Supporting Information for:

Highly Efficient Hydrogenation of Carbon Dioxide to Formate Catalyzed by Iridium(III) Complexes of Imine-diphosphine Ligands

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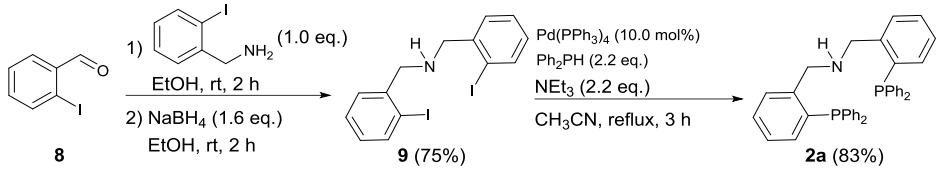
General: Unless otherwise noted, the manipulations which are sensitive to moisture or air were performed in an argon-filled glove box MBRAUN labstar or using standard Schlenk techniques. NMR spectra were recorded on a Bruker AV 400 spectrometer at 400 MHz (^{1}H NMR), 101 MHz (^{13}C NMR) and 162 MHz (^{31}P NMR). Chemical shifts were reported in ppm down field from internal Me_4Si and external 85% H_3PO_4, respectively. Data were presented in the following space: chemical shift, multiplicity, coupling constant in hertz (Hz), and signal area integration in natural numbers. IR spectra were recorded on Nicolet Magna 560 FTIR Spectrometer. High-resolution mass spectra were recorded on an IonSpec FT-ICR mass spectrometer with ESI or MALDI resource.

Hydrogen gas (99.999%) and Carbon oxide gas (99.99%) was purchased from Boc Gas Inc., Tianjin. All the solvents used for reactions were distilled under argon after drying over an appropriate drying agent. $[Ir(COE)_2Cl]_2$ was purchased from Strem Chemicals, Inc. All other commercially available reagents were purchased from Acros, Aldrich and Alfa Aesar Chemical Company. $Pd(PPh_3)_4$ was prepared according to the literature procedure and kept in a refrigerator under argon.[1] $HPPh_2$ were synthesized according to the literature procedure.[2] PNO (**16a, 16b**)[3] and PNN (**14b**)[4] were synthesized according to the literatures.

(A) Preparation and Analytical Data of Ligands

1. Preparation of bis(2-(diphenylphosphino)benzyl)amine 2a



8 **9** (75%) **2a** (83%)

Preparation of bis(2-iodobenzyl)amine 9

To a stirring solution of 2-iodobenzaldehyde **8** (0.6 g, 4.9 mmol) in 15 mL ethanol was added (2-iodophenyl)methanamine (1.2 g, 4.9 mmol). The mixture was stirred at room temperature for 2 h and $NaBH_4$ (0.3 g, 7.9 mmol) was added. The resulting solution was sitrred at this temperature for 2 h to complete the reaction and then was quenched with 10 mL of saturated aqueous $NaHCO_3$, extracted with dichloromethane (3 × 15 mL). The CH_2Cl_2 solution was washed with saturated NaCl solution (30 mL), dried over anhydrous Na_2SO_4 and concentrated in vacuo. The residue was purified by a column chromatography (200-300 mesh silica gel, petroleum ether/ethyl acetate/triethylamine 20:2:1) to provide the desired product bis(2-iodobenzyl)amine **5** as a colorless oil (1.6 g, 75%).

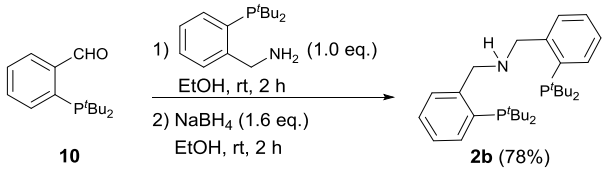
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 7.9, 0.9 Hz, 2H), 7.44 (dd, *J* = 7.6, 1.5 Hz, 2H), 7.34 (td, *J* = 7.5, 1.0 Hz, 2H), 6.97 (td, *J* = 7.7, 1.6 Hz, 2H), 3.85 (s, 4H), 1.92 (brs, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.0, 139.4, 129.8, 128.8, 128.3, 99.8, 57.5. HRMS (ESI) calcd for $C_{14}H_{14}I_2N^+$ ([M + H] $^+$): 449.9210; Found: 449.9205.

Preparation of bis(2-(diphenylphosphino)benzyl)amine 2a

To a stirring solution of bis(2-iodobenzyl)amine **9** (1.8 g, 4.0 mmol) and triethylamine (1.3 mL, 8.8 mmol) in 20 mL degassed acetonitrile was added diphenylphosphine (1.6 g, 8.8 mmol). The reaction mixture was treated with $Pd(PPh_3)_4$ (0.46 g, 0.4 mmol) and stirred under reflux for 3 h. The solution was concentrated to a volume of about 5 mL and diluted with 10 mL diethyl ether. Filtration and washing of the filtercake with diethyl ether /ethyl acetate afforded the desired product bis(2-(diphenylphosphino)benzyl)amine **2a** as a white solid (1.4 g, 88%).

Mp. 149 – 151 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.28 (m, 12H), 7.26 – 7.20 (m, 12H), 7.12 (t, *J* = 7.2 Hz, 2H), 6.84 (dd, *J* = 7.4, 4.6 Hz, 2H), 3.88 (s, 4H), 1.56 (brs, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.4 (d, *J* = 24.2 Hz), 136.8 (d, *J* = 10.7 Hz), 135.6 (d, *J* = 14.0 Hz), 133.9 (d, *J* = 20.0 Hz), 133.4, 129.1 – 128.4 (m), 128.4 – 128.3 (m), 127.0, 51.8 (d, *J* = 21.4 Hz). ^{31}P NMR (162 MHz, $CDCl_3$) δ -15.84 (s). HRMS (ESI) calcd for $C_{38}H_{34}NP_2^+$ ([M + H] $^+$): 566.2161; Found: 566.2165.

2. Preparation of bis(2-(di-*tert*-butylphosphino)benzyl)amine 2b

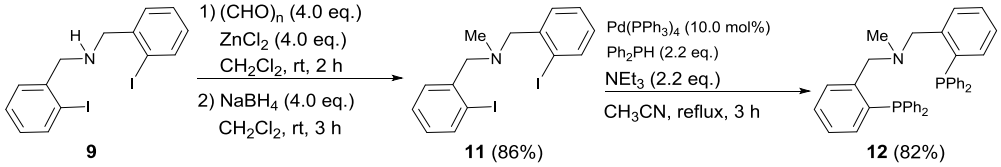


10 **2b** (78%)

Bis(2-(di-*tert*-butylphosphino)benzyl)amine **2b** was prepared according to the procedure for the preparation of bis(2-iodobenzyl)amine **9**.

Colorless oil, 78% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 7.7 Hz, 2H), 7.55 (dd, *J* = 7.2, 3.9 Hz, 2H), 7.33 (t, *J* = 7.4 Hz, 2H), 7.20 (td, *J* = 7.5, 1.0 Hz, 2H), 4.20 (d, *J* = 1.7 Hz, 4H), 2.30 (brs, 1H), 1.18 (d, *J* = 11.9 Hz, 36H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.1, 147.8, 135.4, 135.1, 135.0 (d, *J* = 2.8 Hz), 128.9 (d, *J* = 6.4 Hz), 125.3, 52.9, 52.6, 32.5, 32.3, 30.6 (d, *J* = 15.1 Hz). ^{31}P NMR (162 MHz, $CDCl_3$) δ 13.10 (s). HRMS (ESI) calcd for $C_{30}H_{50}NP_2^+$ ([M + H] $^+$): 486.3413; Found: 486.3425.

3. Preparation of *N*-methyl-bis(2-(diphenylphosphino)benzyl)amine 12



Preparation of *N*-methyl-bis(2-iodobenzyl)amine 11

A mixture of bis(2-iodobenzyl)amine **9** (0.45 g, 1.0 mmol), zinc chloride (0.55 g, 4.0 mmol) and paraformaldehyde (0.12 mg, 4.0 mmol) in dichloromethane (15 mL) was stirred for 2 h at room temperature under dry atmosphere. Sodium borohydride (0.15g. 4.0 mmol) was then added to the reaction mixture and stirring was continued for a further period of 3 h. The reaction was quenched with 10 mL of saturated aqueous $NaHCO_3$ and the whole mixture was stirred for 10 min. The organic layer was separated and the aqueous part was extracted dichloromethane (3 × 15 mL). The CH_2Cl_2 solution was washed with saturated NaCl solution (30 mL), dried over anhydrous Na_2SO_4 and concentrated in vacuo. The residue was purified by a column chromatography (200-300 mesh silica gel, petroleum ether/ethyl acetate 25:1) to provide the desired product *N*-methyl-bis(2-iodobenzyl)amine **11** as a colorless oil (0.4 g, 86%).

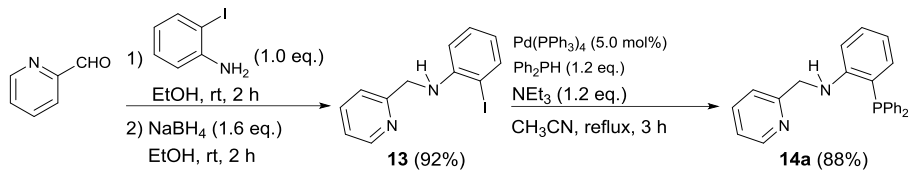
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 7.9, 0.9 Hz, 2H), 7.53 (dd, *J* = 7.7, 1.3 Hz, 2H), 7.32 (td, *J* = 7.5, 0.9 Hz, 2H), 6.94 (td, *J* = 7.7, 1.6 Hz, 2H), 3.65 (s, 4H), 2.25 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.2, 139.4, 130.4, 128.7, 128.1, 100.4, 65.9, 41.9. HRMS (ESI) calcd for $C_{14}H_{14}I_2N^+$ ([M + H] $^+$): 463.9367; Found: 463.9364.

Preparation of *N*-methyl-bis(2-(diphenylphosphino)benzyl)amine 12

N-methyl-bis(2-(diphenylphosphino)benzyl)amine **12** was prepared according to the procedure for the preparation of bis(2-(diphenylphosphino)benzyl)amine **2a**.

Colorless oil, 82% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 – 7.28 (m, 11H), 7.26 – 7.19 (m, 11H), 7.15 (t, *J* = 7.4 Hz, 2H), 7.07 (t, *J* = 7.4 Hz, 2H), 6.81 (dd, *J* = 7.3, 4.5 Hz, 2H), 3.74 (s, 4H), 1.90 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.0 (d, *J* = 22.1 Hz), 137.3 (d, *J* = 10.8 Hz), 135.9 (d, *J* = 14.2 Hz), 133.8 (d, *J* = 19.7 Hz), 133.5, 129.2 (d, *J* = 5.3 Hz), 128.6, 128.4 (d, *J* = 7.0 Hz), 126.8, 60.2 (d, *J* = 21.2 Hz), 40.9. ^{31}P NMR (162 MHz, $CDCl_3$) δ -15.99 (s). HRMS (ESI) calcd for $C_{39}H_{36}NP_2^+$ ([M + H] $^+$): 580.2317; Found: 580.2316.

4. Preparation of 2-(diphenylphosphino)-*N*-(pyridin-2-ylmethyl)aniline 14a



Preparation of 2-iodo-*N*-(pyridin-2-ylmethyl)aniline 13

2-Iodo-*N*-(pyridin-2-ylmethyl)aniline **13** was prepared according to the procedure for the preparation of bis(2-iodobenzyl)amine **9**.

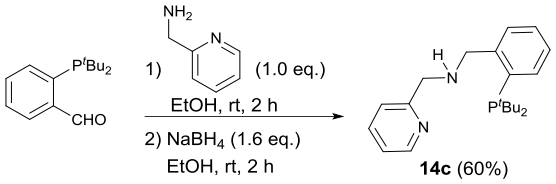
Colorless oil, 92% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.61 (d, *J* = 4.7 Hz, 1H), 7.69 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.64 (td, *J* = 7.7, 1.7 Hz, 1H), 7.31 (d, *J* = 7.8 Hz, 1H), 7.17 (ddd, *J* = 13.7, 8.5, 3.1 Hz, 2H), 6.51 (d, *J* = 8.2 Hz, 1H), 6.49 – 6.40 (m, 1H), 5.29 (brs, 1H), 4.53 (d, *J* = 5.4 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.9, 149.2, 146.9, 139.0, 136.7, 129.4, 122.1, 121.2, 118.9, 111.0, 85.3, 49.5. HRMS (ESI) calcd for $C_{12}H_{12}IN_2^+$ ([M + H] $^+$): 311.0040; Found: 311.0045.

Preparation of 2-(diphenylphosphino)-*N*-(pyridin-2-ylmethyl)aniline 14a

2-(Diphenylphosphino)-*N*-(pyridin-2-ylmethyl)aniline **14a** was prepared according to the procedure for the preparation of bis(2-(diphenylphosphino)benzyl)amine **2a**.

White solid, 88% yield, Mp. 79 – 81 ℃. NMR (400 MHz, $CDCl_3$) δ 8.53 (d, *J* = 4.3 Hz), 7.53 (td, *J* = 7.7, 1.7 Hz), 7.37 (d, *J* = 3.5 Hz), 7.22 – 7.16 (m), 7.15 – 7.05 (m), 6.85 – 6.79 (m), 6.64 (t, *J* = 7.4 Hz), 6.57 (dd, *J* = 8.1, 5.2 Hz), 5.63 (dd, *J* = 12.9, 5.9 Hz), 4.50 (d, *J* = 5.7 Hz). NMR (101 MHz, $CDCl_3$) δ 158.9, 150.3 (d, *J* = 18.3 Hz), 149.1, 136.5, 135.4 (d, *J* = 7.3 Hz), 134.4 (d, *J* = 2.0 Hz), 133.8 (d, *J* = 19.1 Hz), 130.6, 128.8, 128.5 (d, *J* = 7.0 Hz), 121.8, 120.8, 119.3 (d, *J* = 7.7 Hz), 117.5 (d, *J* = 2.1 Hz), 110.6 (d, *J* = 2.5 Hz), 49.4. ^{31}P NMR (162 MHz, $CDCl_3$) δ -21.66 (s). HRMS (ESI) calcd for $C_{24}H_{22}N_2P^+$ ([M + H] $^+$): 369.1515; Found: 369.1508.

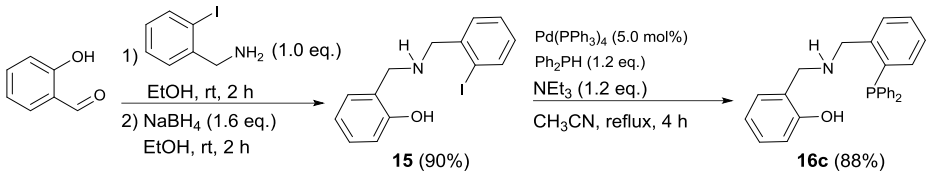
5. Preparation of *N*-(2-(di-*tert*-butylphosphino)benzyl)-1-(pyridin-2-yl)metha-namine 14c



N-(2-(di-tert-butylphosphino)benzyl)-1-(pyridin-2-yl)metha-namine **14c** was prepared according to the procedure for the preparation of bis(2-iodobenzyl)amine **9**.

Colorless oil, 60% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 (s, 1H), 7.74 (d, *J* = 7.1 Hz, 1H), 7.64 (t, *J* = 7.4 Hz, 1H), 7.42 (d, *J* = 7.3 Hz, 2H), 7.32 (t, *J* = 7.3 Hz, 1H), 7.23 (t, *J* = 7.4 Hz, 1H), 7.17 – 7.10 (m, 1H), 4.18 (s, 2H), 3.92 (s, 2H), 1.99 (brs, 1H), 1.19 (d, *J* = 12.0 Hz, 18H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.3, 149.1, 147.3 (d, *J* = 27.0 Hz), 136.3, 135.3 (d, *J* = 3.0 Hz), 129.6 (d, *J* = 3.0 Hz), 129.0, 125.7, 122.1, 121.7, 54.4, 52.9 (d, *J* = 24.2 Hz), 32.5 (d, *J* = 21.9 Hz), 30.6 (d, *J* = 14.7 Hz). ^{31}P NMR (162 MHz, $CDCl_3$) δ 13.43 (s). HRMS (ESI) calcd for $C_{21}H_{32}N_2P^+$ ([M + H] $^+$): 343.2298; Found: 343.2299.

6. Preparation of 2-((2-(diphenylphosphino)benzylamino)methyl) phenol 16c



Preparation of 2-((2-iodobenzylamino)methyl)phenol 15

2-((2-Iodobenzylamino)methyl)phenol **15** was prepared according to the procedure for the preparation of bis(2-iodobenzyl)amine **9**.

Colorless oil, 90% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 7.9 Hz, 1H), 7.33 (t, *J* = 7.4 Hz, 1H), 7.26 (d, *J* = 5.6 Hz, 1H), 7.19 (t, *J* = 7.7 Hz, 1H), 7.00 (dd, *J* = 13.5, 7.3 Hz, 2H), 6.86 (d, *J* = 8.1 Hz, 1H), 6.79 (t, *J* = 7.4 Hz, 1H), 3.97 (s, 2H), 3.87 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.1, 140.2, 139.7, 130.5, 129.5, 128.9, 128.5, 128.6, 122.0, 119.1, 116.4, 99.7, 56.5, 51.4. HRMS (ESI) calcd for $C_{14}H_{15}INO^+$ ([M + H] $^+$): 340.1393; Found: 340.1395.

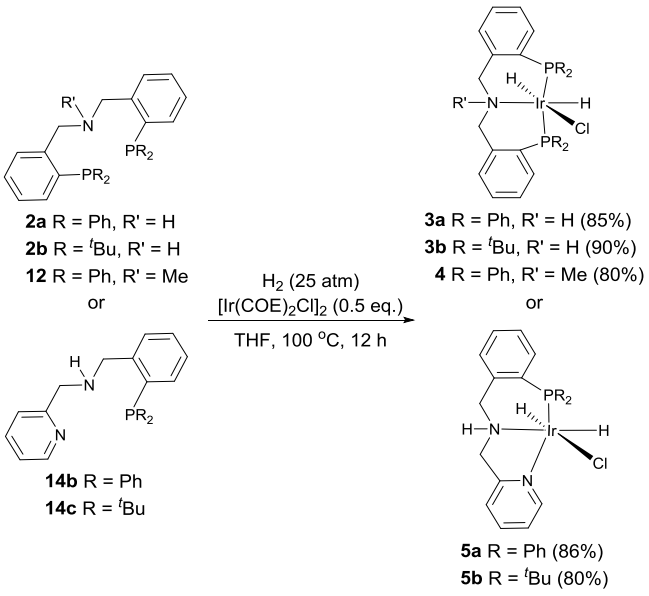
Preparation of 2-((2-(diphenylphosphino)benzylamino)methyl) phenol 16c

2-((2-(Diphenylphosphino)benzylamino)methyl) phenol **16c** was prepared according to the procedure for the preparation of bis(2-(diphenylphosphino)benzyl)amine **2a**.

Colorless oil, 88% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (s, 8H), 7.26 (d, *J* = 4.9 Hz, 5H), 7.21 (t, *J* = 7.1 Hz, 1H), 7.16 (t, *J* = 7.7 Hz, 1H), 6.91 (dd, *J* = 12.9, 6.7 Hz, 2H), 6.83 (d, *J* = 8.0 Hz, 1H), 6.76 (t, *J* = 7.3 Hz, 1H), 3.98 (s, 2H), 3.81 (s, 2H), 1.26 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.2, 142.4, 136.0, 133.9 (d, *J* = 19.8 Hz), 130.3 (d, *J* = 5.2 Hz), 129.1 (d, *J* = 19.2 Hz), 128.7 (dd, *J* = 16.4, 11.3 Hz), 128.0, 122.2, 119.0, 116.3, 51.5, 50.9 (d, *J* = 19.7 Hz). ^{31}P NMR (162 MHz, $CDCl_3$) δ -16.18 (s). HRMS (ESI) calcd for $C_{26}H_{25}NOP^+$ ([M + H] $^+$): 398.1668; Found: 398.1667.

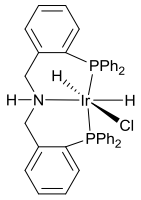
(B) Preparation and Analytical Data of Complexes

1. Preparation and Analytical Data of Complex 3, 4 and 5



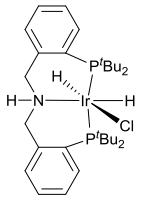
General procedure: To a 50 mL stainless autoclave, $[Ir(COE)_2Cl]_2$ (90 mg, 0.1 mmol), PNP ligand **2a** (113 mg; 0.2 mmol), and THF (6 mL) were charged under argon atmosphere. The mixture was pressurized by hydrogen (25 atm) and stirred at 100 ℃ for 12 hours. The solvent was removed in vacuo and the resulting residue was washed with hexane. Reprecipitation of the residue from THF/hexane gave complex **3a** as a white solid (135 mg, 85%).

Analytical Data of Complex 3a



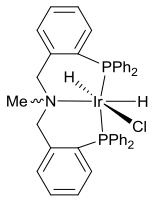
85% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 – 7.80 (m, 3H), 7.53 – 7.28 (m, 23H), 6.93 – 6.85 (m, 2H), 4.54 (t, *J* = 10.5 Hz, 2H), 4.19 (d, *J* = 11.3 Hz, 2H), 3.32 (t, *J* = 8.9 Hz, 1H), -21.14 (td, *J* = 15.9, 7.4 Hz, 1H), -23.95 (td, *J* = 17.3, 8.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.7 (t, *J* = 8.2 Hz), 137.5 (t, *J* = 29.4 Hz), 135.7 (t, *J* = 6.1 Hz), 133.9 (t, *J* = 6.1 Hz), 133.3 (d, *J* = 31.4 Hz), 131.8 (t, *J* = 3.9 Hz), 131.6 (t, *J* = 21.1 Hz), 130.3, 130.0, 129.7, 129.2 (t, *J* = 3.0 Hz), 128.0 (dt, *J* = 10.6, 5.2 Hz), 63.3. ^{31}P NMR (162 MHz, $CDCl_3$) δ 5.24 (t, *J* = 14.1 Hz). HRMS (MALDI) calcd for $C_{38}H_{33}IrNP_2^+$ ($[M - H_2Cl]^+$): 758.1712; Found: 758.1757. IR (KBr, cm^{-1}) ν_{N-H} 3250; ν_{Ir-H} 2242, 2121.

Analytical Data of Complex 3b



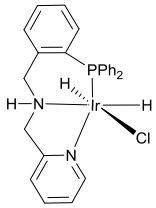
90% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 – 7.92 (m, 2H), 7.43 (t, *J* = 7.4 Hz, 2H), 7.34 (t, *J* = 7.4 Hz, 2H), 7.24 (d, *J* = 7.2 Hz, 2H), 4.49 – 4.25 (m, 4H), 3.81 (brs, 1H), 1.62 (t, *J* = 6.6 Hz, 18H), 1.36 (t, *J* = 6.4 Hz, 18H), -21.87 (td, *J* = 15.8, 7.4 Hz, 1H), -26.04 (td, *J* = 16.9, 7.8 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.7 (t, *J* = 7.1 Hz), 135.0, 132.6, 130.9 (t, *J* = 11.0 Hz), 129.5, 127.1, 63.0, 39.1 (t, *J* = 9.3 Hz), 38.0 (t, *J* = 14.5 Hz), 33.2, 29.9, 26.7. ^{31}P NMR (162 MHz, $CDCl_3$) δ 40.74 (t, *J* = 10.4 Hz). HRMS (MALDI) calcd for $C_{30}H_{47}IrNP_2^+$ ($[M - H_4Cl]^+$): 676.2807; Found: 676.2813. IR (KBr, cm^{-1}) ν_{N-H} 3241; ν_{Ir-H} 2323, 2184.

Analytical Data of Complex 4



80% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 – 7.79 (m, 2H), 7.56 – 7.44 (m, 6H), 7.42 – 7.32 (m, 10H), 7.32 – 7.24 (s, 8H), 7.06 – 6.98 (m, 2H), 6.18 (d, *J* = 12.4 Hz, 1H), 4.83 (d, *J* = 11.7 Hz, 1H), 3.82 (d, *J* = 11.7 Hz, 1H), 3.57 (d, *J* = 12.5 Hz, 1H), 2.38 (s, 1.5H), 2.07 (s, 1.5H), -22.46 – -22.69 (m, 1H), -22.79 (td, *J* = 17.6, 7.8 Hz, 0.5H), -23.78 (td, *J* = 18.7, 7.8 Hz, 0.5H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.0 (t, *J* = 9.1 Hz), 139.9 (t, *J* = 8.6 Hz), 138.2 (t, *J* = 30.7 Hz), 135.5 (t, *J* = 6.2 Hz), 134.5 (t, *J* = 6.0 Hz), 134.3, 134.0 (t, *J* = 6.3 Hz), 133.7 (t, *J* = 6.2 Hz), 133.5 (t, *J* = 3.9 Hz), 133.3 – 133.2 (m), 130.4, 130.2, 129.9, 129.6 (d, *J* = 2.0 Hz), 129.0 (d, *J* = 2.7 Hz), 127.9 – 127.2 (m), 74.0 (t, *J* = 5.3 Hz), 69.2 (t, *J* = 3.8 Hz), 52.5, 46.0. ^{31}P NMR (162 MHz, $CDCl_3$) δ 14.70 (t, *J* = 11.5 Hz), 2.09 (t, *J* = 13.8 Hz). HRMS (MALDI) calcd for $C_{39}H_{33}IrNP_2^+$ ($[M - H_4Cl]^+$): 770.1712; Found: 770.1756. IR (KBr, cm^{-1}) ν_{Ir-H} 2200, 2124.

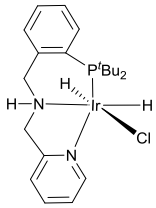
Analytical Data of Complex 5a



86% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.28 (s, 1H), 7.94 – 7.82 (m, 2H), 7.70 (t, *J* = 7.6 Hz 1H), 7.46 – 7.28 (m, 12H), 7.22 – 7.15 (m, 2H), 6.88 (t, *J* = 8.8 Hz,

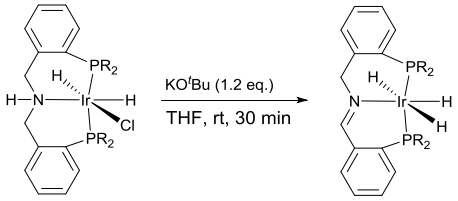
1H), 4.77 (d, *J* = 14.1 Hz, 1H), 4.51 – 4.36 (m, 2H), 4.20 (t, *J* = 11.2 Hz, 1H), 3.88 (t, *J* = 11.2 Hz, 1H), -20.03 (dd, *J* = 21.8, 7.6 Hz, 1H), -23.34 (dd, *J* = 21.3, 8.1 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.4, 156.2, 139.5 (d, *J* = 14.3 Hz), 138.8 (d, *J* = 63.6 Hz) 136.7 (s), 135.3 (d, *J* = 10.7 Hz), 133.9 (d, *J* = 56.4 Hz), 133.3 (d, *J* = 10.7 Hz), 132.5 (d, *J* = 3.3 Hz), 132.0 (d, *J* = 8.5 Hz), 131.6, 130.1 (d, *J* = 9.5 Hz), 129.7, 129.3 (d, *J* = 7.2 Hz), 128.0 (dd, *J* = 14.7, 10.6 Hz), 125.2 (d, *J* = 3.4 Hz), 120.8 (d, *J* = 1.8 Hz), 61.5, 60.3 (d, *J* = 4.8 Hz). ^{31}P NMR (162 MHz, $CDCl_3$) δ 4.60 (d, *J* = 17.6 Hz). HRMS (MALDI) calcd for $C_{25}H_{21}IrN_2P^+$ ([M – H_4Cl] $^+$): 573.1211; Found: 573.1266. IR (KBr, cm^{-1}) $\nu_{N\text{-}H}$ 3162; $\nu_{Ir\text{-}H}$ 2162, 2098.

Analytical Data of Complex 5b



80% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.27 (s, 1H), 7.94 (t, *J* = 7.1 Hz, 1H), 7.69 (t, *J* = 7.6 Hz, 1H), 7.39 (t, *J* = 7.3 Hz, 1H), 7.31 (t, *J* = 7.1 Hz, 2H), 7.22 (d, *J* = 5.2 Hz, 1H), 7.19 – 7.12 (m, 1H), 4.85 (q, *J* = 10.3 Hz, 1H), 4.55 (t, *J* = 11.4 Hz, 1H), 4.40 (d, *J* = 11.9 Hz, 1H), 4.11 (d, *J* = 10.0 Hz, 1H), 1.65 (d, *J* = 13.3 Hz, 9H), 1.30 (d, *J* = 13.2 Hz, 9H), -20.70 (dd, *J* = 19.0, 8.1 Hz, 1H), -24.86 (dd, *J* = 19.8, 8.2 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.3, 156.5, 142.2, 136.3, 134.3, 132.6, 129.6, 127.0 (d, *J* = 5.2 Hz), 124.9, 120.2, 62.6 (d, *J* = 16.7 Hz), 37.5 (dd, *J* = 26.3, 11.2 Hz), 34.6 – 33.7 (m), 28.4. ^{31}P NMR (162 MHz, $CDCl_3$) δ 45.37 (d, *J* = 15.4 Hz). HRMS (MALDI) calcd for $C_{21}H_{29}IrN_2P^+$ ([M – H_4Cl] $^+$): 533.1692; Found: 533.1675. IR (KBr, cm^{-1}) $\nu_{N\text{-}H}$ 3192; $\nu_{Ir\text{-}H}$ 2241, 2146.

2. Preparation and Analytical Data of Complex 1

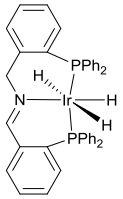


3a R = Ph
3b R = ^{t}Bu

1a R = Ph
1b R = ^{t}Bu

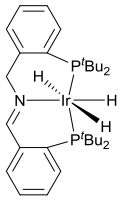
General procedure: Tetrahydrofuran (2 mL) was added to a mixture of $IrH_2Cl[(Ph_2\text{-}PC_6H_4CH_2)_2NH]$ **3a** (80 mg, 0.1 mmol) and KO^{t}Bu (13 mg, 0.12 mmol) and the mixture was stirred for 30 min at room temperature with a color change from green to yellow. Then the mixture was filtered to remove KCl and excess base and the filtrate was evaporated to dryness to afford complex **1a** as solid (57 mg, 75%).

Analytical Data of Complex 1a



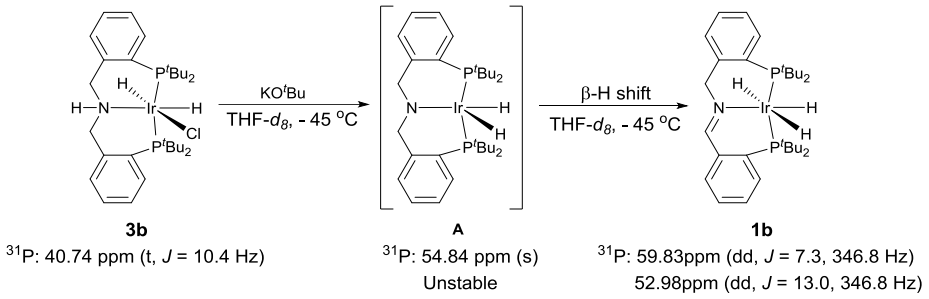
75% yield, ^{1}H NMR (400 MHz, C_6D_6) δ 8.25 – 8.14 (m, 7H), 7.73 (s, 1H), 7.40 – 7.35 (m, 1H), 7.13 – 7.05 (m, 10H), 7.04 – 6.95 (m, 7H), 6.89 – 6.79 (m, 2H), 6.71 (dd, *J* = 7.5, 3.7 Hz, 1H), 5.21 (s, 2H), -9.23 (td, *J* = 18.0, 4.9 Hz, 2H), -18.52 (t, *J* = 18.1 Hz, 1H). ^{31}P NMR (162 MHz, C_6D_6) δ = 22.39 (d, *J* = 367.7 Hz), 12.23 (d, *J* = 367.7 Hz). HRMS (MALDI) calcd for $C_{38}H_{31}IrNP_2^+$ ([M – H_3] $^+$): 756.1555; Found: 756.1570. IR (KBr, cm^{-1}) $\nu_{Ir\text{-}H}$ 2190, 1874, 1720.

Analytical Data of Complex 1b



80% yield, ^{1}H NMR (400 MHz, C_6D_6) δ 8.03 (t, *J* = 5.6 Hz, 1H), 7.94 (t, *J* = 7.2 Hz, 1H), 7.78 (s, 1H), 7.11 (dd, *J* = 7.2, 14.8 Hz, 2H), 6.94 (t, *J* = 5.6 Hz, 2H), 6.90 (t, *J* = 7.2 Hz, 1H), 6.65 (d, *J* = 6.4 Hz, 1H), 5.50 (s, 2H), 1.62 (t, *J* = 13.0 Hz, 36H), -10.77 (t, *J* = 17.4 Hz, 2H), -19.39 (t, *J* = 15.2 Hz, 1H). ^{31}P NMR (162 MHz, THF-d_8) δ 52.98 (dd, *J* = 13.0, 346.8 Hz), 59.83 (dd, *J* = 7.3, 346.8 Hz). ^{13}C NMR (101 MHz, THF-d_8) δ 160.9 (d, *J* = 2.4 Hz), 144.7 (d, *J* = 14.0 Hz), 143.0 (d, *J* = 12.6 Hz), 135.8, 135.3 (t, *J* = 7.1 Hz), 134.5, 133.5, 132.6, 131.5 (d, *J* = 7.5 Hz), 130.2, 129.9 (d, *J* = 3.5 Hz), 129.8, 129.5, 127.7 – 127.5 (m), 81.1 (d, *J* = 7.5 Hz), 36.7 (t, *J* = 18.9 Hz), 34.9 – 31.1 (m), 30.2 (d, *J* = 3.2 Hz). HRMS (MALDI) calcd for $C_{30}H_{47}IrNP_2^+$ ([M – H_3] $^+$): 676.2807; Found: 676.2842. IR (KBr, cm^{-1}) $\nu_{Ir\text{-}H}$ 2207, 1934, 1731.

3. Low-Temperature NMR Spectra of the Reaction of Complex 3b with KO^{t}Bu under -45 °C



3b
^{31}P: 40.74 ppm (t, *J* = 10.4 Hz)

A
^{31}P: 54.84 ppm (s)
Unstable

1b
^{31}P: 59.83ppm (dd, *J* = 7.3, 346.8 Hz)
52.98ppm (dd, *J* = 13.0, 346.8 Hz)

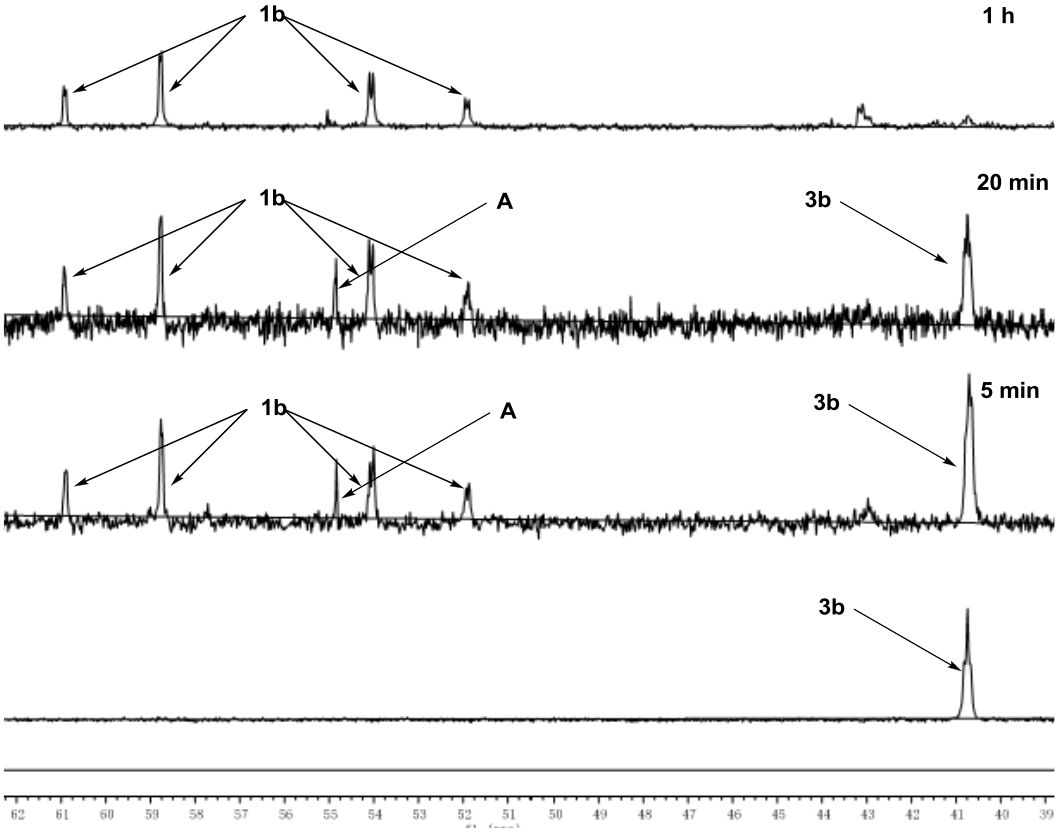


Figure S1. ^{31}P NMR spectra (162 MHz, THF-d_8) of the reaction of complex **3b** with KO^{t}Bu under -45 ^{o}C.

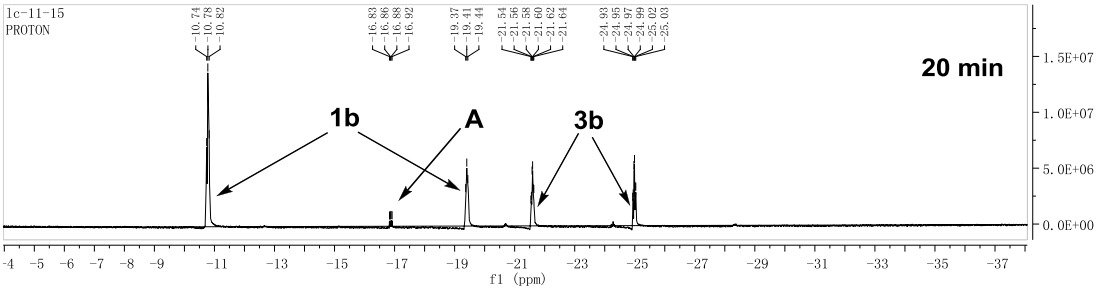
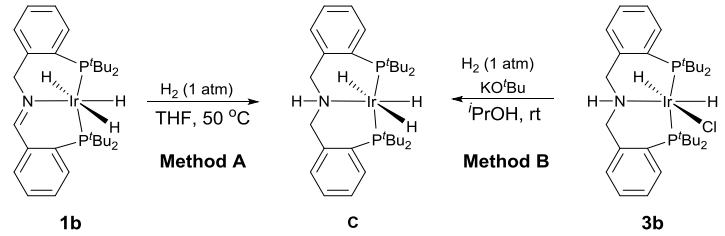


Figure S2. ^{1}H NMR spectra (400 MHz, THF-d_8) of the reaction of complex **3b** with KO^{t}Bu under -45 ^{o}C (hydride region).

4. Preparation and Analytical Data of Complex C

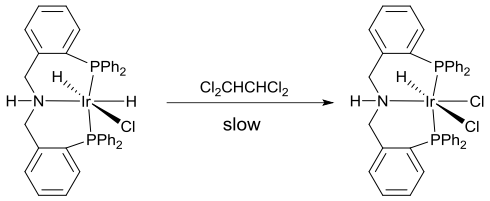


Method A. Exposure of a solution of complex **1b** (68 mg, 0.1 mmol) in THF (3 mL) to 1 atm hydrogen gas for 30 min at 50 ^{o}C resulted in a light-yellow solution. The solvent was removed in vacuo and the resulting residue was washed with hexane. Reprecipitation of the residue from THF/hexane gave complex **C** as a white solid (51 mg, 75%).

Method B. 2-Propanol (3 mL) was added to a mixture of complex **3b** (71 mg, 0.1 mmol) and KO^{t}Bu (13 mg, 0.12 mmol) and the mixture was exposed to 1 atm hydrogen gas for 30 min at room temperature. The mixture was concentrated to 1 mL under reduced pressure. Hexane (2 mL) was then added and the suspension stirred for 20 min. The white solid product was filtered, washed with hexane, and dried under vacuum (54 mg, 80%).

1H NMR (400 MHz, THF-d_8) δ 7.96 (d, J = 6.0 Hz, 2H), 7.29 (t, J = 7.2 Hz, 2H), 7.14 (m, 4H), 4.78 (t, J = 11.5 Hz, 2H), 4.18 (d, J = 11.3 Hz, 2H), 3.83 (t, J = 10.8 Hz, 1H), 1.47 (s, 18H), 1.32 (s, 18H), -11.28 (t, J = 14.3 Hz, 1H), -11.53 (t, J = 18.7 Hz, 1H), -23.80 (t, J = 17.7 Hz, 1H). 31P NMR (162 MHz, THF-d_8) δ 57.70 (d, J = 13.2 Hz). HRMS (MALDI) calcd for $C_{30}H_{47}IrNP_2^+$ ([M – H_5] $^+$): 676.2807; Found: 676.2807. IR (KBr, cm^{-1}) $\nu_{N\text{-}H}$ 3297; $\nu_{Ir\text{-}H}$ 2195, 1736.

5. X-ray Structure of Complex B



3a **B**

In a 20 mL Schlenk tube, 25 mg complex 3a was resolved again with 2.5 mL hot 1,1,2,2-tetrachloroethane. After slowly evaporation of solvent at ambient temperature in an argon-filled glove box, colorless crystal suitable for X-ray diffraction analysis was obtained. The crystal was determined as [IrH(**2a**)Cl_2] by X-ray diffraction analysis at 293 K on a Rigaku 007 Saturn 70 CCD diffractometer. The density of the disordered solvent molecule was flattened by using the SQUEEZE option of PLATON. [5]

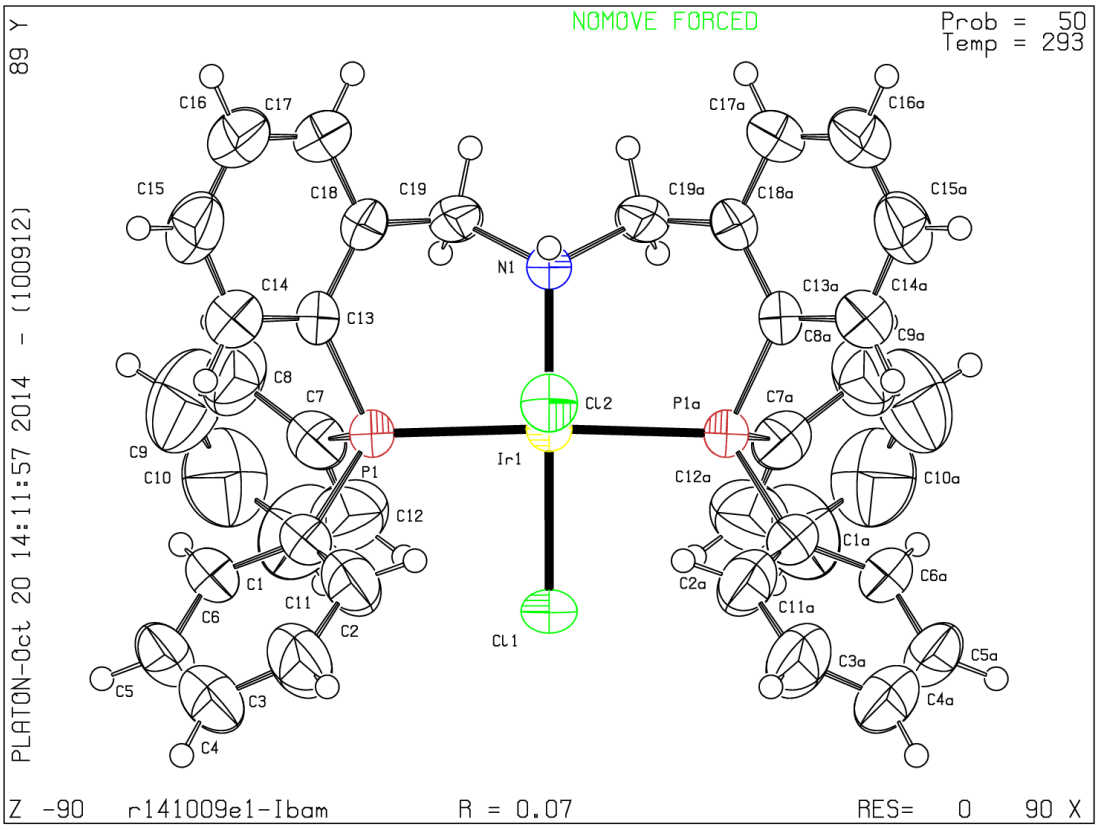


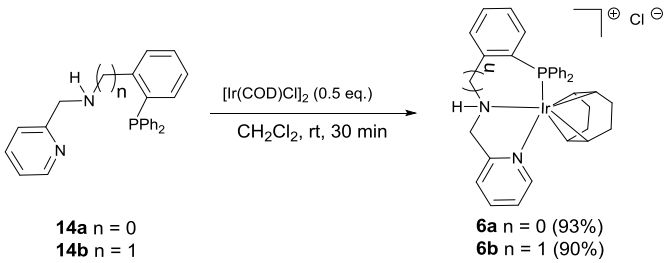
Figure S3. Single-crystal X-ray structure of complex **B**, showing 50% probability displacement ellipsoids and the atom numbering scheme.

Table S1. Crystal data and structure of refinement for complex **B**.

Identification code	R141009e1-sr
Empirical formula	$C_{38}H_{34}Cl_2IrNP_2$
Formula weight	829.70
Temperature	293(2) K
Wavelength	0.71073 Å

Crystal system, space group	Orthorhombic, Ibam
Unit cell dimensions	a = 30.868(6) Å α = 90 deg. b = 17.517(4) Å β = 90 deg. c = 24.155(5) Å γ = 90 deg.
Volume	13061(5) $Å^3$
Z, Calculated density	8, 0.844 Mg/m^3
Absorption coefficient	2.190 mm^{-1}
F(000)	3280
Crystal size	0.20 × 0.18 × 0.16 mm
Theta range for data collection	1.95 to 27.89 deg.
Limiting indices	-40≤h≤40, -22≤k≤22, -31≤l≤31
Reflections collected / unique	79545/7979 [R(int) = 0.0814]
Completeness to theta = 27.89	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7208 and 0.6685
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7979/1/208
Goodness-of-fit on F^2	1.115
Final R indices [I>2σ(I)]	R1 = 0.0719, wR2 = 0.2005
R indices (all data)	R1 = 0.0988, wR2 = 0.2174
Extinction coefficient	0.00033(6)
Largest diff. peak and hole	2.484 and -1.703 e. $Å^{-3}$

6. Preparation and Analytical Data of Complex 6

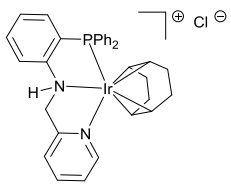


14a n = 0
14b n = 1

6a n = 0 (93%)
6b n = 1 (90%)

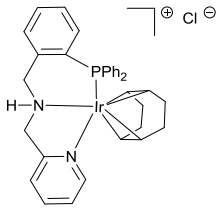
General procedure: $[Ir(COD)Cl]_2$ (34 mg, 0.05 mmol), PNN ligand **14a** (37 mg, 0.1 mmol) and degassed dicholomethane (5 mL) were added to a dry 10 mL Schlenk tube under argon atmosphere and the mixture was stirred at room temperature for 1 h. The reaction mixture was concentrated in vacuo to give complex **6a** as a light yellow solid (65 mg, 93 %).

Analytical Data of Complex 6a



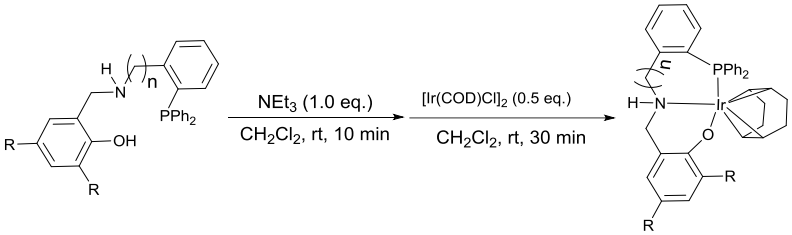
93% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.04 (s, 1H), 8.38 (d, *J* = 4.8 Hz, 1H), 7.83 – 7.75 (m, 2H), 7.51 (d, *J* = 7.6 Hz, 1H), 7.47 – 7.39 (m, 5H), 7.29 (t, *J* = 6.5 Hz, 1H), 7.24 – 7.11 (m, 4H), 7.06 (t, *J* = 7.6 Hz, 1H), 6.70 (s, 1H), 6.63 (t, *J* = 8.3 Hz, 2H), 5.16 (d, *J* = 15.8 Hz, 1H), 4.69 (d, *J* = 16.2 Hz, 1H), 4.08 (s, 2H), 3.93 (s, 2H), 2.38 – 2.30 (m, 2H), 2.15 – 2.00 (m, 4H), 1.63 – 1.51 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.3, 157.1 (d, *J* = 25.1 Hz), 147.9, 136.7, 134.1 (d, *J* = 9.7 Hz), 133.5 – 132.5 (m), 131.6 – 130.9 (m), 130.3 – 129.8 (m), 129.8–128.8 (m), 128.5 (d, *J* = 11.0 Hz), 127.8 (d, *J* = 11.1 Hz), 127.0 (d, *J* = 10.7 Hz), 123.8 (s), 121.6, 68.0, 62.2, 58.8 (d, *J* = 15.8 Hz), 35.9 (d, *J* = 4.7 Hz), 29.6, 27.9. ^{31}P NMR (162 MHz, $CDCl_3$) δ 31.24 (s). HRMS (MALDI) calcd for $C_{32}H_{33}IrN_2P^+$ ([M - Cl] $^+$): 669.2005; Found: 669.2006. IR (KBr, cm^{-1}) $\nu_{N\text{-}H}$ 3340.

Analytical Data of Complex 6b



90% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.56 (d, *J* = 5.3 Hz, 1H), 7.92 – 7.82 (m, 3H), 7.56 (t, *J* = 7.6 Hz, 1H), 7.50 (d, *J* = 6.9 Hz, 1H), 7.47 – 7.43 (m, 2H), 7.43 – 7.35 (m, 3H), 7.29 – 7.26 (m, 1H), 7.19 (dd, *J* = 13.2, 6.8 Hz, 3H), 7.02 – 6.89 (m, 4H), 4.74 (dd, *J* = 17.2, 7.0 Hz, 1H), 4.41 – 4.34 (m, 1H), 4.12 (dd, *J* = 31.2, 15.3 Hz, 2H), 3.72 (t, *J* = 7.0 Hz, 2H), 3.52 – 3.44 (m, 2H), 2.53 – 2.41 (m, 2H), 2.18 – 2.04 (m, 4H), 1.60 – 1.50 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.9, 148.2, 138.1 (d, *J* = 16.5 Hz), 137.2, 134.7 (d, *J* = 13.7 Hz), 132.6 (d, *J* = 9.9 Hz), 132.3 (d, *J* = 7.9 Hz), 131.3 – 131.0 (m), 130.6, 130.2 (d, *J* = 2.3 Hz), 129.9, 129.4 (d, *J* = 5.7 Hz), 128.9 (d, *J* = 10.4 Hz), 128.5 – 128.1 (m), 123.0, 120.6, 62.8, 61.9, 58.7 (dd, *J* = 15.6, 8.1 Hz), 36.2, 29.4. ^{31}P NMR (162 MHz, $CDCl_3$) δ 4.75 (s). HRMS (MALDI) calcd for $C_{33}H_{35}IrN_2P^+$ ([M - Cl] $^+$): 683.2162; Found: 683.2163. IR (KBr, cm^{-1}) $\nu_{N\text{-}H}$ 3327.

7. Preparation and Analytical Data of Complex 7

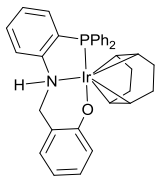


16a n = 0, R = H
16b n = 0, R = ^{t}Bu
16c n = 1, R = H

7a n = 0, R = H (85%)
7b n = 0, R = ^{t}Bu (88%)
7c n = 1, R = H (80%)

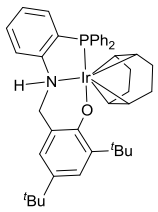
General procedure: To a stirring solution of PNO ligand **16a** (38 mg, 0.1 mmol) in 5 mL degassed dichloromethane was added triethylamine (14.6 μL, 0.1 mmol) under argon atmosphere. The mixture was stirred at room temperature for 10 min and $[Ir(COD)Cl]_2$ (34 mg, 0.05 mmol) in 2 mL degassed dichloromethane was added. The resulting solution was sitrred at this temperature for 30 min to complete the reaction. The reaction mixture was filtered and the filtrate was concentrated in vacuo to give complex **7a** as a brownish red solid (58 mg, 85 %).

Analytical Data of Complex 7a



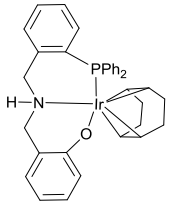
85% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.00 (brs, 1H), 7.74 – 7.51 (m, 4H), 7.41 (m, 6H), 7.16 (d, *J* = 7.4 Hz, 1H), 7.05 (dd, *J* = 17.5, 9.6 Hz, 2H), 6.98 (t, *J* = 7.2 Hz, 1H), 6.81 (t, *J* = 7.3 Hz, 1H), 6.68 (d, *J* = 7.8 Hz, 1H), 6.65 – 6.56 (m, 1H), 6.42 – 6.32 (m, 1H), 5.31 – 4.71 (m, 4H), 3.00 – 2.65 (m, 2H), 2.34 – 2.11 (m, 4H), 1.99 – 1.76 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.7, 133.1, 130.6, 128.7, 128.6, 128.4, 127.2, 125.3, 120.1 (d, *J* = 55.4 Hz), 119.5, 116.5, 116.3, 113.8, 94.0, 60.4, 55.9, 54.8, 32.7, 31.9, 30.1, 28.0. ^{31}P NMR (162 MHz, $CDCl_3$) δ 27.72 (s). HRMS (MALDI) calcd for $C_{33}H_{34}IrNOP^+$ ([M + H] $^+$): 684.2002; Found: 684.2001. IR (KBr, cm^{-1}) $\nu_{N\text{-}H}$ 3198.

Analytical Data of Complex 7b



88% yield.^{1}H NMR (400 MHz, $CDCl_3$) δ 8.88 (brs, 1H), 7.74 – 7.56 (m, 4H), 7.45 – 7.37 (m, 7H), 7.12 – 6.93 (m, 5H), 6.67 (dd, J = 8.2, 5.7 Hz, 1H), 6.33 (t, J = 7.1 Hz, 1H), 5.43 – 4.63 (m, 4H), 2.35 – 2.26 (m, 2H), 2.24 – 2.13 (m, 2H), 1.99 – 1.83 (m, 4H), 1.34 – 1.30 (m, 18H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.6 (d, *J* = 24.0 Hz), 153.9, 140.4, 135.4, 133.1, 132.7, 130.49 (s), 128.62 (d, *J* = 10.3 Hz), 124.2, 123.6, 121.5, 120.5 (d, *J* = 55.6 Hz), 115.9 (d, *J* = 7.6 Hz), 113.9 (d, *J* =12.3 Hz), 56.60 (s), 54.7 – 53.9 (m), 34.9, 34.2, 32.8, 31.7, 31.6, 30.0, 29.6, 28.0, 26.9. ^{31}P NMR (162 MHz, $CDCl_3$) δ 28.51 (s). HRMS (MALDI) calcd for $C_{41}H_{50}IrNOP^+$ ([M + H] $^+$): 796.3254; Found: 796.3252. IR (KBr, cm^{-1}) $\nu_{N\text{-}H}$ 3178.

Analytical Data of Complex 7c



80% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 – 7.65 (m, 2H), 7.53 – 7.43 (m, 6H), 7.43 – 7.32 (m, 3H), 7.20 (d, *J* = 7.8 Hz, 1H), 7.13 (t, *J* = 7.2 Hz, 1H), 7.08 – 7.01 (m, 1H), 6.82 (d, J = 6.9 Hz, 1H), 6.69 (t, J = 7.2 Hz, 1H), 4.12 (s, 2H), 4.07 – 3.70 (m, 4H), 2.33 – 2.08 (m, 4H), 1.88 – 1.59 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.7 (d, *J* = 15.5 Hz), 134.2 (d, *J* = 9.3 Hz), 133.3 (d, *J* = 9.0 Hz), 132.4, 131.8 (d, *J* = 9.8 Hz), 131.2, 130.9, 130.7, 130.0, 129.8 (d, *J* = 6.5 Hz), 128.9 (d, *J* = 10.5 Hz), 128.6, 121.2, 120.2 – 118.3 (m), 53.0, 31.4 – 30.8 (m), 27.9. ^{31}P NMR (162 MHz, $CDCl_3$) δ 8.97 (s). HRMS (MALDI) calcd for $C_{34}H_{36}IrNOP^+$ ([M + H] $^+$): 698.2158; Found: 698.2160. IR (KBr, cm^{-1}) $\nu_{N\text{-}H}$ 3290.

(C) General Procedure for Hydrogenation of Carbon Dioxide

Hydrogenation of CO_2 at S/C = 100,000. A stock solution of complex **1b** (5.0×10^{-4} mmol/mL) was made by dissolving complex **1b** (1.8 mg, 0.0025 mmol) in degassed dry THF (5 mL). To the 30 mL stainless autoclave the solution of catalyst (100 μL) and degassed aqueous KOH (1.00 M, 5.00 mL) were charged. Then the autoclave was tightened and purged three times with argon and three times with CO_2 before it was pressurized by CO_2 and then by H_2 so that the CO_2/H_2 ratio to be 1/1 with 60 atm total initial pressure. The reaction mixture was stirred at 140 ^{o}C for 20 h. Sodium 3-(trimethylsilyl)-1-propanesulfonate (14.0 mg, 64.0 μmol) was added to the reaction mixture as an internal standard and an aliquot (0.5mL) of the reaction mixture was removed and the solvent evaporated in vacuo. The obtained white solid was dissolved in D_2O for an estimation of the yield by using ^{1}H NMR spectrum. The same reaction was repeated at least twice to confirm the reproducibility.

Hydrogenation of CO_2 at S/C = 1,000,000. A stock solution of complex **1b** (2.5×10^{-4}

mmol/mL) was made by dissolving complex **1b** (1.8 mg, 0.0025 mmol) in degassed dry THF (10 mL). To the 30 mL stainless autoclave the solution of catalyst (100 μL) and degassed aqueous KOH (5.00 M, 5.00 mL) were charged. Then the autoclave was tightened and pressurized by CO_2 to 20 atm and then by H_2 so that the total pressure to 60 atm. The reaction mixture was stirred at 140 ^oC for 20 h. Sodium 3-(trimethylsilyl)-1-propanesulfonate (35.0 mg, 0.16 mmol) was added to the reaction mixture as an internal standard and an aliquot (0.5 mL) of the reaction mixture was removed and the solvent evaporated in vacuo. The obtained white solid was dissolved in D_2O for an estimation of the yield by using ^1H NMR spectrum. A representative spectrum of the reaction mixture is shown in (**E**). The same reaction was repeated at least twice to confirm the reproducibility.

References

[1] D. R. Coulson, L. C. Satek, S. O. Grim, in *Inorg. Synth.*, John Wiley & Sons, Inc., **2007**, pp. 121-124.

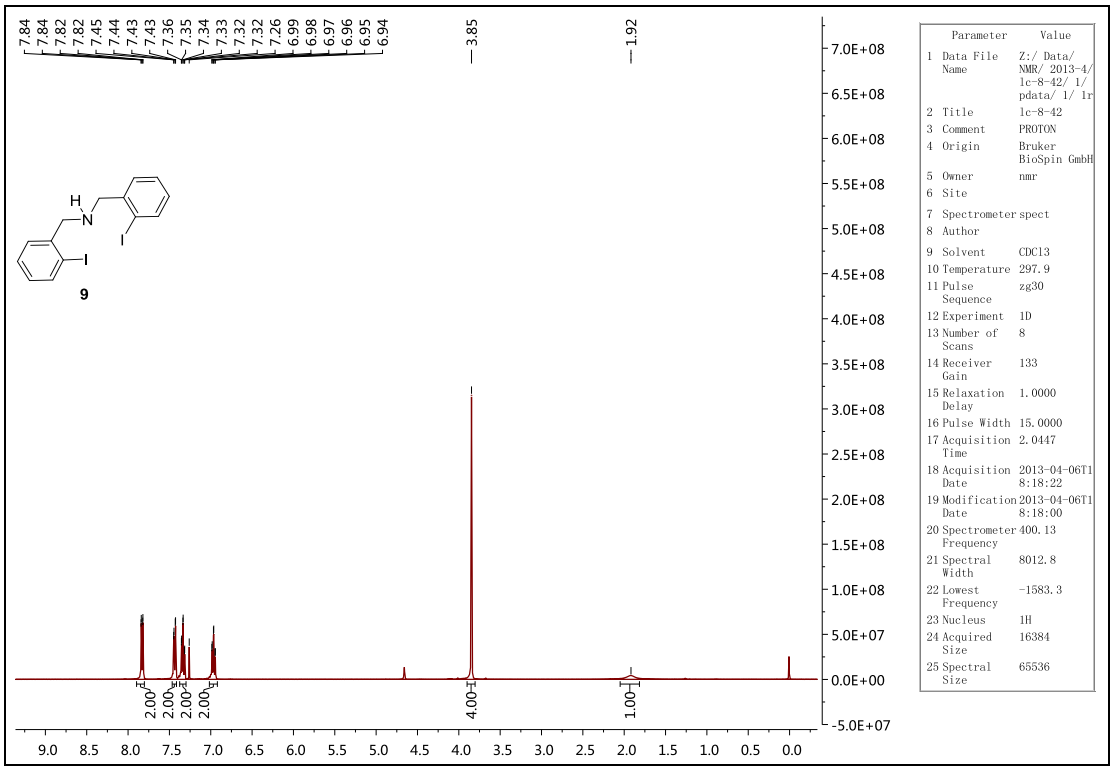
[2] J. Meiners, A. Friedrich, E. Herdtweck, S. Schneider, *Organometallics* **2009**, *28*, 6331-6338.

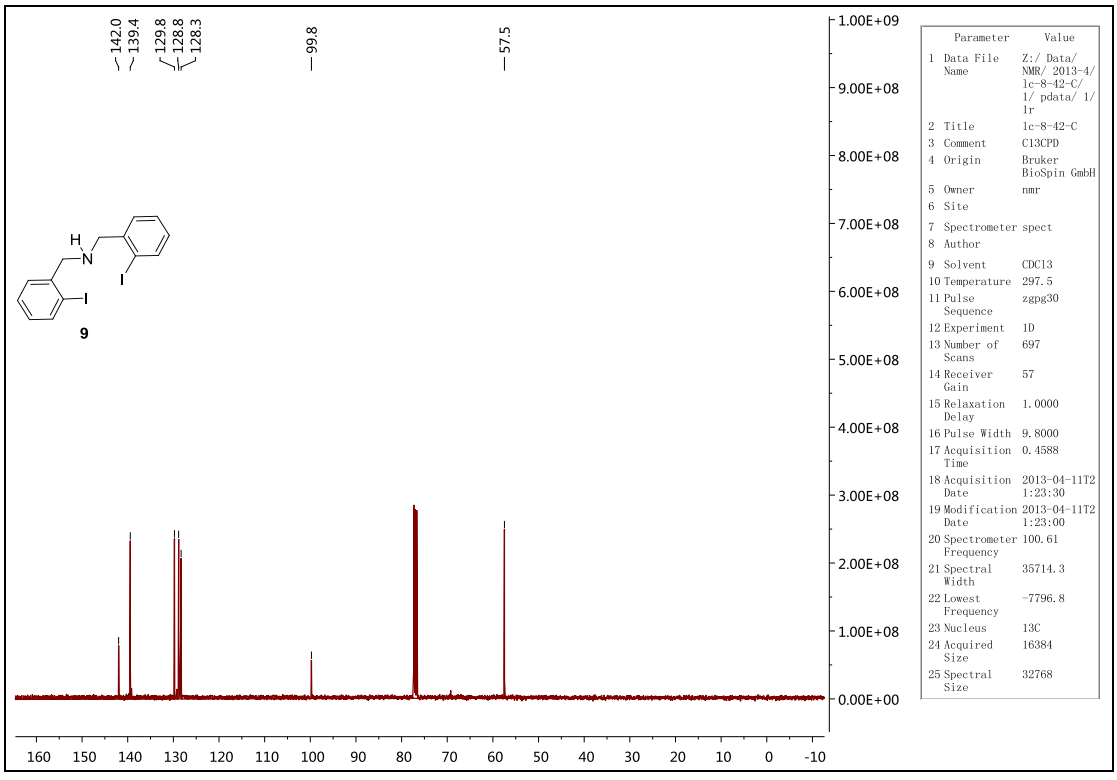
[3] W.-G. Hu, X.-L. Sun, C. Wang, Y. Gao, Y. Tang, L.-P. Shi, W. Xie, J. Sun, H.-L. Dai, X.-Q. Li, X.-L. Yao, X.-R. Wang, *Organometallics* **2004**, *23*, 1684-1688.

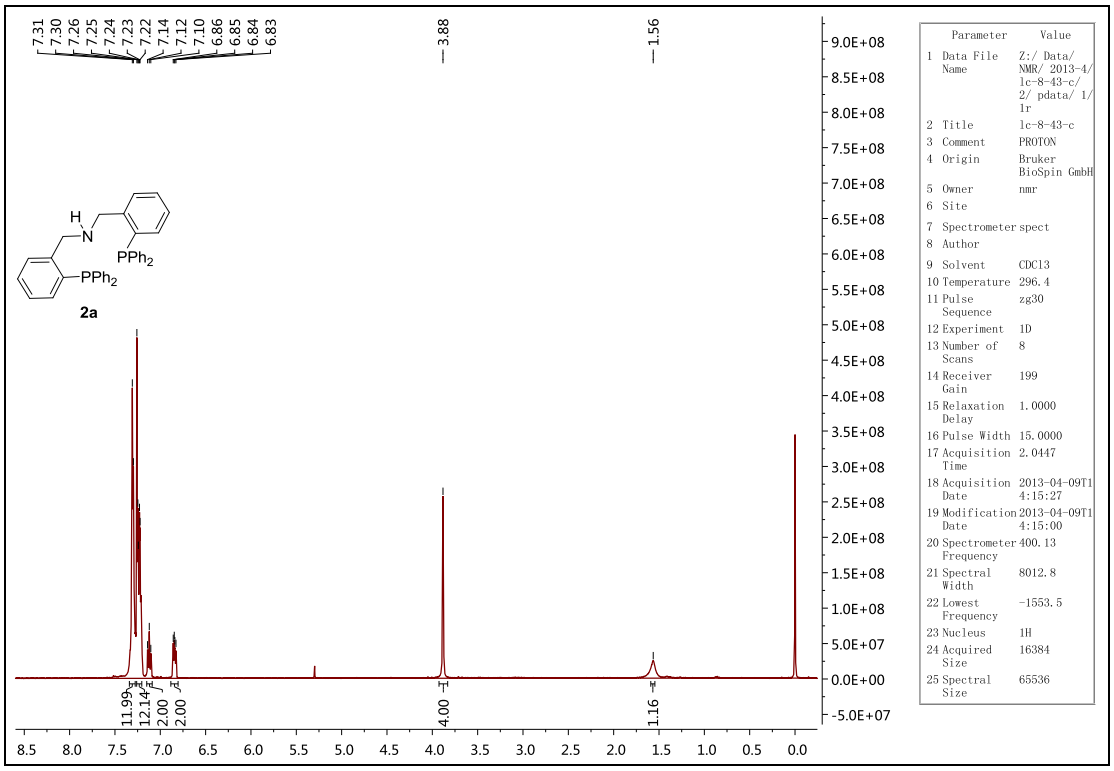
[4] A. Del Zotto, W. Baratta, M. Ballico, E. Herdtweck, P. Rigo, *Organometallics* **2007**, *26*, 5636-5640.

[5] P. v. d. Sluis, A. L. Spek, *Acta Crystallogr. Sect. A* **1990**, *46*, 194-201.

(D) NMR Spectra of New Compounds







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8	Author	
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11	Pulse Sequence	zg30
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16	Pulse Width	15.0000
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22	Lowest Frequency	-1553.5
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24	Acquired Size	16384
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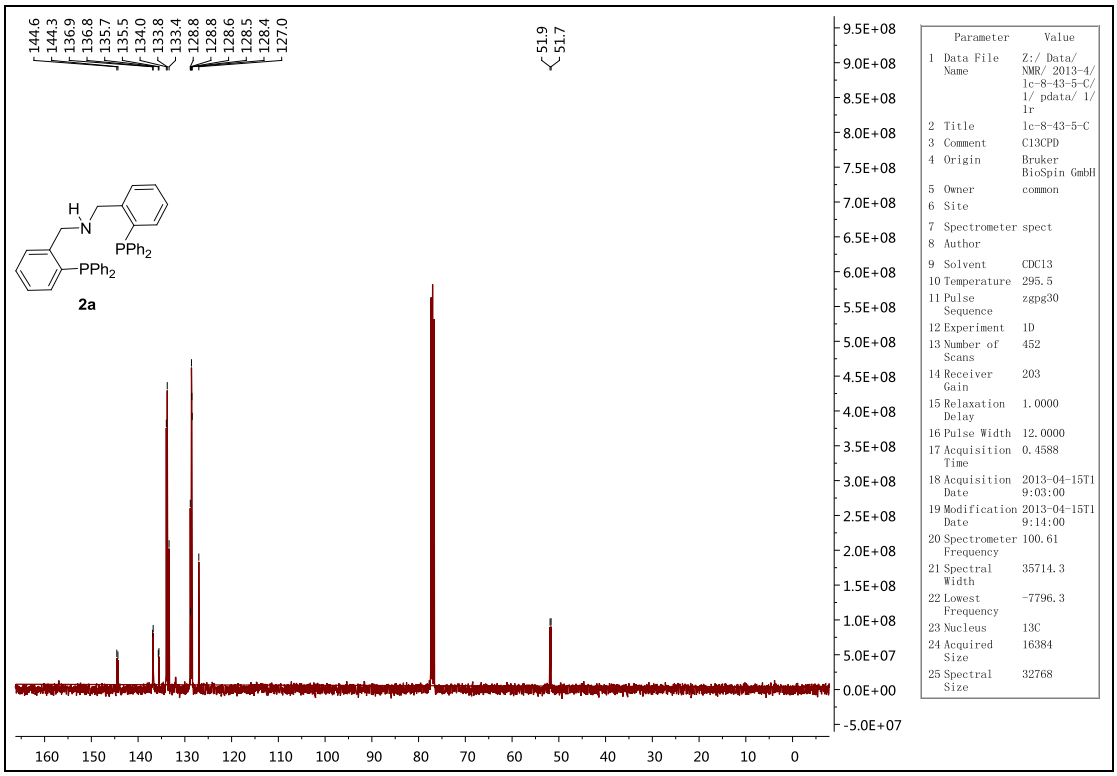

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24	Acquired Size	16384
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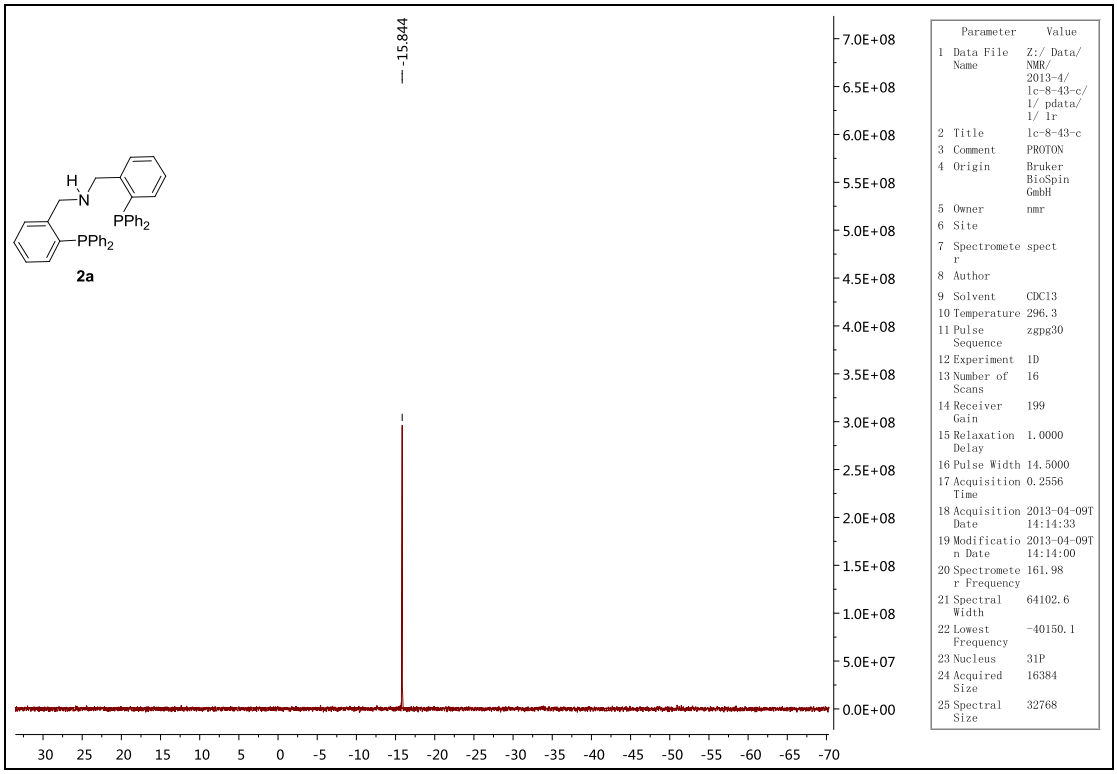

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7 Spectrometer	spect
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23 Nucleus	31P
24 Acquired Size	16384
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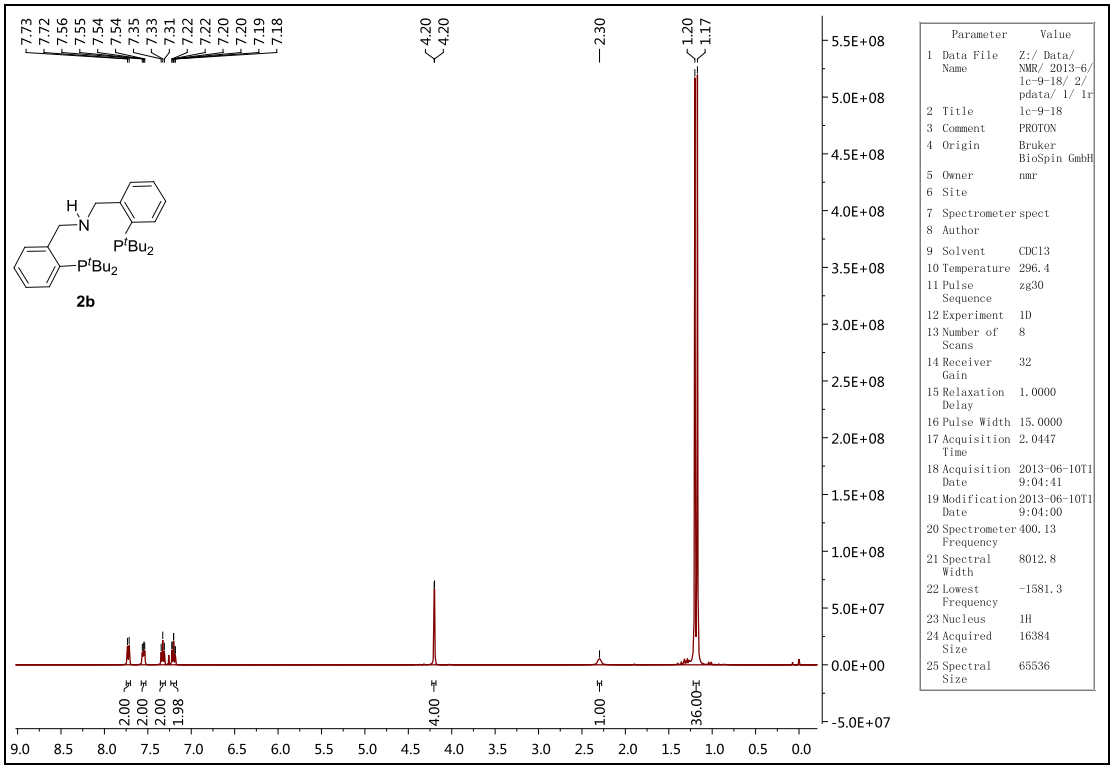

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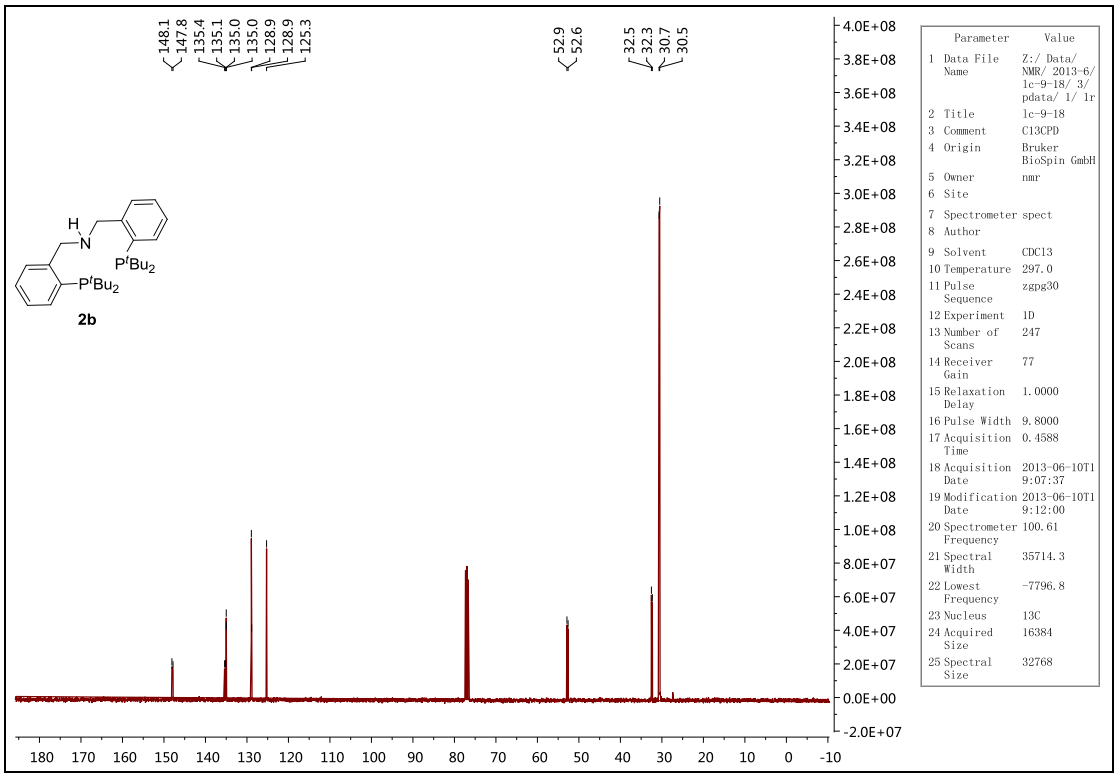
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7 Spectrometer spect
8 Author
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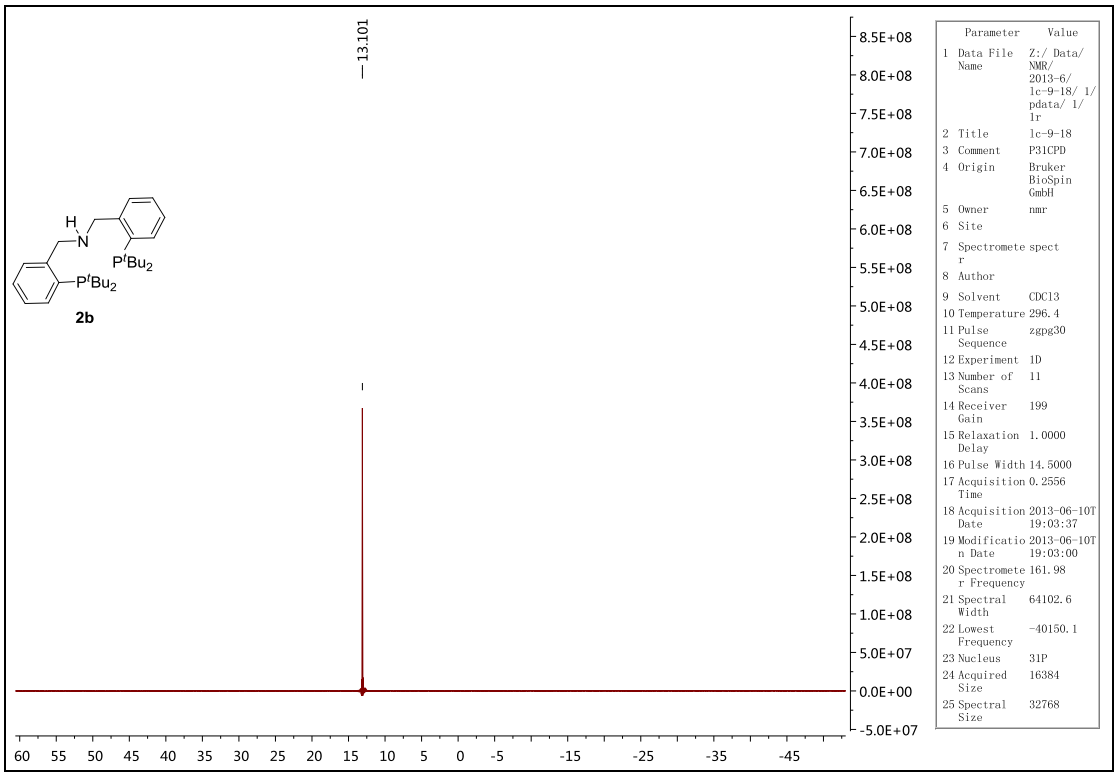
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8 Author
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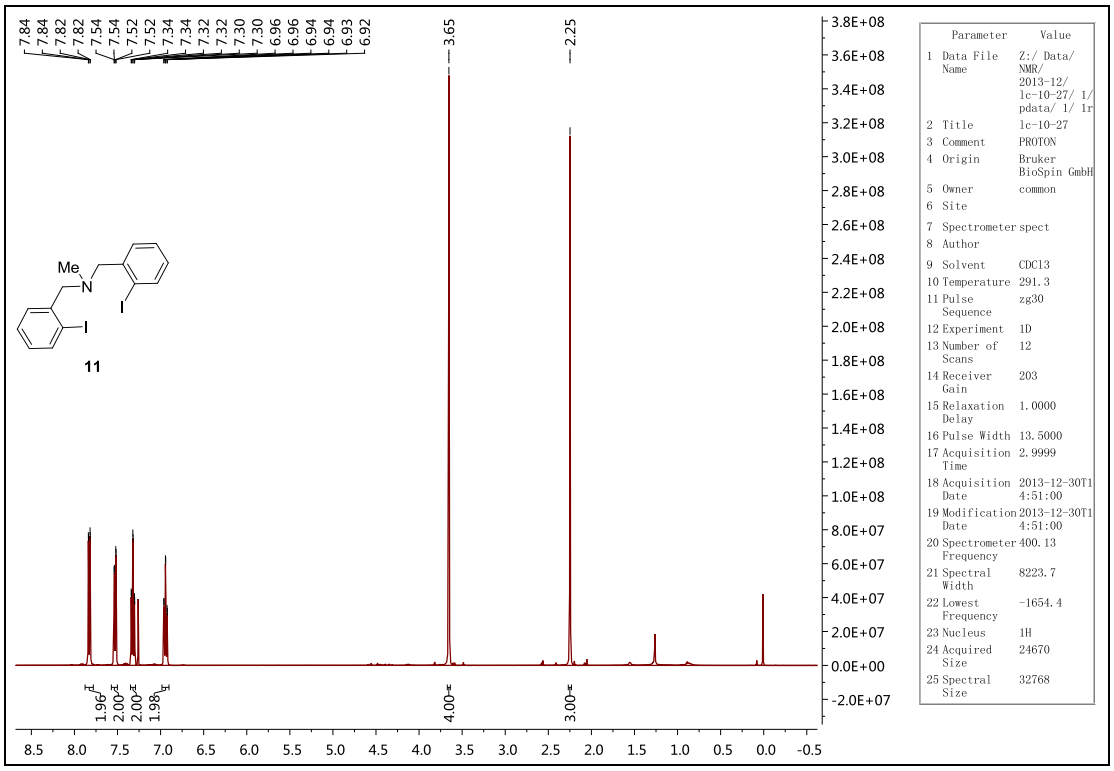

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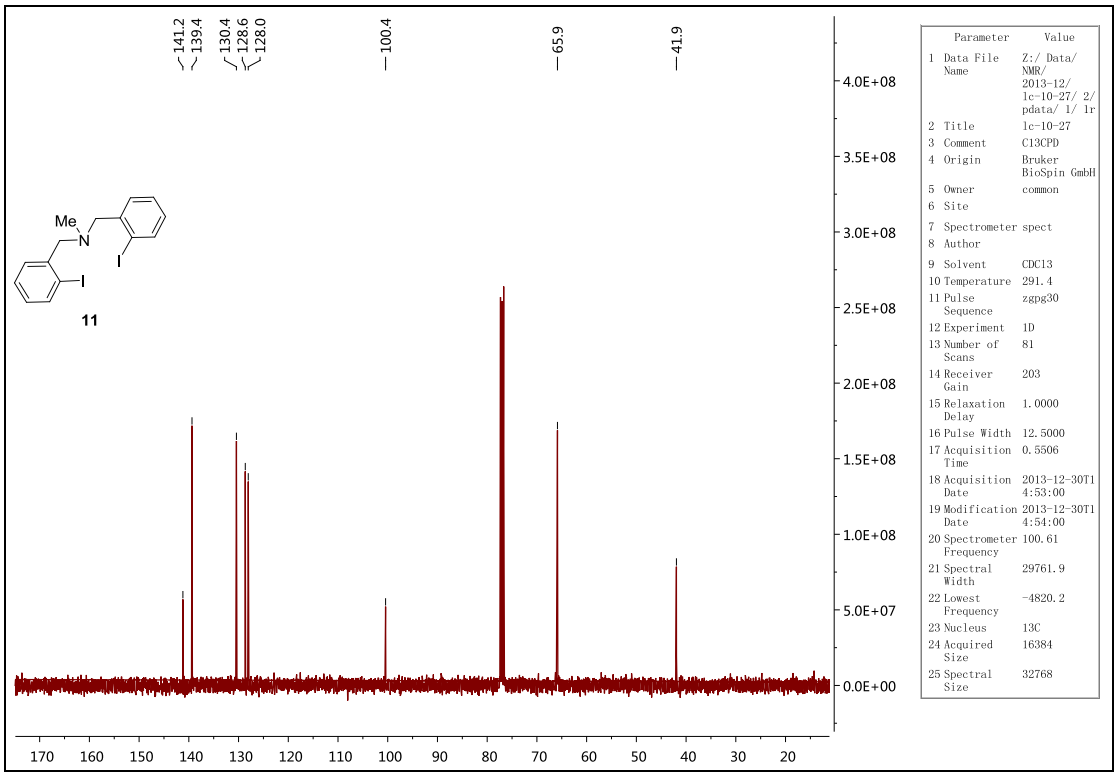

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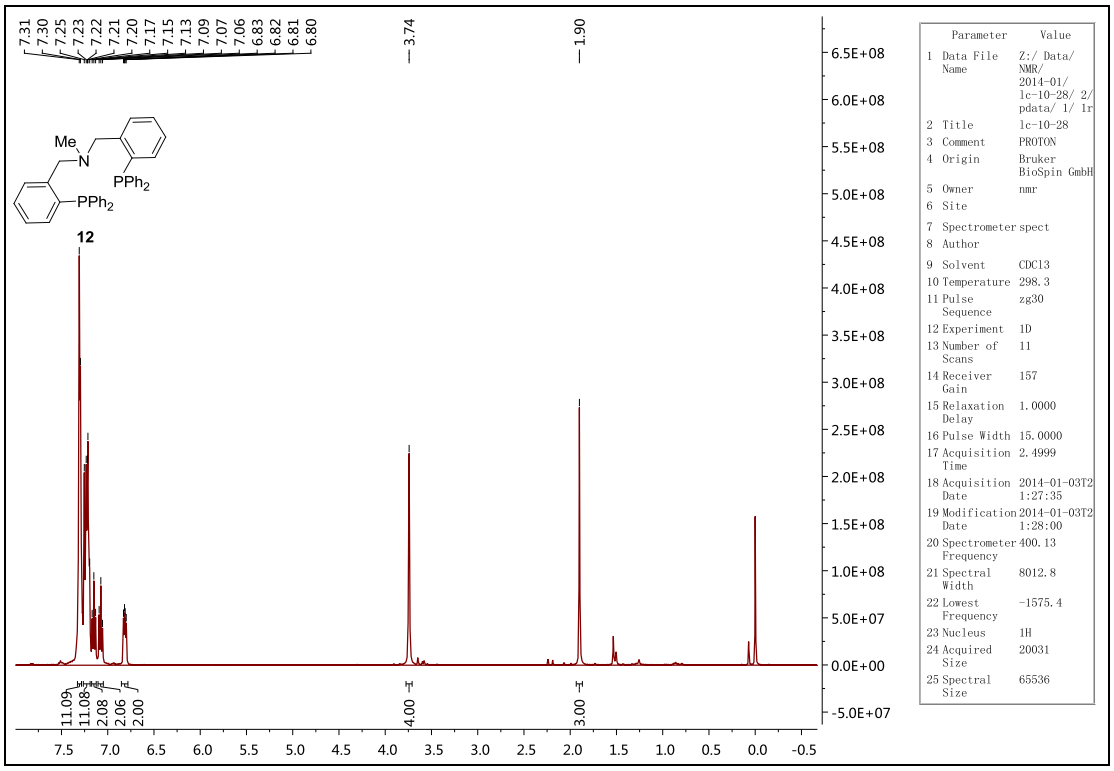

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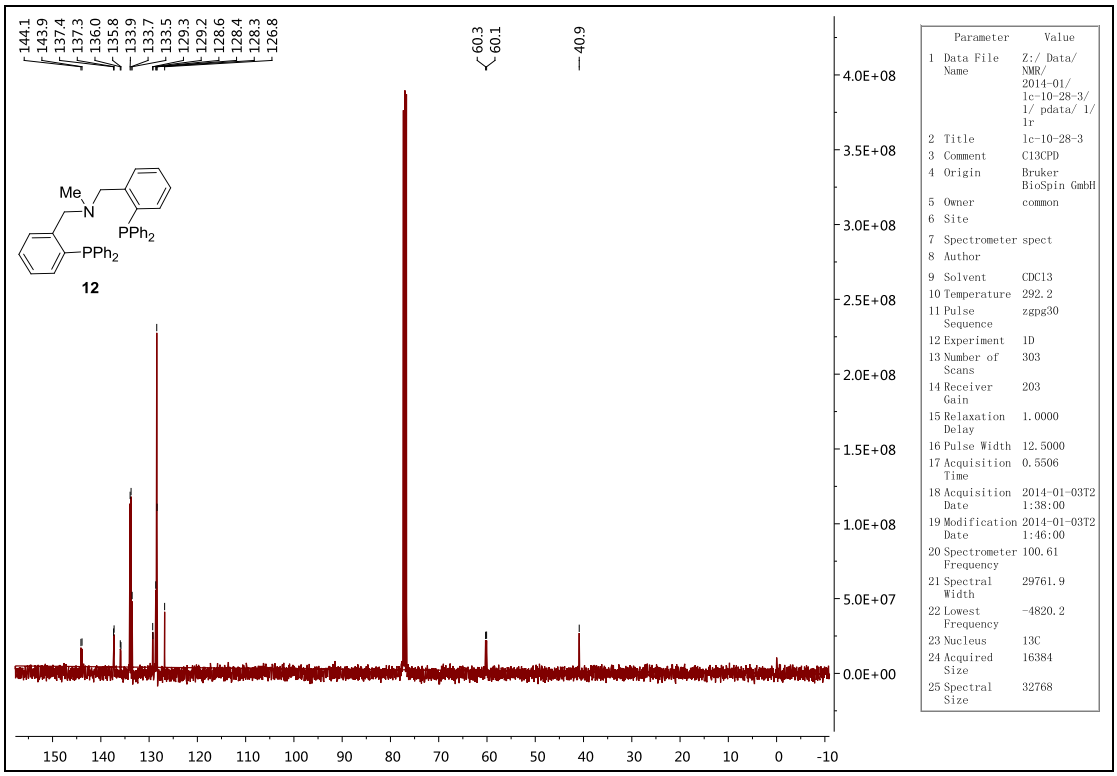

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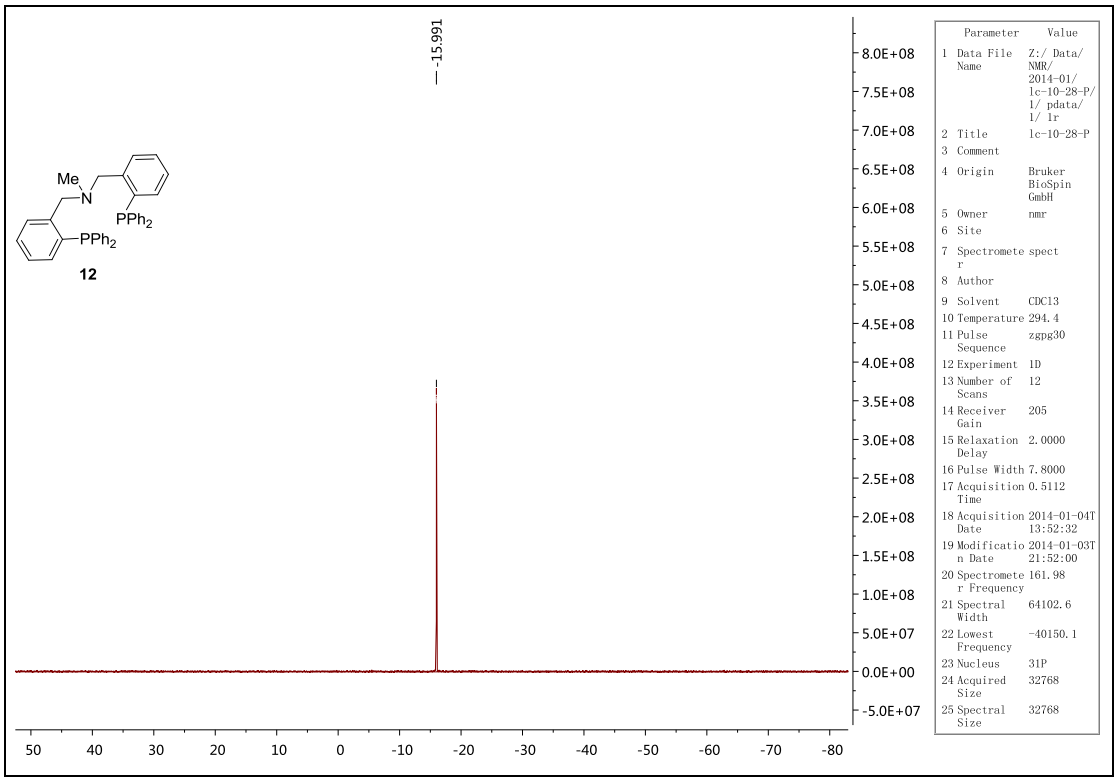

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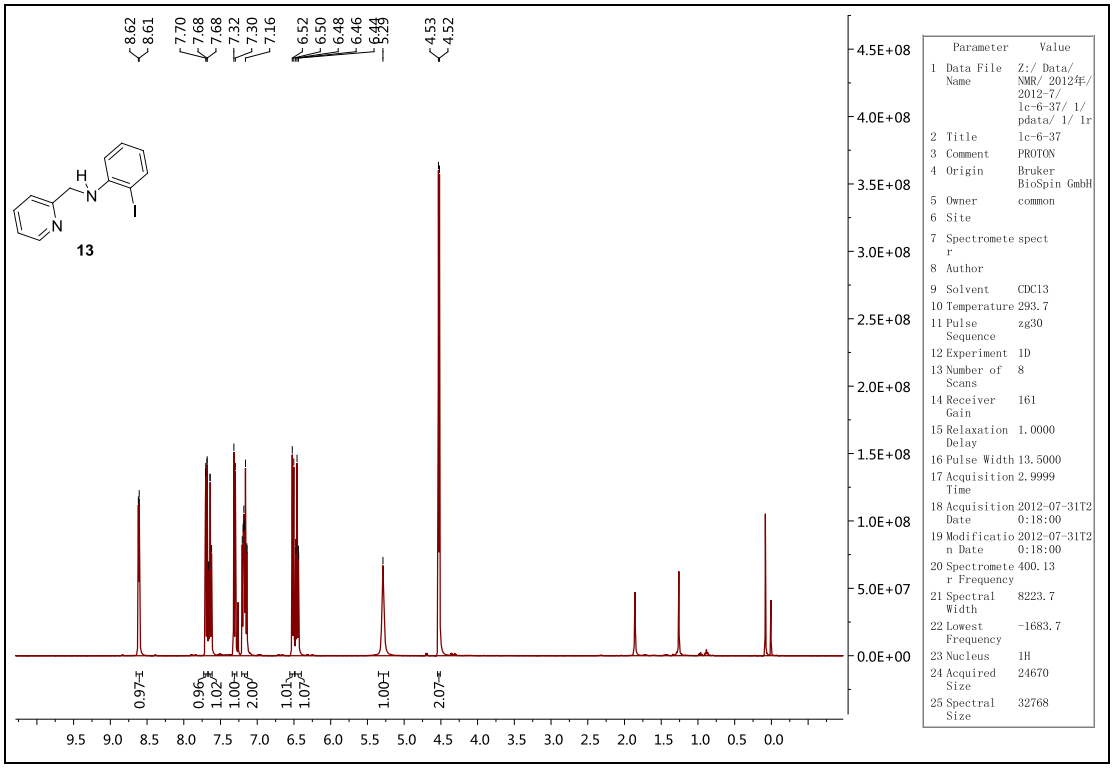

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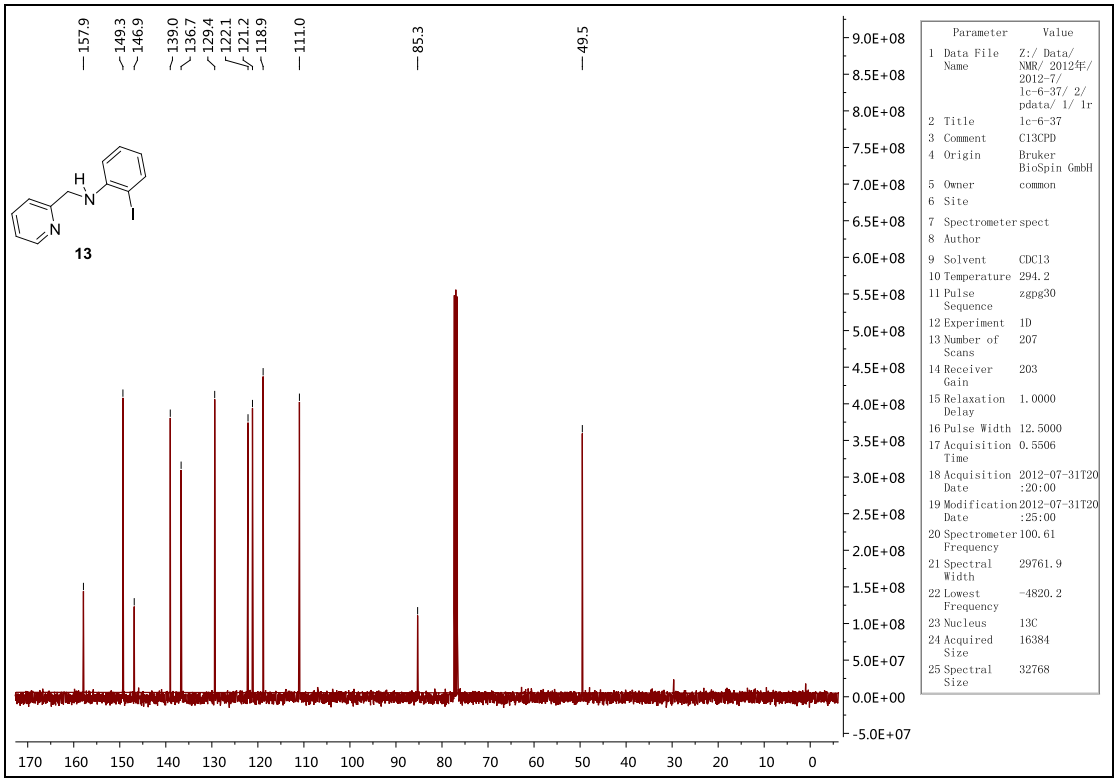
25	Spectral Size	32768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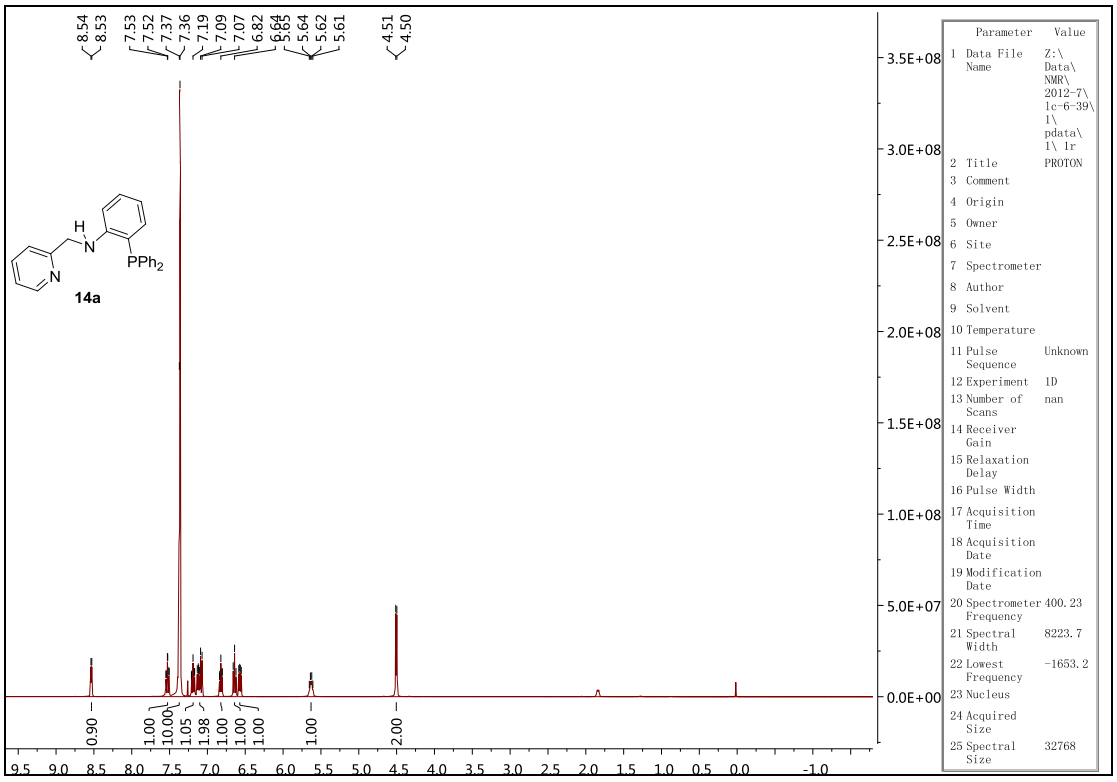
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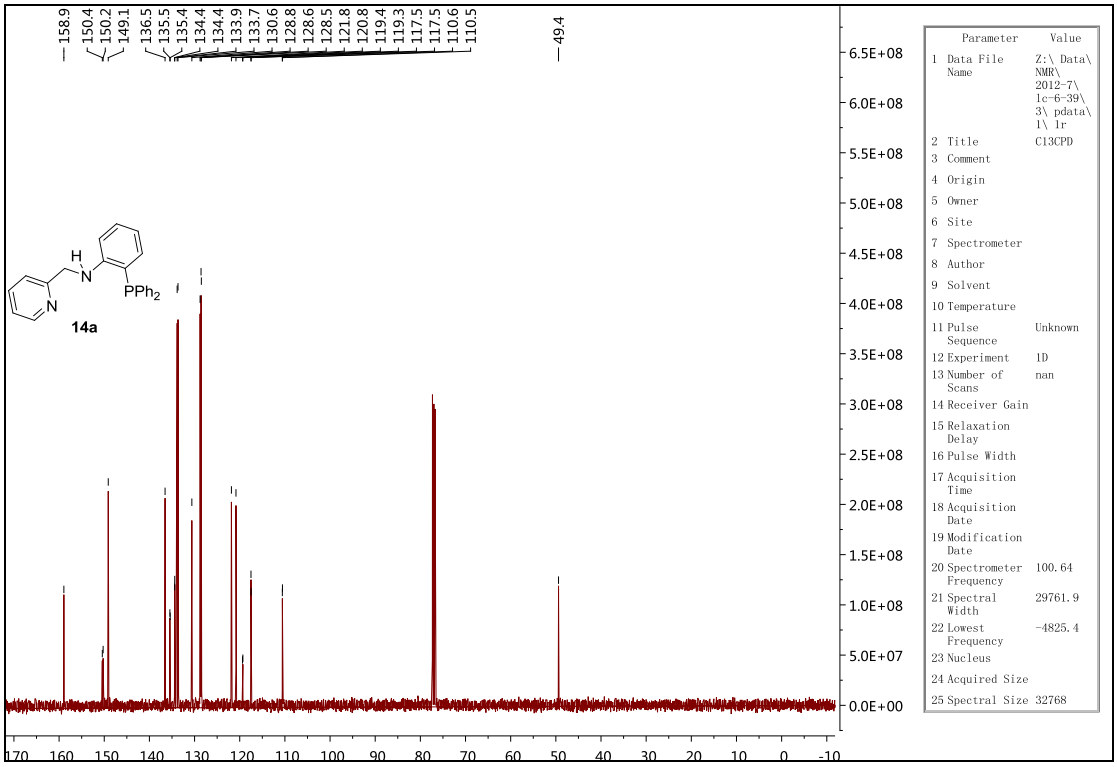
4 Origin
5 Owner
6 Site
7 Spectrometer
8 Author
9 Solvent
10 Temperature
11 Pulse Sequence Unknown
12 Experiment 1D
13 Number of Scans nan
14 Receiver Gain
15 Relaxation Delay
16 Pulse Width
17 Acquisition Time
18 Acquisition Date
19 Modification Date
20 Spectrometer Frequency 400.23
21 Spectral Width 8223.7
22 Lowest Frequency -1653.2
23 Nucleus
24 Acquired Size
25 Spectral Size 32768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49.4
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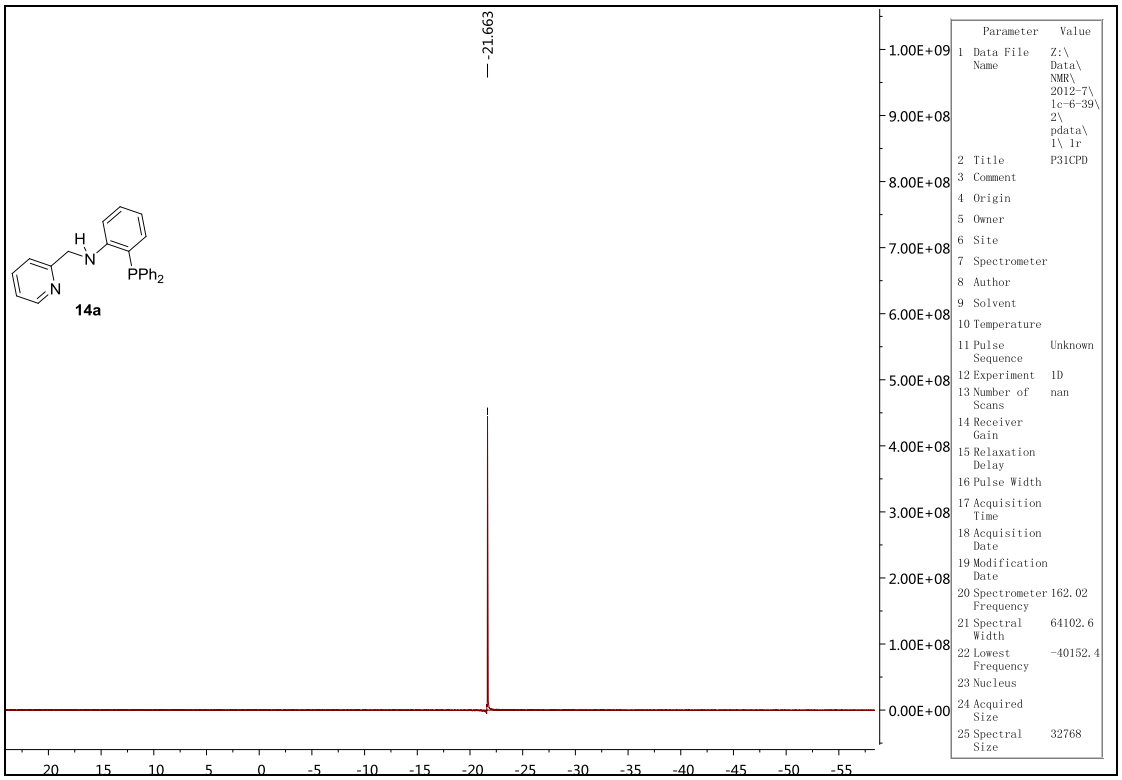
2 Title C13CPD
3 Comment
4 Origin
5 Owner
6 Site
7 Spectrometer
8 Author
9 Solvent
10 Temperature
11 Pulse Sequence Unknown
12 Experiment 1D
13 Number of Scans nan
14 Receiver Gain
15 Relaxation Delay
16 Pulse Width
17 Acquisition Time
18 Acquisition Date
19 Modification Date
20 Spectrometer Frequency 100.64
21 Spectral Width 29761.9
22 Lowest Frequency -4825.4
23 Nucleus
24 Acquired Size
25 Spectral Size 32768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3 Comment
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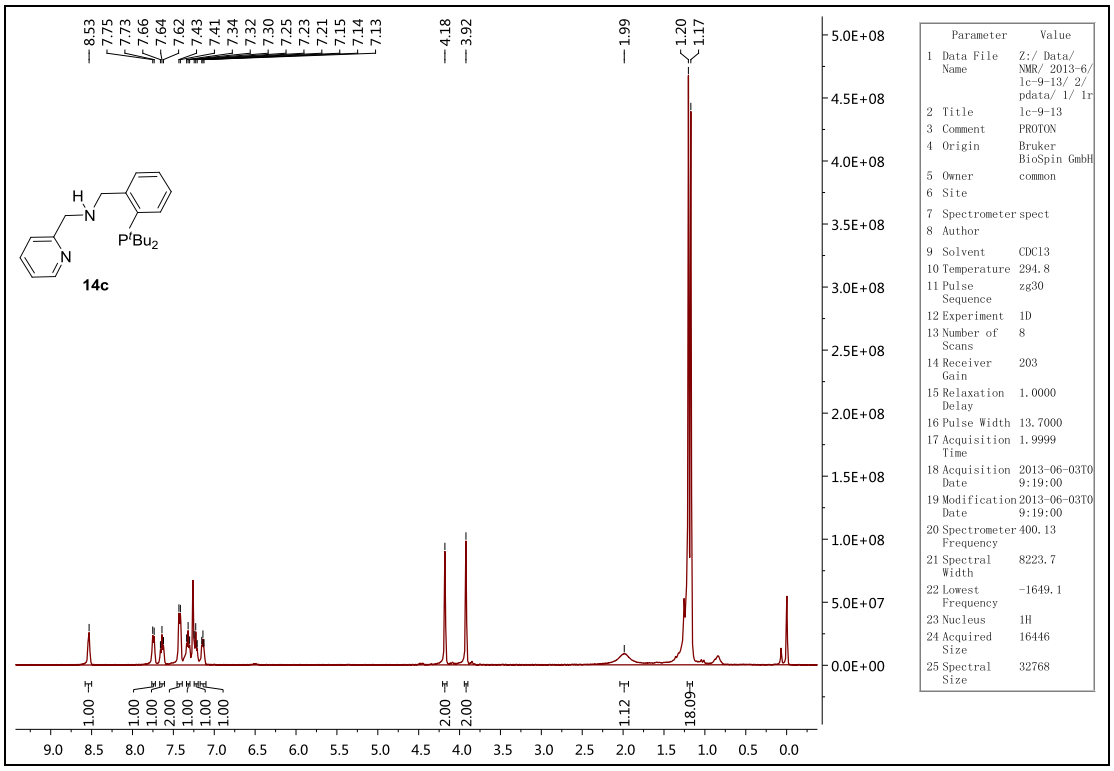
7 Spectrometer
8 Author
9 Solvent
10 Temperature
11 Pulse Sequence Unknown
12 Experiment 1D
13 Number of Scans nan
14 Receiver Gain
15 Relaxation Delay
16 Pulse Width
17 Acquisition Time
18 Acquisition Date
19 Modification Date
20 Spectrometer Frequency 162.02
21 Spectral Width 64102.6
22 Lowest Frequency -40152.4
23 Nucleus
24 Acquired Size
25 Spectral Size 32768



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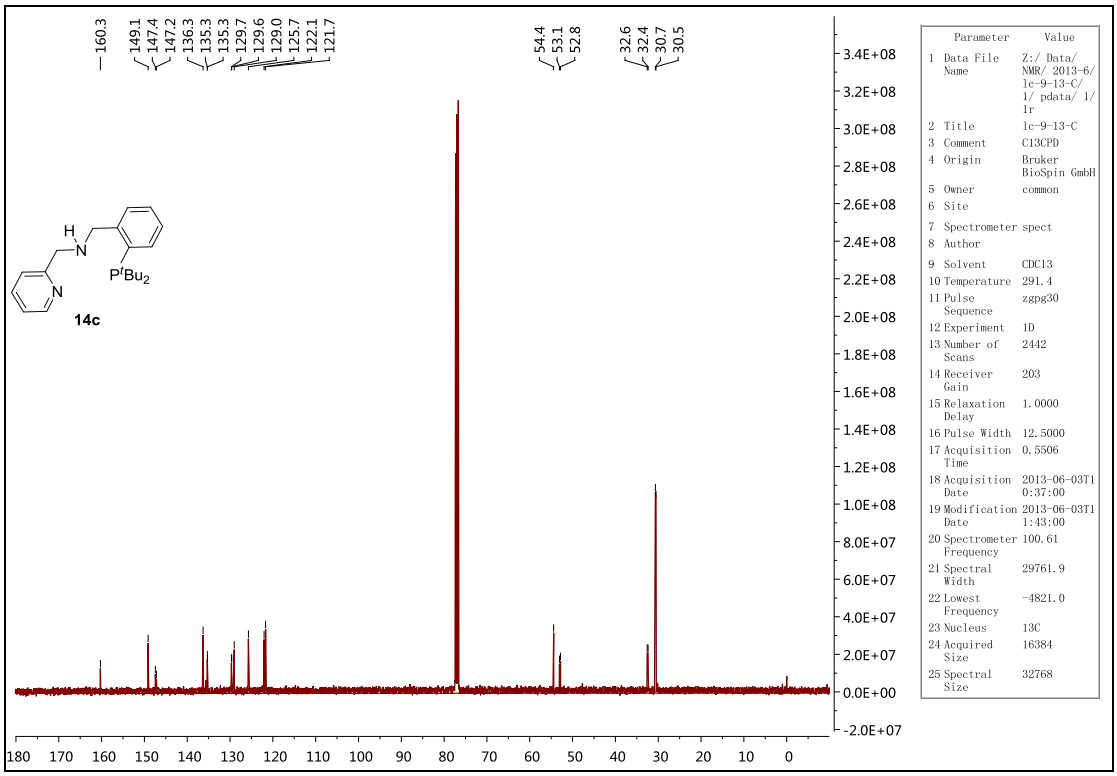
2	Title	lc-9-13
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	294.8
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	13.7000
17	Acquisition Time	1.9999
18	Acquisition Date	2013-06-03T09:19:00
19	Modification Date	2013-06-03T09:19:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8223.7
22	Lowest Frequency	-1649.1
23	Nucleus	1H
24	Acquired Size	16446
25	Spectral Size	32768



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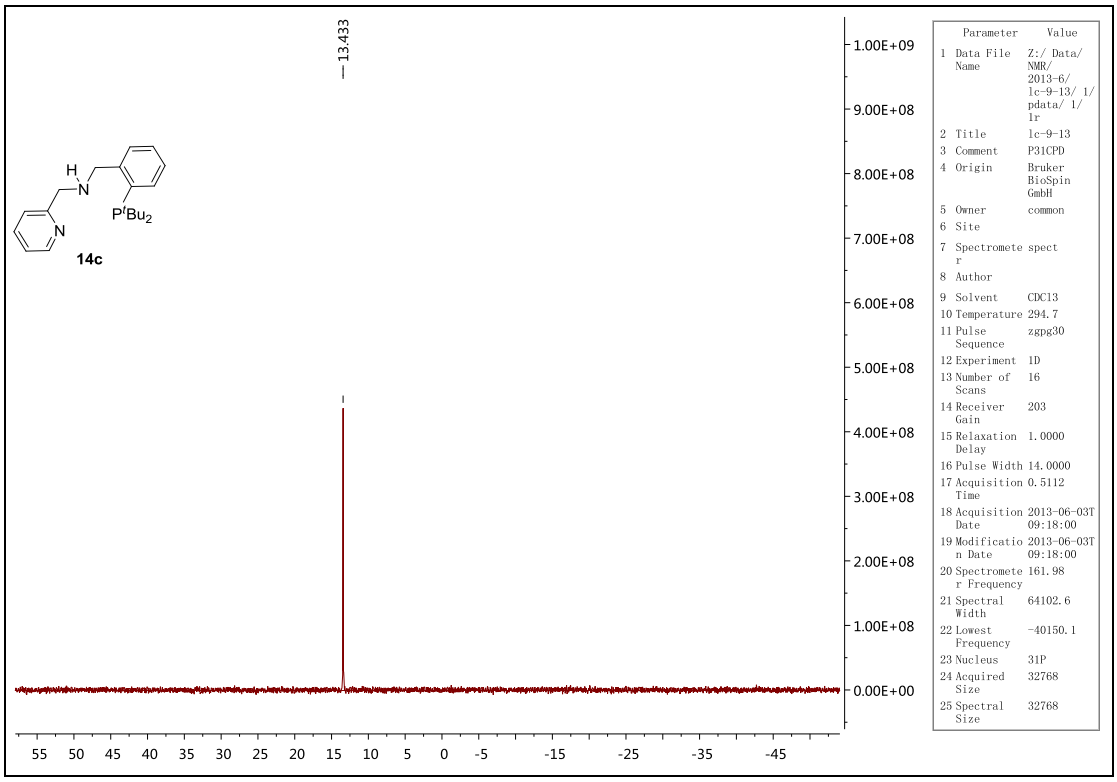
2	Title	lc-9-13-C
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	291.4
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	2442
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	12.5000
17	Acquisition Time	0.5506
18	Acquisition Date	2013-06-03T10:37:00
19	Modification Date	2013-06-03T11:43:00
20	Spectrometer Frequency	100.61
21	Spectral Width	29761.9
22	Lowest Frequency	-4821.0
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768



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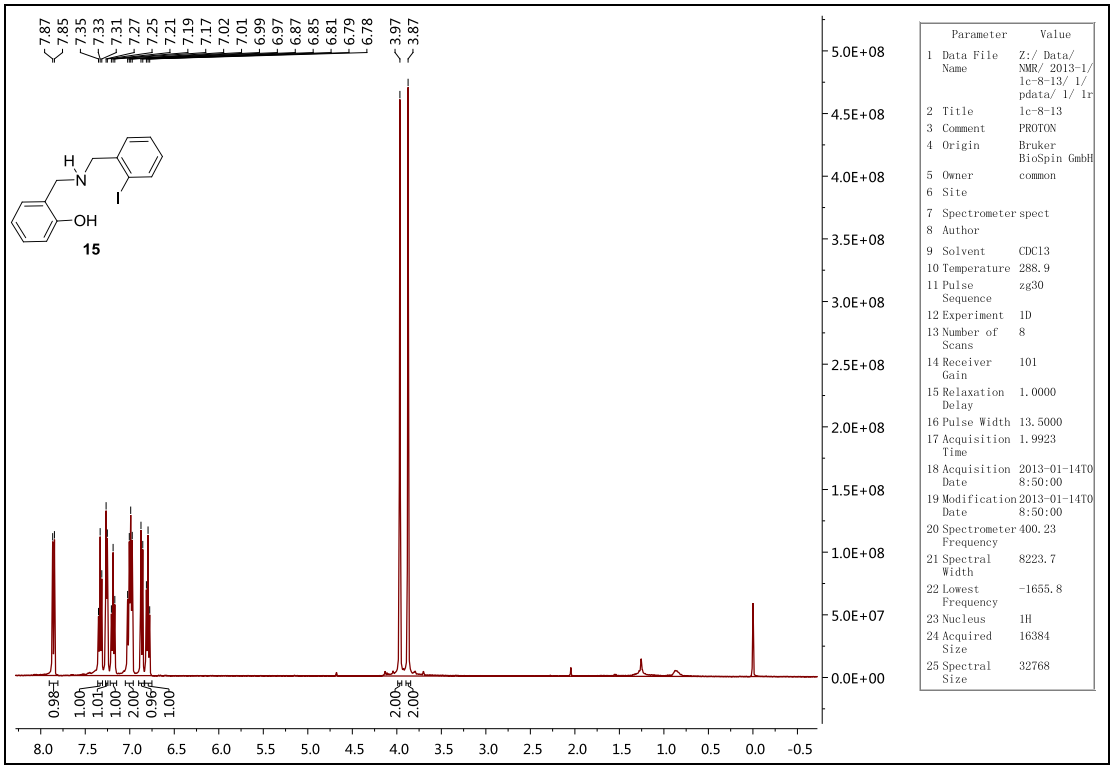
1	Data File Name	Z:/ Data/ NMR/ 2013-6/ lc-9-13/ 1/ pdata/ 1/ 1r
2	Title	lc-9-13
3	Comment	P31CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect r
8	Author	
9	Solvent	CDCl3
10	Temperature	294.7
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	16
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	14.0000
17	Acquisition Time	0.5112
18	Acquisition Date	2013-06-03T 09:18:00
19	Modification Date	2013-06-03T 09:18:00
20	Spectrometer Frequency	161.98
21	Spectral Width	64102.6
22	Lowest Frequency	-40150.1
23	Nucleus	31P
24	Acquired Size	32768
25	Spectral Size	32768



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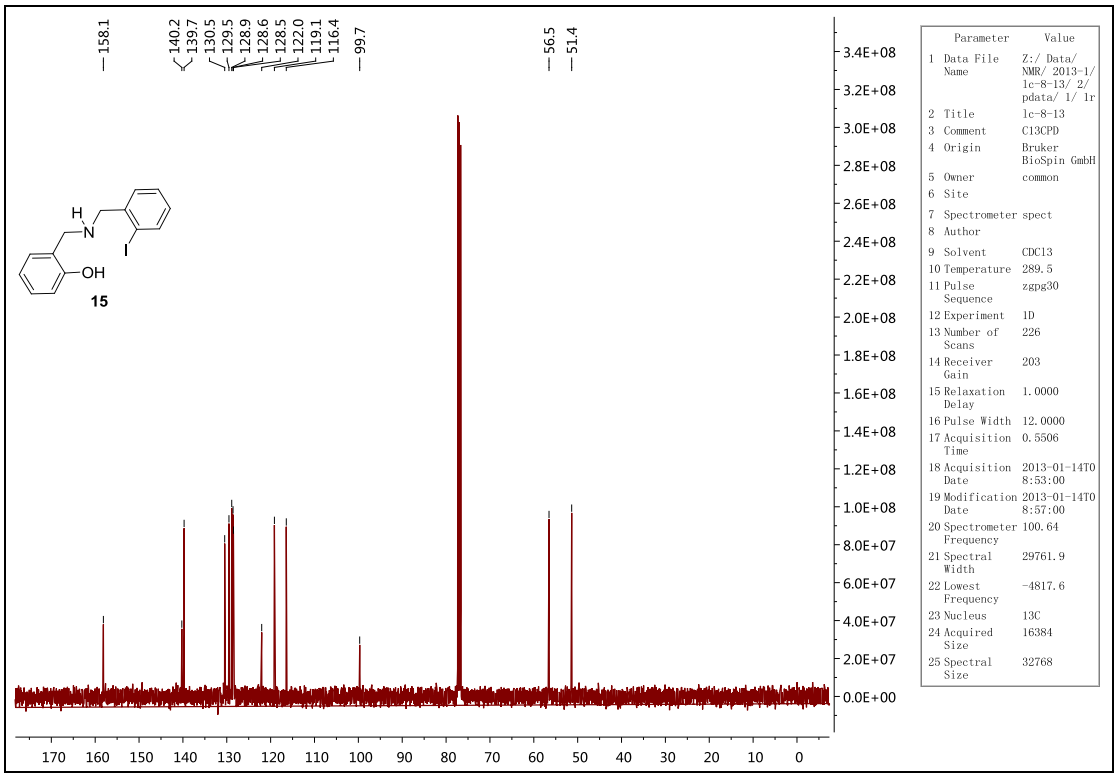
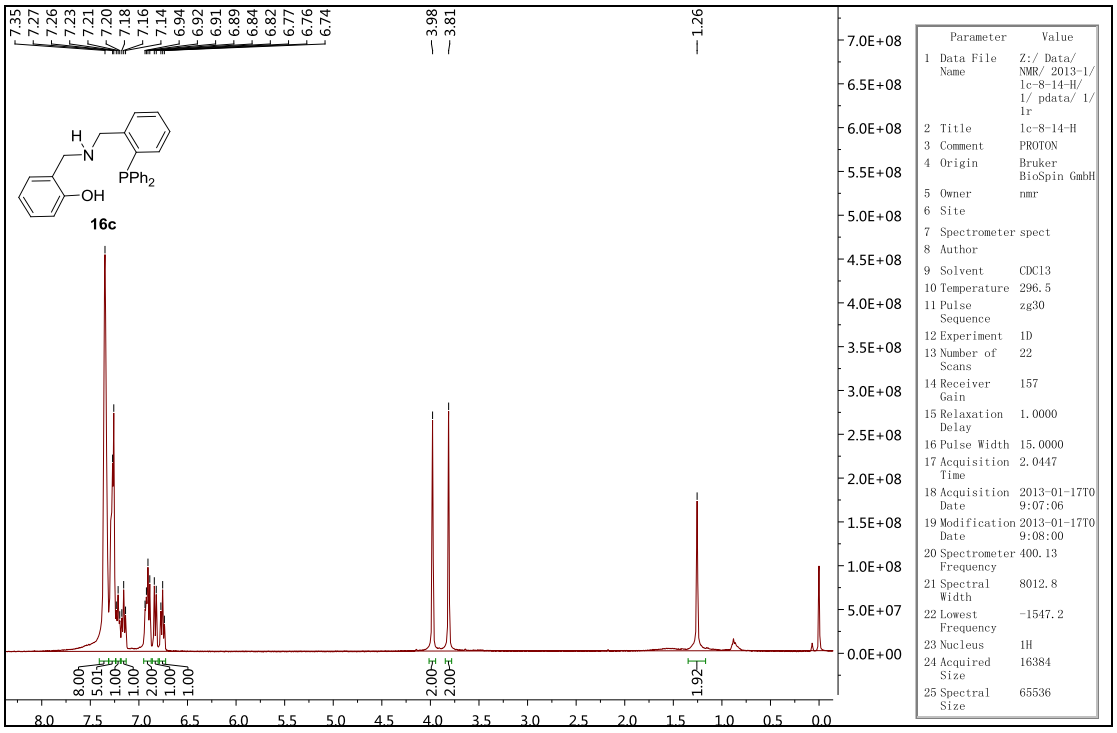
1	Data File Name	Z:/ Data/ NMR/ 2013-1/ lc-8-13/ 1/ pdata/ 1/ 1r
2	Title	lc-8-13
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	288.9
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	101
15	Relaxation Delay	1.0000
16	Pulse Width	13.5000
17	Acquisition Time	1.9923
18	Acquisition Date	2013-01-14T0 8:50:00
19	Modification Date	2013-01-14T0 8:50:00
20	Spectrometer Frequency	400.23
21	Spectral Width	8223.7
22	Lowest Frequency	-1655.8
23	Nucleus	1H
24	Acquired Size	16384
25	Spectral Size	32768



	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2013-1/ 1c-8-13/ 2/ pdata/ 1/ 1r
2	Title	1c-8-13
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDC13
10	Temperature	289.5
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	226
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	12.0000
17	Acquisition Time	0.5506
18	Acquisition Date	2013-01-14T08:53:00
19	Modification Date	2013-01-14T08:57:00
20	Spectrometer Frequency	100.64
21	Spectral Width	29761.9
22	Lowest Frequency	-4817.6
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768



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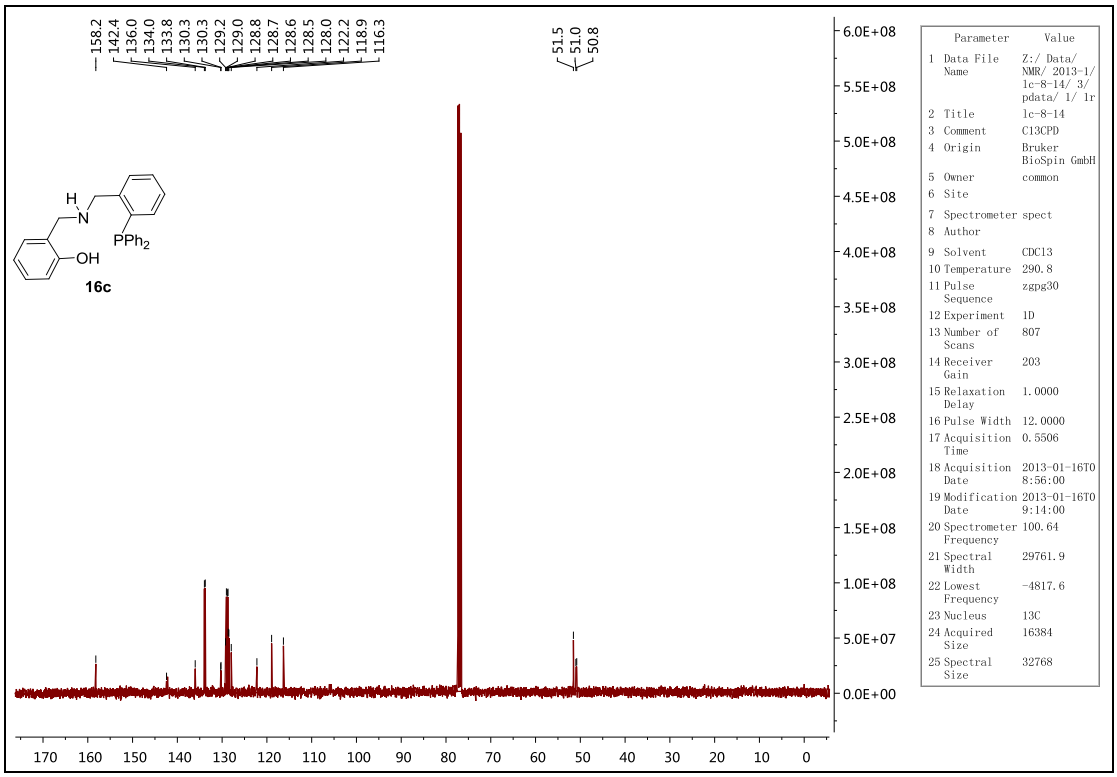
1	Data File Name	Z:/ Data/ NMR/ 2013-1/ 1c-8-14-H/ 1/ pdata/ 1/ 1r
2	Title	1c-8-14-H
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	296.5
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	22
14	Receiver Gain	157
15	Relaxation Delay	1.0000
16	Pulse Width	15.0000
17	Acquisition Time	2.0447
18	Acquisition Date	2013-01-17T09:07:06
19	Modification Date	2013-01-17T09:08:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8012.8
22	Lowest Frequency	-1547.2
23	Nucleus	1H
24	Acquired Size	16384
25	Spectral Size	65536



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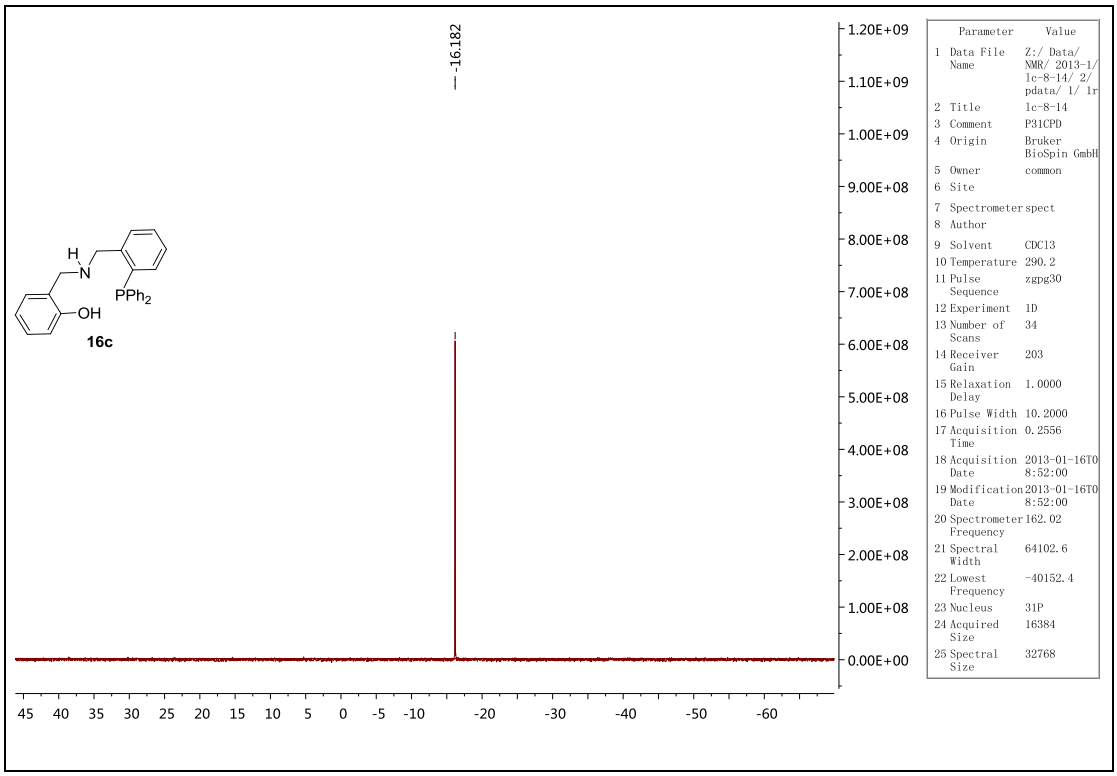
1	Data File Name	Z:/ Data/ NMR/ 2013-1/ 1c-8-14/ 3/ pdata/ 1/ 1r
2	Title	1c-8-14
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDC13
10	Temperature	290.8
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	807
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	12.0000
17	Acquisition Time	0.5506
18	Acquisition Date	2013-01-16T0 8:56:00
19	Modification Date	2013-01-16T0 9:14:00
20	Spectrometer Frequency	100.64
21	Spectral Width	29761.9
22	Lowest Frequency	-4817.6
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768



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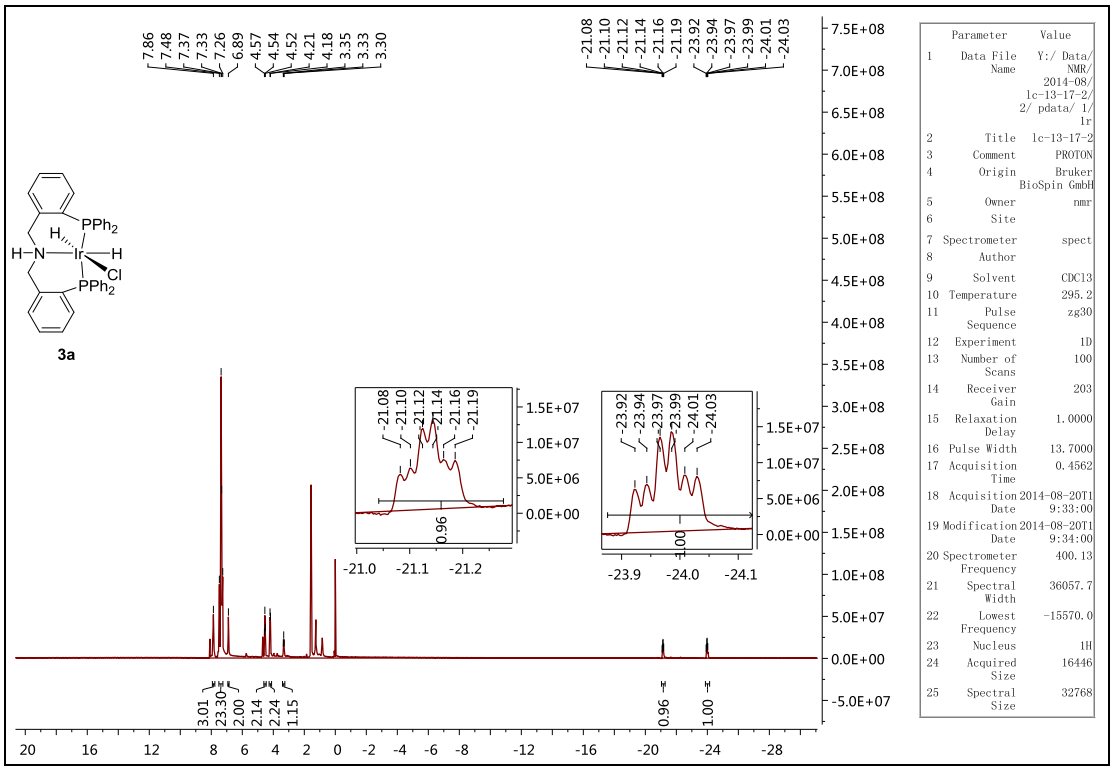
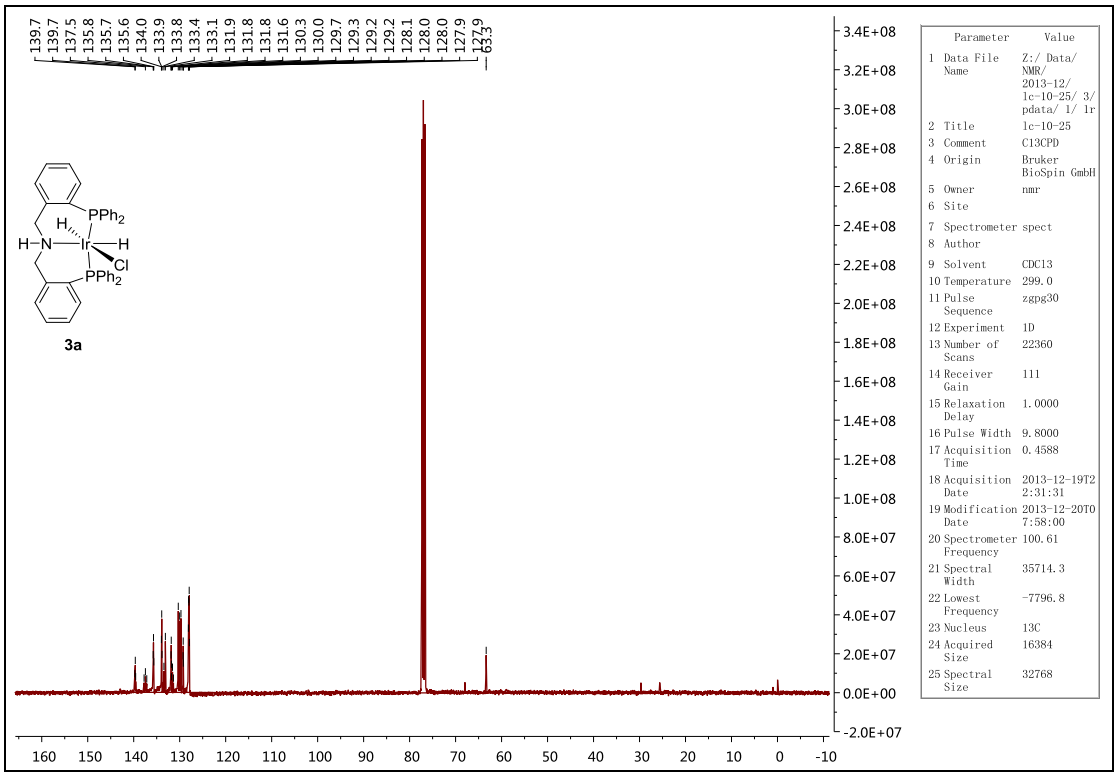
1	Data File Name	Z:/ Data/ NMR/ 2013-1/ 1c-8-14/ 2/ pdata/ 1/ 1r
2	Title	1c-8-14
3	Comment	P31CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDC13
10	Temperature	290.2
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	34
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	10.2000
17	Acquisition Time	0.2556
18	Acquisition Date	2013-01-16T0 8:52:00
19	Modification Date	2013-01-16T0 8:52:00
20	Spectrometer Frequency	162.02
21	Spectral Width	64102.6
22	Lowest Frequency	-40152.4
23	Nucleus	31P
24	Acquired Size	16384
25	Spectral Size	32768



	Parameter	Value
1	Data File Name	Y:/ Data/ NMR/ 2014-08/ 1c-13-17-2/ 2/ pdata/ 1/ 1r
2	Title	1c-13-17-2
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	295.2
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	100
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	13.7000
17	Acquisition Time	0.4562
18	Acquisition Date	2014-08-20T1 9:33:00
19	Modification Date	2014-08-20T1 9:34:00
20	Spectrometer Frequency	400.13
21	Spectral Width	36057.7
22	Lowest Frequency	-15570.0
23	Nucleus	1H
24	Acquired Size	16446
25	Spectral Size	32768



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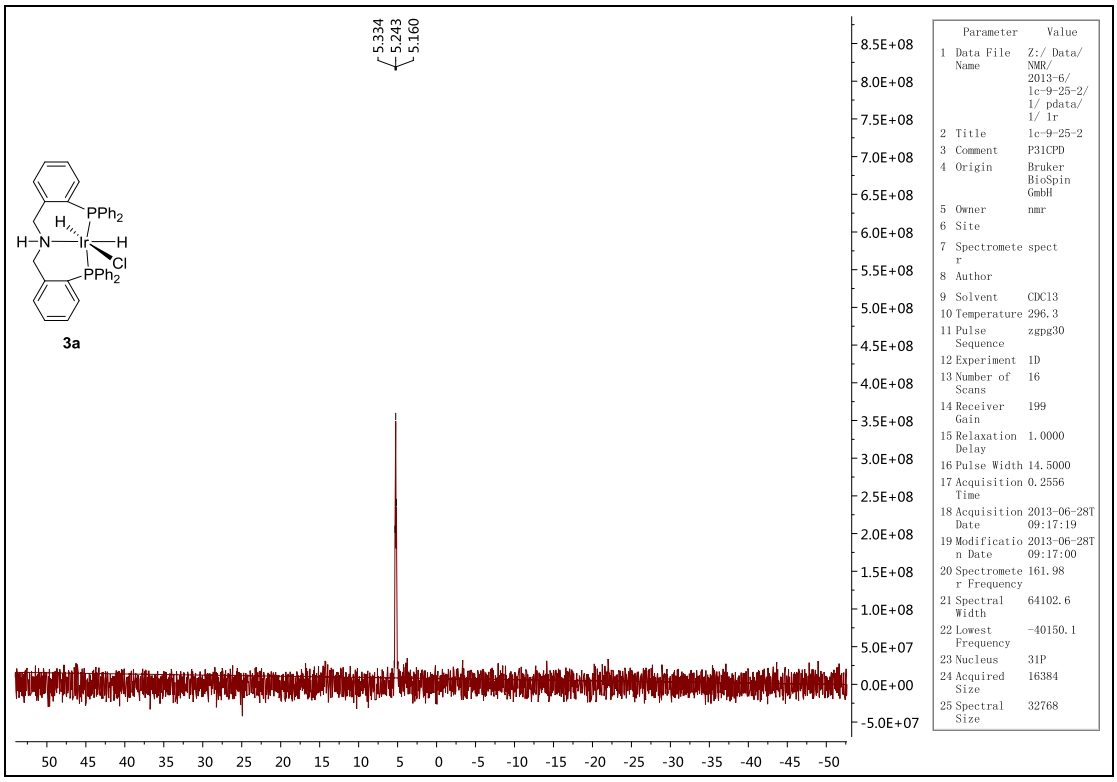
2	Title	1c-10-25
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	299.0
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	22360
14	Receiver Gain	111
15	Relaxation Delay	1.0000
16	Pulse Width	9.8000
17	Acquisition Time	0.4588
18	Acquisition Date	2013-12-19T2 2:31:31
19	Modification Date	2013-12-20T0 7:58:00
20	Spectrometer Frequency	100.61
21	Spectral Width	35714.3
22	Lowest Frequency	-7796.8
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768



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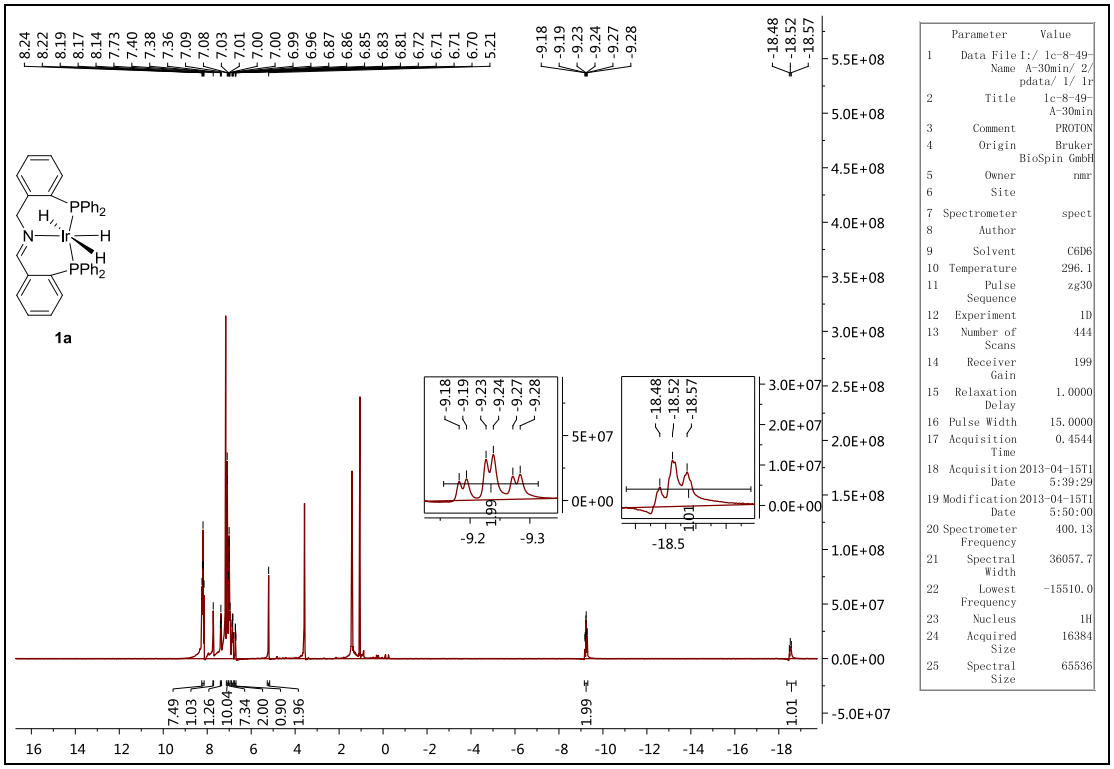
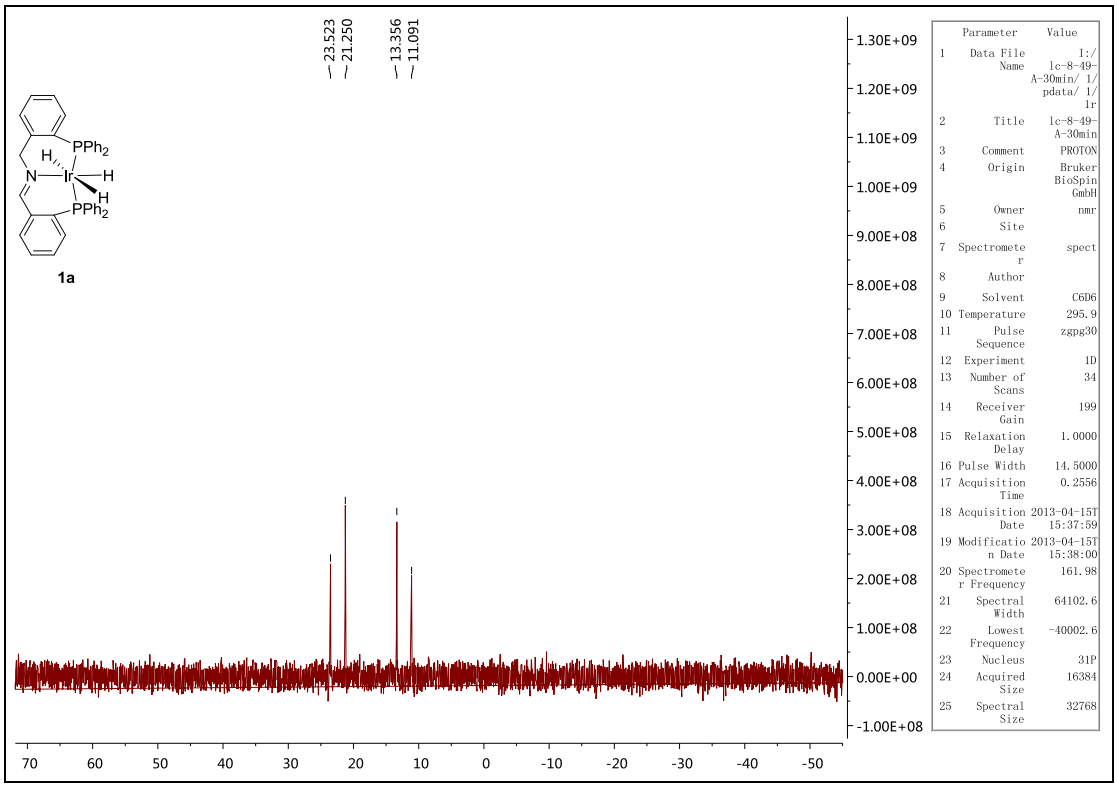
2	Title	lc-9-25-2
3	Comment	P31CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect r
8	Author	
9	Solvent	CDCl3
10	Temperature	296.3
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	16
14	Receiver Gain	199
15	Relaxation Delay	1.0000
16	Pulse Width	14.5000
17	Acquisition Time	0.2556
18	Acquisition Date	2013-06-28T 09:17:19
19	Modificatio n Date	2013-06-28T 09:17:00
20	Spectrometer Frequency	161.98
21	Spectral Width	64102.6
22	Lowest Frequency	-40150.1
23	Nucleus	31P
24	Acquired Size	16384
25	Spectral Size	32768



	Parameter	Value
1	Data File Name	I:/ lc-8-49-A-30min/ 2/ pdata/ 1/ 1r
2	Title	lc-8-49-A-30min
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	C6D6
10	Temperature	296.1
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	444
14	Receiver Gain	199
15	Relaxation Delay	1.0000
16	Pulse Width	15.0000
17	Acquisition Time	0.4544
18	Acquisition Date	2013-04-15T1 5:39:29
19	Modification Date	2013-04-15T1 5:50:00
20	Spectrometer Frequency	400.13
21	Spectral Width	36057.7
22	Lowest Frequency	-15510.0
23	Nucleus	1H
24	Acquired Size	16384
25	Spectral Size	65536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11.091
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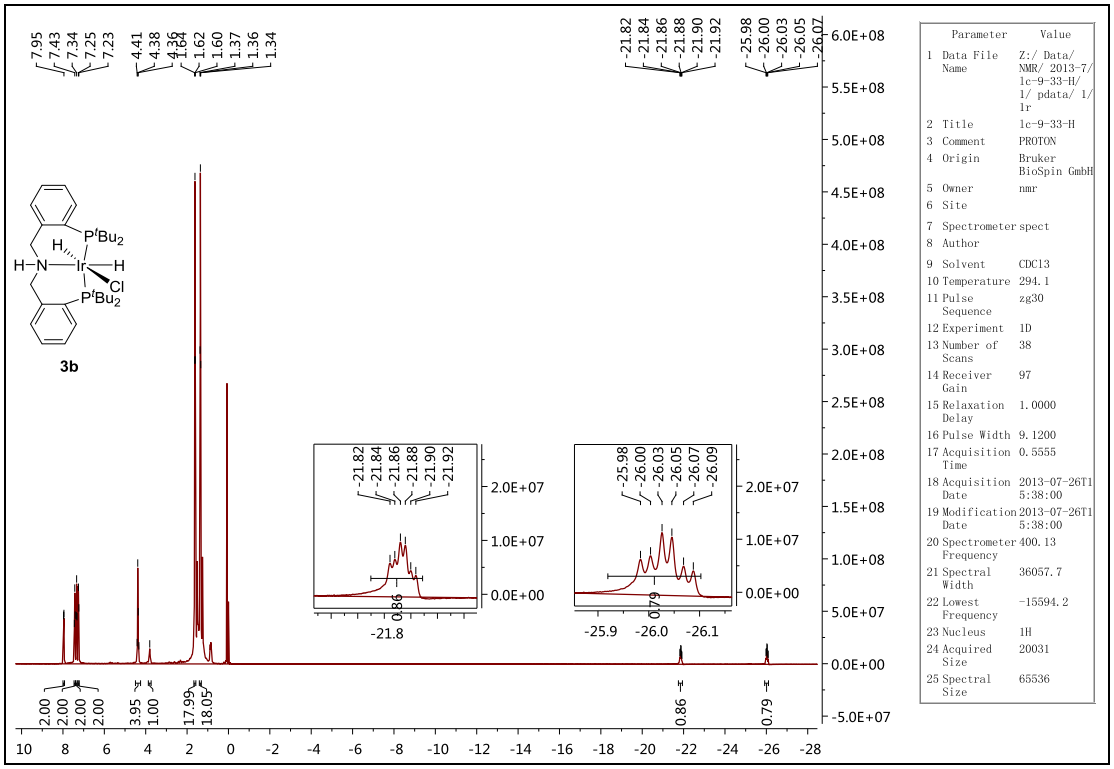
2 Title lc-8-49-A-30min
3 Comment PROTON
4 Origin Bruker BioSpin GmbH
5 Owner nmr
6 Site
7 Spectrometer spect
8 Author
9 Solvent C6D6
10 Temperature 295.9
11 Pulse Sequence zgpg30
12 Experiment 1D
13 Number of Scans 34
14 Receiver Gain 199
15 Relaxation Delay 1.0000
16 Pulse Width 14.5000
17 Acquisition Time 0.2556
18 Acquisition Date 2013-04-15T 15:37:59
19 Modification Date 2013-04-15T 15:38:00
20 Spectrometer Frequency 161.98
21 Spectral Width 64102.6
22 Lowest Frequency -40002.6
23 Nucleus 31P
24 Acquired Size 16384
25 Spectral Size 32768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7.23
4.41
4.38
1.62
1.60
1.37
1.36
1.34
-21.82
-21.84
-21.86
-21.88
-21.90
-21.92
-25.98
-26.00
-26.03
-26.05
-26.07
3b
2.00
2.00
2.00
2.00
3.95
1.00
17.99
18.05
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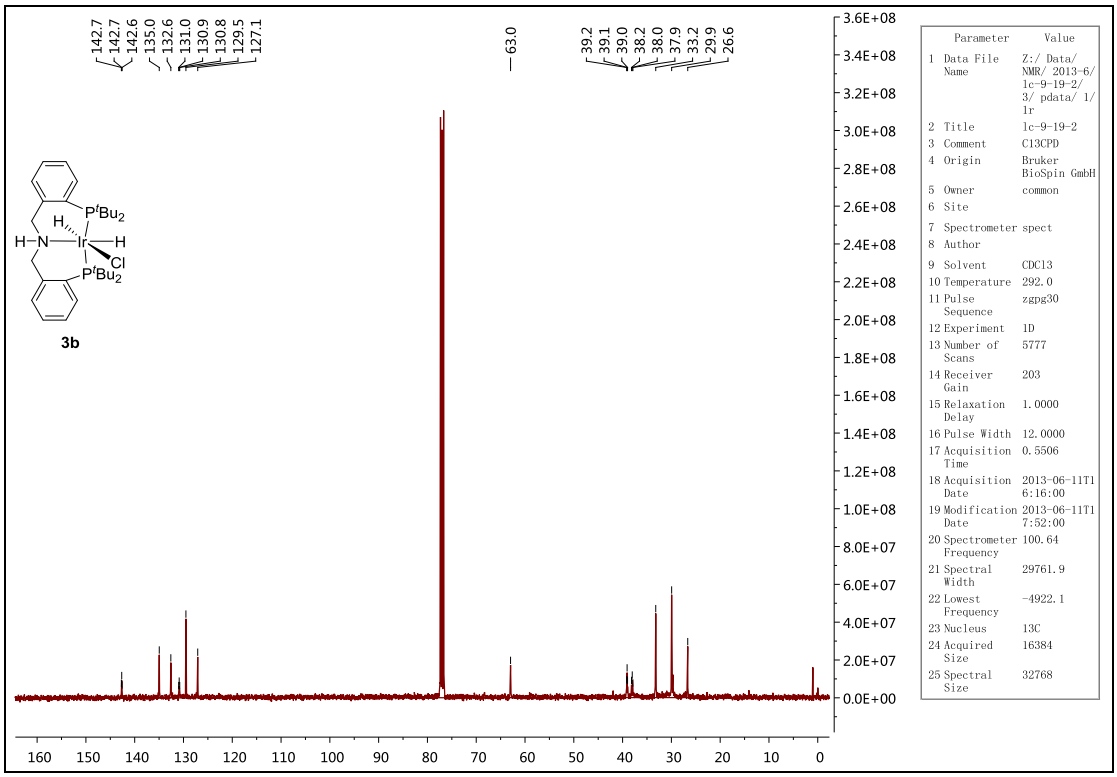
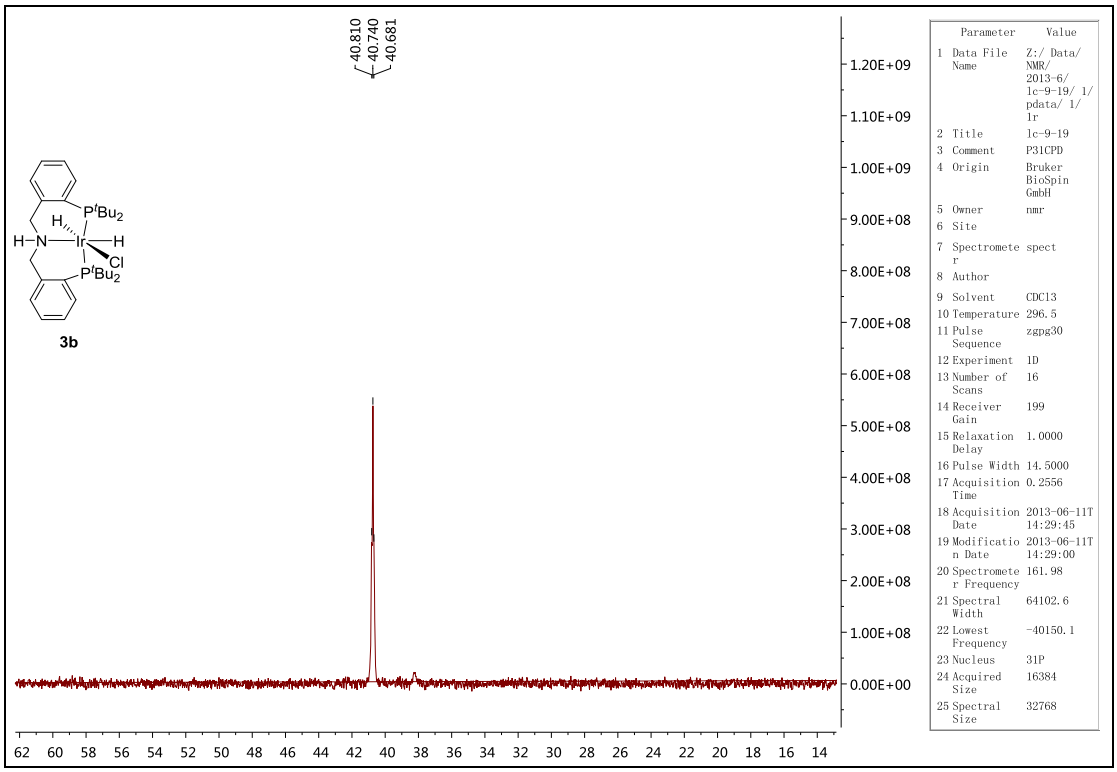
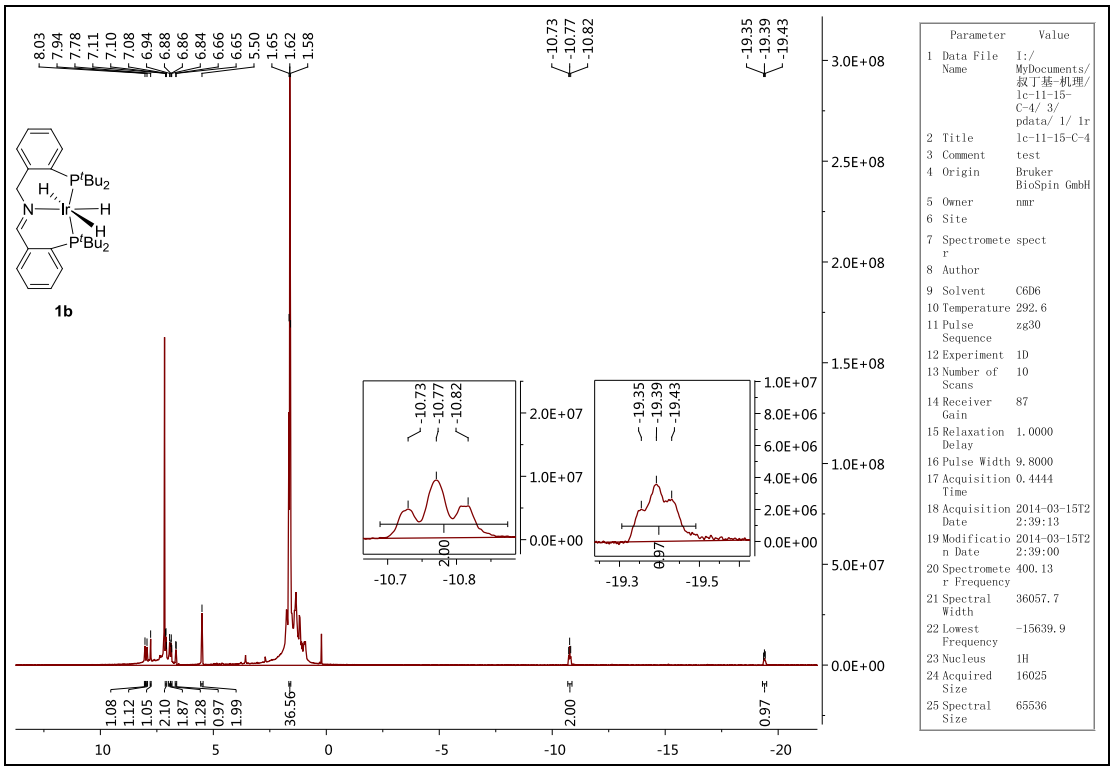
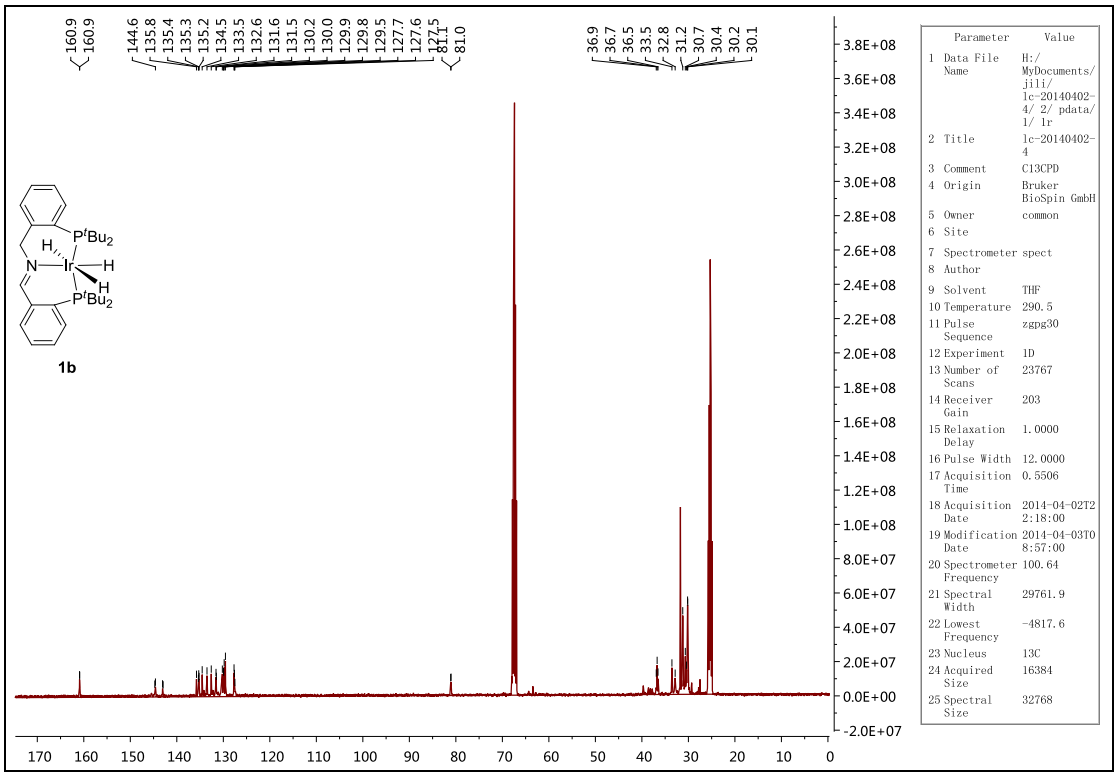
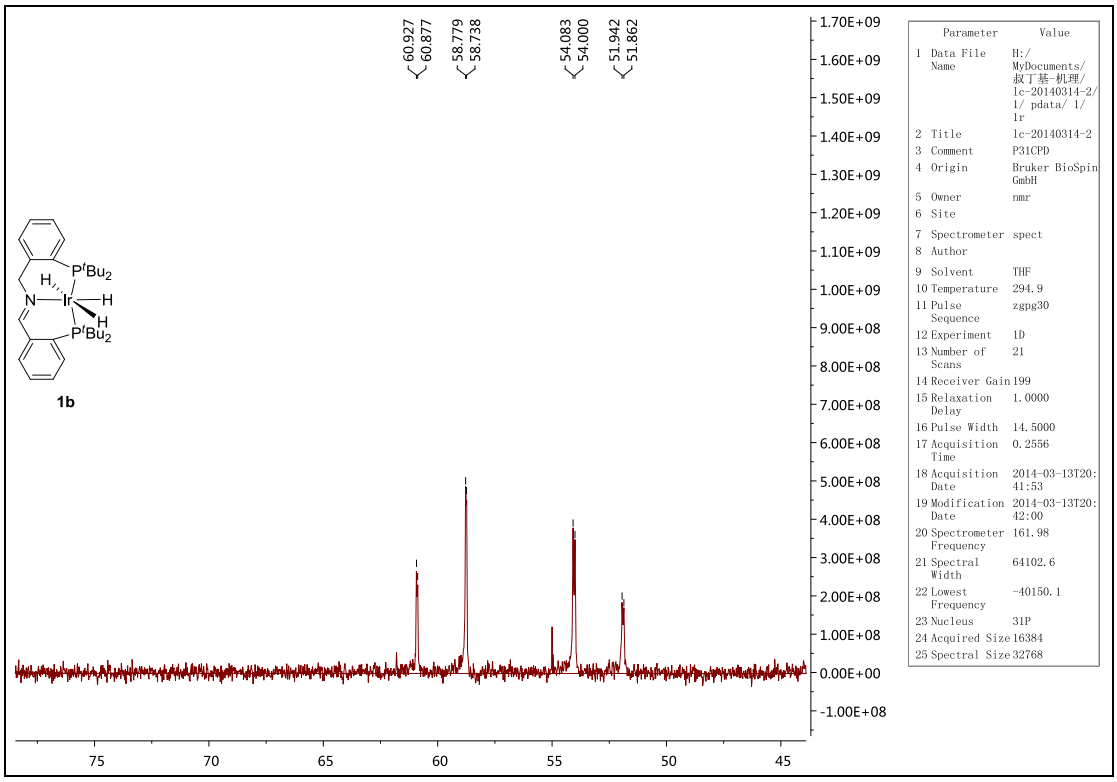
1 Data File Name Z:/ Data/ NMR/ 2013-7/ lc-9-33-H/ 1/ pdata/ 1/ 1r
2 Title lc-9-33-H
3 Comment PROTON
4 Origin Bruker BioSpin GmbH
5 Owner nmr
6 Site
7 Spectrometer spect
8 Author
9 Solvent CDCl3
10 Temperature 294.1
11 Pulse Sequence zg30
12 Experiment 1D
13 Number of Scans 38
14 Receiver Gain 97
15 Relaxation Delay 1.0000
16 Pulse Width 9.1200
17 Acquisition Time 0.5555
18 Acquisition Date 2013-07-26T15:38:00
19 Modification Date 2013-07-26T15:38:00
20 Spectrometer Frequency 400.13
21 Spectral Width 36057.7
22 Lowest Frequency -15594.2
23 Nucleus 1H
24 Acquired Size 20031
25 Spectral Size 65536


142.7
142.7
142.6
135.0
132.6
131.0
130.9
130.8
129.5
127.1
63.0
39.2
39.1
39.0
38.2
38.0
37.9
33.2
29.9
26.6
3b
Parameter Value
1 Data File Name Z:/ Data/ NMR/ 2013-6/ 1c-9-19-2/ 3/ pdata/ 1/ 1r
2 Title 1c-9-19-2
3 Comment C13CPD
4 Origin Bruker BioSpin GmbH
5 Owner common
6 Site
7 Spectrometer spect
8 Author
9 Solvent CDCl3
10 Temperature 292.0
11 Pulse Sequence zgpg30
12 Experiment 1D
13 Number of Scans 5777
14 Receiver Gain 203
15 Relaxation Delay 1.0000
16 Pulse Width 12.0000
17 Acquisition Time 0.5506
18 Acquisition Date 2013-06-11T16:16:00
19 Modification Date 2013-06-11T17:52:00
20 Spectrometer Frequency 100.64
21 Spectral Width 29761.9
22 Lowest Frequency -4922.1
23 Nucleus 13C
24 Acquired Size 16384
25 Spectral Size 32768


40.810
40.740
40.681
3b
Parameter Value
1 Data File Name Z:/ Data/ NMR/ 2013-6/ 1c-9-19/ 1/ pdata/ 1/ 1r
2 Title 1c-9-19
3 Comment P31CPD
4 Origin Bruker BioSpin GmbH
5 Owner nmr
6 Site
7 Spectrometer spect
8 Author
9 Solvent CDCl3
10 Temperature 296.5
11 Pulse Sequence zgpg30
12 Experiment 1D
13 Number of Scans 16
14 Receiver Gain 199
15 Relaxation Delay 1.0000
16 Pulse Width 14.5000
17 Acquisition Time 0.2556
18 Acquisition Date 2013-06-11T14:29:45
19 Modification Date 2013-06-11T14:29:00
20 Spectrometer Frequency 161.98
21 Spectral Width 64102.6
22 Lowest Frequency -40150.1
23 Nucleus 31P
24 Acquired Size 16384
25 Spectral Size 32768


8.03
7.94
7.78
7.11
7.10
7.08
6.94
6.88
6.86
6.84
6.66
6.65
5.50
1.65
1.62
1.58
-10.73
-10.77
-10.82
-19.35
-19.39
-19.43
1b
1.08
1.12
1.05
2.10
1.87
1.28
0.97
1.99
36.56
2.00
0.97
Parameter Value
1 Data File Name I:/MyDocuments/叔丁基-机理/lc-11-15-C-4/3/pdata/1/1r
2 Title lc-11-15-C-4
3 Comment test
4 Origin Bruker BioSpin GmbH
5 Owner nmr
6 Site
7 Spectrometer spect
8 Author
9 Solvent C6D6
10 Temperature 292.6
11 Pulse Sequence zg30
12 Experiment 1D
13 Number of Scans 10
14 Receiver Gain 87
15 Relaxation Delay 1.0000
16 Pulse Width 9.8000
17 Acquisition Time 0.4444
18 Acquisition Date 2014-03-15T12:39:13
19 Modification Date 2014-03-15T12:39:00
20 Spectrometer Frequency 400.13
21 Spectral Width 36057.7
22 Lowest Frequency -15639.9
23 Nucleus 1H
24 Acquired Size 16025
25 Spectral Size 65536


160.9
160.9
144.6
135.8
135.4
135.3
135.2
134.5
133.5
132.6
131.6
131.5
130.2
130.0
129.9
129.8
129.5
127.7
127.6
127.5
81.1
81.0
36.9
36.7
36.5
33.5
32.8
31.2
30.7
30.4
30.2
30.1
1b
Parameter Value
1 Data File Name H:/MyDocuments/jili/lc-20140402-4/2/pdata/1/1r
2 Title lc-20140402-4
3 Comment C13CPD
4 Origin Bruker BioSpin GmbH
5 Owner common
6 Site
7 Spectrometer spect
8 Author
9 Solvent THF
10 Temperature 290.5
11 Pulse Sequence zgpg30
12 Experiment 1D
13 Number of Scans 23767
14 Receiver Gain 203
15 Relaxation Delay 1.0000
16 Pulse Width 12.0000
17 Acquisition Time 0.5506
18 Acquisition Date 2014-04-02T22:18:00
19 Modification Date 2014-04-03T08:57:00
20 Spectrometer Frequency 100.64
21 Spectral Width 29761.9
22 Lowest Frequency -4817.6
23 Nucleus 13C
24 Acquired Size 16384
25 Spectral Size 32768



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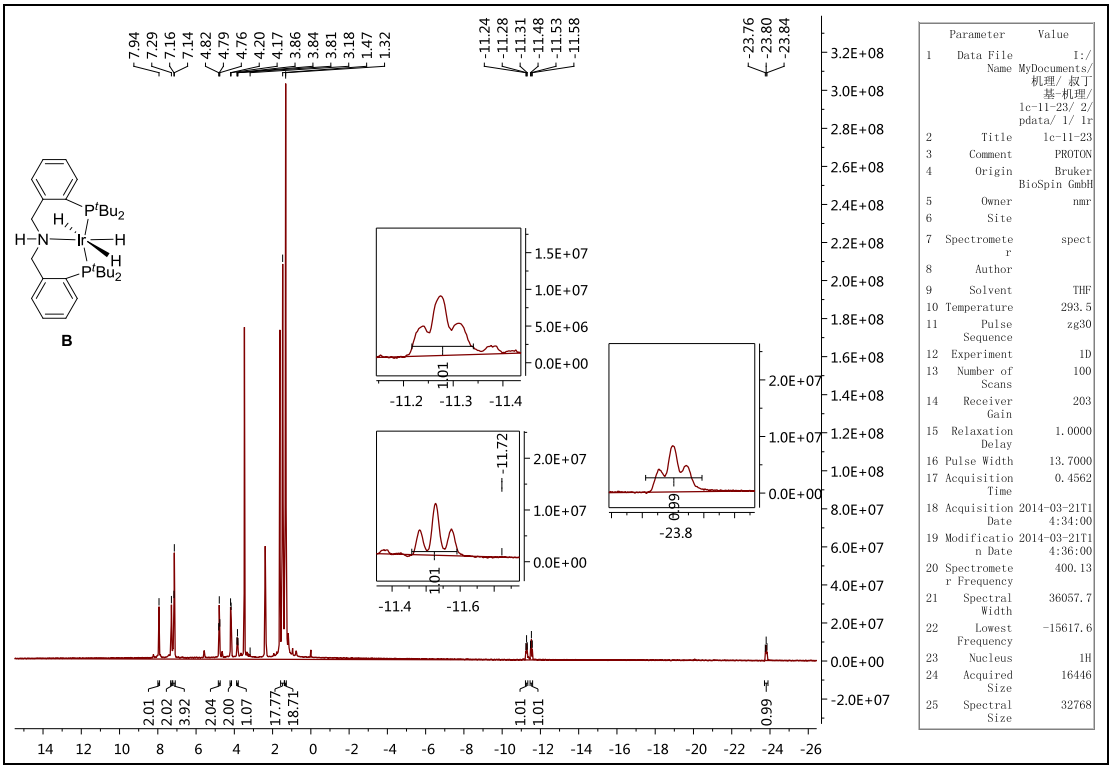
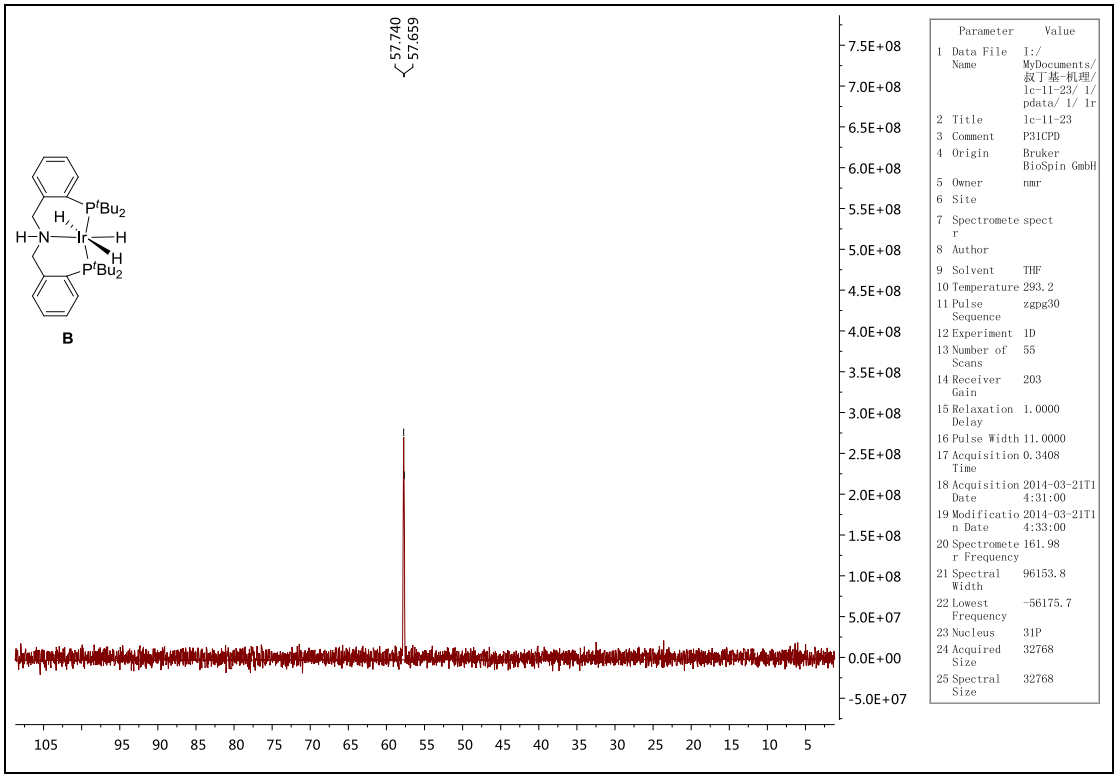
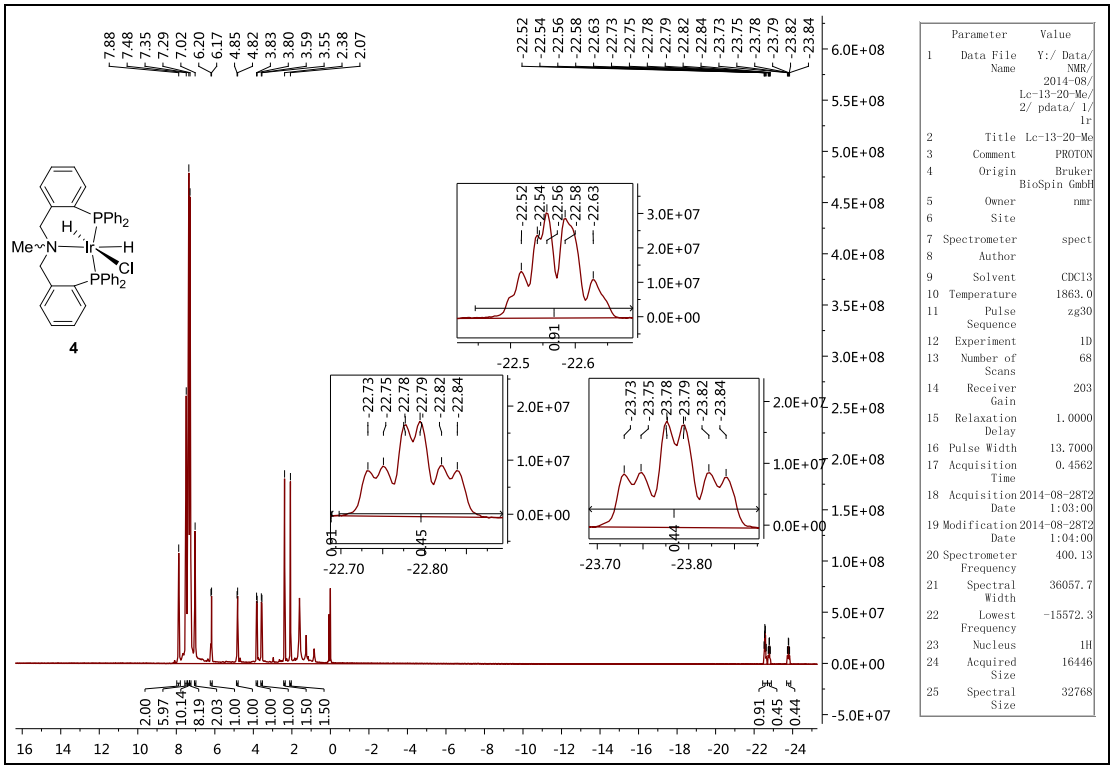
1	Data File Name	H:/MyDocuments/叔丁基-机理/lc-20140314-2/1/pdata/1/1r
2	Title	lc-20140314-2
3	Comment	P31CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	THF
10	Temperature	294.9
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	21
14	Receiver Gain	199
15	Relaxation Delay	1.0000
16	Pulse Width	14.5000
17	Acquisition Time	0.2556
18	Acquisition Date	2014-03-13T20:41:53
19	Modification Date	2014-03-13T20:42:00
20	Spectrometer Frequency	161.98
21	Spectral Width	64102.6
22	Lowest Frequency	-40150.1
23	Nucleus	31P
24	Acquired Size	16384
25	Spectral Size	32768



	Parameter	Value
1	Data File Name	I:/MyDocuments/机理/叔丁基-机理/lc-11-23/2/pdata/1/1r
2	Title	lc-11-23
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	THF
10	Temperature	293.5
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	100
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	13.7000
17	Acquisition Time	0.4562
18	Acquisition Date	2014-03-21T14:34:00
19	Modification Date	2014-03-21T14:36:00
20	Spectrometer Frequency	400.13
21	Spectral Width	36057.7
22	Lowest Frequency	-15617.6
23	Nucleus	1H
24	Acquired Size	16446
25	Spectral Size	32768



	Parameter	Value
1	Data File Name	I:/MyDocuments/叔丁基-机理/lc-11-23/1/pdata/1/1r
2	Title	lc-11-23
3	Comment	P31CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	THF
10	Temperature	293.2
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	55
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	11.0000
17	Acquisition Time	0.3408
18	Acquisition Date	2014-03-21T14:31:00
19	Modification Date	2014-03-21T14:33:00
20	Spectrometer Frequency	161.98
21	Spectral Width	96153.8
22	Lowest Frequency	-56175.7
23	Nucleus	31P
24	Acquired Size	32768
25	Spectral Size	32768



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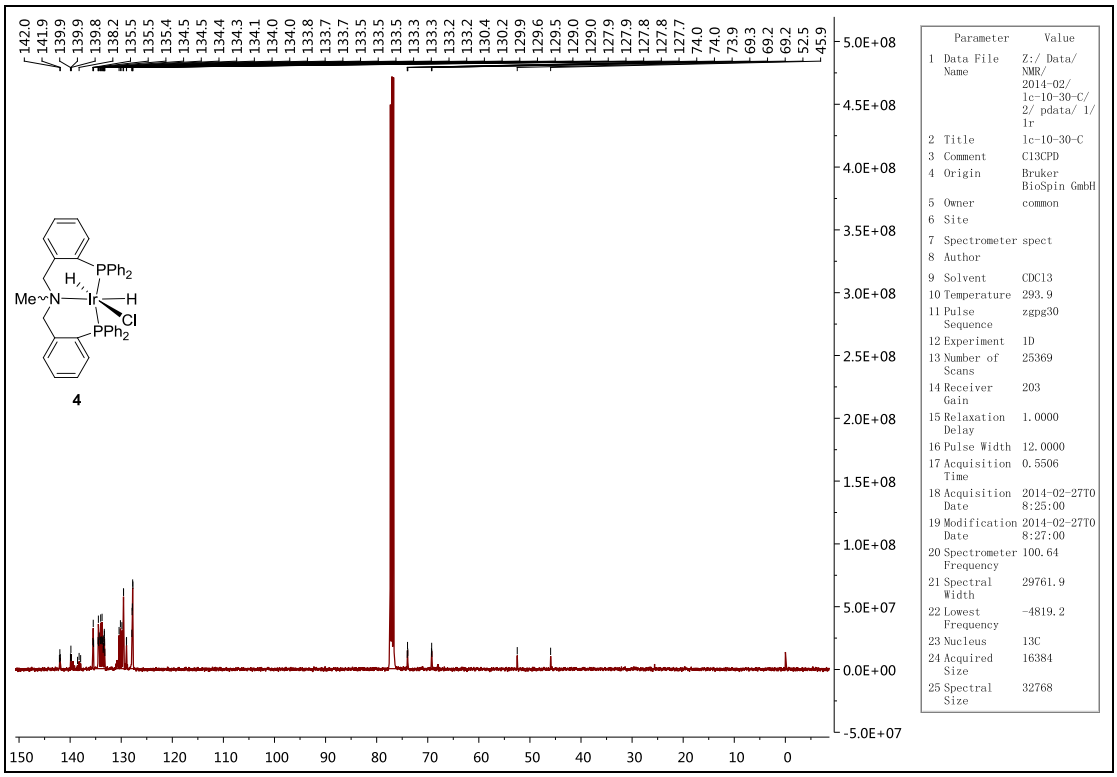
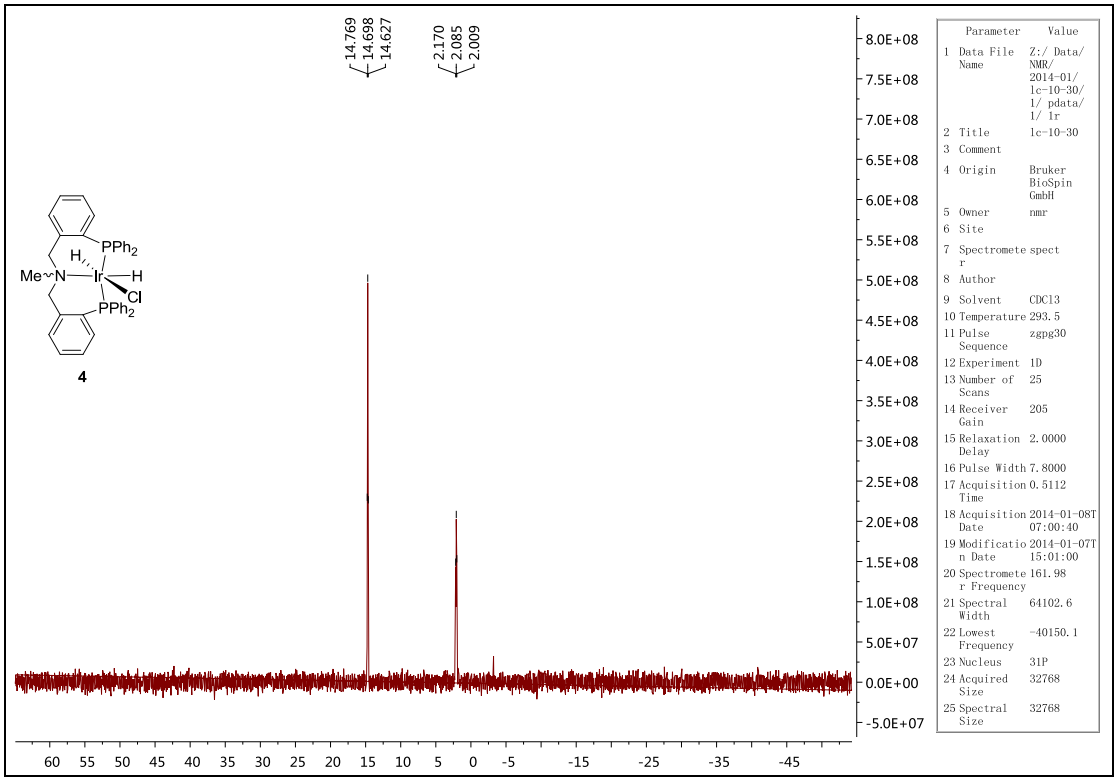
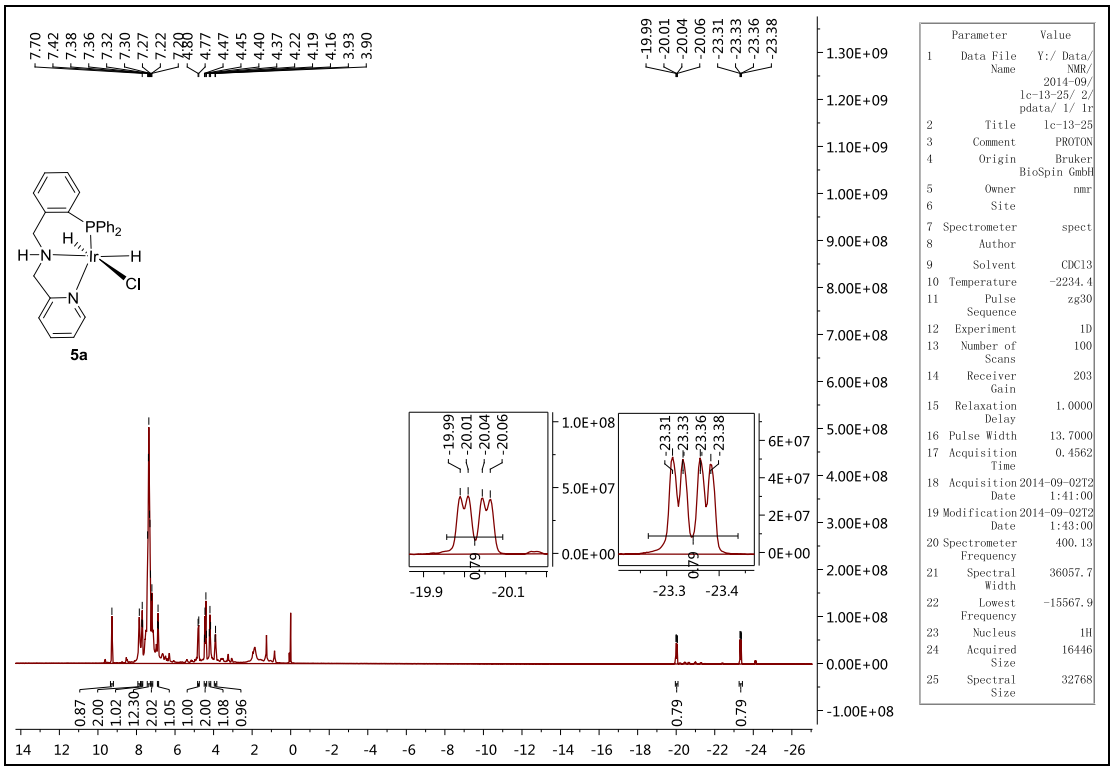
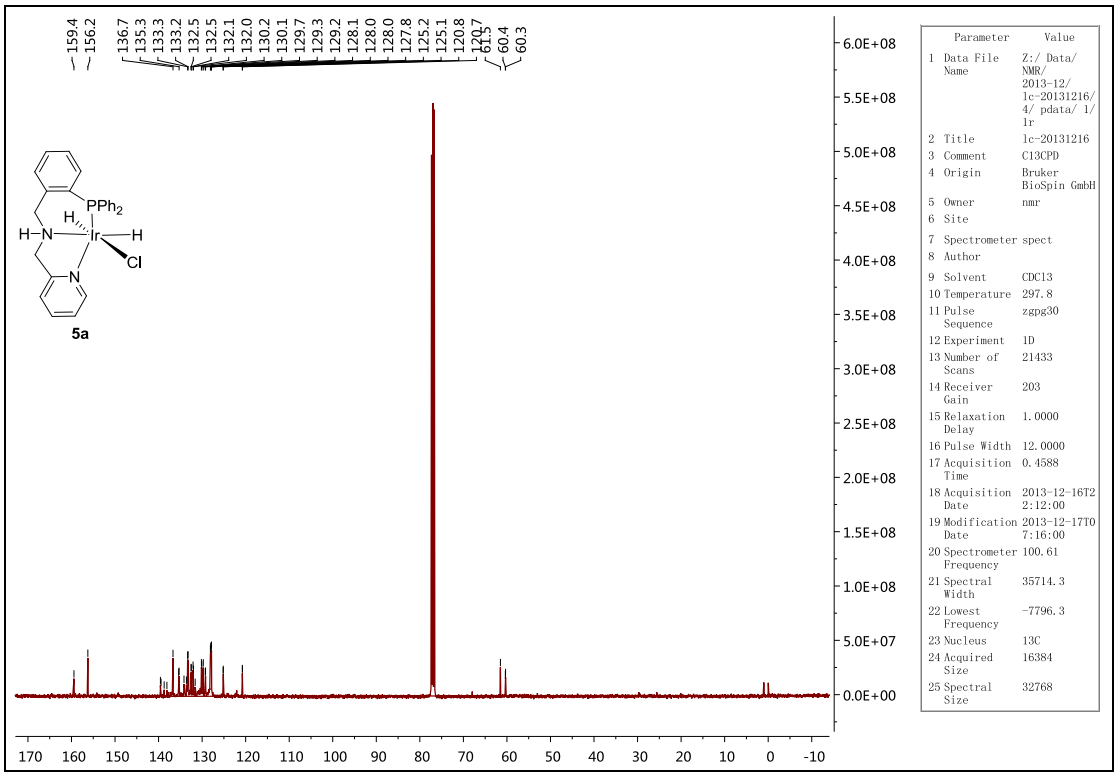
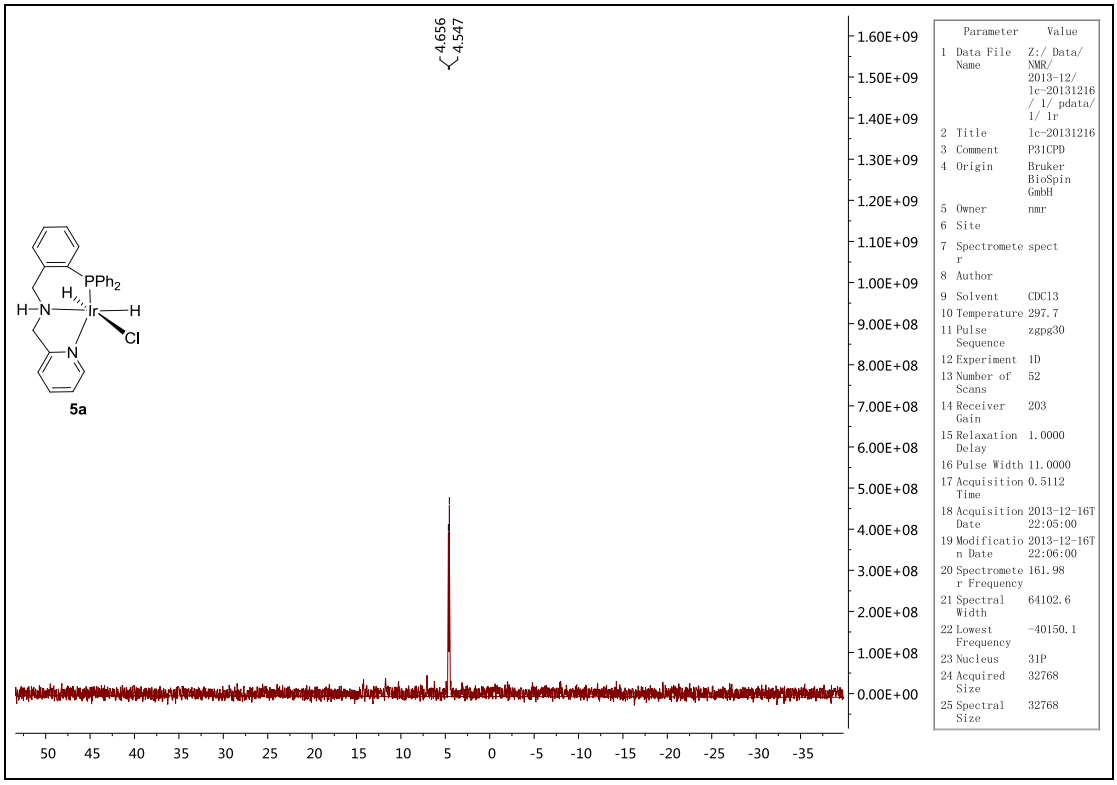
1	Data File Name	Y:/Data/NMR/2014-08/Lc-13-20-Me/2/pdata/1/1r
2	Title	Lc-13-20-Me
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	1863.0
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	68
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	13.7000
17	Acquisition Time	0.4562
18	Acquisition Date	2014-08-28T21:03:00
19	Modification Date	2014-08-28T21:04:00
20	Spectrometer Frequency	400.13
21	Spectral Width	36057.7
22	Lowest Frequency	-15572.3
23	Nucleus	1H
24	Acquired Size	16446
25	Spectral Size	32768


142.0 141.9 139.9 139.9 139.8 138.2 135.5 135.5 135.4 134.5 134.5 134.4 134.3 134.1 134.0 134.0 133.8 133.7 133.7 133.5 133.5 133.5 133.3 133.3 133.2 133.2 130.4 130.2 129.9 129.6 129.5 129.0 129.0 127.9 127.9 127.8 127.8 127.7 74.0 73.9 69.3 69.2 52.5 45.9
PPh2
H
Me
N
Ir
H
Cl
PPh2
4
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
-5.0E+07
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
Parameter Value
1 Data File Name Z:/ Data/ NMR/ 2014-02/ 1c-10-30-C/ 2/ pdata/ 1/ 1r
2 Title 1c-10-30-C
3 Comment C13CPD
4 Origin Bruker BioSpin GmbH
5 Owner common
6 Site
7 Spectrometer spect
8 Author
9 Solvent CDCl3
10 Temperature 293.9
11 Pulse Sequence zgpg30
12 Experiment 1D
13 Number of Scans 25369
14 Receiver Gain 203
15 Relaxation Delay 1.0000
16 Pulse Width 12.0000
17 Acquisition Time 0.5506
18 Acquisition Date 2014-02-27T08:25:00
19 Modification Date 2014-02-27T08:27:00
20 Spectrometer Frequency 100.64
21 Spectral Width 29761.9
22 Lowest Frequency -4819.2
23 Nucleus 13C
24 Acquired Size 16384
25 Spectral Size 32768

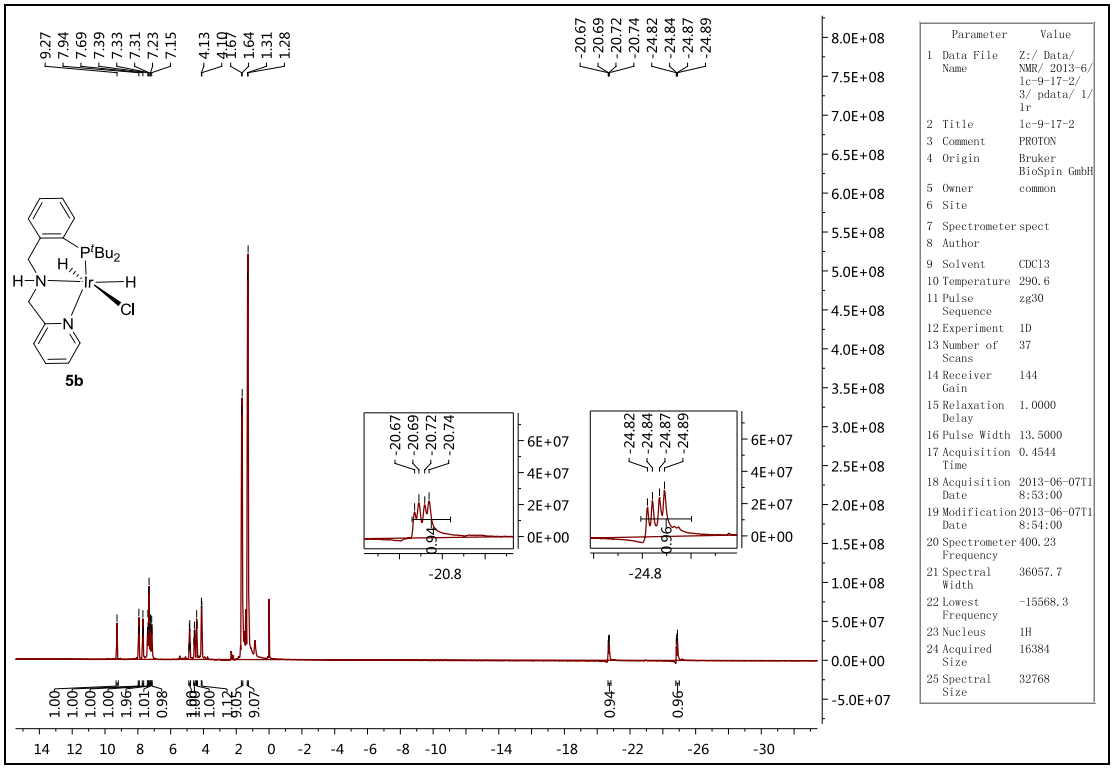

14.769
14.698
14.627
2.170
2.085
2.009
PPh2
H
Me
N
Ir
H
Cl
PPh2
4
8.0E+08
7.5E+08
7.0E+08
6.5E+08
6.0E+08
5.5E+08
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
-5.0E+07
60 55 50 45 40 35 30 25 20 15 10 5 0 -5 -15 -25 -35 -45
Parameter Value
1 Data File Name Z:/ Data/ NMR/ 2014-01/ 1c-10-30/ 1/ pdata/ 1/ 1r
2 Title 1c-10-30
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmr
6 Site
7 Spectrometer spect r
8 Author
9 Solvent CDCl3
10 Temperature 293.5
11 Pulse Sequence zgpg30
12 Experiment 1D
13 Number of Scans 25
14 Receiver Gain 205
15 Relaxation Delay 2.0000
16 Pulse Width 7.8000
17 Acquisition Time 0.5112
18 Acquisition Date 2014-01-08T07:00:40
19 Modification Date 2014-01-07T15:01:00
20 Spectrometer Frequency 161.98
21 Spectral Width 64102.6
22 Lowest Frequency -40150.1
23 Nucleus 31P
24 Acquired Size 32768
25 Spectral Size 32768


7.70
7.42
7.38
7.36
7.32
7.30
7.27
7.22
7.20
4.80
4.77
4.47
4.45
4.40
4.37
4.22
4.19
4.16
3.93
3.90
-19.99
-20.01
-20.04
-20.06
-23.31
-23.33
-23.36
-23.38
PPh2
H
H–N
Ir
H
Cl
N
5a
0.87
2.00
1.02
12.30
2.02
1.05
1.00
2.00
1.08
0.96
0.79
0.79
14 12 10 8 6 4 2 0 -2 -4 -6 -8 -10 -12 -14 -16 -18 -20 -22 -24 -26
-19.9
-20.1
-23.3
-23.4
Parameter Value
1 Data File Name Y:/ Data/ NMR/ 2014-09/ lc-13-25/ 2/ pdata/ 1/ 1r
2 Title lc-13-25
3 Comment PROTON
4 Origin Bruker BioSpin GmbH
5 Owner nmr
6 Site
7 Spectrometer spect
8 Author
9 Solvent CDCl3
10 Temperature -2234.4
11 Pulse Sequence zg30
12 Experiment 1D
13 Number of Scans 100
14 Receiver Gain 203
15 Relaxation Delay 1.0000
16 Pulse Width 13.7000
17 Acquisition Time 0.4562
18 Acquisition Date 2014-09-02T21:41:00
19 Modification Date 2014-09-02T21:43:00
20 Spectrometer Frequency 400.13
21 Spectral Width 36057.7
22 Lowest Frequency -15567.9
23 Nucleus 1H
24 Acquired Size 16446
25 Spectral Size 32768

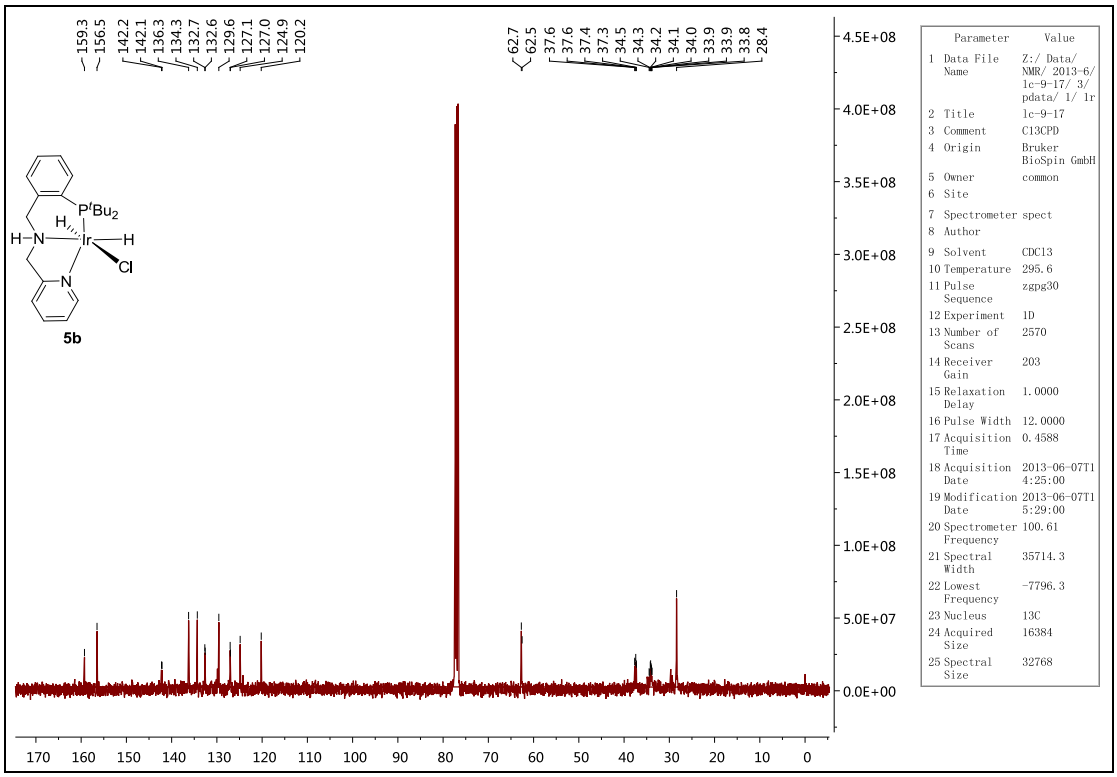

159.4
156.2
136.7
135.3
133.3
133.2
132.5
132.5
132.1
132.0
130.2
130.1
129.7
129.3
129.2
128.1
128.0
128.0
127.8
125.2
125.1
120.8
120.7
61.5
60.4
60.3
PPh2
H
H–N
Ir
H
Cl
N
5a
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
Parameter Value
1 Data File Name Z:/ Data/ NMR/ 2013-12/ lc-20131216/ 4/ pdata/ 1/ 1r
2 Title lc-20131216
3 Comment C13CPD
4 Origin Bruker BioSpin GmbH
5 Owner nmr
6 Site
7 Spectrometer spect
8 Author
9 Solvent CDCl3
10 Temperature 297.8
11 Pulse Sequence zgpg30
12 Experiment 1D
13 Number of Scans 21433
14 Receiver Gain 203
15 Relaxation Delay 1.0000
16 Pulse Width 12.0000
17 Acquisition Time 0.4588
18 Acquisition Date 2013-12-16T22:12:00
19 Modification Date 2013-12-17T07:16:00
20 Spectrometer Frequency 100.61
21 Spectral Width 35714.3
22 Lowest Frequency -7796.3
23 Nucleus 13C
24 Acquired Size 16384
25 Spectral Size 32768

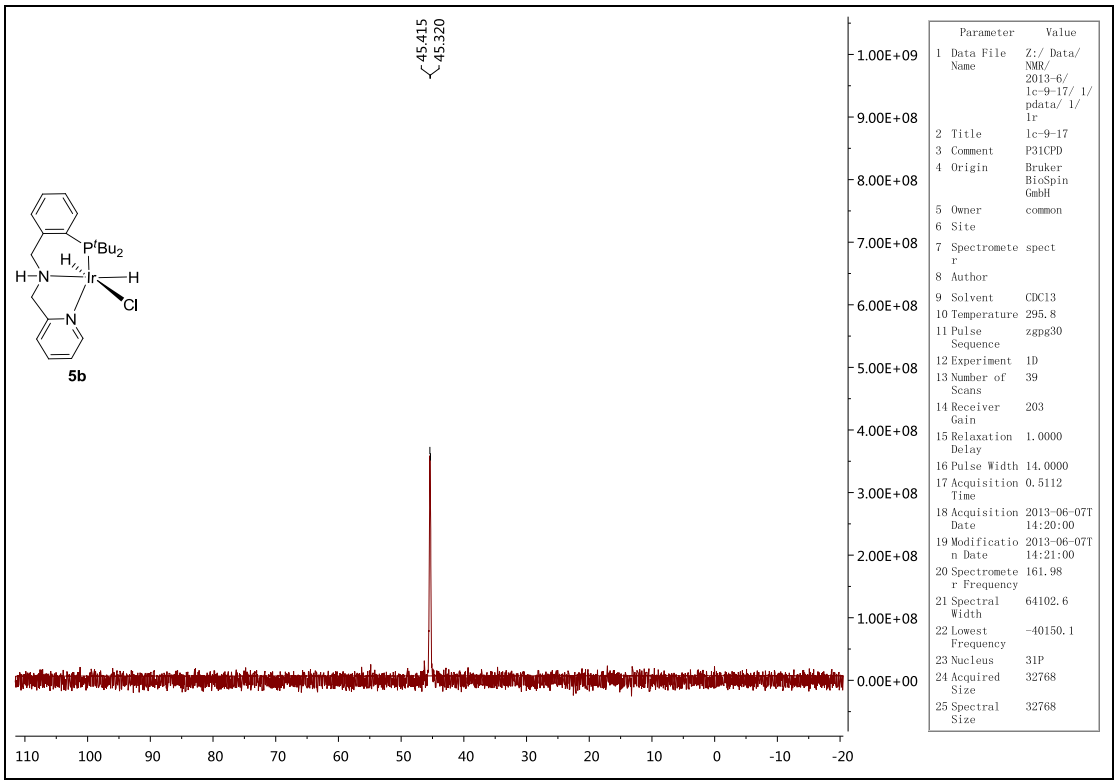


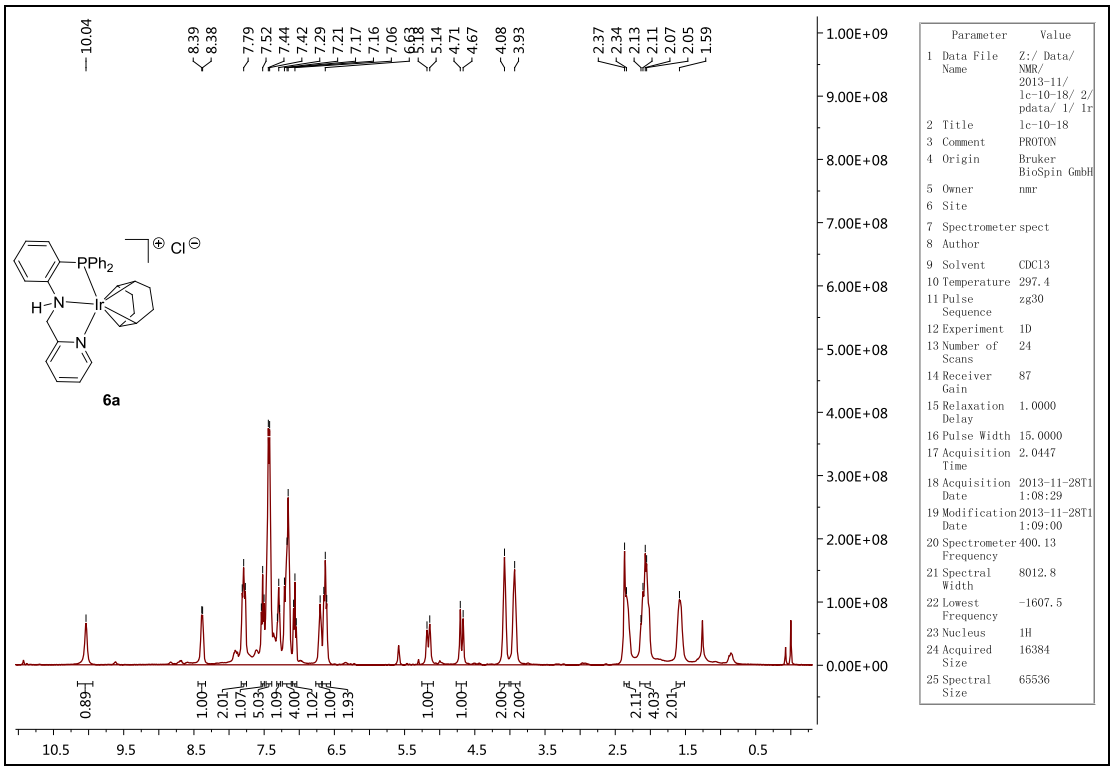
Parameter	Value
1 Data File Name	Z:/ Data/ NMR/ 2013-12/ lc-20131216 / 1/ pdata/ 1/ 1r
2 Title	lc-20131216
3 Comment	P31CPD
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect r
8 Author	
9 Solvent	CDCl3
10 Temperature	297.7
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	52
14 Receiver Gain	203
15 Relaxation Delay	1.0000
16 Pulse Width	11.0000
17 Acquisition Time	0.5112
18 Acquisition Date	2013-12-16T 22:05:00
19 Modificatio n Date	2013-12-16T 22:06:00
20 Spectrometer r Frequency	161.98
21 Spectral Width	64102.6
22 Lowest Frequency	-40150.1
23 Nucleus	31P
24 Acquired Size	32768
25 Spectral Size	32768



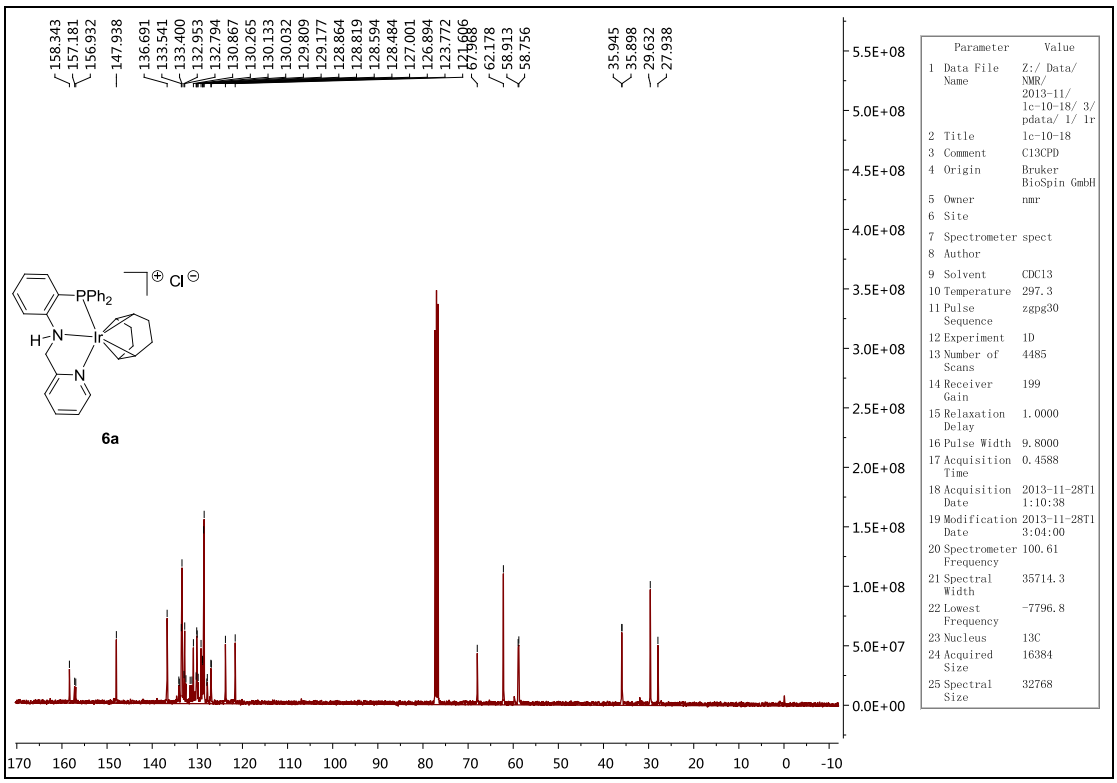
Parameter	Value
1 Data File Name	Z:/ Data/ NMR/ 2013-6/ lc-9-17-2/ 3/ pdata/ 1/ 1r
2 Title	lc-9-17-2
3 Comment	PROTON
4 Origin	Bruker BioSpin GmbH
5 Owner	common
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	290.6
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	37
14 Receiver Gain	144
15 Relaxation Delay	1.0000
16 Pulse Width	13.5000
17 Acquisition Time	0.4544
18 Acquisition Date	2013-06-07T1 8:53:00
19 Modification Date	2013-06-07T1 8:54:00
20 Spectrometer Frequency	400.23
21 Spectral Width	36057.7
22 Lowest Frequency	-15568.3
23 Nucleus	1H
24 Acquired Size	16384
25 Spectral Size	32768


159.3
156.5
142.2
142.1
136.3
134.3
132.7
132.6
129.6
127.1
127.0
124.9
120.2
62.7
62.5
37.6
37.6
37.4
37.3
34.5
34.3
34.2
34.1
34.0
33.9
33.9
33.8
28.4
P^{t}Bu$_2$
H
H–N
Ir
H
Cl
N
5b
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
Parameter Value
1 Data File Name Z:/ Data/ NMR/ 2013-6/ 1c-9-17/ 3/ pdata/ 1/ 1r
2 Title 1c-9-17
3 Comment C13CPD
4 Origin Bruker BioSpin GmbH
5 Owner common
6 Site
7 Spectrometer spect
8 Author
9 Solvent CDCl3
10 Temperature 295.6
11 Pulse Sequence zgpg30
12 Experiment 1D
13 Number of Scans 2570
14 Receiver Gain 203
15 Relaxation Delay 1.0000
16 Pulse Width 12.0000
17 Acquisition Time 0.4588
18 Acquisition Date 2013-06-07T14:25:00
19 Modification Date 2013-06-07T15:29:00
20 Spectrometer Frequency 100.61
21 Spectral Width 35714.3
22 Lowest Frequency -7796.3
23 Nucleus 13C
24 Acquired Size 16384
25 Spectral Size 32768

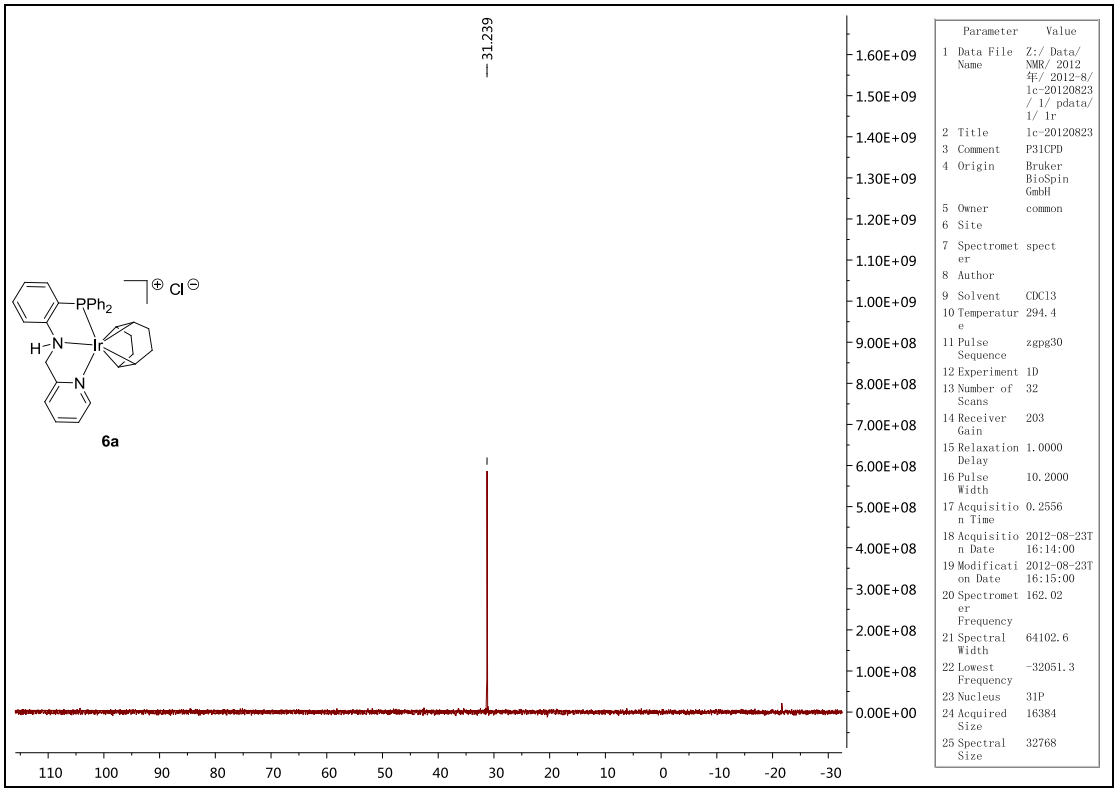

45.415
45.320
P^{t}Bu$_2$
H
H–N
Ir
H
Cl
N
5b
1.00E+09
9.00E+08
8.00E+08
7.00E+08
6.00E+08
5.00E+08
4.00E+08
3.00E+08
2.00E+08
1.00E+08
0.00E+00
110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
Parameter Value
1 Data File Name Z:/ Data/ NMR/ 2013-6/ 1c-9-17/ 1/ pdata/ 1/ 1r
2 Title 1c-9-17
3 Comment P31CPD
4 Origin Bruker BioSpin GmbH
5 Owner common
6 Site
7 Spectrometer spect
8 Author
9 Solvent CDCl3
10 Temperature 295.8
11 Pulse Sequence zgpg30
12 Experiment 1D
13 Number of Scans 39
14 Receiver Gain 203
15 Relaxation Delay 1.0000
16 Pulse Width 14.0000
17 Acquisition Time 0.5112
18 Acquisition Date 2013-06-07T14:20:00
19 Modification Date 2013-06-07T14:21:00
20 Spectrometer Frequency 161.98
21 Spectral Width 64102.6
22 Lowest Frequency -40150.1
23 Nucleus 31P
24 Acquired Size 32768
25 Spectral Size 32768



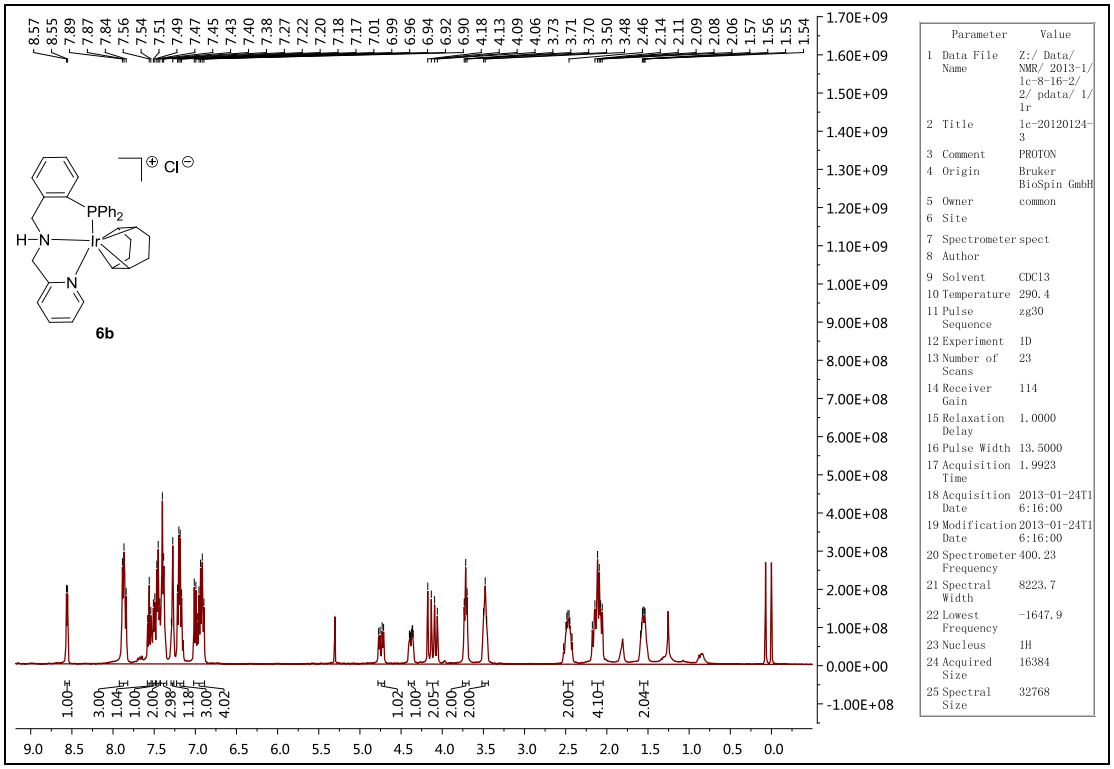
	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2013-11/ 1c-10-18/ 2/ pdata/ 1/ 1r
2	Title	1c-10-18
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	297.4
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	24
14	Receiver Gain	87
15	Relaxation Delay	1.0000
16	Pulse Width	15.0000
17	Acquisition Time	2.0447
18	Acquisition Date	2013-11-28T11:08:29
19	Modification Date	2013-11-28T11:09:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8012.8
22	Lowest Frequency	-1607.5
23	Nucleus	1H
24	Acquired Size	16384
25	Spectral Size	65536



	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2013-11/ 1c-10-18/ 3/ pdata/ 1/ 1r
2	Title	1c-10-18
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	297.3
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	4485
14	Receiver Gain	199
15	Relaxation Delay	1.0000
16	Pulse Width	9.8000
17	Acquisition Time	0.4588
18	Acquisition Date	2013-11-28T11:10:38
19	Modification Date	2013-11-28T13:04:00
20	Spectrometer Frequency	100.61
21	Spectral Width	35714.3
22	Lowest Frequency	-7796.8
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768



	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2012 4F/ 2012-8/ lc-20120823 / 1/ pdata/ 1/ 1r
2	Title	lc-20120823
3	Comment	P31CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	294.4
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	32
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	10.2000
17	Acquisition Time	0.2556
18	Acquisition Date	2012-08-23T 16:14:00
19	Modification Date	2012-08-23T 16:15:00
20	Spectrometer Frequency	162.02
21	Spectral Width	64102.6
22	Lowest Frequency	-32051.3
23	Nucleus	31P
24	Acquired Size	16384
25	Spectral Size	32768



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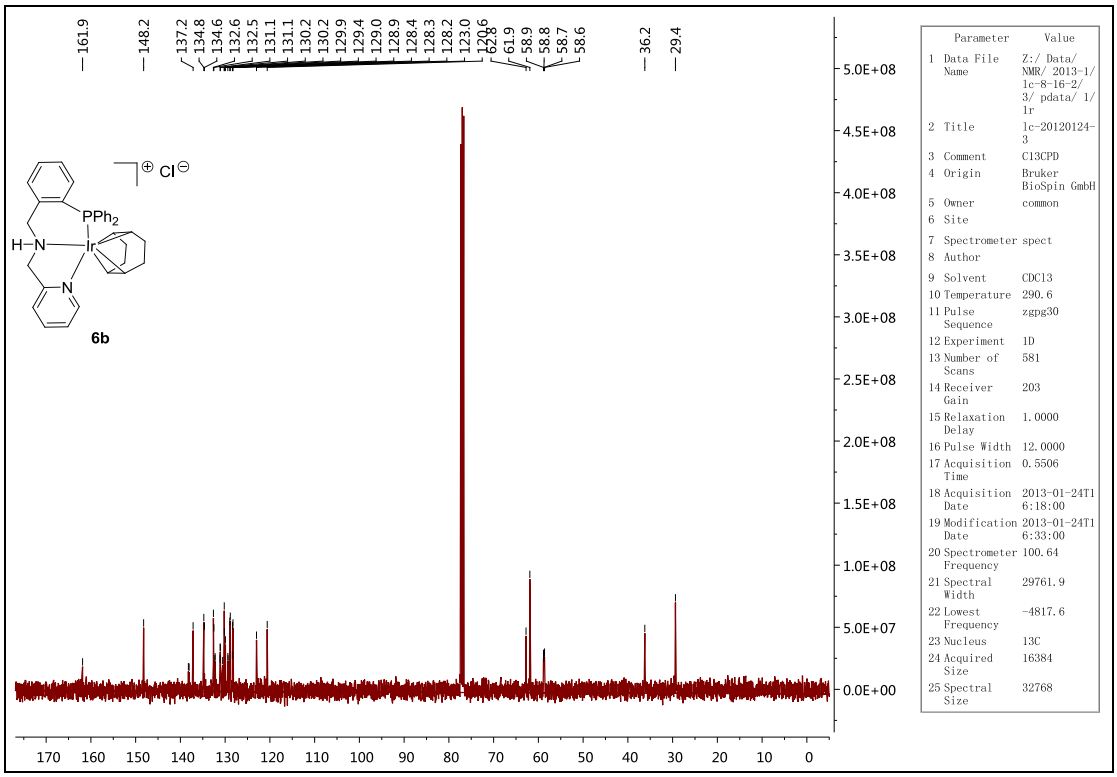
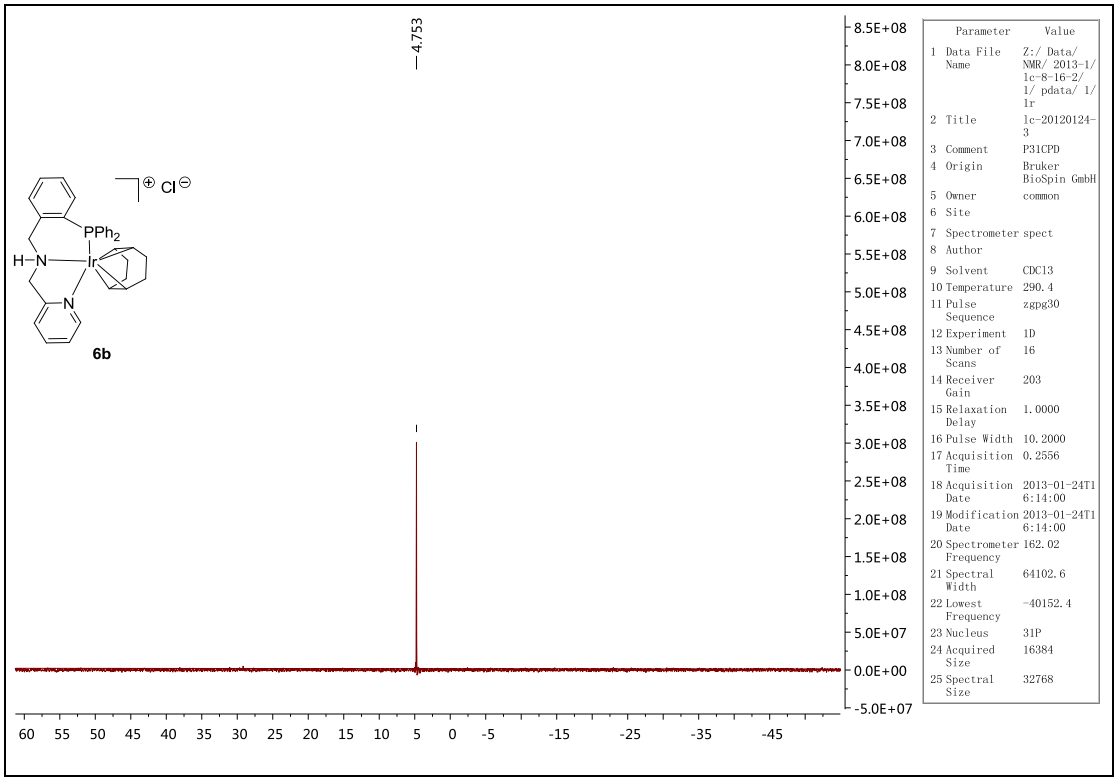
1	Data File Name	Z:/ Data/ NMR/ 2013-1/ lc-8-16-2/ 2/ pdata/ 1/ 1r
2	Title	lc-20120124-3
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	290.4
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	23
14	Receiver Gain	114
15	Relaxation Delay	1.0000
16	Pulse Width	13.5000
17	Acquisition Time	1.9923
18	Acquisition Date	2013-01-24T1 6:16:00
19	Modification Date	2013-01-24T1 6:16:00
20	Spectrometer Frequency	400.23
21	Spectral Width	8223.7
22	Lowest Frequency	-1647.9
23	Nucleus	1H
24	Acquired Size	16384
25	Spectral Size	32768



	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2013-1/ 1c-8-16-2/ 3/ pdata/ 1/ 1r
2	Title	1c-20120124-3
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	290.6
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	581
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	12.0000
17	Acquisition Time	0.5506
18	Acquisition Date	2013-01-24T16:18:00
19	Modification Date	2013-01-24T16:33:00
20	Spectrometer Frequency	100.64
21	Spectral Width	29761.9
22	Lowest Frequency	-4817.6
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768



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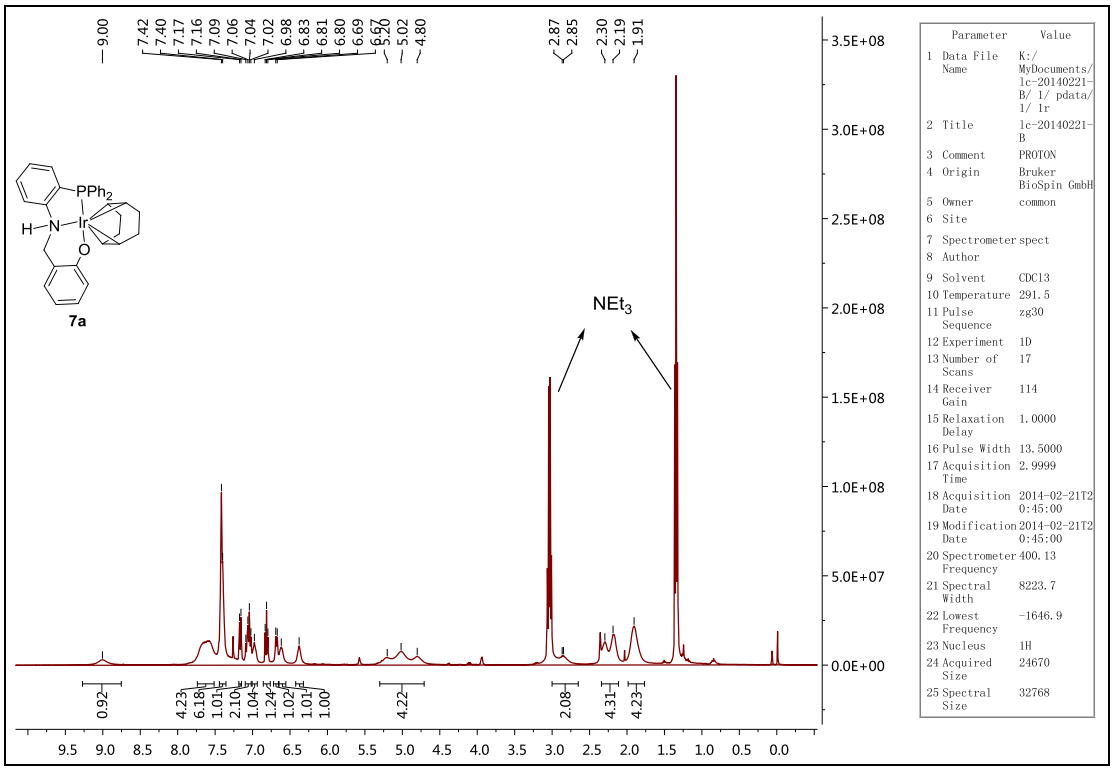
1	Data File Name	Z:/ Data/ NMR/ 2013-1/ 1c-8-16-2/ 1/ pdata/ 1/ 1r
2	Title	1c-20120124-3
3	Comment	P31CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	290.4
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	16
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	10.2000
17	Acquisition Time	0.2556
18	Acquisition Date	2013-01-24T16:14:00
19	Modification Date	2013-01-24T16:14:00
20	Spectrometer Frequency	162.02
21	Spectral Width	64102.6
22	Lowest Frequency	-40152.4
23	Nucleus	31P
24	Acquired Size	16384
25	Spectral Size	32768


9.00
7.42
7.40
7.17
7.16
7.09
7.06
7.04
7.02
6.98
6.83
6.81
6.80
6.69
6.67
5.20
5.02
4.80
2.87
2.85
2.30
2.19
1.91
PPh2
H
N
Ir
O
7a
NEt3
0.92
4.23
6.18
1.01
2.10
1.04
1.24
1.02
1.01
1.00
4.22
2.08
4.31
4.23
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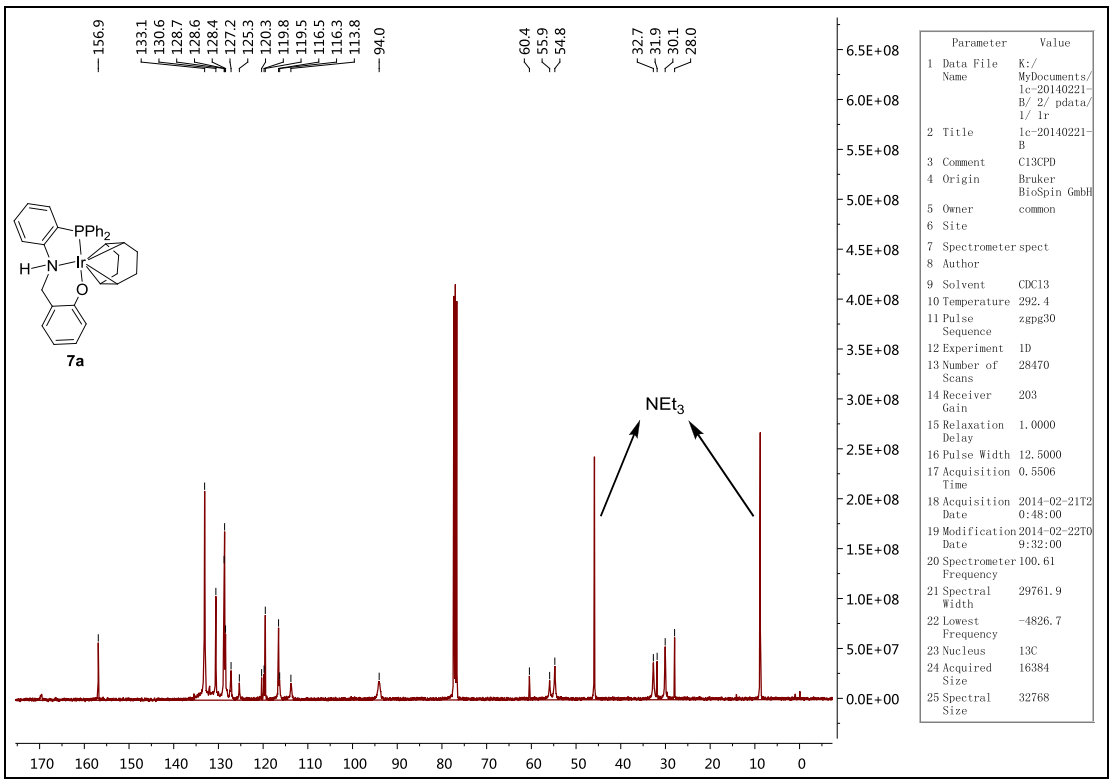
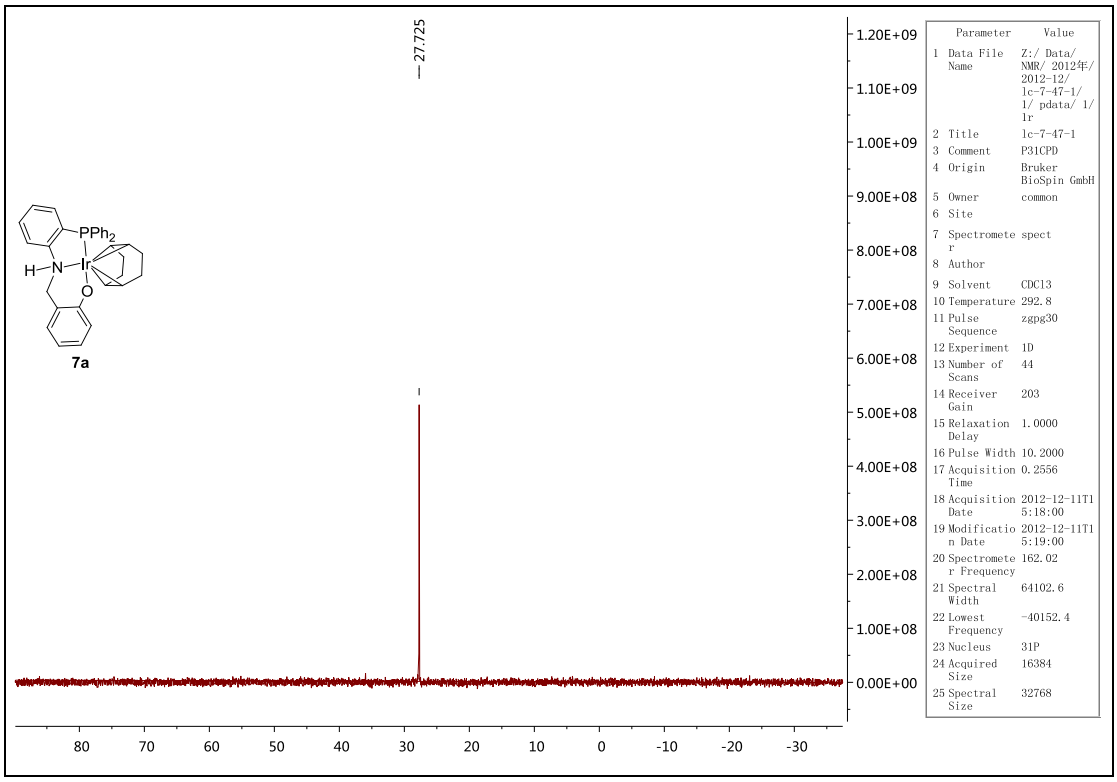
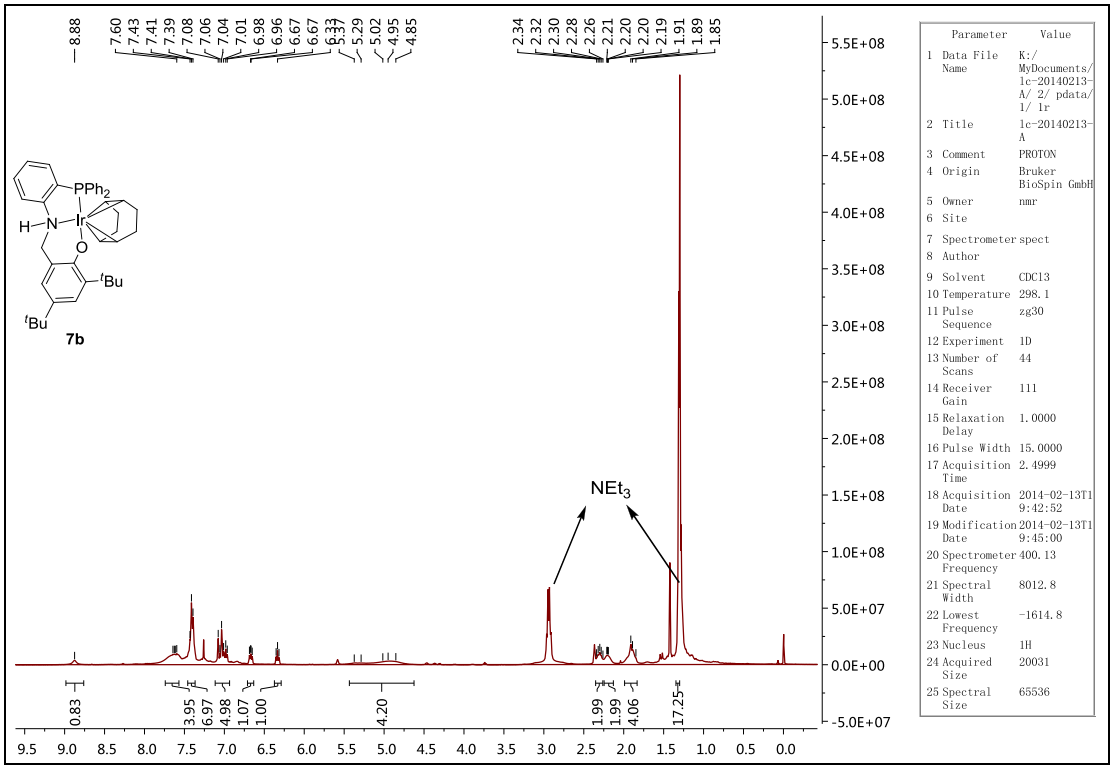
1 Data File Name K:/MyDocuments/1c-20140221-B/1/pdata/1/1r
2 Title 1c-20140221-B
3 Comment PROTON
4 Origin Bruker BioSpin GmbH
5 Owner common
6 Site
7 Spectrometer spect
8 Author
9 Solvent CDCl3
10 Temperature 291.5
11 Pulse Sequence zg30
12 Experiment 1D
13 Number of Scans 17
14 Receiver Gain 114
15 Relaxation Delay 1.0000
16 Pulse Width 13.5000
17 Acquisition Time 2.9999
18 Acquisition Date 2014-02-21T20:45:00
19 Modification Date 2014-02-21T20:45:00
20 Spectrometer Frequency 400.13
21 Spectral Width 8223.7
22 Lowest Frequency -1646.9
23 Nucleus 1H
24 Acquired Size 24670
25 Spectral Size 32768

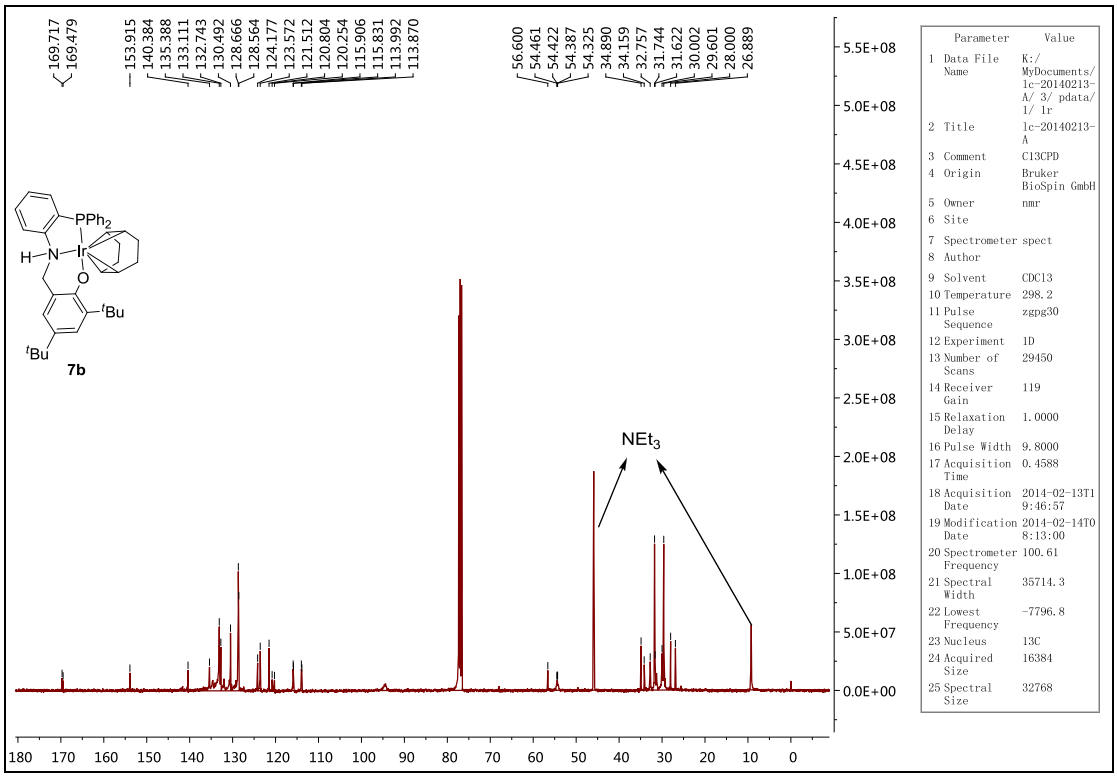

156.9
133.1
130.6
128.7
128.6
128.4
127.2
125.3
120.3
119.8
119.5
116.5
116.3
113.8
94.0
60.4
55.9
54.8
32.7
31.9
30.1
28.0
PPh2
H
N
Ir
O
7a
NEt3
Parameter Value
1 Data File Name K:/MyDocuments/1c-20140221-B/2/pdata/1/1r
2 Title 1c-20140221-B
3 Comment C13CPD
4 Origin Bruker BioSpin GmbH
5 Owner common
6 Site
7 Spectrometer spect
8 Author
9 Solvent CDCl3
10 Temperature 292.4
11 Pulse Sequence zgpg30
12 Experiment 1D
13 Number of Scans 28470
14 Receiver Gain 203
15 Relaxation Delay 1.0000
16 Pulse Width 12.5000
17 Acquisition Time 0.5506
18 Acquisition Date 2014-02-21T20:48:00
19 Modification Date 2014-02-22T09:32:00
20 Spectrometer Frequency 100.61
21 Spectral Width 29761.9
22 Lowest Frequency -4826.7
23 Nucleus 13C
24 Acquired Size 16384
25 Spectral Size 32768

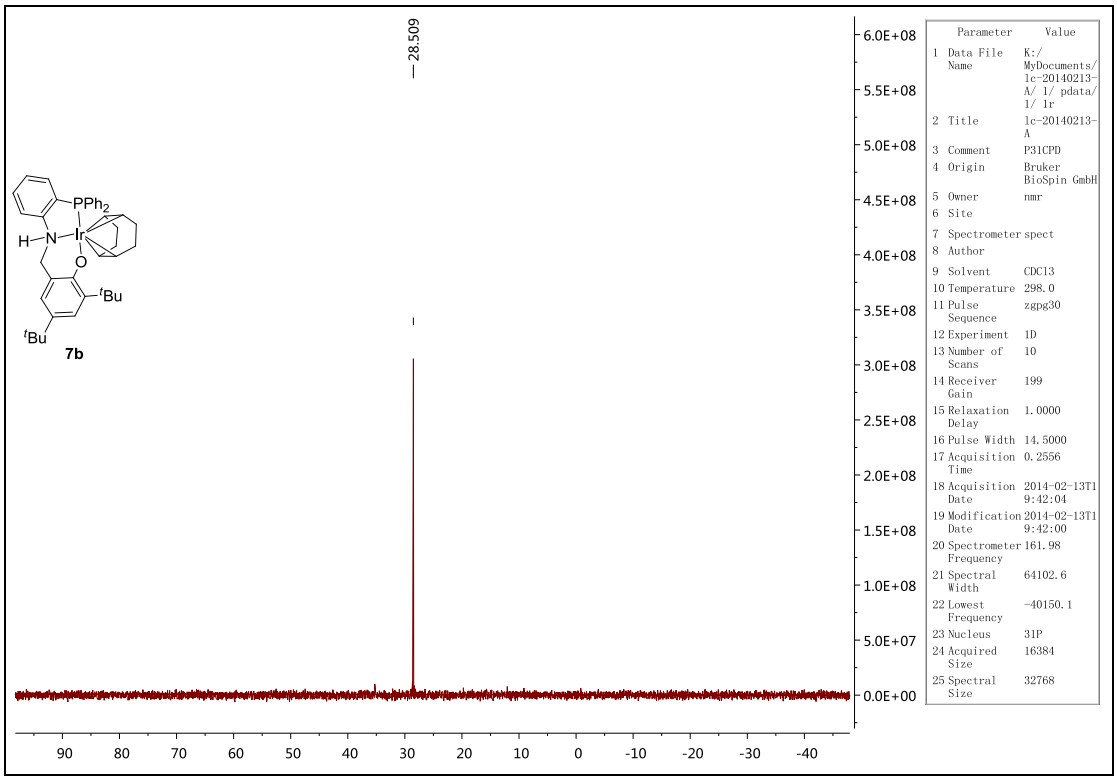


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2012年/ 2012-12/ 1c-7-47-1/ 1/ pdata/ 1/ 1r
2	Title	1c-7-47-1
3	Comment	P31CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect r
8	Author	
9	Solvent	CDCl3
10	Temperature	292.8
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	44
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	10.2000
17	Acquisition Time	0.2556
18	Acquisition Date	2012-12-11T1 5:18:00
19	Modification Date	2012-12-11T1 5:19:00
20	Spectrometer Frequency	162.02
21	Spectral Width	64102.6
22	Lowest Frequency	-40152.4
23	Nucleus	31P
24	Acquired Size	16384
25	Spectral Size	32768



	Parameter	Value
1	Data File Name	K:/ MyDocuments/ 1c-20140213-A/ 2/ pdata/ 1/ 1r
2	Title	1c-20140213-A
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	298.1
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	44
14	Receiver Gain	111
15	Relaxation Delay	1.0000
16	Pulse Width	15.0000
17	Acquisition Time	2.4999
18	Acquisition Date	2014-02-13T1 9:42:52
19	Modification Date	2014-02-13T1 9:45:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8012.8
22	Lowest Frequency	-1614.8
23	Nucleus	1H
24	Acquired Size	20031
25	Spectral Size	65536


169.717
169.479
153.915
140.384
135.388
133.111
132.743
130.492
128.666
128.564
124.177
123.572
121.512
120.804
120.254
115.906
115.831
113.992
113.870
56.600
54.461
54.422
54.387
54.325
34.890
34.159
32.757
31.744
31.622
30.002
29.601
28.000
26.889
NEt3
7b
Parameter Value
1 Data File Name K:/MyDocuments/1c-20140213-A/3/pdata/1/1r
2 Title 1c-20140213-A
3 Comment C13CPD
4 Origin Bruker BioSpin GmbH
5 Owner nmr
6 Site
7 Spectrometer spect
8 Author
9 Solvent CDCl3
10 Temperature 298.2
11 Pulse Sequence zgpg30
12 Experiment 1D
13 Number of Scans 29450
14 Receiver Gain 119
15 Relaxation Delay 1.0000
16 Pulse Width 9.8000
17 Acquisition Time 0.4588
18 Acquisition Date 2014-02-13T19:46:57
19 Modification Date 2014-02-14T08:13:00
20 Spectrometer Frequency 100.61
21 Spectral Width 35714.3
22 Lowest Frequency -7796.8
23 Nucleus 13C
24 Acquired Size 16384
25 Spectral Size 32768


28.509
7b
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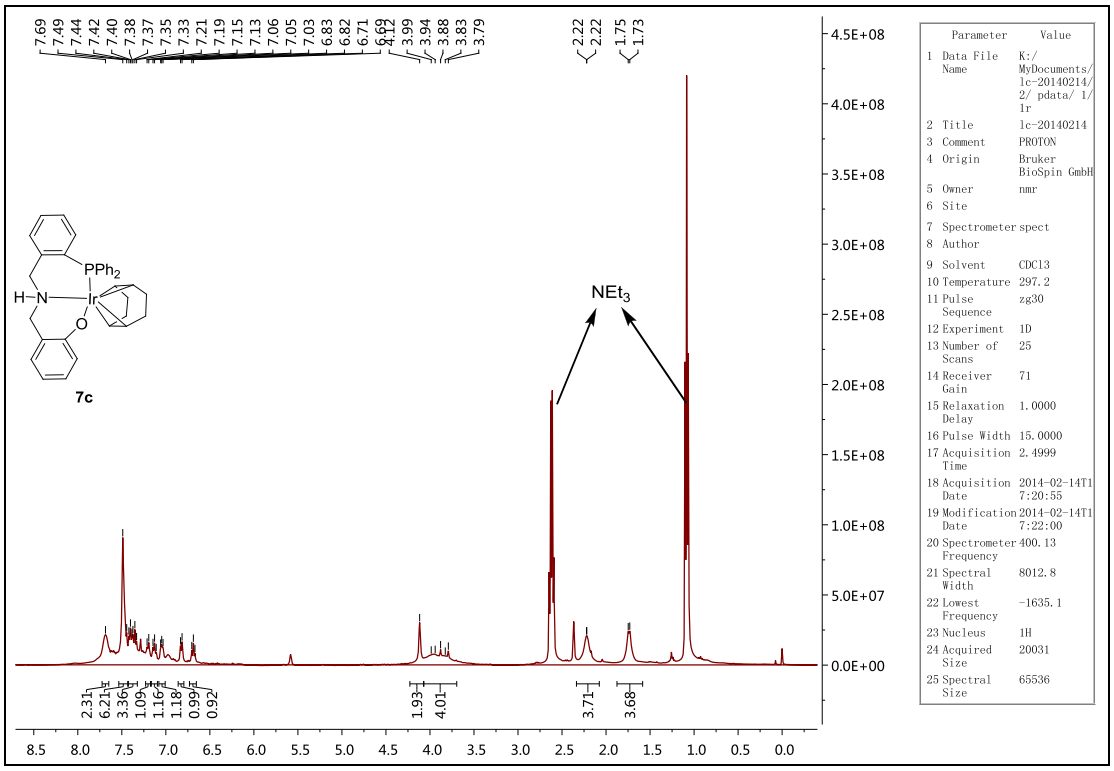
1 Data File Name K:/MyDocuments/1c-20140213-A/1/pdata/1/1r
2 Title 1c-20140213-A
3 Comment P31CPD
4 Origin Bruker BioSpin GmbH
5 Owner nmr
6 Site
7 Spectrometer spect
8 Author
9 Solvent CDCl3
10 Temperature 298.0
11 Pulse Sequence zgpg30
12 Experiment 1D
13 Number of Scans 10
14 Receiver Gain 199
15 Relaxation Delay 1.0000
16 Pulse Width 14.5000
17 Acquisition Time 0.2556
18 Acquisition Date 2014-02-13T19:42:04
19 Modification Date 2014-02-13T19:42:00
20 Spectrometer Frequency 161.98
21 Spectral Width 64102.6
22 Lowest Frequency -40150.1
23 Nucleus 31P
24 Acquired Size 16384
25 Spectral Size 32768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7.49
7.44
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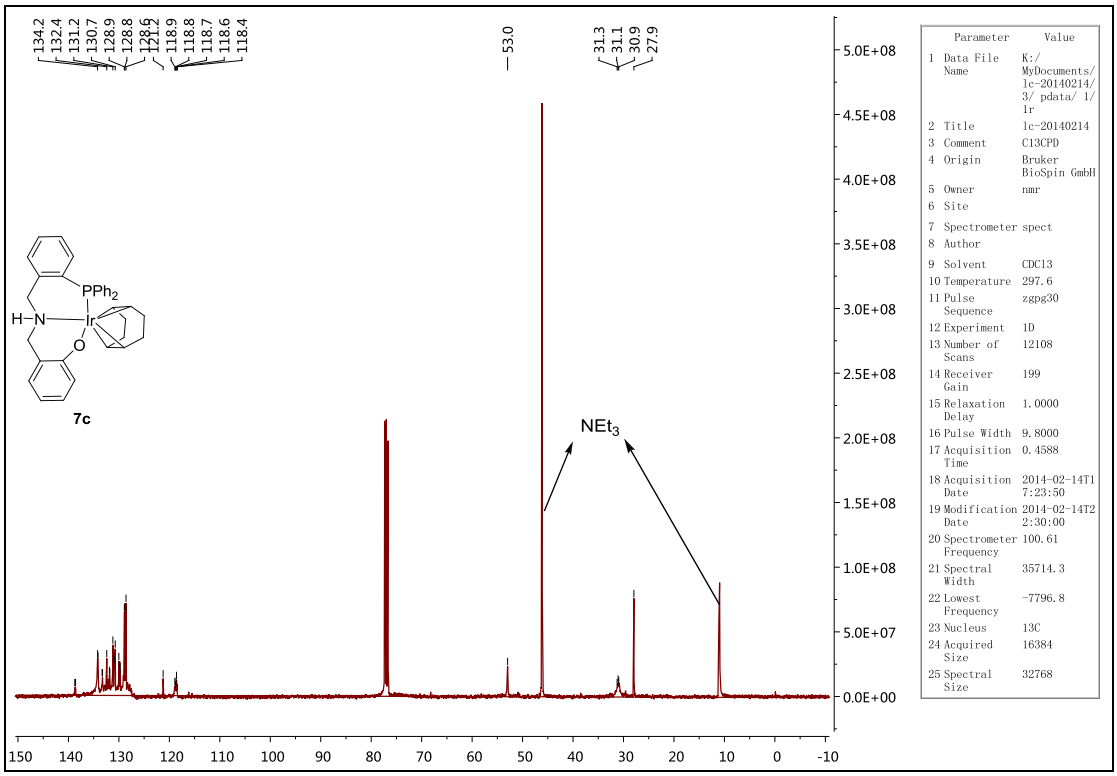
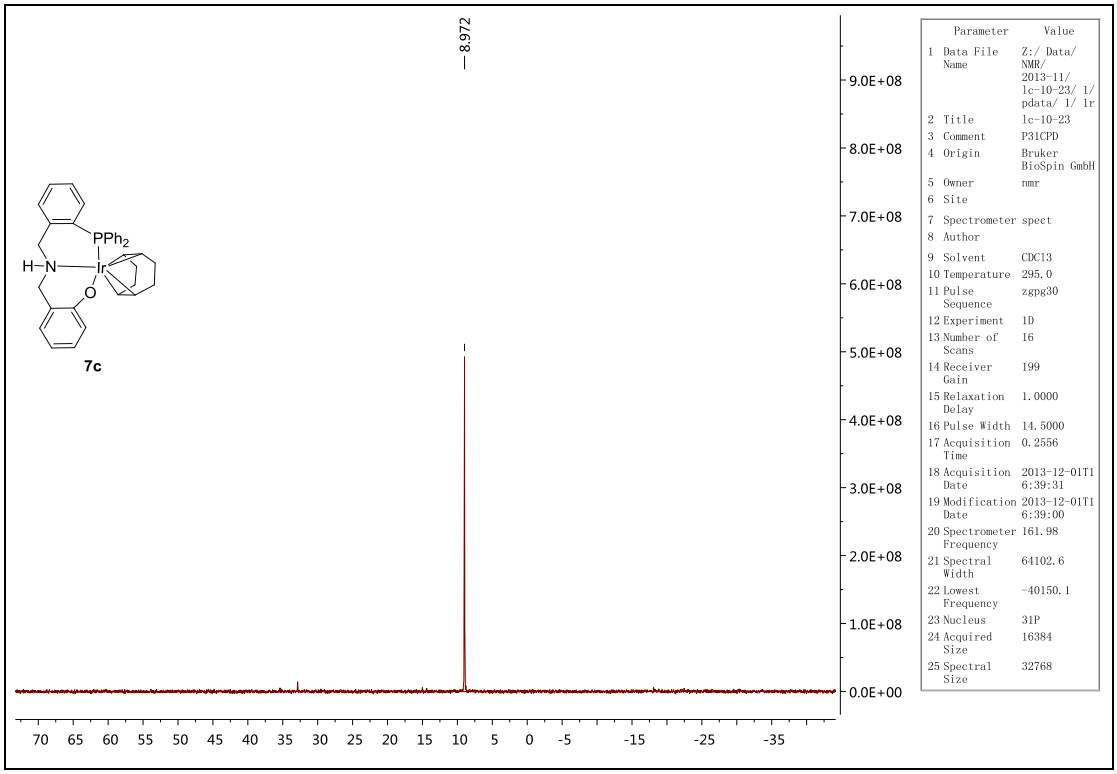
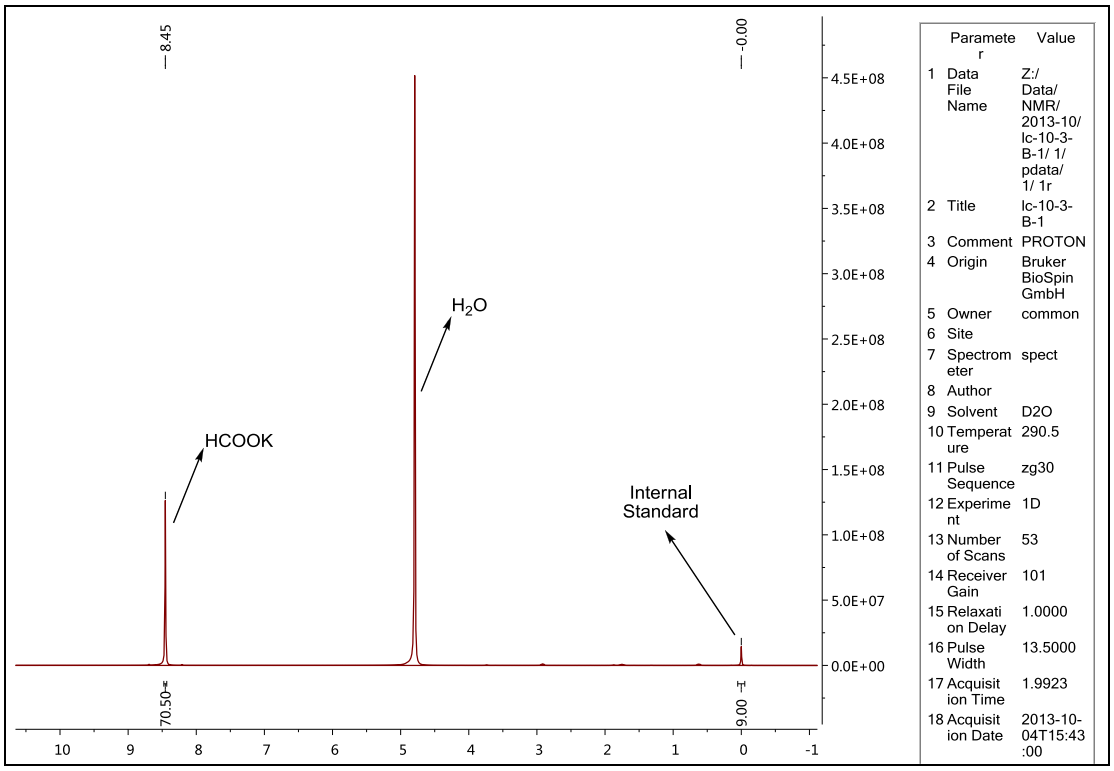
7.40
7.38
7.37
7.35
7.33
7.21
7.19
7.15
7.13
7.06
7.05
7.03
6.83
6.82
6.71
4.12
3.99
3.94
3.88
3.83
3.79
2.22
2.22
1.75
1.73
PPh2
H–N
Ir
O
7c
NEt3
2.31
6.21
3.36
1.09
1.16
1.18
0.99
0.92
1.93
4.01
3.71
3.68
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
Parameter Value
1 Data File Name K:/ MyDocuments/ 1c-20140214/ 2/ pdata/ 1/ 1r
2 Title 1c-20140214
3 Comment PROTON
4 Origin Bruker BioSpin GmbH
5 Owner nmr
6 Site
7 Spectrometer spect
8 Author
9 Solvent CDCl3
10 Temperature 297.2
11 Pulse Sequence zg30
12 Experiment 1D
13 Number of Scans 25
14 Receiver Gain 71
15 Relaxation Delay 1.0000
16 Pulse Width 15.0000
17 Acquisition Time 2.4999
18 Acquisition Date 2014-02-14T1 7:20:55
19 Modification Date 2014-02-14T1 7:22:00
20 Spectrometer Frequency 400.13
21 Spectral Width 8012.8
22 Lowest Frequency -1635.1
23 Nucleus 1H
24 Acquired Size 20031
25 Spectral Size 65536


134.2
132.4
131.2
130.7
128.9
128.8
128.6
128.2
118.9
118.8
118.7
118.6
118.4
53.0
31.3
31.1
30.9
27.9
PPh2
H–N
Ir
O
7c
NEt3
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
Parameter Value
1 Data File Name K:/ MyDocuments/ 1c-20140214/ 3/ pdata/ 1/ 1r
2 Title 1c-20140214
3 Comment C13CPD
4 Origin Bruker BioSpin GmbH
5 Owner nmr
6 Site
7 Spectrometer spect
8 Author
9 Solvent CDCl3
10 Temperature 297.6
11 Pulse Sequence zgpg30
12 Experiment 1D
13 Number of Scans 12108
14 Receiver Gain 199
15 Relaxation Delay 1.0000
16 Pulse Width 9.8000
17 Acquisition Time 0.4588
18 Acquisition Date 2014-02-14T1 7:23:50
19 Modification Date 2014-02-14T2 2:30:00
20 Spectrometer Frequency 100.61
21 Spectral Width 35714.3
22 Lowest Frequency -7796.8
23 Nucleus 13C
24 Acquired Size 16384
25 Spectral Size 32768



	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2013-11/ 1c-10-23/ 1/ pdata/ 1/ 1r
2	Title	1c-10-23
3	Comment	P31CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	295.0
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	16
14	Receiver Gain	199
15	Relaxation Delay	1.0000
16	Pulse Width	14.5000
17	Acquisition Time	0.2556
18	Acquisition Date	2013-12-01T16:39:31
19	Modification Date	2013-12-01T16:39:00
20	Spectrometer Frequency	161.98
21	Spectral Width	64102.6
22	Lowest Frequency	-40150.1
23	Nucleus	31P
24	Acquired Size	16384
25	Spectral Size	32768

(E) Representative ^{1}H NMR Spectra of Reaction Mixture



	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2013-10/ lc-10-3-B-1/ 1/ pdata/ 1/ 1r
2	Title	lc-10-3-B-1
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	D2O
10	Temperature	290.5
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	53
14	Receiver Gain	101
15	Relaxation Delay	1.0000
16	Pulse Width	13.5000
17	Acquisition Time	1.9923
18	Acquisition Date	2013-10-04T15:43:00