.363(5)
C(10)-H(10A)	0.9300
C(11)-C(12)	1.387(5)
C(11)-H(11A)	0.9300
C(12)-H(12A)	0.9300

C(13)-C(14)	1.396(4)
C(13)-C(18)	1.399(4)
C(14)-C(15)	1.384(4)
C(14)-H(14A)	0.9300
C(15)-C(16)	1.366(5)
C(15)-H(15A)	0.9300
C(16)-C(17)	1.385(4)
C(16)-H(16A)	0.9300
C(17)-C(18)	1.390(4)
C(17)-H(17A)	0.9300
C(18)-C(19)	1.504(4)
C(19)-C(20)	1.364(4)
C(19)-C(28)	1.414(4)
C(20)-C(21)	1.431(4)
C(20)-H(20A)	0.9300
C(21)-C(26)	1.407(4)
C(21)-C(22)	1.410(4)
C(22)-C(23)	1.370(5)
C(22)-H(22A)	0.9300
C(23)-C(24)	1.398(6)
C(23)-H(23A)	0.9300
C(24)-C(25)	1.342(6)
C(24)-H(24A)	0.9300
C(25)-C(26)	1.439(5)
C(25)-H(25A)	0.9300
C(26)-C(27)	1.396(5)
C(27)-C(28)	1.372(5)
C(27)-H(27A)	0.9300
C(28)-H(28A)	0.9300
C(29)-Cl(4)	1.698(5)
C(29)-Cl(5)	1.712(5)
C(29)-H(29A)	0.9700
C(29)-H(29B)	0.9700

P(1)-Pd(1)-Cl(1)	87.83(3)
P(1)-Pd(1)-Cl(3)	96.18(3)
Cl(1)-Pd(1)-Cl(3)	173.89(3)
P(1)-Pd(1)-Cl(2)	179.65(2)
Cl(1)-Pd(1)-Cl(2)	92.09(4)
Cl(3)-Pd(1)-Cl(2)	83.93(3)
Pd(1)#1-Cl(2)-Pd(1)	93.09(4)
Pd(1)-Cl(3)-Pd(1)#1	99.06(4)
C(1)-P(1)-C(13)	106.77(13)
C(1)-P(1)-C(7)	101.29(13)

C(13)-P(1)-C(7) 106.90(13)
C(1)-P(1)-Pd(1) 117.12(9)
C(13)-P(1)-Pd(1) 108.83(9)
C(7)-P(1)-Pd(1) 115.14(10)
C(6)-C(1)-C(2) 118.7(3)
C(6)-C(1)-P(1) 121.5(2)
C(2)-C(1)-P(1) 119.6(2)
C(3)-C(2)-C(1) 120.2(3)
C(3)-C(2)-H(2A) 119.9
C(1)-C(2)-H(2A) 119.9
C(4)-C(3)-C(2) 120.5(3)
C(4)-C(3)-H(3A) 119.7
C(2)-C(3)-H(3A) 119.7
C(5)-C(4)-C(3) 119.7(3)
C(5)-C(4)-H(4A) 120.1
C(3)-C(4)-H(4A) 120.1
C(4)-C(5)-C(6) 120.3(3)
C(4)-C(5)-H(5A) 119.9
C(6)-C(5)-H(5A) 119.9
C(5)-C(6)-C(1) 120.4(3)
C(5)-C(6)-H(6A) 119.8
C(1)-C(6)-H(6A) 119.8
C(8)-C(7)-C(12) 118.6(3)
C(8)-C(7)-P(1) 122.0(2)
C(12)-C(7)-P(1) 119.3(2)
C(7)-C(8)-C(9) 119.7(3)
C(7)-C(8)-H(8A) 120.2
C(9)-C(8)-H(8A) 120.2
C(10)-C(9)-C(8) 120.8(4)
C(10)-C(9)-H(9A) 119.6
C(8)-C(9)-H(9A) 119.6
C(11)-C(10)-C(9) 120.2(3)
C(11)-C(10)-H(10A) 119.9
C(9)-C(10)-H(10A) 119.9
C(10)-C(11)-C(12) 119.8(3)
C(10)-C(11)-H(11A) 120.1
C(12)-C(11)-H(11A) 120.1
C(7)-C(12)-C(11) 120.9(3)
C(7)-C(12)-H(12A) 119.5
C(11)-C(12)-H(12A) 119.5
C(14)-C(13)-C(18) 119.4(3)
C(14)-C(13)-P(1) 119.5(2)
C(18)-C(13)-P(1) 121.0(2)
C(15)-C(14)-C(13) 120.8(3)

C(15)-C(14)-H(14A)	119.6
C(13)-C(14)-H(14A)	119.6
C(16)-C(15)-C(14)	119.9(3)
C(16)-C(15)-H(15A)	120.1
C(14)-C(15)-H(15A)	120.1
C(15)-C(16)-C(17)	120.1(3)
C(15)-C(16)-H(16A)	119.9
C(17)-C(16)-H(16A)	119.9
C(16)-C(17)-C(18)	121.2(3)
C(16)-C(17)-H(17A)	119.4
C(18)-C(17)-H(17A)	119.4
C(17)-C(18)-C(13)	118.7(3)
C(17)-C(18)-C(19)	117.7(3)
C(13)-C(18)-C(19)	123.6(2)
C(20)-C(19)-C(28)	119.0(3)
C(20)-C(19)-C(18)	121.1(3)
C(28)-C(19)-C(18)	119.7(3)
C(19)-C(20)-C(21)	121.2(3)
C(19)-C(20)-H(20A)	119.4
C(21)-C(20)-H(20A)	119.4
C(26)-C(21)-C(22)	120.1(3)
C(26)-C(21)-C(20)	118.7(3)
C(22)-C(21)-C(20)	121.2(3)
C(23)-C(22)-C(21)	120.0(3)
C(23)-C(22)-H(22A)	120.0
C(21)-C(22)-H(22A)	120.0
C(22)-C(23)-C(24)	120.3(4)
C(22)-C(23)-H(23A)	119.8
C(24)-C(23)-H(23A)	119.8
C(25)-C(24)-C(23)	121.1(3)
C(25)-C(24)-H(24A)	119.5
C(23)-C(24)-H(24A)	119.5
C(24)-C(25)-C(26)	120.8(4)
C(24)-C(25)-H(25A)	119.6
C(26)-C(25)-H(25A)	119.6
C(27)-C(26)-C(21)	119.4(3)
C(27)-C(26)-C(25)	123.0(3)
C(21)-C(26)-C(25)	117.6(3)
C(28)-C(27)-C(26)	120.8(3)
C(28)-C(27)-H(27A)	119.6
C(26)-C(27)-H(27A)	119.6
C(27)-C(28)-C(19)	120.9(3)
C(27)-C(28)-H(28A)	119.6
C(19)-C(28)-H(28A)	119.6

Cl(4)-C(29)-Cl(5) 115.8(3)
Cl(4)-C(29)-H(29A) 108.3
Cl(5)-C(29)-H(29A) 108.3
Cl(4)-C(29)-H(29B) 108.3
Cl(5)-C(29)-H(29B) 108.3
H(29A)-C(29)-H(29B) 107.4

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,y,-z+1/2

Table S4. Torsion angles [deg] for ALS1702.

P(1)-Pd(1)-Cl(2)-Pd(1)#1	107(5)
Cl(1)-Pd(1)-Cl(2)-Pd(1)#1	-175.36(2)
Cl(3)-Pd(1)-Cl(2)-Pd(1)#1	0.0
P(1)-Pd(1)-Cl(3)-Pd(1)#1	-179.66(2)
Cl(1)-Pd(1)-Cl(3)-Pd(1)#1	49.5(3)
Cl(2)-Pd(1)-Cl(3)-Pd(1)#1	0.0
Cl(1)-Pd(1)-P(1)-C(1)	173.04(10)
Cl(3)-Pd(1)-P(1)-C(1)	-2.34(10)
Cl(2)-Pd(1)-P(1)-C(1)	-109(5)
Cl(1)-Pd(1)-P(1)-C(13)	51.90(10)
Cl(3)-Pd(1)-P(1)-C(13)	-123.48(9)
Cl(2)-Pd(1)-P(1)-C(13)	130(5)
Cl(1)-Pd(1)-P(1)-C(7)	-68.06(11)
Cl(3)-Pd(1)-P(1)-C(7)	116.56(10)
Cl(2)-Pd(1)-P(1)-C(7)	10(5)
C(13)-P(1)-C(1)-C(6)	-14.4(3)
C(7)-P(1)-C(1)-C(6)	97.3(2)
Pd(1)-P(1)-C(1)-C(6)	-136.6(2)
C(13)-P(1)-C(1)-C(2)	171.2(2)
C(7)-P(1)-C(1)-C(2)	-77.1(2)
Pd(1)-P(1)-C(1)-C(2)	49.0(2)
C(6)-C(1)-C(2)-C(3)	4.0(4)
P(1)-C(1)-C(2)-C(3)	178.5(2)
C(1)-C(2)-C(3)-C(4)	-2.0(4)
C(2)-C(3)-C(4)-C(5)	-2.0(5)
C(3)-C(4)-C(5)-C(6)	3.9(5)
C(4)-C(5)-C(6)-C(1)	-1.9(5)
C(2)-C(1)-C(6)-C(5)	-2.1(4)
P(1)-C(1)-C(6)-C(5)	-176.5(2)
C(1)-P(1)-C(7)-C(8)	149.4(3)
C(13)-P(1)-C(7)-C(8)	-99.0(3)
Pd(1)-P(1)-C(7)-C(8)	22.0(3)
C(1)-P(1)-C(7)-C(12)	-30.1(3)
C(13)-P(1)-C(7)-C(12)	81.5(3)
Pd(1)-P(1)-C(7)-C(12)	-157.4(2)
C(12)-C(7)-C(8)-C(9)	-0.1(5)
P(1)-C(7)-C(8)-C(9)	-179.5(3)
C(7)-C(8)-C(9)-C(10)	0.3(6)
C(8)-C(9)-C(10)-C(11)	-0.2(6)
C(9)-C(10)-C(11)-C(12)	0.0(6)
C(8)-C(7)-C(12)-C(11)	-0.2(5)
P(1)-C(7)-C(12)-C(11)	179.3(3)

C(10)-C(11)-C(12)-C(7)	0.2(6)
C(1)-P(1)-C(13)-C(14)	105.3(2)
C(7)-P(1)-C(13)-C(14)	-2.5(3)
Pd(1)-P(1)-C(13)-C(14)	-127.5(2)
C(1)-P(1)-C(13)-C(18)	-79.5(2)
C(7)-P(1)-C(13)-C(18)	172.8(2)
Pd(1)-P(1)-C(13)-C(18)	47.8(2)
C(18)-C(13)-C(14)-C(15)	-0.9(5)
P(1)-C(13)-C(14)-C(15)	174.4(3)
C(13)-C(14)-C(15)-C(16)	-0.2(5)
C(14)-C(15)-C(16)-C(17)	0.5(5)
C(15)-C(16)-C(17)-C(18)	0.4(5)
C(16)-C(17)-C(18)-C(13)	-1.5(5)
C(16)-C(17)-C(18)-C(19)	179.1(3)
C(14)-C(13)-C(18)-C(17)	1.7(4)
P(1)-C(13)-C(18)-C(17)	-173.5(2)
C(14)-C(13)-C(18)-C(19)	-178.9(3)
P(1)-C(13)-C(18)-C(19)	5.8(4)
C(17)-C(18)-C(19)-C(20)	-99.0(3)
C(13)-C(18)-C(19)-C(20)	81.6(4)
C(17)-C(18)-C(19)-C(28)	75.8(4)
C(13)-C(18)-C(19)-C(28)	-103.6(3)
C(28)-C(19)-C(20)-C(21)	0.4(4)
C(18)-C(19)-C(20)-C(21)	175.3(3)
C(19)-C(20)-C(21)-C(26)	1.4(4)
C(19)-C(20)-C(21)-C(22)	-177.6(3)
C(26)-C(21)-C(22)-C(23)	1.5(5)
C(20)-C(21)-C(22)-C(23)	-179.5(3)
C(21)-C(22)-C(23)-C(24)	0.4(5)
C(22)-C(23)-C(24)-C(25)	-1.3(6)
C(23)-C(24)-C(25)-C(26)	0.2(6)
C(22)-C(21)-C(26)-C(27)	177.0(3)
C(20)-C(21)-C(26)-C(27)	-2.0(4)
C(22)-C(21)-C(26)-C(25)	-2.5(4)
C(20)-C(21)-C(26)-C(25)	178.5(3)
C(24)-C(25)-C(26)-C(27)	-177.8(4)
C(24)-C(25)-C(26)-C(21)	1.7(5)
C(21)-C(26)-C(27)-C(28)	0.8(5)
C(25)-C(26)-C(27)-C(28)	-179.7(3)
C(26)-C(27)-C(28)-C(19)	1.0(6)
C(20)-C(19)-C(28)-C(27)	-1.7(5)
C(18)-C(19)-C(28)-C(27)	-176.6(3)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,y,-z+1/2

Figure S7: Crystalline structure of $Pd(C_{27}H_{20}NP)(CH_3CO_2)_2$, Pd-NP-1 complex

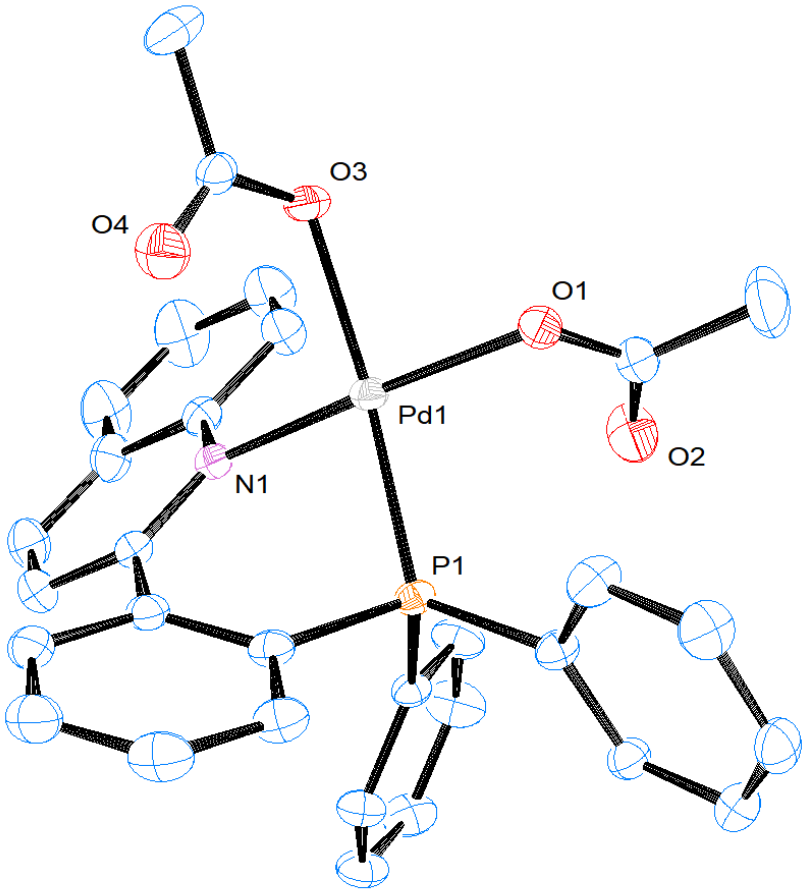


Table S3. Crystal data and structure refinement for $Pd(C_{27}H_{20}NP)(CH_3CO_2)_2$, Pd-NP-1 complex.

Identification code	yoy6	
Empirical formula	$Pd(C_{27}H_{20}NP)(CH_3CO_2)_2 .CH_2Cl_2$	
Formula weight	698.82	
Temperature	297(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.0468(5) Å	◎= 81.570(2)°.
	b = 12.3263(7) Å	◎= 75.746(2)°.
	c = 13.6449(8) Å	◎ = 69.269(2)°.
Volume	1528.42(15) $Å^3$	
Z	2	
Density (calculated)	1.518 Mg/m^3	
Absorption coefficient	0.872 mm^{-1}	
F(000)	708	
Crystal size	0.12 x 0.06 x 0.04 mm^3	
Theta range for data collection	2.22 to 30.61°.	
Index ranges	-14<=h<=14, -17<=k<=17, -19<=l<=19	
Reflections collected	135040	
Independent reflections	9404 [R(int) = 0.0355]	
Completeness to theta = 30.61°	99.7 %	
Absorption correction	None	
Max. and min. transmission	0.7461 and 0.7084	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9404 / 0 / 386	
Goodness-of-fit on F^2	1.004	
Final R indices [I>2sigma(I)]	R1 = 0.0377, wR2 = 0.1031	
R indices (all data)	R1 = 0.0498, wR2 = 0.1175	
Largest diff. peak and hole	1.080 and -0.961 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for YOY6. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pd(1)	4058(1)	2545(1)	2262(1)	32(1)
P(1)	2214(1)	3634(1)	1591(1)	31(1)
O(1)	4557(1)	3896(1)	2554(1)	47(1)
O(2)	2383(2)	4511(2)	3583(1)	67(1)
O(3)	5983(1)	1448(1)	2684(1)	45(1)
O(4)	6770(2)	1053(2)	1068(1)	61(1)
N(1)	3368(2)	1194(1)	2137(1)	34(1)
C(1)	3044(2)	996(2)	1306(1)	37(1)
C(2)	2518(2)	78(2)	1296(2)	50(1)
C(3)	2310(3)	-611(2)	2143(2)	57(1)
C(4)	2604(2)	-407(2)	3040(2)	51(1)
C(5)	2384(4)	-1084(2)	3961(2)	77(1)
C(6)	2693(4)	-858(3)	4808(2)	89(1)
C(7)	3209(3)	53(2)	4788(2)	69(1)
C(8)	3434(3)	732(2)	3919(2)	51(1)
C(9)	3142(2)	510(2)	3021(1)	39(1)
C(10)	3187(2)	1766(2)	369(1)	38(1)
C(11)	2768(2)	2979(2)	382(1)	37(1)
C(12)	2862(2)	3644(2)	-533(2)	47(1)
C(13)	3357(2)	3122(2)	-1450(2)	58(1)
C(14)	3757(3)	1935(2)	-1462(2)	60(1)
C(15)	3659(2)	1257(2)	-558(2)	50(1)
C(16)	465(2)	3482(1)	2177(1)	32(1)
C(17)	-496(2)	3468(2)	1604(2)	44(1)
C(18)	-1829(2)	3355(2)	2079(2)	52(1)
C(19)	-2208(2)	3255(2)	3109(2)	57(1)
C(20)	-1261(3)	3259(3)	3682(2)	64(1)
C(21)	80(2)	3371(2)	3223(2)	50(1)
C(22)	1930(2)	5163(2)	1272(1)	35(1)
C(23)	544(2)	5971(2)	1362(2)	40(1)

C(24)	362(2)	7123(2)	1030(2)	50(1)
C(25)	1546(3)	7470(2)	618(2)	52(1)
C(26)	2929(3)	6684(2)	538(2)	56(1)
C(27)	3136(2)	5527(2)	869(2)	50(1)
C(28)	3591(2)	4572(2)	3207(2)	50(1)
C(29)	4032(3)	5536(2)	3453(3)	93(1)
C(30)	6949(2)	957(2)	1935(2)	40(1)
C(31)	8394(3)	218(3)	2192(3)	77(1)
C(32)	-1263(5)	-3615(4)	4140(3)	111(1)
Cl(1)	-3158(2)	-2997(2)	4085(1)	194(1)
Cl(2)	-478(2)	-2605(1)	3974(1)	143(1)

Table 3. Bond lengths [Å] and angles [°] for YOY6.

Pd(1)-O(1)	2.0164(15)
Pd(1)-N(1)	2.0601(16)
Pd(1)-O(3)	2.0901(13)
Pd(1)-P(1)	2.1885(4)
P(1)-C(16)	1.8052(16)
P(1)-C(22)	1.8065(18)
P(1)-C(11)	1.8166(19)
O(1)-C(28)	1.284(2)
O(2)-C(28)	1.220(3)
O(3)-C(30)	1.276(2)
O(4)-C(30)	1.223(3)
N(1)-C(1)	1.331(2)
N(1)-C(9)	1.385(2)
C(1)-C(2)	1.411(3)
C(1)-C(10)	1.485(3)
C(2)-C(3)	1.349(3)
C(2)-H(2A)	0.94(3)
C(3)-C(4)	1.404(4)
C(3)-H(3A)	0.9300
C(4)-C(9)	1.409(3)
C(4)-C(5)	1.419(3)
C(5)-C(6)	1.357(5)
C(5)-H(5A)	0.9300
C(6)-C(7)	1.387(5)
C(6)-H(6A)	0.9300
C(7)-C(8)	1.367(3)
C(7)-H(7A)	0.9300
C(8)-C(9)	1.413(3)
C(8)-H(8A)	0.9300
C(10)-C(15)	1.394(3)
C(10)-C(11)	1.404(3)
C(11)-C(12)	1.391(3)
C(12)-C(13)	1.389(3)

C(12)-H(12A)	0.9300
C(13)-C(14)	1.375(4)
C(13)-H(13A)	0.9300
C(14)-C(15)	1.388(3)
C(14)-H(14A)	0.9300
C(15)-H(15A)	0.9300
C(16)-C(21)	1.383(3)
C(16)-C(17)	1.390(3)
C(17)-C(18)	1.383(3)
C(17)-H(17A)	0.95(2)
C(18)-C(19)	1.361(3)
C(18)-H(18A)	0.9300
C(19)-C(20)	1.374(4)
C(19)-H(19A)	0.9300
C(20)-C(21)	1.384(3)
C(20)-H(20A)	0.9300
C(21)-H(21A)	0.9300
C(22)-C(23)	1.385(2)
C(22)-C(27)	1.399(3)
C(23)-C(24)	1.388(3)
C(23)-H(23A)	0.9300
C(24)-C(25)	1.369(3)
C(24)-H(24A)	1.03(3)
C(25)-C(26)	1.374(3)
C(25)-H(25A)	0.93(2)
C(26)-C(27)	1.388(3)
C(26)-H(26A)	0.9300
C(27)-H(27A)	0.9300
C(28)-C(29)	1.512(4)
C(29)-H(29A)	0.9600
C(29)-H(29B)	0.9600
C(29)-H(29C)	0.9600
C(30)-C(31)	1.511(3)
C(31)-H(31A)	0.9600
C(31)-H(31B)	0.9600

C(31)-H(31C)	0.9600
C(32)-Cl(2)	1.658(5)
C(32)-Cl(1)	1.799(5)
C(32)-H(32A)	0.9700
C(32)-H(32B)	0.9700

O(1)-Pd(1)-N(1)	172.84(6)
O(1)-Pd(1)-O(3)	87.72(6)
N(1)-Pd(1)-O(3)	93.76(6)
O(1)-Pd(1)-P(1)	94.60(4)
N(1)-Pd(1)-P(1)	84.95(4)
O(3)-Pd(1)-P(1)	171.50(4)
C(16)-P(1)-C(22)	107.64(8)
C(16)-P(1)-C(11)	106.12(9)
C(22)-P(1)-C(11)	105.15(9)
C(16)-P(1)-Pd(1)	116.67(6)
C(22)-P(1)-Pd(1)	120.49(6)
C(11)-P(1)-Pd(1)	98.70(5)
C(28)-O(1)-Pd(1)	115.41(14)
C(30)-O(3)-Pd(1)	112.74(12)
C(1)-N(1)-C(9)	119.49(17)
C(1)-N(1)-Pd(1)	124.92(12)
C(9)-N(1)-Pd(1)	115.43(13)
N(1)-C(1)-C(2)	121.37(18)
N(1)-C(1)-C(10)	120.37(17)
C(2)-C(1)-C(10)	118.23(18)
C(3)-C(2)-C(1)	120.2(2)
C(3)-C(2)-H(2A)	122.4(18)
C(1)-C(2)-H(2A)	117.4(18)
C(2)-C(3)-C(4)	119.9(2)
C(2)-C(3)-H(3A)	120.0
C(4)-C(3)-H(3A)	120.0
C(3)-C(4)-C(9)	118.4(2)
C(3)-C(4)-C(5)	122.8(2)
C(9)-C(4)-C(5)	118.9(2)

C(6)-C(5)-C(4)	120.6(3)
C(6)-C(5)-H(5A)	119.7
C(4)-C(5)-H(5A)	119.7
C(5)-C(6)-C(7)	120.4(3)
C(5)-C(6)-H(6A)	119.8
C(7)-C(6)-H(6A)	119.8
C(8)-C(7)-C(6)	121.2(3)
C(8)-C(7)-H(7A)	119.4
C(6)-C(7)-H(7A)	119.4
C(7)-C(8)-C(9)	120.0(2)
C(7)-C(8)-H(8A)	120.0
C(9)-C(8)-H(8A)	120.0
N(1)-C(9)-C(4)	120.62(19)
N(1)-C(9)-C(8)	120.33(19)
C(4)-C(9)-C(8)	119.05(19)
C(15)-C(10)-C(11)	119.43(18)
C(15)-C(10)-C(1)	117.74(18)
C(11)-C(10)-C(1)	122.66(16)
C(12)-C(11)-C(10)	119.04(18)
C(12)-C(11)-P(1)	121.65(16)
C(10)-C(11)-P(1)	119.23(13)
C(13)-C(12)-C(11)	120.8(2)
C(13)-C(12)-H(12A)	119.6
C(11)-C(12)-H(12A)	119.6
C(14)-C(13)-C(12)	120.1(2)
C(14)-C(13)-H(13A)	120.0
C(12)-C(13)-H(13A)	120.0
C(13)-C(14)-C(15)	120.0(2)
C(13)-C(14)-H(14A)	120.0
C(15)-C(14)-H(14A)	120.0
C(14)-C(15)-C(10)	120.6(2)
C(14)-C(15)-H(15A)	119.7
C(10)-C(15)-H(15A)	119.7
C(21)-C(16)-C(17)	119.40(17)
C(21)-C(16)-P(1)	118.99(15)

C(17)-C(16)-P(1)	121.61(14)
C(18)-C(17)-C(16)	120.06(19)
C(18)-C(17)-H(17A)	120.5(16)
C(16)-C(17)-H(17A)	119.2(16)
C(19)-C(18)-C(17)	120.3(2)
C(19)-C(18)-H(18A)	119.8
C(17)-C(18)-H(18A)	119.8
C(18)-C(19)-C(20)	120.1(2)
C(18)-C(19)-H(19A)	120.0
C(20)-C(19)-H(19A)	120.0
C(19)-C(20)-C(21)	120.6(2)
C(19)-C(20)-H(20A)	119.7
C(21)-C(20)-H(20A)	119.7
C(16)-C(21)-C(20)	119.5(2)
C(16)-C(21)-H(21A)	120.2
C(20)-C(21)-H(21A)	120.2
C(23)-C(22)-C(27)	119.36(17)
C(23)-C(22)-P(1)	121.35(14)
C(27)-C(22)-P(1)	119.17(13)
C(22)-C(23)-C(24)	119.89(19)
C(22)-C(23)-H(23A)	120.1
C(24)-C(23)-H(23A)	120.1
C(25)-C(24)-C(23)	120.48(19)
C(25)-C(24)-H(24A)	117.4(17)
C(23)-C(24)-H(24A)	122.1(17)
C(24)-C(25)-C(26)	120.4(2)
C(24)-C(25)-H(25A)	115.9(14)
C(26)-C(25)-H(25A)	123.8(14)
C(25)-C(26)-C(27)	120.1(2)
C(25)-C(26)-H(26A)	119.9
C(27)-C(26)-H(26A)	119.9
C(26)-C(27)-C(22)	119.77(18)
C(26)-C(27)-H(27A)	120.1
C(22)-C(27)-H(27A)	120.1
O(2)-C(28)-O(1)	125.3(2)

O(2)-C(28)-C(29)	120.5(2)
O(1)-C(28)-C(29)	114.1(2)
C(28)-C(29)-H(29A)	109.5
C(28)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(28)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
O(4)-C(30)-O(3)	124.87(18)
O(4)-C(30)-C(31)	120.6(2)
O(3)-C(30)-C(31)	114.6(2)
C(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
Cl(2)-C(32)-Cl(1)	111.9(3)
Cl(2)-C(32)-H(32A)	109.2
Cl(1)-C(32)-H(32A)	109.2
Cl(2)-C(32)-H(32B)	109.2
Cl(1)-C(32)-H(32B)	109.2
H(32A)-C(32)-H(32B)	107.9

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for YOY6. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pd(1)	25(1)	32(1)	39(1)	-2(1)	-10(1)	-8(1)
P(1)	24(1)	32(1)	35(1)	1(1)	-6(1)	-8(1)
O(1)	33(1)	43(1)	69(1)	-9(1)	-11(1)	-16(1)
O(2)	59(1)	76(1)	68(1)	-22(1)	6(1)	-32(1)
O(3)	33(1)	49(1)	49(1)	-6(1)	-16(1)	-4(1)
O(4)	61(1)	70(1)	50(1)	-9(1)	-7(1)	-20(1)
N(1)	31(1)	32(1)	39(1)	-3(1)	-10(1)	-8(1)
C(1)	31(1)	35(1)	43(1)	-7(1)	-10(1)	-5(1)
C(2)	51(1)	46(1)	59(1)	-12(1)	-19(1)	-17(1)
C(3)	66(1)	44(1)	73(1)	-7(1)	-17(1)	-28(1)
C(4)	59(1)	37(1)	58(1)	-1(1)	-9(1)	-20(1)
C(5)	116(2)	56(1)	71(2)	12(1)	-14(2)	-51(1)
C(6)	145(2)	70(1)	58(2)	21(1)	-18(2)	-56(2)
C(7)	99(2)	69(1)	44(1)	10(1)	-19(1)	-38(1)
C(8)	65(1)	50(1)	41(1)	3(1)	-14(1)	-25(1)
C(9)	39(1)	35(1)	42(1)	0(1)	-8(1)	-10(1)
C(10)	29(1)	45(1)	37(1)	-6(1)	-9(1)	-6(1)
C(11)	27(1)	45(1)	36(1)	-1(1)	-7(1)	-9(1)
C(12)	40(1)	55(1)	41(1)	6(1)	-7(1)	-13(1)
C(13)	48(1)	85(2)	34(1)	6(1)	-6(1)	-18(1)
C(14)	47(1)	85(2)	39(1)	-17(1)	-7(1)	-6(1)
C(15)	41(1)	58(1)	45(1)	-15(1)	-12(1)	-2(1)
C(16)	25(1)	33(1)	38(1)	2(1)	-6(1)	-10(1)
C(17)	38(1)	54(1)	45(1)	4(1)	-15(1)	-18(1)
C(18)	40(1)	61(1)	66(1)	7(1)	-22(1)	-25(1)
C(19)	35(1)	66(1)	72(1)	13(1)	-9(1)	-27(1)
C(20)	52(1)	100(2)	45(1)	8(1)	-2(1)	-39(1)
C(21)	40(1)	76(1)	39(1)	1(1)	-8(1)	-28(1)
C(22)	33(1)	34(1)	37(1)	4(1)	-7(1)	-11(1)
C(23)	35(1)	38(1)	45(1)	-3(1)	-9(1)	-9(1)

C(24)	51(1)	37(1)	60(1)	-2(1)	-16(1)	-8(1)
C(25)	70(1)	36(1)	53(1)	4(1)	-17(1)	-21(1)
C(26)	58(1)	52(1)	60(1)	9(1)	-7(1)	-32(1)
C(27)	38(1)	45(1)	61(1)	7(1)	-3(1)	-16(1)
C(28)	50(1)	43(1)	61(1)	-6(1)	-16(1)	-17(1)
C(29)	83(2)	71(1)	139(3)	-48(2)	-6(2)	-39(1)
C(30)	37(1)	30(1)	54(1)	-2(1)	-12(1)	-10(1)
C(31)	45(1)	69(2)	97(2)	-14(2)	-21(1)	11(1)
C(32)	119(3)	111(3)	83(2)	-22(2)	-15(2)	-13(2)
Cl(1)	217(2)	275(2)	144(1)	20(1)	-109(1)	-110(1)
Cl(2)	159(1)	109(1)	137(1)	-2(1)	-26(1)	-20(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for YOY6.

	x	y	z	U(eq)
H(2A)	2310(30)	-20(20)	690(20)	68(8)
H(3A)	1972	-1220	2132	69
H(5A)	2025	-1689	3985	93
H(6A)	2558	-1315	5405	107
H(7A)	3404	204	5376	83
H(8A)	3780	1339	3920	61
H(12A)	2589	4447	-531	57
H(13A)	3419	3576	-2056	70
H(14A)	4092	1586	-2076	72
H(15A)	3910	456	-570	60
H(17A)	-190(30)	3460(20)	889(19)	52(7)
H(18A)	-2471	3348	1694	63
H(19A)	-3108	3185	3425	68
H(20A)	-1523	3186	4385	77
H(21A)	717	3371	3615	60
H(23A)	-265	5741	1644	48
H(24A)	-650(30)	7750(20)	1070(20)	70(8)
H(25A)	1340(20)	8248(19)	394(17)	41(6)
H(26A)	3729	6926	262	67
H(27A)	4073	4996	823	59
H(29A)	4623	5245	3952	190(20)
H(29B)	3177	6163	3714	230
H(29C)	4577	5813	2850	230
H(31A)	9034	-165	1604	142(17)
H(31B)	8248	-353	2728	170
H(31C)	8820	704	2407	170
H(32A)	-1172	-4035	4793	133
H(32B)	-764	-4166	3620	133

Table 6. Torsion angles [°] for YOY6.

O(1)-Pd(1)-P(1)-C(16)	-121.62(8)
N(1)-Pd(1)-P(1)-C(16)	51.21(8)
O(3)-Pd(1)-P(1)-C(16)	132.8(3)
O(1)-Pd(1)-P(1)-C(22)	11.96(8)
N(1)-Pd(1)-P(1)-C(22)	-175.21(8)
O(3)-Pd(1)-P(1)-C(22)	-93.6(3)
O(1)-Pd(1)-P(1)-C(11)	125.35(8)
N(1)-Pd(1)-P(1)-C(11)	-61.82(8)
O(3)-Pd(1)-P(1)-C(11)	19.8(3)
N(1)-Pd(1)-O(1)-C(28)	-21.0(5)
O(3)-Pd(1)-O(1)-C(28)	-123.09(16)
P(1)-Pd(1)-O(1)-C(28)	65.11(15)
O(1)-Pd(1)-O(3)-C(30)	-110.24(14)
N(1)-Pd(1)-O(3)-C(30)	76.78(14)
P(1)-Pd(1)-O(3)-C(30)	-4.2(4)
O(1)-Pd(1)-N(1)-C(1)	135.3(4)
O(3)-Pd(1)-N(1)-C(1)	-123.03(13)
P(1)-Pd(1)-N(1)-C(1)	48.54(12)
O(1)-Pd(1)-N(1)-C(9)	-40.1(5)
O(3)-Pd(1)-N(1)-C(9)	61.63(12)
P(1)-Pd(1)-N(1)-C(9)	-126.80(11)
C(9)-N(1)-C(1)-C(2)	-2.1(2)
Pd(1)-N(1)-C(1)-C(2)	-177.26(13)
C(9)-N(1)-C(1)-C(10)	176.07(14)
Pd(1)-N(1)-C(1)-C(10)	0.9(2)
N(1)-C(1)-C(2)-C(3)	1.1(3)
C(10)-C(1)-C(2)-C(3)	-177.09(18)
C(1)-C(2)-C(3)-C(4)	0.6(3)
C(2)-C(3)-C(4)-C(9)	-1.2(3)
C(2)-C(3)-C(4)-C(5)	178.8(2)
C(3)-C(4)-C(5)-C(6)	179.6(3)
C(9)-C(4)-C(5)-C(6)	-0.4(4)
C(4)-C(5)-C(6)-C(7)	1.0(5)

C(5)-C(6)-C(7)-C(8)	-0.8(5)
C(6)-C(7)-C(8)-C(9)	0.0(4)
C(1)-N(1)-C(9)-C(4)	1.4(2)
Pd(1)-N(1)-C(9)-C(4)	177.02(14)
C(1)-N(1)-C(9)-C(8)	-177.90(17)
Pd(1)-N(1)-C(9)-C(8)	-2.3(2)
C(3)-C(4)-C(9)-N(1)	0.3(3)
C(5)-C(4)-C(9)-N(1)	-179.8(2)
C(3)-C(4)-C(9)-C(8)	179.58(19)
C(5)-C(4)-C(9)-C(8)	-0.5(3)
C(7)-C(8)-C(9)-N(1)	180.0(2)
C(7)-C(8)-C(9)-C(4)	0.7(3)
N(1)-C(1)-C(10)-C(15)	143.99(18)
C(2)-C(1)-C(10)-C(15)	-37.8(2)
N(1)-C(1)-C(10)-C(11)	-40.8(2)
C(2)-C(1)-C(10)-C(11)	137.42(19)
C(15)-C(10)-C(11)-C(12)	-1.2(3)
C(1)-C(10)-C(11)-C(12)	-176.38(18)
C(15)-C(10)-C(11)-P(1)	-177.94(15)
C(1)-C(10)-C(11)-P(1)	6.9(2)
C(16)-P(1)-C(11)-C(12)	112.26(16)
C(22)-P(1)-C(11)-C(12)	-1.64(18)
Pd(1)-P(1)-C(11)-C(12)	-126.61(15)
C(16)-P(1)-C(11)-C(10)	-71.13(16)
C(22)-P(1)-C(11)-C(10)	174.97(14)
Pd(1)-P(1)-C(11)-C(10)	49.99(15)
C(10)-C(11)-C(12)-C(13)	0.1(3)
P(1)-C(11)-C(12)-C(13)	176.76(17)
C(11)-C(12)-C(13)-C(14)	0.3(4)
C(12)-C(13)-C(14)-C(15)	0.3(4)
C(13)-C(14)-C(15)-C(10)	-1.4(4)
C(11)-C(10)-C(15)-C(14)	1.9(3)
C(1)-C(10)-C(15)-C(14)	177.2(2)
C(22)-P(1)-C(16)-C(21)	-98.30(17)
C(11)-P(1)-C(16)-C(21)	149.53(16)

Pd(1)-P(1)-C(16)-C(21)	40.78(17)
C(22)-P(1)-C(16)-C(17)	82.06(17)
C(11)-P(1)-C(16)-C(17)	-30.11(17)
Pd(1)-P(1)-C(16)-C(17)	-138.86(14)
C(21)-C(16)-C(17)-C(18)	0.7(3)
P(1)-C(16)-C(17)-C(18)	-179.71(16)
C(16)-C(17)-C(18)-C(19)	-0.1(3)
C(17)-C(18)-C(19)-C(20)	-0.4(4)
C(18)-C(19)-C(20)-C(21)	0.4(4)
C(17)-C(16)-C(21)-C(20)	-0.6(3)
P(1)-C(16)-C(21)-C(20)	179.70(19)
C(19)-C(20)-C(21)-C(16)	0.1(4)
C(16)-P(1)-C(22)-C(23)	-8.39(19)
C(11)-P(1)-C(22)-C(23)	104.44(17)
Pd(1)-P(1)-C(22)-C(23)	-145.60(14)
C(16)-P(1)-C(22)-C(27)	175.58(17)
C(11)-P(1)-C(22)-C(27)	-71.59(19)
Pd(1)-P(1)-C(22)-C(27)	38.37(19)
C(27)-C(22)-C(23)-C(24)	1.5(3)
P(1)-C(22)-C(23)-C(24)	-174.49(17)
C(22)-C(23)-C(24)-C(25)	-0.3(3)
C(23)-C(24)-C(25)-C(26)	-0.7(4)
C(24)-C(25)-C(26)-C(27)	0.5(4)
C(25)-C(26)-C(27)-C(22)	0.8(4)
C(23)-C(22)-C(27)-C(26)	-1.8(3)
P(1)-C(22)-C(27)-C(26)	174.34(19)
Pd(1)-O(1)-C(28)-O(2)	-6.5(3)
Pd(1)-O(1)-C(28)-C(29)	176.7(2)
Pd(1)-O(3)-C(30)-O(4)	-3.6(3)
Pd(1)-O(3)-C(30)-C(31)	176.06(17)

Symmetry transformations used to generate equivalent atoms:

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