Supporting Information

$Rh_2(OAc)_4$-Catalyzed 2,3-Migration of β-Ferrocenecarboxyl α-Diazocarbonyl Compounds: An Efficient Synthesis of Ferrocene-Containing α,β-Unsaturated Esters

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CONTENTS

1. General information All reagents were used as received from commercial sources, unless specified otherwise, or prepared as described in the literature. All solvents were distilled under a nitrogen atmosphere prior to use. CH_2Cl_2 was dried over CaH_2. For chromatography, 200-300 mesh silica gel (Qingdao, China) was employed. ^1H and ^{13}C NMR spectra were recorded at 500 MHz and 125 MHz FT-NMR spectrometer. Chemical shifts are reported in *ppm* using tetramethylsilane as internal standard when $CDCl_3$ was used as solvent. IR spectra were recorded on a FT-IR instrument. The HRMS analysis was obtained on a GCTOF mass spectrometer. Melting points were determined with melting points apparatus and are uncorrected.

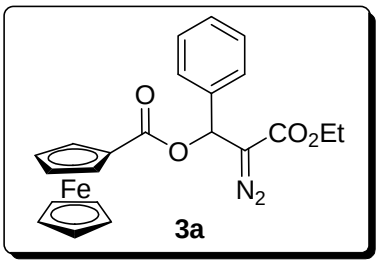
2. General Procedure for the preparation of β-ferrocenecarboxyl substituted diazo compounds 3

In a dried three-necked round-bottom flask, ferrocenoyl chloride (1.1 mmol) in 2 mL of anhydrous CH_2Cl_2 was added dropwise to a solution of β-hydroxy α-diazo ester **2** (1.0 mmol) with pyridine (2.0 mmol) in 5 mL of anhydrous CH_2Cl_2 at 0 ℃ under N_2. The resulting mixture was stirred at 0 °C and the progress of the reaction was monitored by TLC. After completion of the esterification reaction, saturated $NaHCO_3$ was added at 0 °C. the organic phase was dried using Na_2SO_4, and solvent was removed under reduced pressure. Next, the residue was subjected to chromatography on silica gel to afford the products **3a-j**.

3. General Procedure for the $Rh_2(OAc)_4$-catalyzed reaction of 3a-j

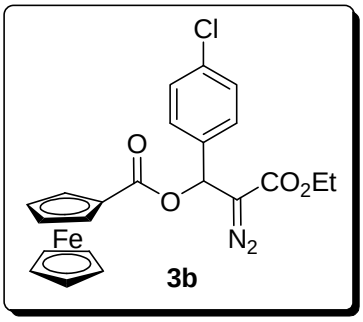
In a dried three-necked round-bottom flask, $Rh_2(OAc)_4$ (0.1 mol %) was dissolved into 5 mL of anhydrous CH_2Cl_2. A solution of diazo substrates **3a-j** in anhydrous CH_2Cl_2 was added dropwise at 0 °C over the course of 30 min. The reaction mixture was stirred until TLC analysis indicated the complete disappearance of the diazo compound. The solvent was then removed under reduced pressure, and the crude residue was purified by column chromatography to give the corresponding 2,3-migration products.

4. β-ferrocenecarboxyl substituted diazo compounds 3



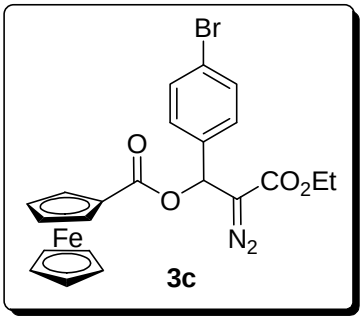
3a

Red solid; Mp**:** 83-84 ^{o}C; IR (KBr) 3110, 2098, 1701, 1404, 1122, 1025, 829 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.29 (t, *J* = 7.0 Hz, 3H), 4.17 (s, 5H), 4.28 (q, *J* = 7.0 Hz, 2H), 4.44 (s, 2H), 4.88 (s, 2H), 6.98 (s, 1H), 7.34-7.45 (m, 5H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.5, 61.4, 70.0, 70.3, 70.5, 70.6, 71.7, 125.9, 128.6, 128.9, 136.9, 170.2; EI-MS (*m/z*, relative intensity): 404 [(M-28)$^{+}$, 100]; Anal. calcd for $C_{22}H_{20}FeN_2O_4$: C, 61.13; H, 4.66; N, 6.48; Found: C, 61.35; H, 4.93; N, 6.31.



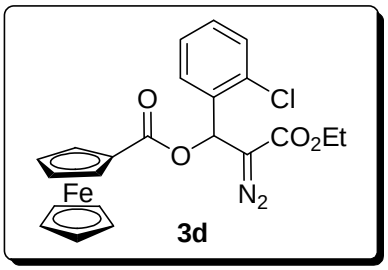
3b

Red solid; Mp**:** 98-100 ^{o}C; IR (KBr) 3110, 2104, 1715, 1121, 1005, 824 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.29 (t, *J* = 7.0 Hz, 3H), 4.18 (s, 5H), 4.28 (q, *J* = 7.0 Hz, 2H), 4.45 (t, *J* = 2.0 Hz, 2H), 4.87 (d, *J* = 2.0 Hz, 2H), 6.93 (s, 1H), 7.39 (s, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.5, 61.4, 69.4, 69.9, 70.2, 70.3, 71.7, 127.4, 129.1, 134.5, 135.5, 170.3; EI-MS (*m/z*, relative intensity): 438 [(M-28)$^{+}$, 33], 461 (100); Anal. calcd for $C_{22}H_{19}ClFeN_2O_4$: C, 56.62; H, 4.10; N, 6.00; Found: C, 57.01; H, 4.09; N, 6.03.



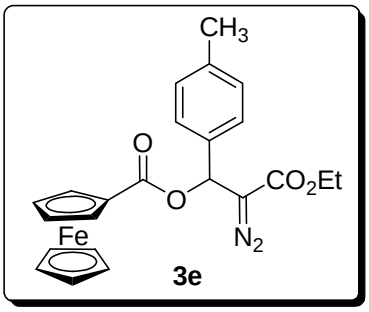
3c

Red solid; Mp**:** 100-101 ^{o}C; IR (KBr) 3086, 2102, 1701, 1125, 1006, 819 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.29 (t, *J* = 7.0 Hz, 3H), 4.18 (s, 5H), 4.28 (q, *J* = 7.0 Hz, 2H), 4.45 (t, *J* = 2.0 Hz, 2H), 4.87 (d, *J* = 2.0 Hz, 2H), 6.91 (s, 1H), 7.34 (d, *J* = 10.0 Hz, 2H), 7.55 (d, *J* = 10.0 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.5, 61.4, 69.5, 69.9, 70.3, 70.4, 71.8, 122.6, 127.6, 132.0, 136.0, 170.3; EI-MS (*m/z*, relative intensity): 465 (100), 505 [(M+Na-28)$^{+}$, 58]; Anal. calcd for $C_{22}H_{19}BrFeN_2O_4$: C, 51.69; H, 3.75; N, 5.48; Found: C, 51.80; H, 4.04; N, 5.54.



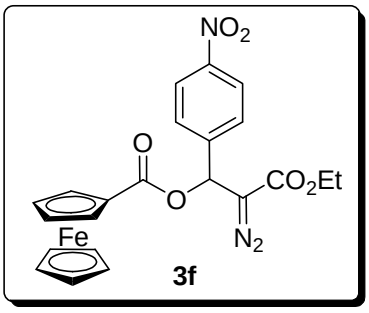
3d

Red solid; Mp**:** 103-105 ^{o}C; IR (KBr) 3109, 2099, 1708, 1113, 1025, 826 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.27 (t, *J* = 7.0 Hz, 3H), 4.20 (s, 5H), 4.23-4.27 (m, 2H), 4.46 (t, *J* = 1.0 Hz, 2H), 4.90 (dd, *J* = 2.0 Hz, *J* = 1.0 Hz, 2H), 7.12 (s, 1H), 7.28-7.34 (m, 2H), 7.44 (d, *J* = 1.5 Hz, 1H), 7.60 (d, *J* = 7.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.5, 61.2, 68.4, 69.9, 70.2, 70.4, 71.7, 126.9, 127.4，129.7, 130.0, 132.1, 134.4, 170.3; EI-MS (*m/z*, relative intensity): 466 (M^+, 73), 455 (100); Anal. calcd for $C_{22}H_{19}ClFeN_2O_4$: C, 56.62; H, 4.10; N, 6.00; Found: C, 57.00; H, 4.11; N, 6.03.



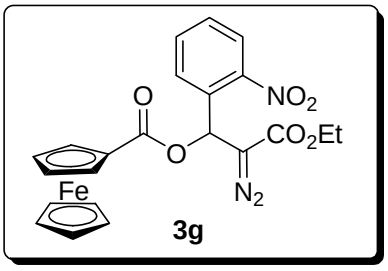
3e

Red solid; Mp**:** 74-75 ^{o}C; IR (KBr) 3111, 2097, 1702, 1404, 1122, 1025, 829 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.29 (t, *J* = 7.0 Hz, 3H), 1.42 (s, 3H), 4.17 (s, 5H), 4.28 (q, *J* = 7.0 Hz, 2H), 4.43 (t, *J* = 1.5 Hz, 2H), 4.88 (dd, *J* = 2.0 Hz, *J* = 1.5 Hz, 2H), 6.99 (s, 1H), 7.44 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.5, 61.6, 69.4, 69.6, 70.0, 70.2, 70.4, 72.0, 124.1, 126.9, 144.1, 147.9, 164.2, 170.5; EI-MS (*m/z*, relative intensity): 418 [$(M-28)^+$, 8], 421 (100); Anal. calcd for $C_{23}H_{22}FeN_2O_4$: C, 61.90; H, 4.97; N, 6.28; Found: C, 62.23; H, 5.04; N, 6.33.



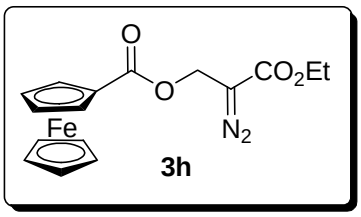
3f

Red solid; Mp**:** 61-63 ^{o}C; IR (KBr) 3115, 2101, 1714, 1606, 1118, 1003, 847 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.29 (t, *J* = 7.5 Hz, 3H), 4.20 (s, 5H), 4.28 (q, *J* = 7.5 Hz, 2H), 4.49 (t, *J* = 1.5 Hz, 2H), 4.90 (d, *J* = 2.0 Hz, 2H), 7.00 (s, 1H), 7.64 (d, *J* = 10.5 Hz, 2H), 8.28 (d, *J* = 10.5 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.5, 61.6, 69.3, 69.6, 70.0, 72.0, 124.1, 126.9, 144.1, 147.9, 164.2, 170.5; EI-MS (*m/z*, relative intensity): 477 (M^+, 48), 499 (100); Anal. calcd for $C_{22}H_{19}FeN_3O_6$: C, 55.37; H, 4.01; N, 8.80; Found: C, 55.03; H, 4.11; N,8.71.



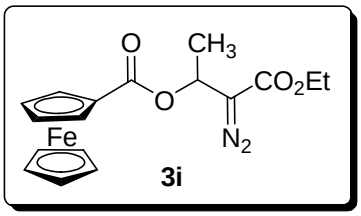
3g

Red solid; Mp**:** 105-107 ^{o}C; IR (KBr) 3108, 2096, 1709, 1112, 1023, 850, 826 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.26 (t, *J* = 7.0 Hz, 3H), 4.21 (s, 5H), 4.26 (q, *J* = 7.0 Hz, 2H), 4.47 (s, 2H), 4.89 (d, *J* = 1.5 Hz, 2H), 7.40 (s, 1H), 7.54 (t, *J* = 7.0 Hz, 1H), 7.71 (t, *J* = 7.5 Hz, 1H), 7.89 (d, *J* = 7.0 Hz, 1H), 8.12 (d, *J* = 7.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.5, 61.4, 70.0, 70.3, 70.4, 71.9, 72.0, 125.5, 128.9，129.6, 131.0, 132.5, 146.9, 167.8, 170.6; EI-MS (*m/z*, relative intensity): 449 [(M-28)$^{+}$, 82], 494 (100); Anal. calcd for $C_{22}H_{19}FeN_3O_6$: C, 55.37; H, 4.01; N, 8.80; Found: C, 55.12; H, 4.10; N,8.74.



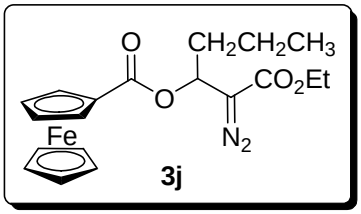
3h

Orange solid; Mp**:** 74-75 ^{o}C; IR (KBr) 3104, 2111, 1688, 1117, 1025, 824 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.29 (t, *J* = 7.0 Hz, 3H), 4.18 (s, 5H), 4.26 (q, *J* = 7.0 Hz, 2H), 4.41 (s, 2H), 4.82 (s, 2H), 5.05 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.5, 59.2, 61.1, 69.8, 70.1, 70.3, 71.6, 165.5, 172.6; EI-MS (*m/z*, relative intensity): 329 (100), 356 (M^{+}, 45); Anal. calcd for $C_{16}H_{16}FeN_2O_4$: C, 53.96; H, 4.53; N, 7.78; Found: C, 53.61; H, 4.53; N, 7.61.



3i

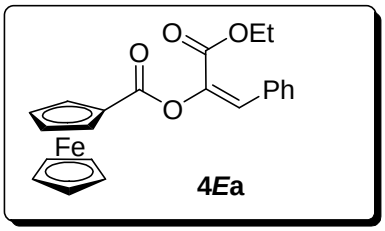
Orange oil; IR (KBr) 3104, 2103, 1763, 1712, 1127, 1004, 826 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.28 (t, *J* = 7.0 Hz, 3H), 1.59 (d, *J* = 7.0 Hz, 3H), 4.19 (s, 5H), 4.26 (q, *J* = 7.0 Hz, 2H), 4.40 (dt, *J* = 3.5 Hz, *J* = 1.5 Hz, 2H), 4.80 (dt, *J* = 15.5 Hz, *J* = 1.5 Hz, 2H), 5.90 (q, *J* = 7.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.5, 18.8, 61.1, 66.0, 69.9, 70.2, 70.8, 71.5, 165.0, 171.0; Anal. calcd for $C_{17}H_{18}FeN_2O_4$: C, 55.16; H, 4.90; N, 7.57; Found: C, 55.39; H, 4.72; N, 7.63.



3j

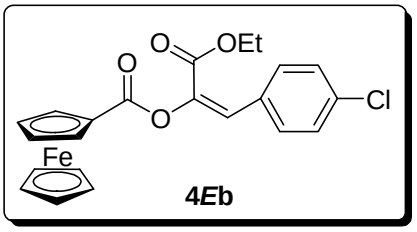
Orange oil; IR (KBr) 3101, 2101, 1712, 1099, 1024, 824 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$) δ 1.00 (t, *J* = 7.5 Hz, 3H), 1.27 (t, *J* = 7.0 Hz, 3H), 1.42-1.50 (m, 2H), 1.79-1.86 (m, 1H), 1.98-2.06 (m, 1H), 4.18 (s, 5H), 4.24 (q, *J* = 7.0 Hz, 2H), 4.40 (dd, *J* = 4.0 Hz, *J* = 1.5 Hz, 2H), 4.81 (dt, *J* = 13.0 Hz, *J* = 1.5 Hz, 2H), 5.72 (t, *J* = 7.5 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 13.6, 14.5, 18.9, 34.1, 61.0, 69.4, 69.8, 70.2, 71.8, 71.4, 165.0, 171.1; EI-MS (*m/z*, relative intensity): 370 (100), 384 (M^+, 7); Anal. calcd for $C_{19}H_{22}FeN_2O_4$: C, 57.30; H, 5.57; N, 7.03; Found: C, 57.55; H, 5.53; N, 7.03.

5. Spectral data for 2,3-migration products



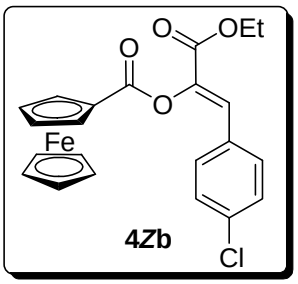
4*E*a

Orange oil; IR (KBr) 3100, 1724, 1105, 1022, 824 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$) δ 1.13 (t, *J* = 7.0 Hz, 3H), 4.22 (q, *J* = 7.0 Hz, 2H), 4.37 (s, 5H), 4.49 (d, *J* = 2.0 Hz, 2H), 4.92 (t, *J* = 2.0 Hz, 2H), 6.90 (s, 1H), 7.33-7.41 (m, 5H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 13.7, 61.4, 69.1, 70.1, 70.6, 72.0, 127.9, 128.0, 128.4, 129.2, 132.7, 138.5, 162.5, 170.4; EI-MS (*m/z*, relative intensity): 404 (M^+, 100); Anal. calcd for $C_{22}H_{20}FeO_4$: C, 65.37; H, 4.99; Found: C, 65.66; H, 5.02.



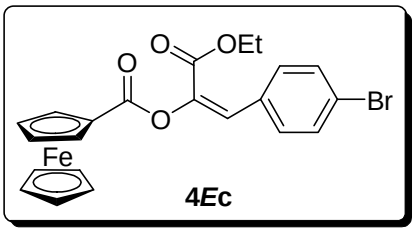
4*E*b

Orange solid; Mp**:** 111-112 °C; IR (KBr) 3111, 1725, 1098, 1011, 849, 810 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$) δ 1.17 (t, *J* = 7.0 Hz, 3H), 4.22 (q, *J* = 7.0 Hz, 2H), 4.36 (s, 5H), 4.50 (t, *J* = 2.0 Hz, 2H), 4.91 (t, *J* = 2.0 Hz, 2H), 6.82 (s, 1H), 7.32-7.36 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 13.8, 61.5, 68.9, 70.1, 70.6, 72.1, 126.9, 128.2, 130.6, 131.1, 134.4, 138.8, 162.2, 170.4; EI-MS (*m/z*, relative intensity): 438 (M^+, 100); Anal. calcd for $C_{22}H_{19}ClFeO_4$: C, 60.23; H, 4.37; Found: C,60.52; H, 4.52.



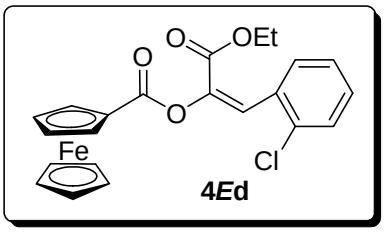
4Zb

Orange solid; Mp**:** 102-103 ^{o}C; IR (KBr) 3098, 1725, 1098, 1010, 849, 810 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.37 (t, *J* = 7.0 Hz, 3H), 4.36 (m, 7H), 4.54 (t, *J* = 1.5 Hz, 2H), 4.95 (t, *J* = 1.5 Hz, 2H), 7.27 (s, 1H), 7.35-7.58 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.3, 61.8, 69.2, 70.2, 70.6, 72.1, 125.4, 129.0, 130.8, 131.4, 135.5, 137.8, 162.5, 169.4; EI-MS (*m/z*, relative intensity): 438 (M^+, 100); Anal. calcd for $C_{22}H_{19}ClFeO_4$: C, 60.23; H, 4.37; Found: C,60.47; H, 4.55.



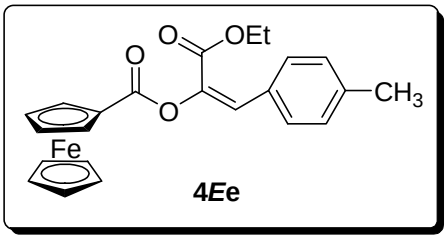
4Ec

Orange solid; Mp**:** 104-106 ^{o}C; IR (KBr) 3108, 1725, 1100, 1007, 824 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.17 (t, *J* = 7.0 Hz, 3H), 4.22 (q, *J* = 7.0 Hz, 2H), 4.36 (s, 5H), 4.50 (t, *J* = 2.0 Hz, 2H), 4.91 (t, *J* = 2.0 Hz, 2H), 6.80 (s, 1H), 7.27 (t, *J* = 7.0 Hz, 2H), 7.47 (d, *J* = 10.5 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 13.8, 61.5, 68.9, 70.1, 70.6, 72.1, 122.6, 126.9, 130.9, 131.2, 131.6, 138.8, 162.2, 170.4; EI-MS (*m/z*, relative intensity): 482 (M^+, 100); Anal. calcd for $C_{22}H_{19}BrFeO_4$: C, 54.69; H, 3.96; Found: C, 54.49; H, 4.26.



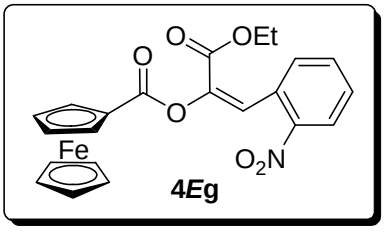
4Ed

Orange oil; IR (KBr) 3110, 1727, 1102, 1022, 824 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$) δ1.38 (t, *J* = 7.0 Hz, 3H), 4.30 (s, 5H), 4.36 (q, *J* = 7.0 Hz, 2H), 4.49 (t, *J* = 2.0 Hz, 2H), 4.90 (t, *J* = 2.0 Hz, 2H), 7.24-7.28 (m, 2H), 742-7.44 (m, 1H), 6.69 (s, 1H), 7.80 (q, *J* = 7.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.3, 61.9, 69.1, 70.1, 70.6, 72.0, 122.8, 126.7, 129.8, 130.4, 130.5, 130.6, 134.7, 138.8, 162.4, 169.5; EI-MS (*m/z*, relative intensity): 438 (M^+, 100); Anal. calcd for $C_{22}H_{19}ClFeO_4$: C, 60.23; H, 4.37; Found: C, 60.44; H, 4.44.



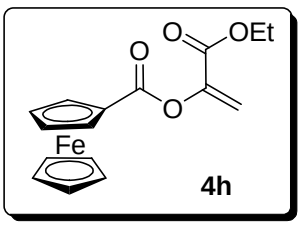
4*E*e

Orange oil; IR (KBr) 3096, 1724, 1104, 1022, 824 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$) δ 1.13 (t, *J* = 7.0 Hz, 3H), 1.25 (s, 3H), 4.20 (q, *J* = 7.0 Hz, 2H), 4.37 (s, 5H), 4.50 (t, *J* = 1.5 Hz, 2H), 4.92 (t, *J* = 1.5 Hz, 2H), 6.90 (s, 1H), 7.32-7.40 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 13.7, 29.7, 61,4, 69.1, 70.1, 70.6, 72.0, 127.9, 128.0, 128.4, 129.2, 132.7, 138.5, 162.5, 170.4; EI-MS (*m/z*, relative intensity): 418 (M^+, 5), 381 (100); Anal. calcd for $C_{23}H_{22}FeO_4$: C, 66.05; H, 5.30; Found: C, 65.94; H, 5.06.



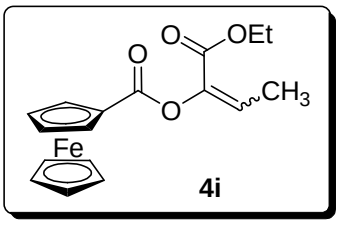
4*E*g

Orange oil; IR (KBr) 3106, 1727, 1101, 1021, 824 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$) δ 1.38 (t, *J* = 7.0 Hz, 3H), 4.23 (s, 5H), 4.37 (q, *J* = 7.0 Hz, 2H), 4.46 (t, *J* = 1.5 Hz, 2H), 4.81 (t, *J* = 1.5 Hz, 2H), 7.48-7.51 (m, 1H), 7.60-7.63 (m, 2H), 7.75 (s, 1H), 8.10 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.2, 62.1, 68.7, 70.1, 70.6, 72.1, 123.2, 124.9, 127.7, 129.7, 131.1, 133.2, 139.4, 148.0, 161.8, 170.0; EI-MS (*m/z*, relative intensity): 449 (M^+, 100); Anal. calcd for: $C_{22}H_{19}FeNO_6$: C, 58.82; H, 4.26; N, 3.12; Found: C, 59.17; H, 4.51; N, 2.96.



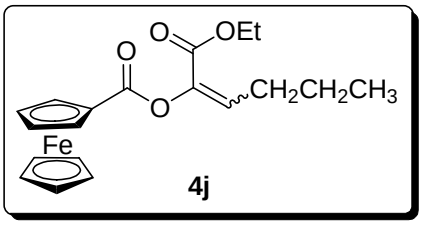
4h

Orange oil; IR (KBr) 3106, 1732, 1647, 1107, 1024, 825 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$) δ 1.35 (t, *J* = 7.0 Hz, 3H), 4.32 (q, *J* = 7.0 Hz, 2H), 4.35 (s, 5H), 4.47 (s, 2H), 4.88 (s, 2H), 5.50 (s, 1H), 6.08 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.2, 61.7, 69.2, 70.1, 70.6, 71.9, 113.6, 144.9, 161.7, 169.9; EI-MS (*m/z*, relative intensity): 328 (M^+, 42), 346 (100); Anal. calcd for $C_{16}H_{16}FeO_4$: C, 58.56; H, 4.91; Found: C, 58.81; H, 4.94.



4i

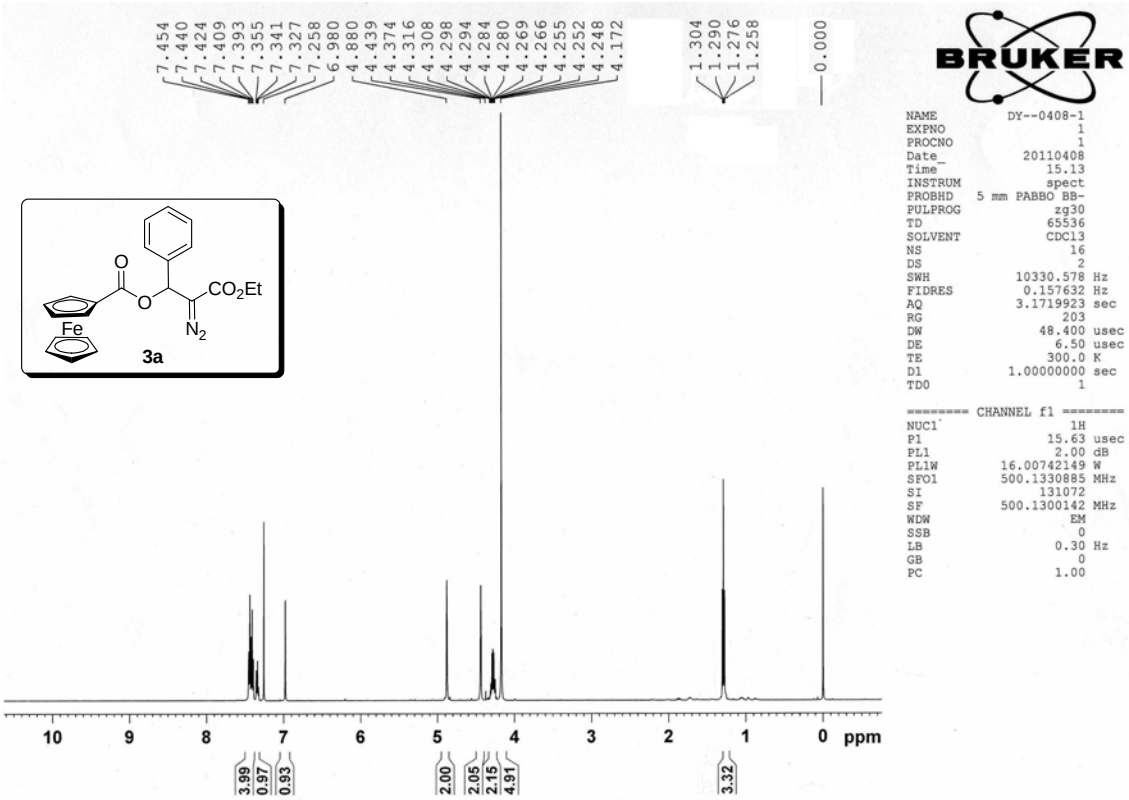
Orange solid; Mp**:** 76-78 ^{o}C; IR (KBr) 3106, 1720, 1118, 1022, 822 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.34 (t, *J* = 7.0 Hz, 3H), 2.12 (d, *J* = 7.5 Hz, 3H), 4.30-4.35 (m, 7H), 4.46 (t, *J* = 2.0 Hz, 2H), 4.87 (t, *J* = 2.0 Hz, 2H), 6.05 (q, *J* = 7.5 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 13.0, 14.3, 61.1, 69.6, 70.0, 70.5, 71.8, 128.6, 138.3, 162.3, 170.6; EI-MS (*m/z*, relative intensity): 342 (M^+, 100); Anal. calcd for $C_{17}H_{18}FeO_4$: C, 59.67; H, 5.30; Found: C, 59.95; H, 5.54.



4j

Orange oil; IR (KBr) 3106, 1726, 1122, 1025, 823 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$) δ 0.98 (t, *J* = 7.5 Hz, 3H), 1.33 (t, *J* = 7.0 Hz, 3H), 1.51 (q, *J* = 7.0 Hz, 2H), 2.58 (q, *J* = 7.5 Hz, 2H), 4.28-4.35 (m, 7H), 4.45 (t, *J* = 2.0 Hz, 2H), 4.87 (t, *J* = 2.0 Hz, 2H), 5.96 (t, *J* = 8.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 13.8, 14.3, 22.5, 29.0, 61.2, 69.7, 70.1, 70.6, 71.8, 133.7, 137.7, 162.4, 170.6; EI-MS (*m/z*, relative intensity): 356 (M^+, 4), 387 (100); Anal. calcd for $C_{19}H_{22}FeO_4$: C, 61.64; H, 5.99; Found: C, 61.35; H, 6.01.

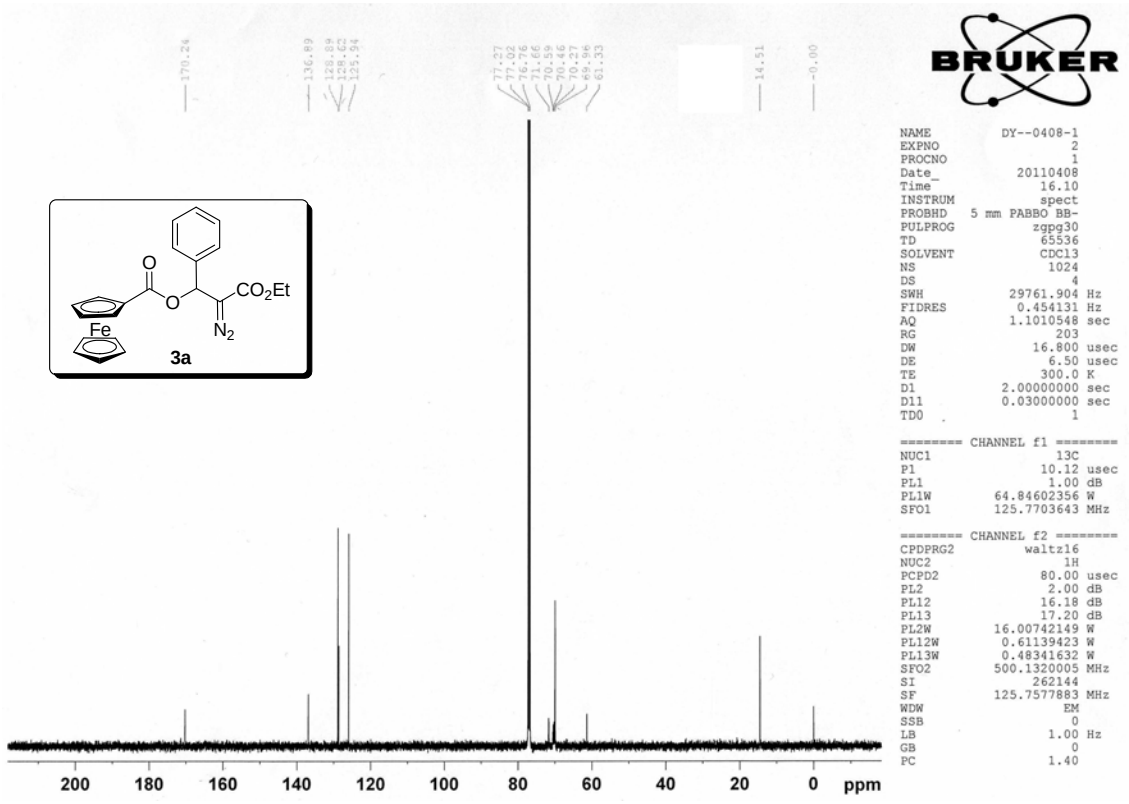
6. ^{1}H and $^{13}CNMR$ spectra



BRUKER

```
NAME            DY--0408-1
EXPNO                    1
PROCNO                   1
Date_             20110408
Time                 15.13
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH              10330.578 Hz
FIDRES               0.157632 Hz
AQ                3.1719923 sec
RG                     203
DW                  48.400 usec
DE                   6.50 usec
TE                  300.0 K
D1               1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   15.63 usec
PL1                   2.00 dB
PL1W            16.00742149 W
SFO1           500.1330885 MHz
SI                   131072
SF             500.1300142 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

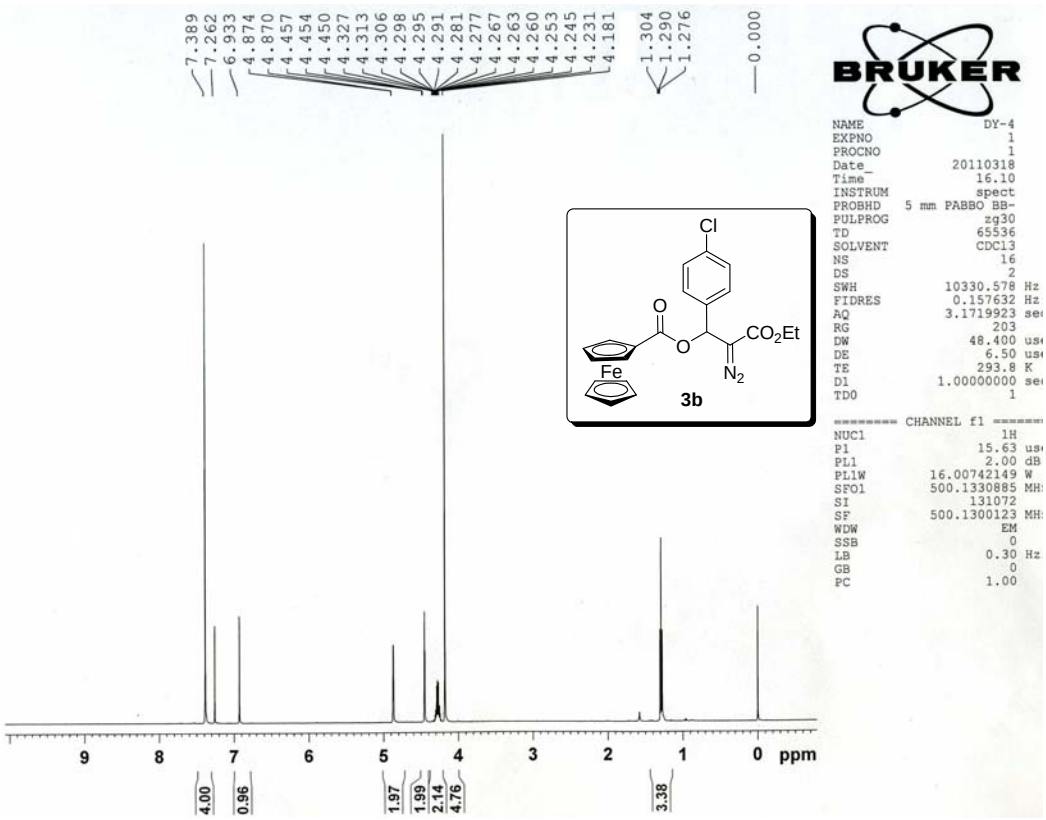


BRUKER

```
NAME            DY--0408-1
EXPNO                    2
PROCNO                   1
Date_             20110408
Time                 16.10
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1024
DS                       4
SWH              29761.904 Hz
FIDRES               0.454131 Hz
AQ                1.1010548 sec
RG                     203
DW                  16.800 usec
DE                   6.50 usec
TE                  300.0 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                   10.12 usec
PL1                   1.00 dB
PL1W            64.84602356 W
SFO1           125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                   2.00 dB
PL12                 16.18 dB
PL13                 17.20 dB
PL2W            16.00742149 W
PL12W            0.61139423 W
PL13W            0.48341632 W
SFO2           500.1320005 MHz
SI                   262144
SF             125.7577883 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```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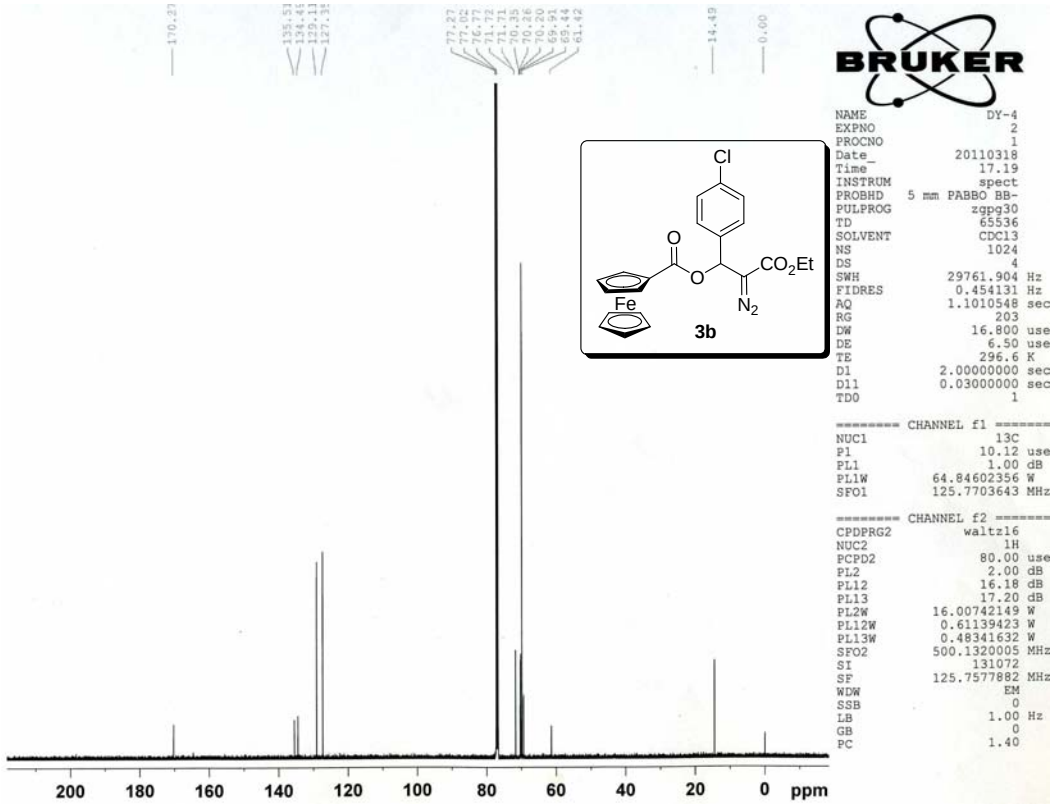
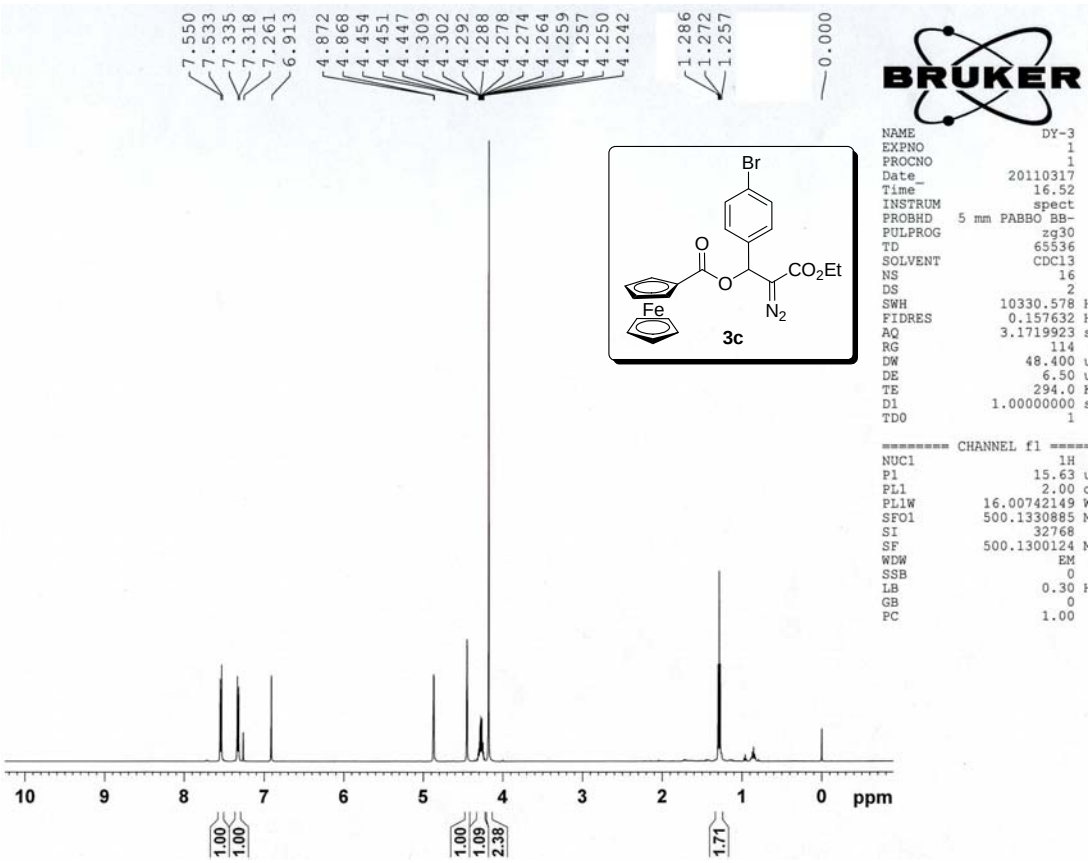
7.262
6.933
4.874
4.870
4.457
4.454
4.450
4.327
4.313
4.306
4.298
4.295
4.291
4.281
4.277
4.267
4.263
4.260
4.253
4.245
4.231
4.181
1.304
1.290
1.276
0.000
Cl
O
O
CO2Et
N2
Fe
3b
9
8
7
6
5
4
3
2
1
0
ppm
4.00
0.96
1.97
1.99
2.14
4.76
3.38
BRUKER
NAME DY-4
EXPNO 1
PROCNO 1
Date_ 20110318
Time_ 16.10
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 se
RG 203
DW 48.400 us
DE 6.50 us
TE 293.8 K
D1 1.00000000 se
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 15.63 us
PL1 2.00 dB
PL1W 16.00742149 W
SFO1 500.1330885 MH
SI 131072
SF 500.1300123 MH
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


170.23
135.53
134.45
129.11
127.31
77.27
77.02
76.77
71.72
71.71
70.35
70.26
70.20
69.91
69.44
61.42
14.49
0.00
Cl
O
O
CO2Et
N2
Fe
3b
200
180
160
140
120
100
80
60
40
20
0
ppm
BRUKER
NAME DY-4
EXPNO 2
PROCNO 1
Date_ 20110318
Time_ 17.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 use
DE 6.50 use
TE 296.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.12 use
PL1 1.00 dB
PL1W 64.84602356 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 use
PL2 2.00 dB
PL12 16.18 dB
PL13 17.20 dB
PL2W 16.00742149 W
PL12W 0.61139423 W
PL13W 0.48341632 W
SFO2 500.1320005 MHz
SI 131072
SF 125.7577882 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40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7.318
7.261
6.913
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4.868
4.454
4.451
4.447
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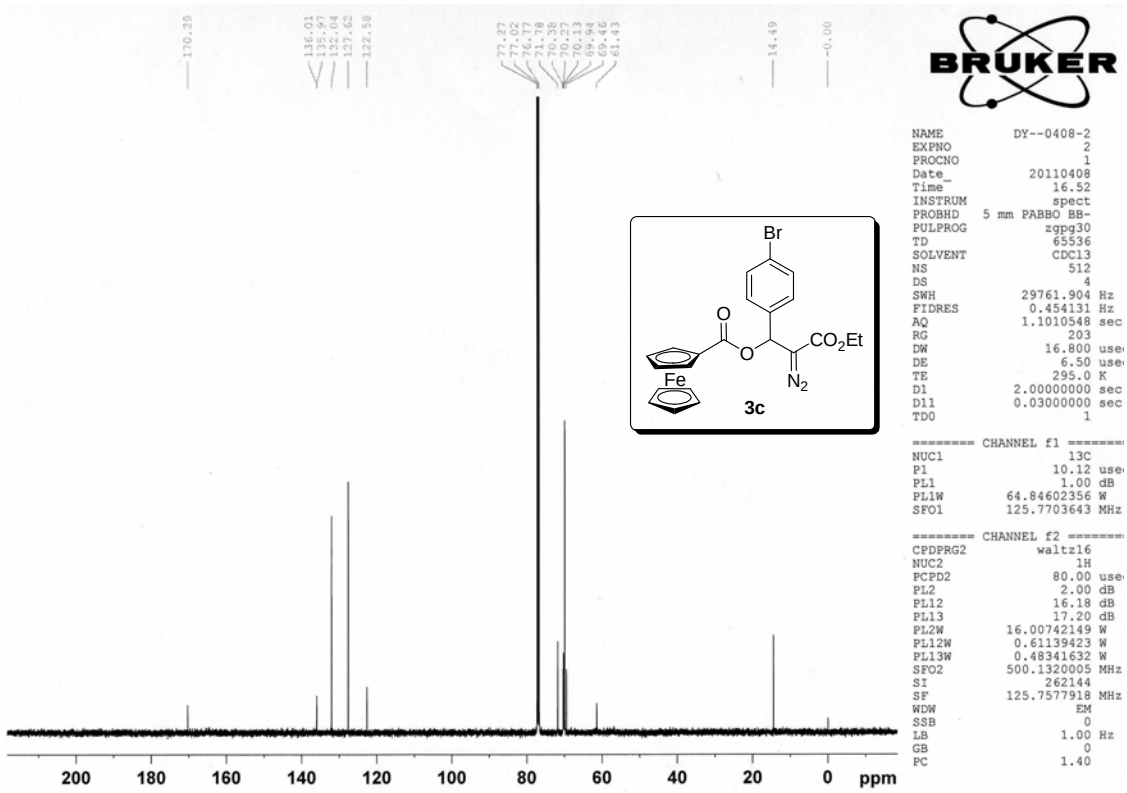
4.292
4.288
4.278
4.274
4.264
4.259
4.257
4.250
4.242
1.286
1.272
1.257
0.000
Br
O
O
CO2Et
N2
Fe
3c
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.00
1.00
1.09
2.38
1.71
BRUKER
NAME DY-3
EXPNO 1
PROCNO 1
Date_ 20110317
Time 16.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578
FIDRES 0.157632
AQ 3.1719923
RG 114
DW 48.400
DE 6.50
TE 294.0
D1 1.00000000
TD0 1
======== CHANNEL f1 ======
NUC1 1H
P1 15.63
PL1 2.00
PL1W 16.00742149
SFO1 500.1330885
SI 32768
SF 500.1300124
WDW EM
SSB 0
LB 0.30
GB 0
PC 1.00


170.29
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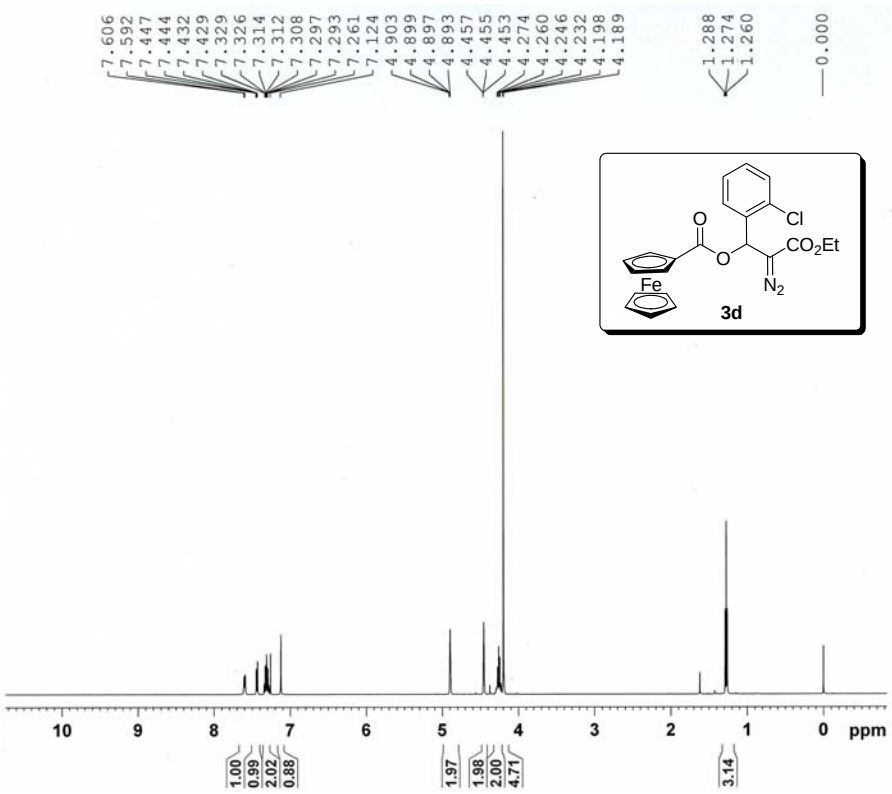
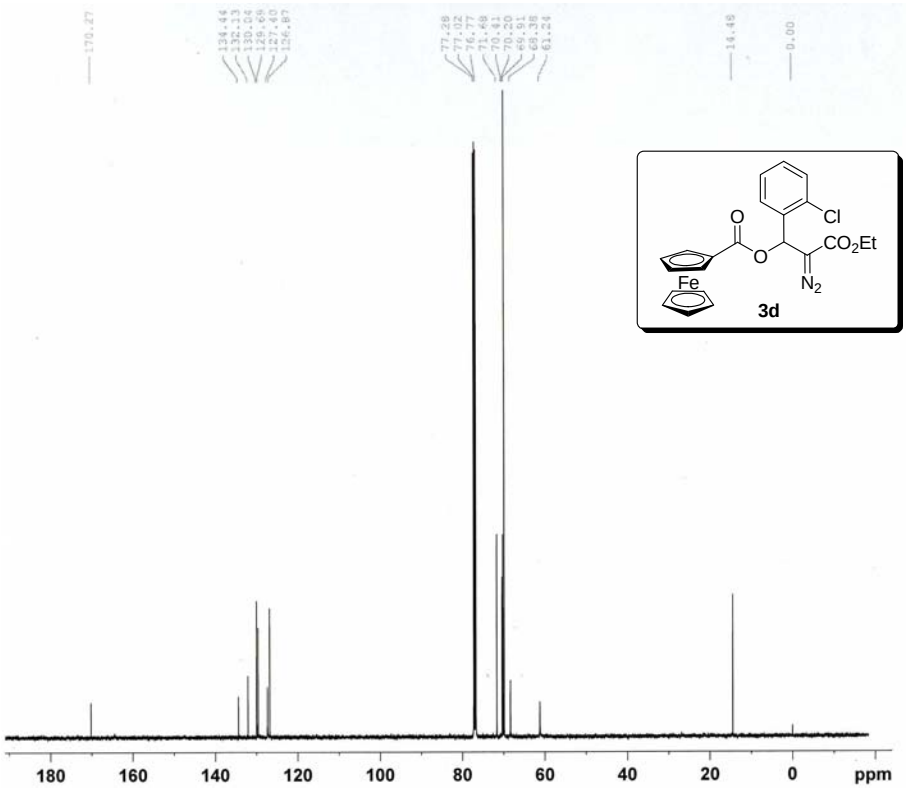
132.67
132.04
127.62
122.58
77.27
77.02
76.77
71.78
70.38
70.27
70.13
69.94
69.46
61.43
14.49
0.00
Br
O
O
CO2Et
N2
Fe
3c
200
180
160
140
120
100
80
60
40
20
0
ppm
BRUKER
NAME DY--0408-2
EXPNO 2
PROCNO 1
Date_ 20110408
Time 16.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 use
DE 6.50 use
TE 295.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ======
NUC1 13C
P1 10.12 use
PL1 1.00 dB
PL1W 64.84602356 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 use
PL2 2.00 dB
PL12 16.18 dB
PL13 17.20 dB
PL2W 16.00742149 W
PL12W 0.61139423 W
PL13W 0.48341632 W
SFO2 500.1320005 MHz
SI 262144
SF 125.7577918 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



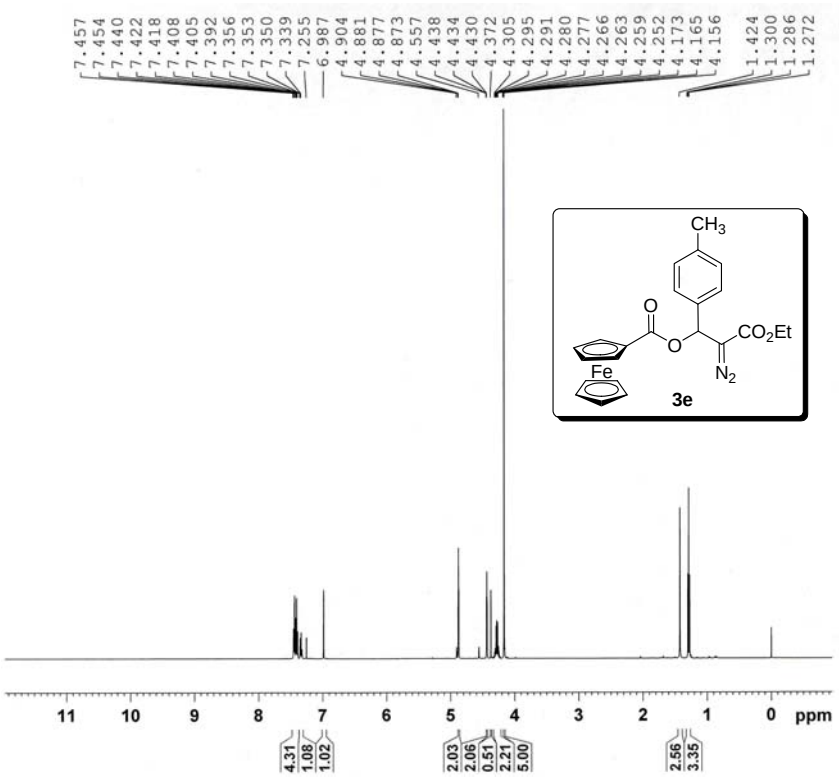
BRUKER

```
NAME                DY-04291
EXPNO                      1
PROCNO                     1
Date_               20110429
Time                   10.20
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        16
DS                         2
SWH               10330.578 Hz
FIDRES            0.157632 Hz
AQ                3.1719923 sec
RG                       181
DW                  48.400 usec
DE                   6.50 usec
TE                   293.7 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                  15.63 usec
PL1                  2.00 dB
PL1W             16.00742149 W
SFO1             500.1330885 MHz
SI                     131072
SF               500.1300130 MHz
WDW                       EM
SSB                        0
LB                   0.30 Hz
GB                         0
PC                      1.00
```

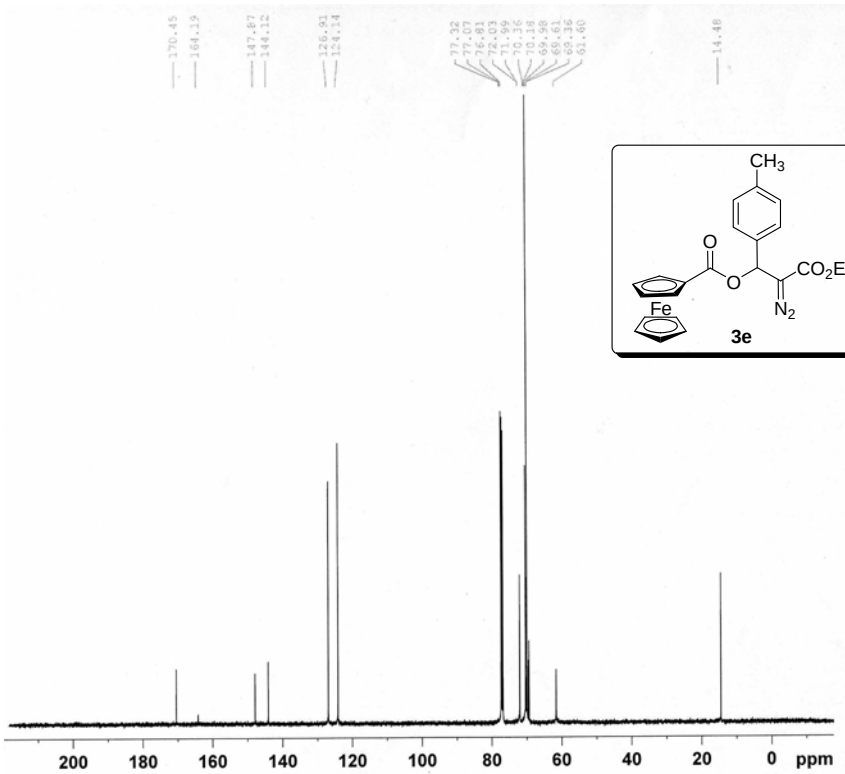


BRUKER

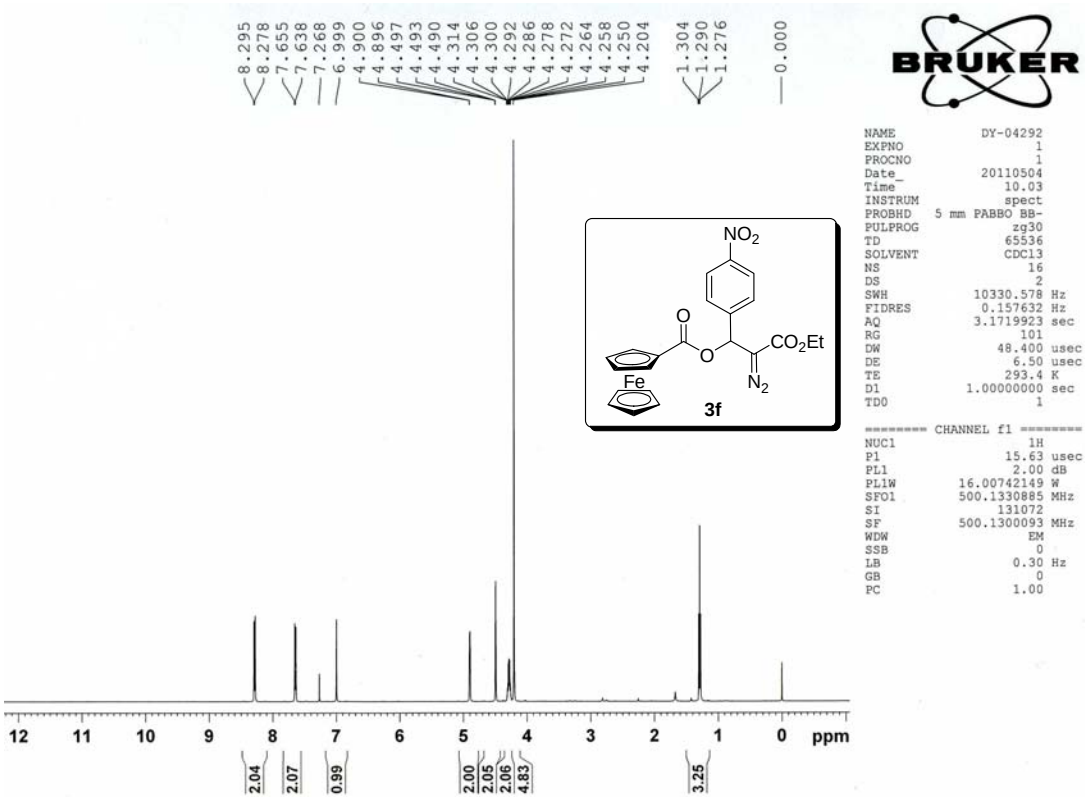
```
NAME                DY-04291
EXPNO                      2
PROCNO                     1
Date_               20110429
Time                   11.18
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      1024
DS                         4
SWH               29761.904 Hz
FIDRES            0.454131 Hz
AQ                1.1010548 sec
RG                       203
DW                  16.800 usec
DE                   6.50 usec
TE                   295.9 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      13C
P1                  10.12 usec
PL1                  1.00 dB
PL1W             64.84602356 W
SFO1             125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2               80.00 usec
PL2                  2.00 dB
PL12                16.18 dB
PL13                17.20 dB
PL2W             16.00742149 W
PL12W             0.61139423 W
PL13W             0.48341632 W
SFO2             500.1320005 MHz
SI                     131072
SF               125.7577915 MHz
WDW                       EM
SSB                        0
LB                   1.00 Hz
GB                         0
PC                      1.40
```



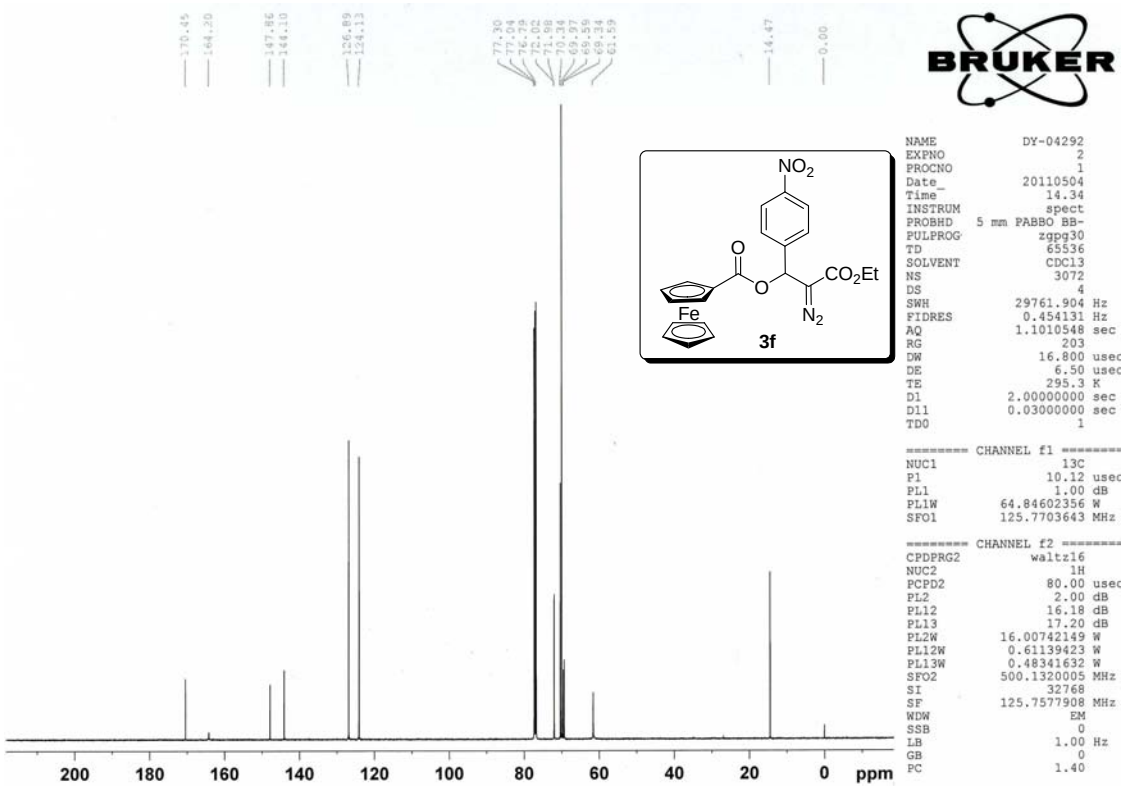
```
NAME                DY-PCH3
EXPNO                     1
PROCNO                    1
Date_              20110511
Time                  9.47
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH               10330.578 Hz
FIDRES            0.157632 Hz
AQ                3.1719923 sec
RG                       57
DW                  48.400 usec
DE                   6.50 usec
TE                   294.0 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                  15.63 usec
PL1                  2.00 dB
PL1W            16.00742149 W
SFO1           500.1330885 MHz
SI                    262144
SF             500.1300154 MHz
WDW                      EM
SSB                       0
LB                   0.30 Hz
GB                        0
PC                     1.00
```



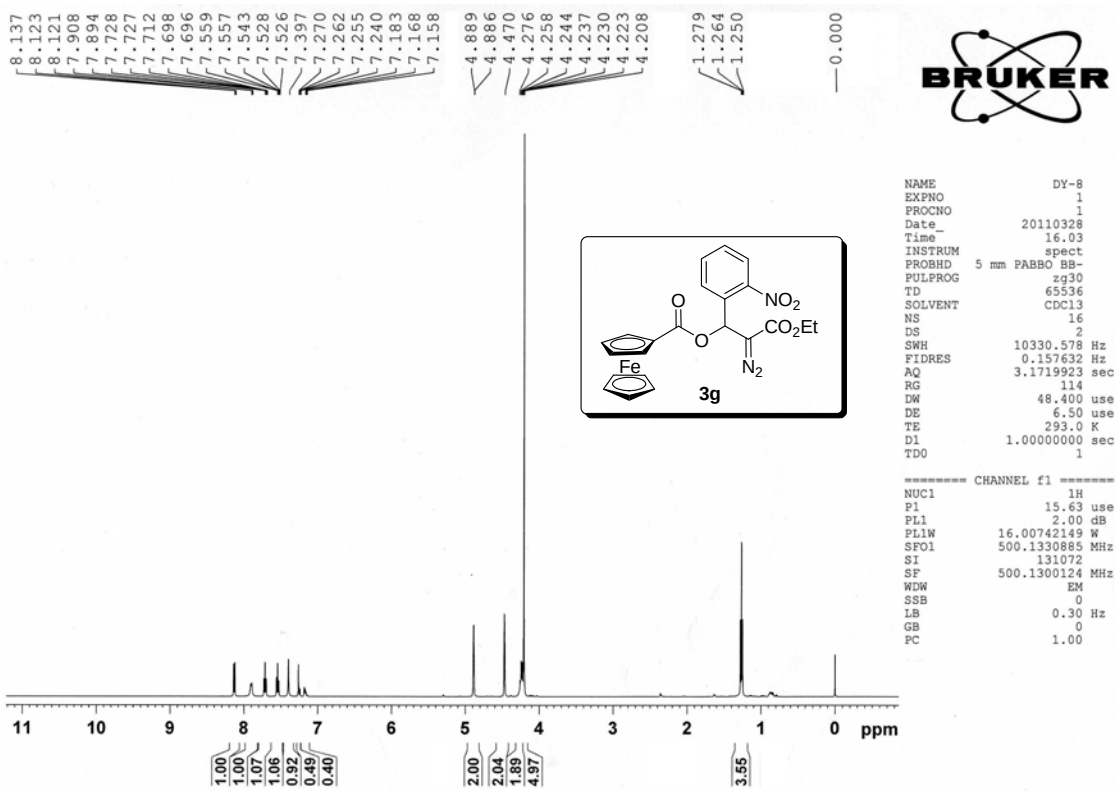
```
NAME                DY-PCH3
EXPNO                     2
PROCNO                    1
Date_              20110511
Time                 15.02
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      822
DS                        4
SWH               29761.904 Hz
FIDRES            0.454131 Hz
AQ                1.1010548 sec
RG                      203
DW                  16.800 usec
DE                   6.50 usec
TE                   296.0 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                  10.12 usec
PL1                  1.00 dB
PL1W            64.84602356 W
SFO1           125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                     1H
PCPD2               80.00 usec
PL2                  2.00 dB
PL12                16.18 dB
PL13                17.20 dB
PL2W            16.00742149 W
PL12W            0.61139423 W
PL13W            0.48341632 W
SFO2           500.1320005 MHz
SI                     32768
SF             125.7577890 MHz
WDW                      EM
SSB                       0
LB                   1.00 Hz
GB                        0
PC                     1.40
```




```
NAME            DY-04292
EXPNO                  1
PROCNO                 1
Date_           20110504
Time                10.03
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDC13
NS                    16
DS                     2
SWH           10330.578 Hz
FIDRES        0.157632 Hz
AQ            3.1719923 sec
RG                   101
DW              48.400 usec
DE               6.50 usec
TE              293.4 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1             15.63 usec
PL1             2.00 dB
PL1W       16.00742149 W
SFO1       500.1330885 MHz
SI              131072
SF         500.1300093 MHz
WDW                EM
SSB                 0
LB              0.30 Hz
GB                  0
PC              1.00
```




```
NAME            DY-04292
EXPNO                  2
PROCNO                 1
Date_           20110504
Time                14.34
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 65536
SOLVENT            CDC13
NS                  3072
DS                     4
SWH           29761.904 Hz
FIDRES        0.454131 Hz
AQ            1.1010548 sec
RG                   203
DW              16.800 usec
DE               6.50 usec
TE              295.3 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1             10.12 usec
PL1             1.00 dB
PL1W       64.84602356 W
SFO1       125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2          80.00 usec
PL2             2.00 dB
PL12           16.18 dB
PL13           17.20 dB
PL2W       16.00742149 W
PL12W       0.61139423 W
PL13W       0.48341632 W
SFO2       500.1320005 MHz
SI               32768
SF         125.7577908 MHz
WDW                EM
SSB                 0
LB              1.00 Hz
GB                  0
PC              1.40
```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8.123
8.121
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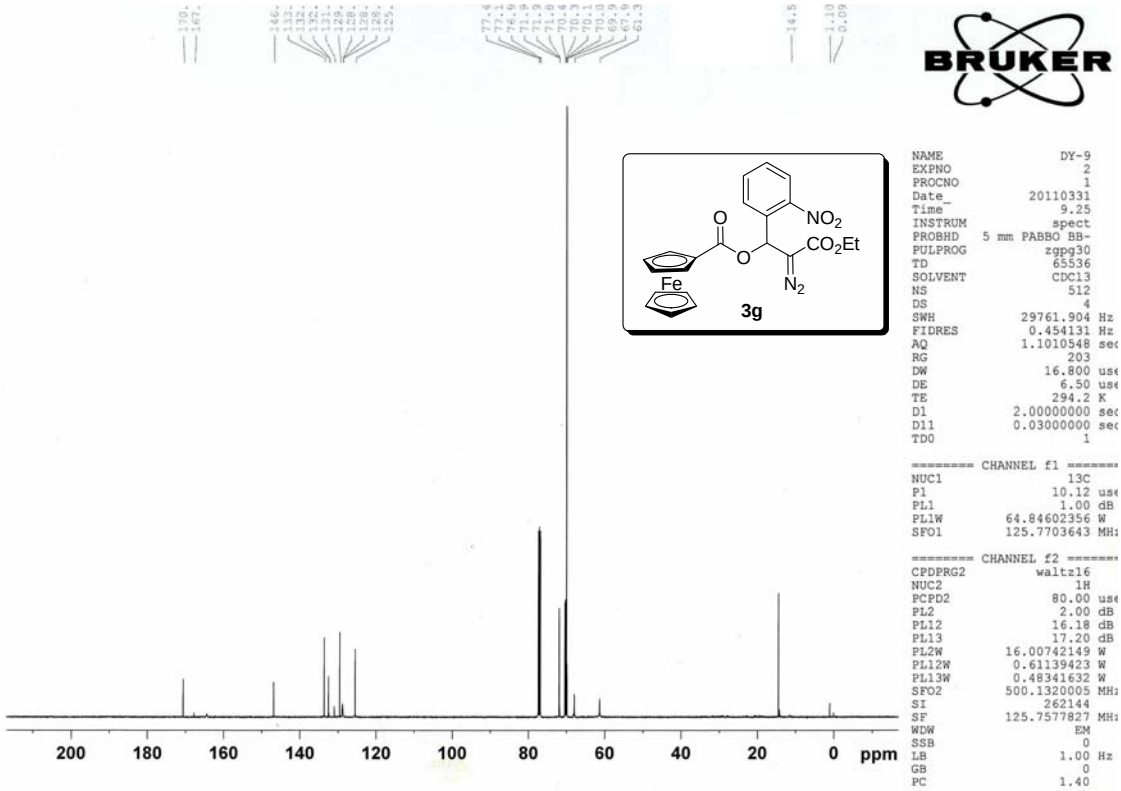
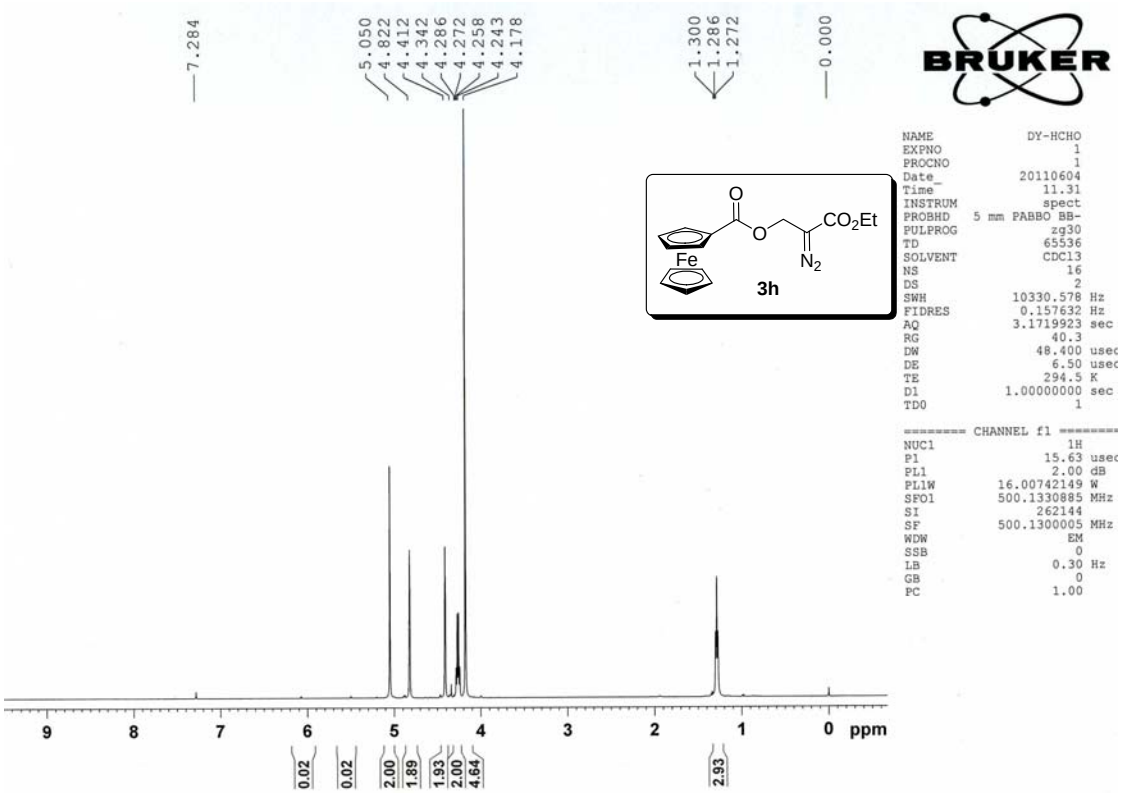
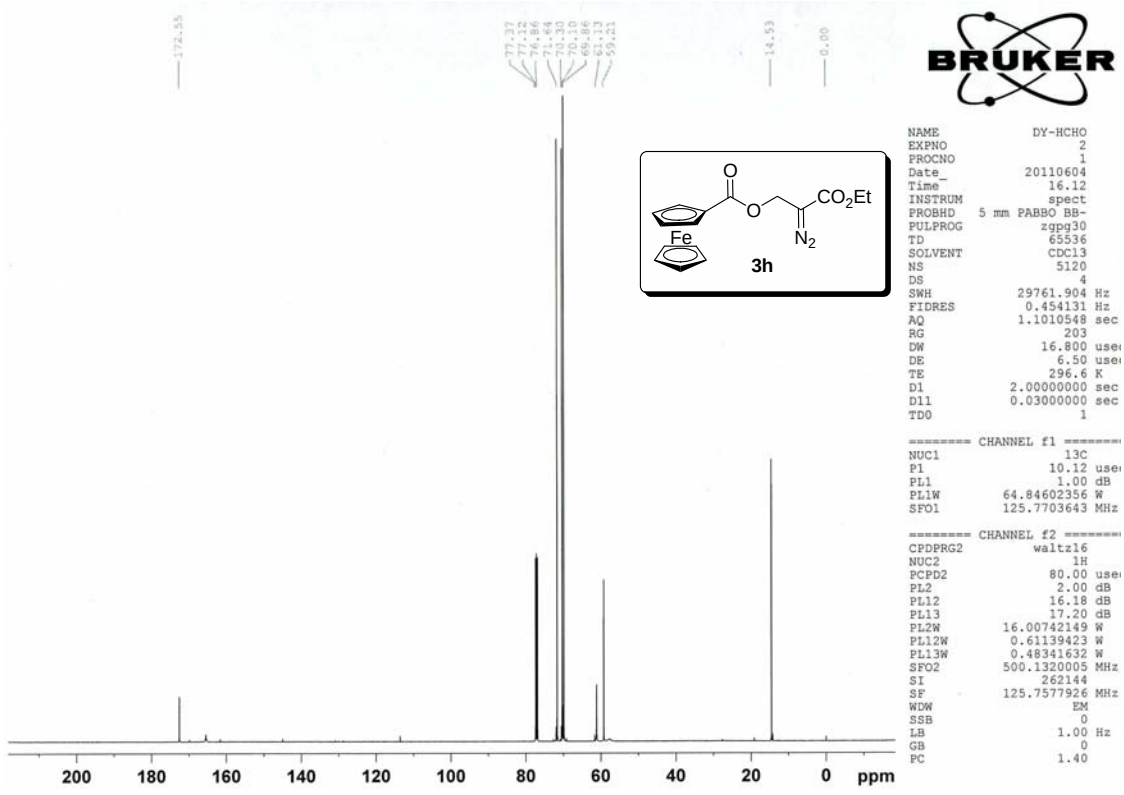
7.894
7.728
7.727
7.712
7.698
7.696
7.559
7.557
7.543
7.528
7.526
7.397
7.270
7.262
7.255
7.240
7.183
7.168
7.158
4.889
4.886
4.470
4.276
4.258
4.244
4.237
4.230
4.223
4.208
1.279
1.264
1.250
0.000
BRUKER
NAME DY-8
EXPNO 1
PROCNO 1
Date_ 20110328
Time 16.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 114
DW 48.400 use
DE 6.50 use
TE 293.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 15.63 use
PL1 2.00 dB
PL1W 16.00742149 W
SFO1 500.1330885 MHz
SI 131072
SF 500.1300124 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
NO2
CO2Et
O
O
N2
Fe
3g
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.00
1.07
1.06
0.92
0.49
0.40
2.00
2.04
1.89
4.97
3.55

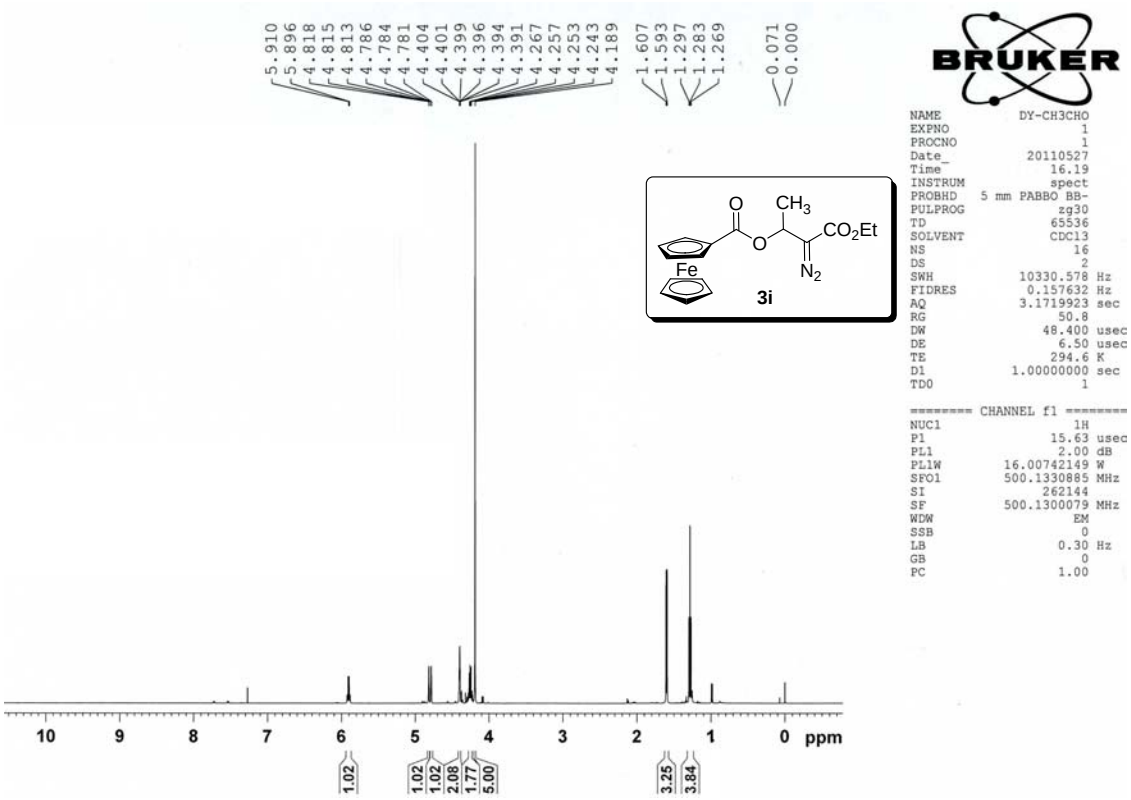

170.
167.
146.
133.
132.
132.
131.
129.
128.
128.
128.
120.
77.4
77.1
76.9
71.9
71.9
71.8
70.4
70.3
70.1
70.0
69.9
67.9
61.3
14.5
11.10
6.09
BRUKER
NAME DY-9
EXPNO 2
PROCNO 1
Date_ 20110331
Time 9.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 use
DE 6.50 use
TE 294.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.12 use
PL1 1.00 dB
PL1W 64.84602356 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 use
PL2 2.00 dB
PL12 16.18 dB
PL13 17.20 dB
PL2W 16.00742149 W
PL12W 0.61139423 W
PL13W 0.48341632 W
SFO2 500.1320005 MHz
SI 262144
SF 125.7577827 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
NO2
CO2Et
O
O
N2
Fe
3g
200
180
160
140
120
100
80
60
40
20
0
ppm




```
NAME                DY-HCHO
EXPNO                     1
PROCNO                    1
Date_              20110604
Time                 11.31
INSTRUM              spect
PROBHD     5 mm PABBO BB-
PULPROG              zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH              10330.578 Hz
FIDRES           0.157632 Hz
AQ               3.1719923 sec
RG                    40.3
DW                 48.400 usec
DE                  6.50 usec
TE                 294.5 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   1H
P1                 15.63 usec
PL1                2.00 dB
PL1W        16.00742149 W
SFO1        500.1330885 MHz
SI                262144
SF          500.1300005 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```

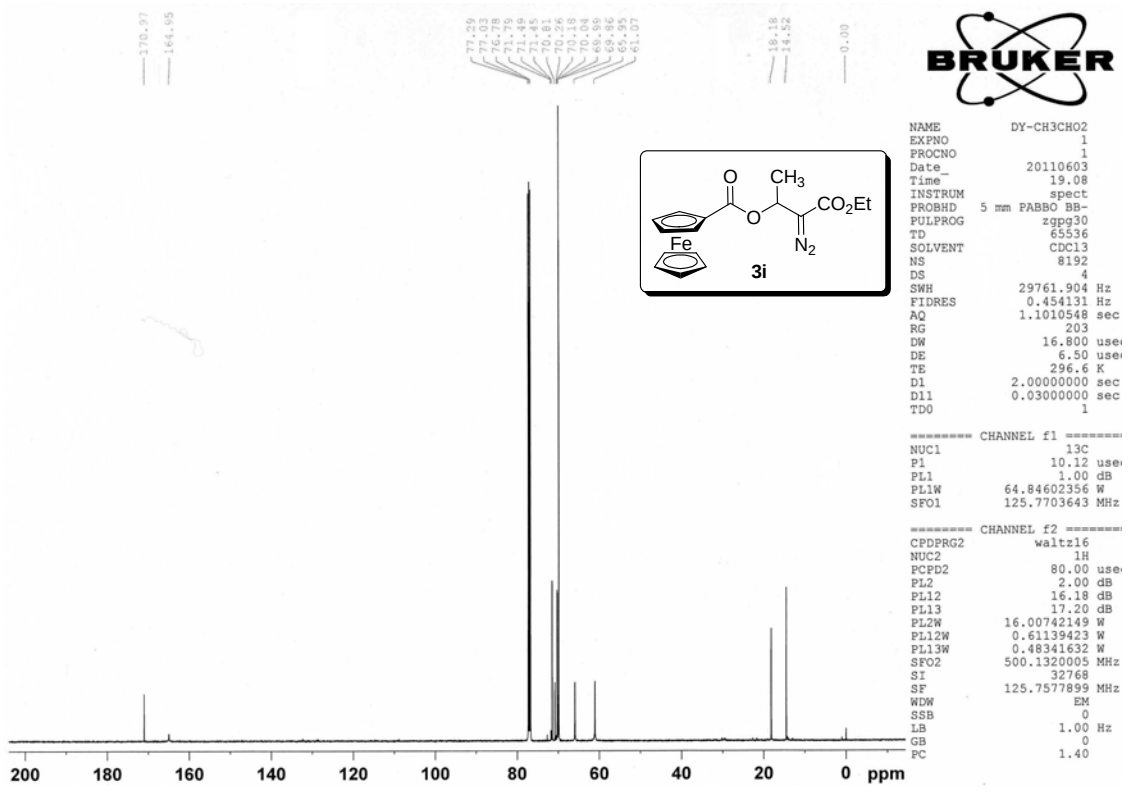



```
NAME                DY-HCHO
EXPNO                     2
PROCNO                    1
Date_              20110604
Time                 16.12
INSTRUM              spect
PROBHD     5 mm PABBO BB-
PULPROG            zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    5120
DS                       4
SWH              29761.904 Hz
FIDRES           0.454131 Hz
AQ               1.1010548 sec
RG                     203
DW                 16.800 usec
DE                  6.50 usec
TE                 296.6 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                  13C
P1                 10.12 usec
PL1                1.00 dB
PL1W        64.84602356 W
SFO1        125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                   1H
PCPD2              80.00 usec
PL2                2.00 dB
PL12               16.18 dB
PL13               17.20 dB
PL2W        16.00742149 W
PL12W        0.61139423 W
PL13W        0.48341632 W
SFO2        500.1320005 MHz
SI                262144
SF          125.7577926 MHz
WDW                   EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                1.40
```



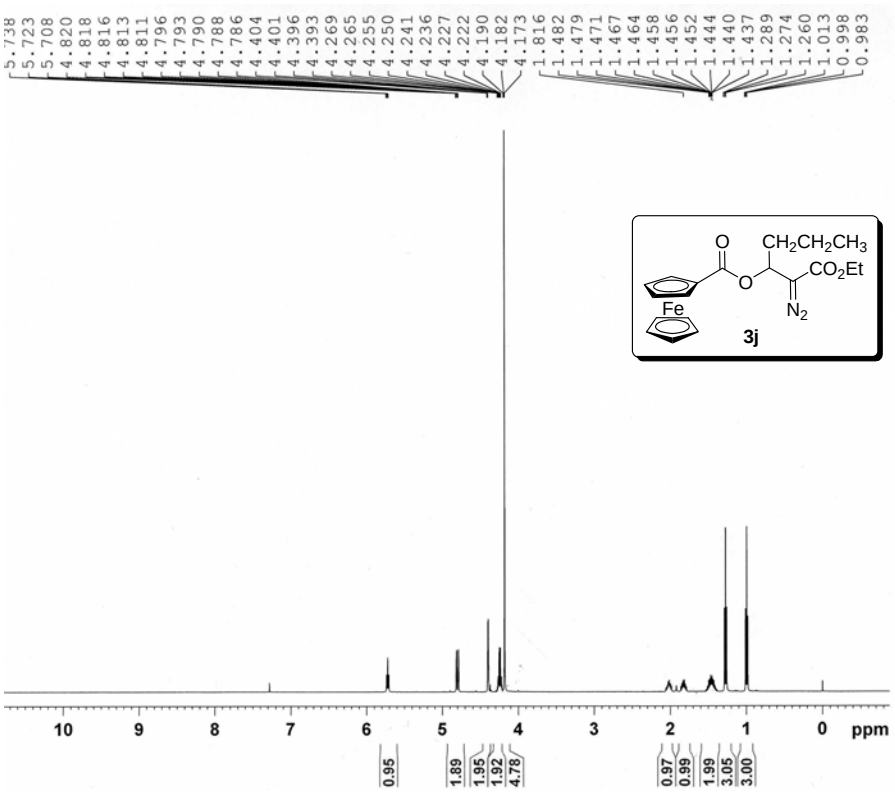
BRUKER

```
NAME            DY-CH3CHO
EXPNO                   1
PROCNO                  1
Date_            20110527
Time                16.19
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH             10330.578 Hz
FIDRES          0.157632 Hz
AQ              3.1719923 sec
RG                   50.8
DW                 48.400 usec
DE                  6.50 usec
TE                 294.6 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  15.63 usec
PL1                  2.00 dB
PL1W           16.00742149 W
SFO1           500.1330885 MHz
SI                  262144
SF             500.1300079 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

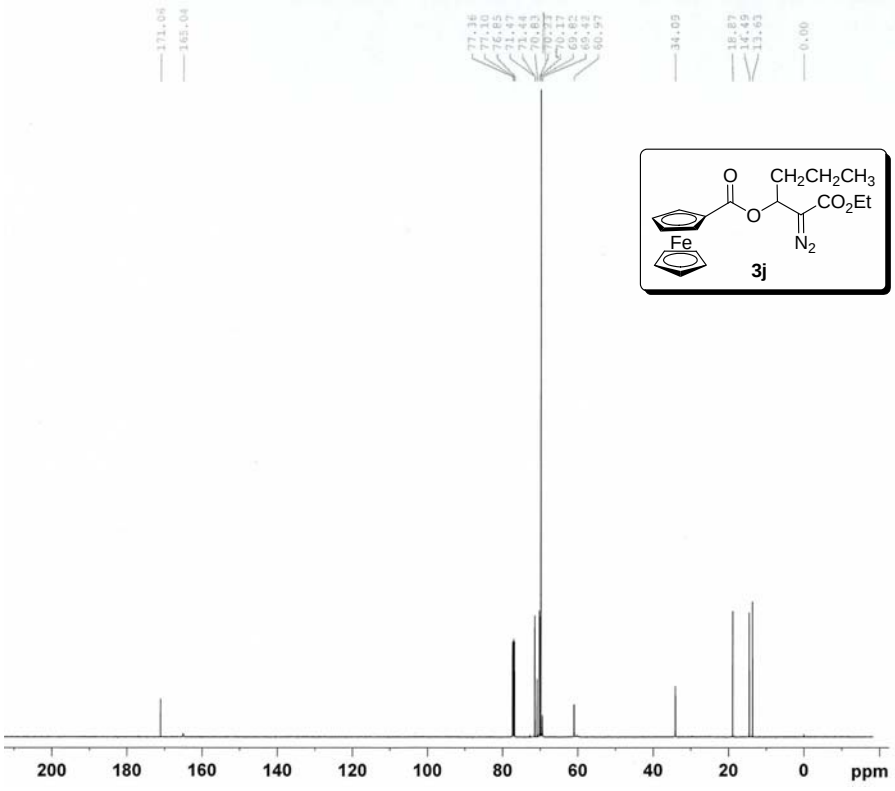


BRUKER

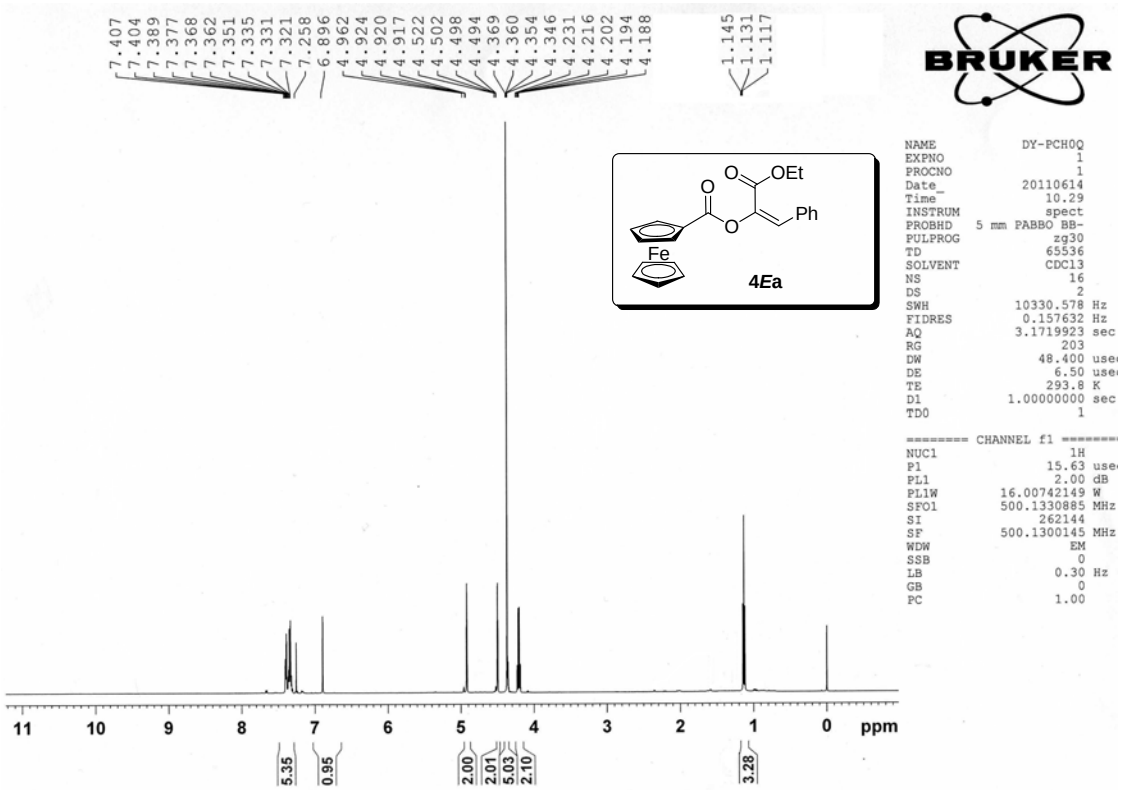
```
NAME           DY-CH3CHO2
EXPNO                   1
PROCNO                  1
Date_            20110603
Time                19.08
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   8192
DS                      4
SWH             29761.904 Hz
FIDRES          0.454131 Hz
AQ              1.1010548 sec
RG                    203
DW                 16.800 use
DE                  6.50 use
TE                 296.6 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                  10.12 use
PL1                  1.00 dB
PL1W           64.84602356 W
SFO1           125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               80.00 use
PL2                  2.00 dB
PL12                16.18 dB
PL13                17.20 dB
PL2W           16.00742149 W
PL12W           0.61139423 W
PL13W           0.48341632 W
SFO2           500.1320005 MHz
SI                  32768
SF             125.7577899 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```




```
NAME          DY-CH3CH2CH2CHO
EXPNO                       1
PROCNO                      1
Date_              20110624
Time                    9.49
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                CDC13
NS                        16
DS                         2
SWH               10330.578 Hz
FIDRES            0.157632 Hz
AQ                3.1719923 sec
RG                        36
DW                  48.400 usec
DE                   6.50 usec
TE                   294.3 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                   15.63 usec
PL1                   2.00 dB
PL1W             16.00742149 W
SFO1             500.1330885 MHz
SI                     262144
SF               500.1300031 MHz
WDW                       EM
SSB                        0
LB                   0.30 Hz
GB                         0
PC                      1.00
```




```
NAME          DY-CH3CH2CH2CHO
EXPNO                       2
PROCNO                      1
Date_              20110624
Time                   10.32
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG              zgpg30
TD                     65536
SOLVENT                CDC13
NS                       728
DS                         4
SWH               29761.904 Hz
FIDRES            0.454131 Hz
AQ                1.1010548 sec
RG                       203
DW                  16.800 usec
DE                   6.50 usec
TE                   295.9 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     13C
P1                   10.12 usec
PL1                   1.00 dB
PL1W             64.84602356 W
SFO1             125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                80.00 usec
PL2                   2.00 dB
PL12                 16.18 dB
PL13                 17.20 dB
PL2W             16.00742149 W
PL12W             0.61139423 W
PL13W             0.48341632 W
SFO2             500.1320005 MHz
SI                     262144
SF               125.7577918 MHz
WDW                       EM
SSB                        0
LB                   1.00 Hz
GB                         0
PC                      1.40
```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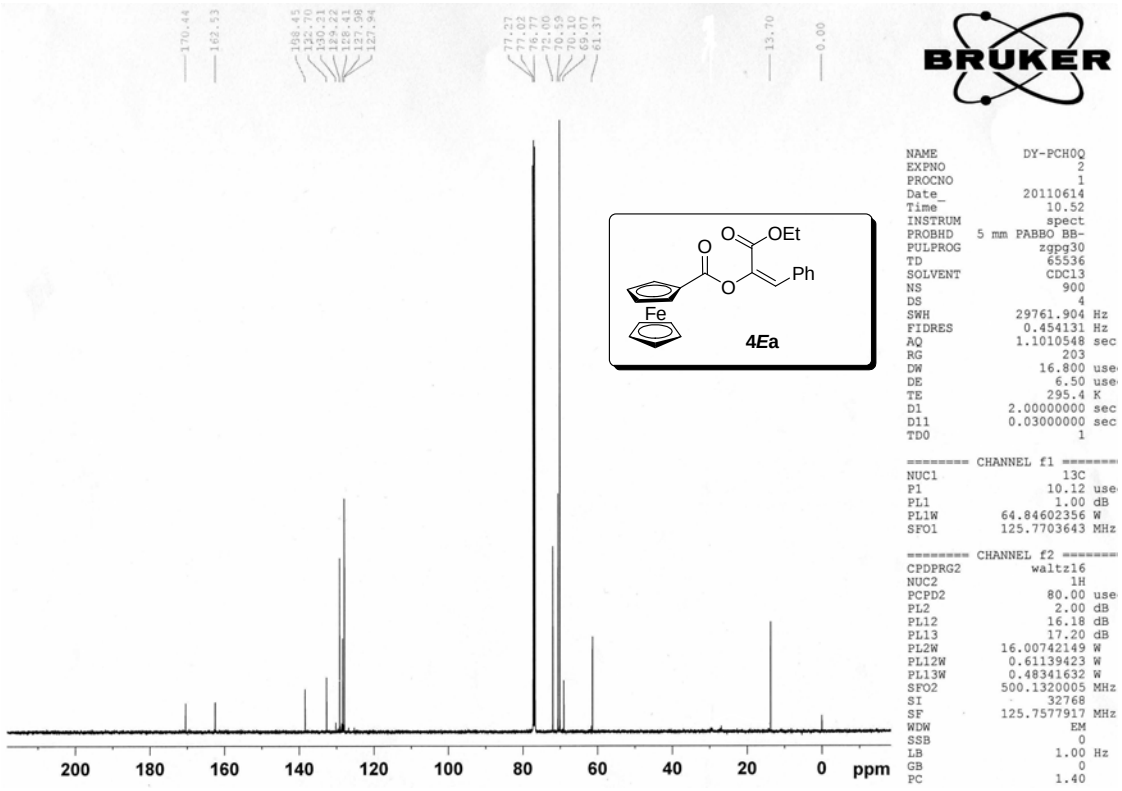
7.377
7.368
7.362
7.351
7.335
7.331
7.321
7.258
6.896
4.962
4.924
4.920
4.917
4.522
4.502
4.498
4.494
4.369
4.360
4.354
4.346
4.231
4.216
4.202
4.194
4.188
1.145
1.131
1.117
O
OEt
O
Ph
O
Fe
4Ea
11
10
9
8
7
6
5
4
3
2
1
0
ppm
5.35
0.95
2.00
2.01
5.03
2.10
3.28
BRUKER
NAME DY-PCH0Q
EXPNO 1
PROCNO 1
Date_ 20110614
Time 10.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 203
DW 48.400 use
DE 6.50 use
TE 293.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 15.63 use
PL1 2.00 dB
PL1W 16.00742149 W
SFO1 500.1330885 MHz
SI 262144
SF 500.1300145 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00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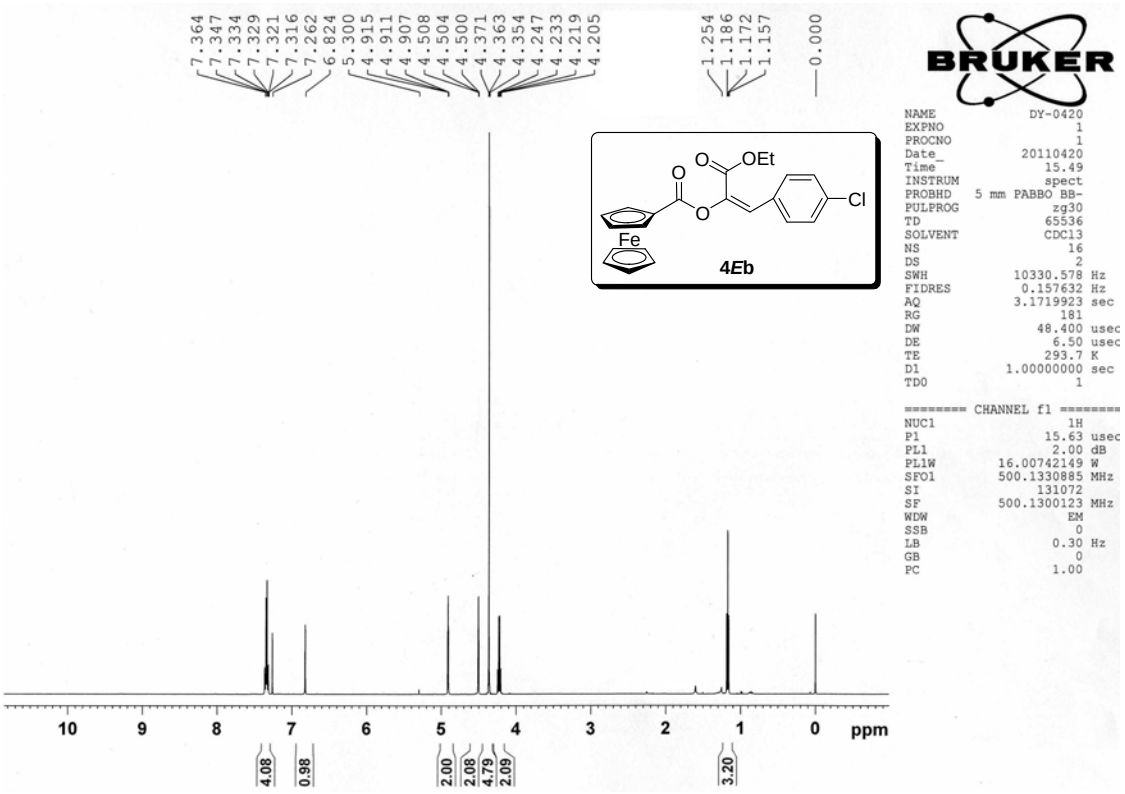
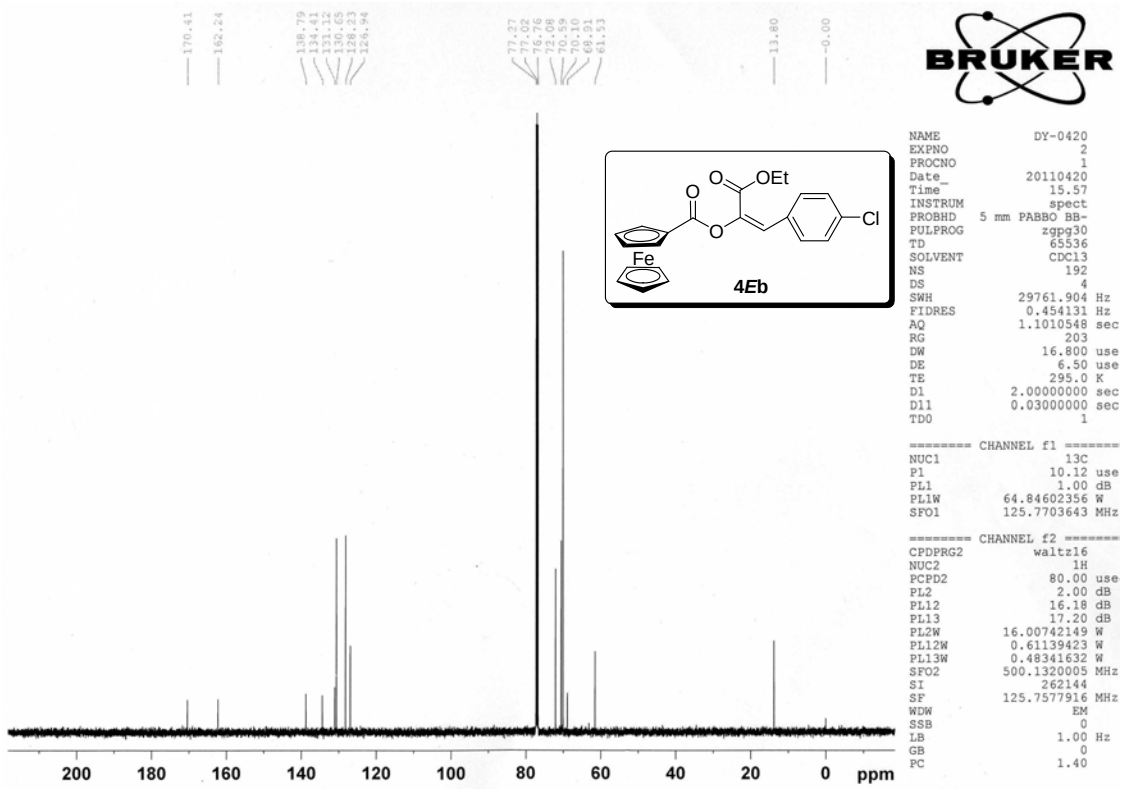
132.31
129.22
128.41
127.98
127.94
77.27
77.02
76.77
72.60
70.59
70.10
69.07
61.37
13.70
0.00
O
OEt
O
Ph
O
Fe
4Ea
200
180
160
140
120
100
80
60
40
20
0
ppm
BRUKER
NAME DY-PCH0Q
EXPNO 2
PROCNO 1
Date_ 20110614
Time 10.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 900
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 use
DE 6.50 use
TE 295.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.12 use
PL1 1.00 dB
PL1W 64.84602356 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 use
PL2 2.00 dB
PL12 16.18 dB
PL13 17.20 dB
PL2W 16.00742149 W
PL12W 0.61139423 W
PL13W 0.48341632 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577917 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



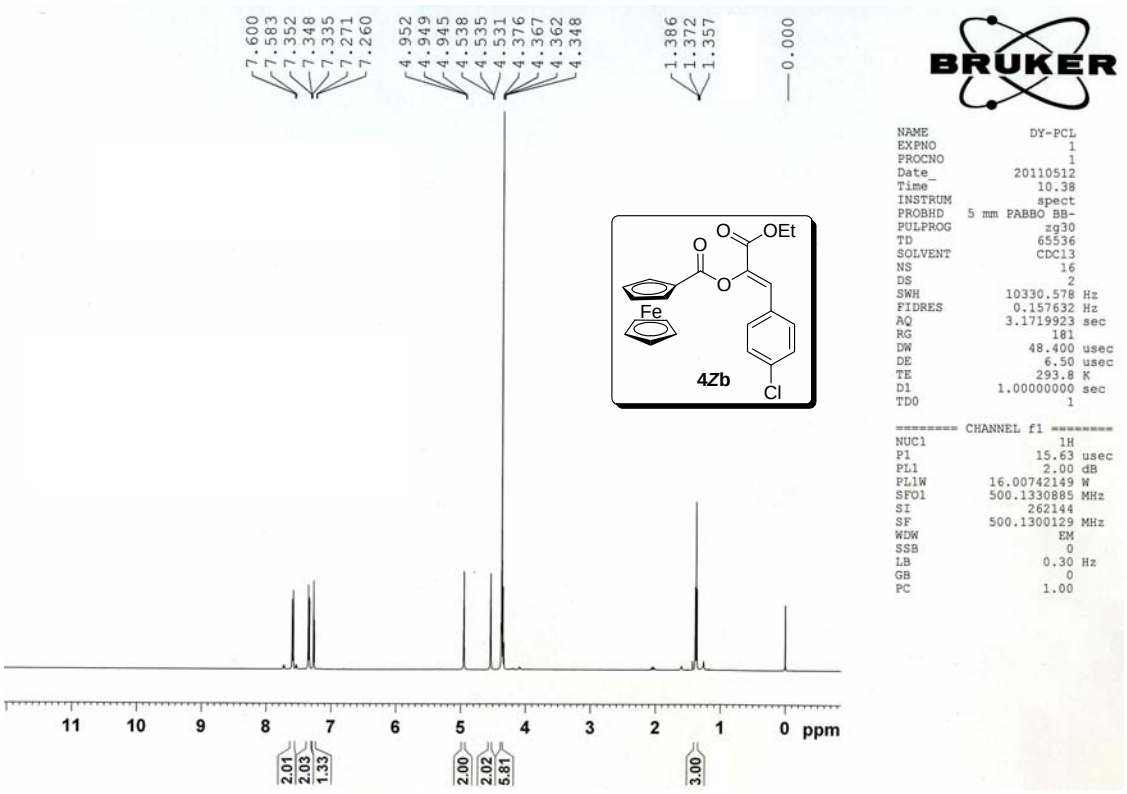
BRUKER

NAME	DY-0420
EXPNO	1
PROCNO	1
Date_	20110420
Time	15.49
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	181
DW	48.400 usec
DE	6.50 usec
TE	293.7 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	15.63 usec
PL1	2.00 dB
PL1W	16.00742149 W
SFO1	500.1330885 MHz
SI	131072
SF	500.1300123 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



BRUKER

NAME	DY-0420
EXPNO	2
PROCNO	1
Date_	20110420
Time	15.57
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	192
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	203
DW	16.800 use
DE	6.50 use
TE	295.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	10.12 use
PL1	1.00 dB
PL1W	64.84602356 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 use
PL2	2.00 dB
PL12	16.18 dB
PL13	17.20 dB
PL2W	16.00742149 W
PL12W	0.61139423 W
PL13W	0.48341632 W
SFO2	500.1320005 MHz
SI	262144
SF	125.7577916 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

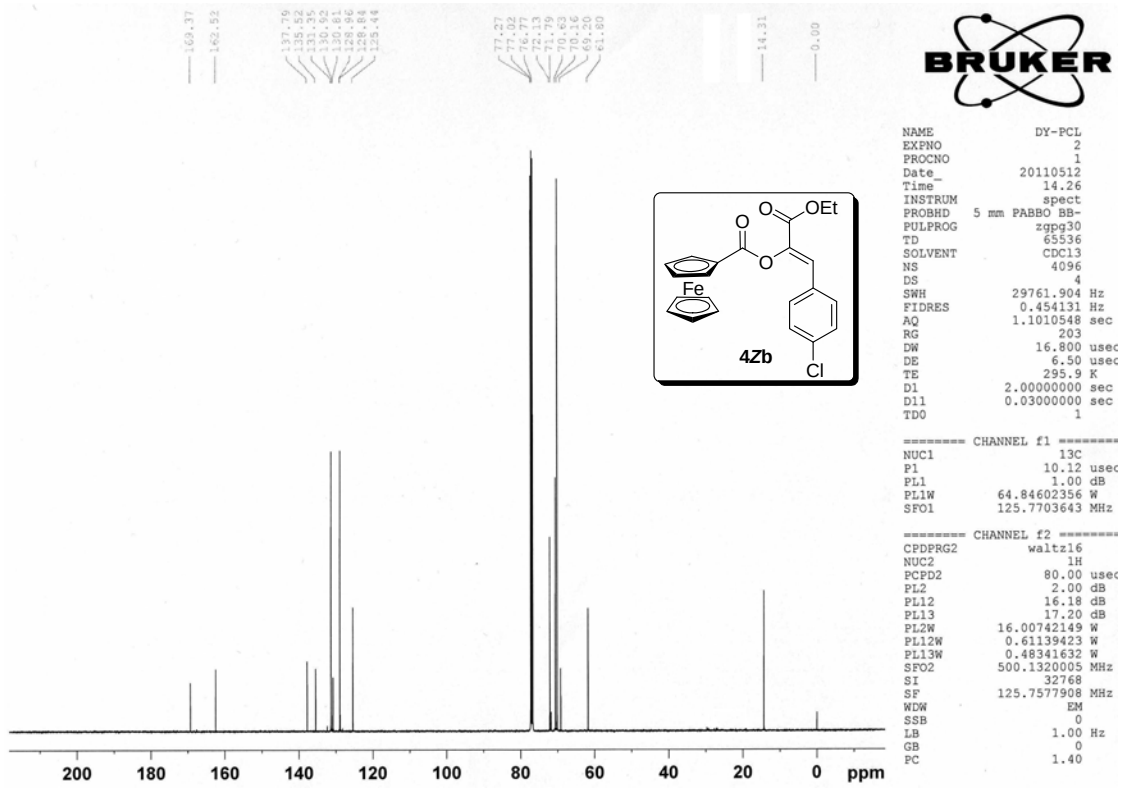


BRUKER

NAME	DY-PCL
EXPNO	1
PROCNO	1
Date_	20110512
Time	10.38
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	181
DW	48.400 usec
DE	6.50 usec
TE	293.8 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========

NUC1	1H
P1	15.63 usec
PL1	2.00 dB
PL1W	16.00742149 W
SFO1	500.1330885 MHz
SI	262144
SF	500.1300129 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



BRUKER

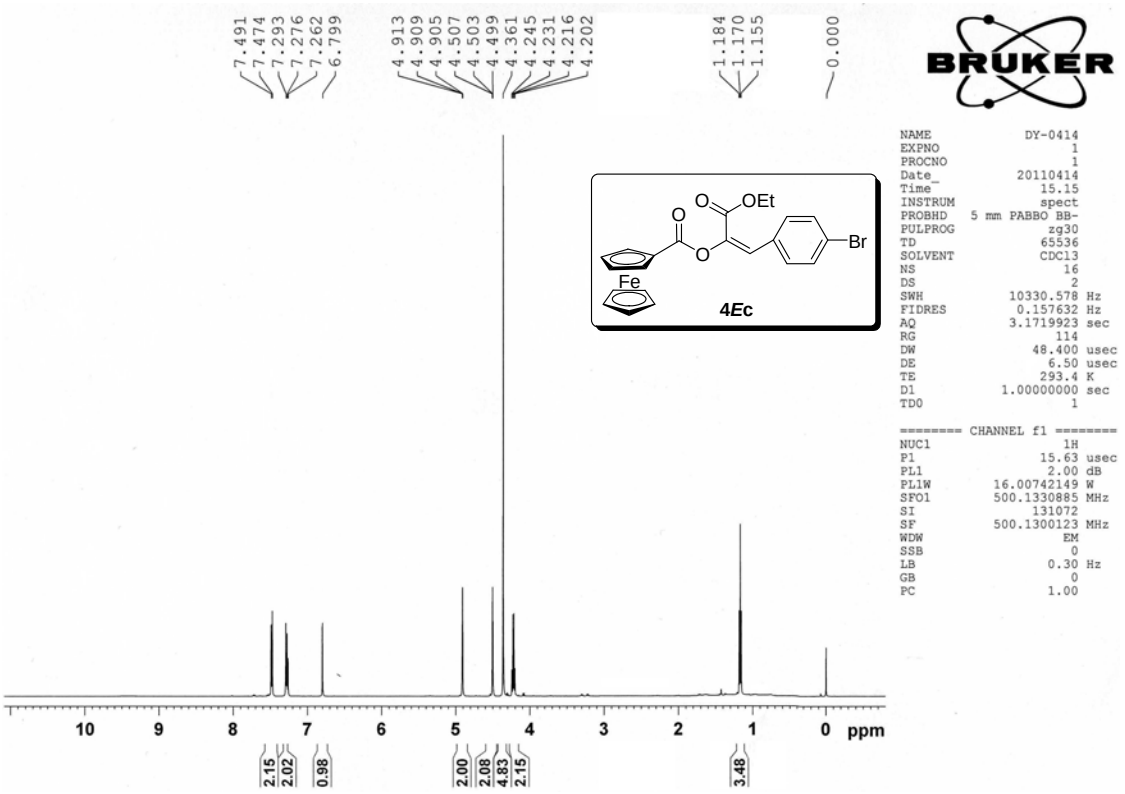
NAME	DY-PCL
EXPNO	2
PROCNO	1
Date_	20110512
Time	14.26
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	4096
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	295.9 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1

======== CHANNEL f1 ========

NUC1	13C
P1	10.12 usec
PL1	1.00 dB
PL1W	64.84602356 W
SFO1	125.7703643 MHz

======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	2.00 dB
PL12	16.18 dB
PL13	17.20 dB
PL2W	16.00742149 W
PL12W	0.61139423 W
PL13W	0.48341632 W
SFO2	500.1320005 MHz
SI	32768
SF	125.7577908 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40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6.799
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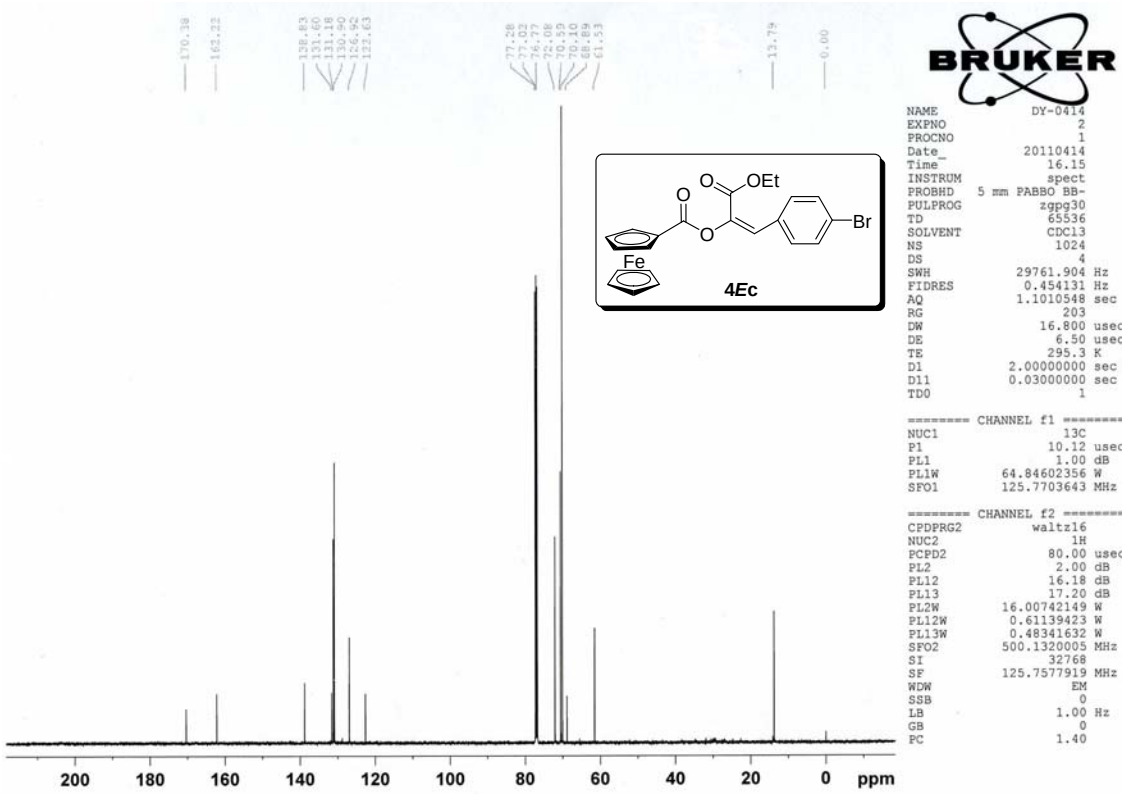
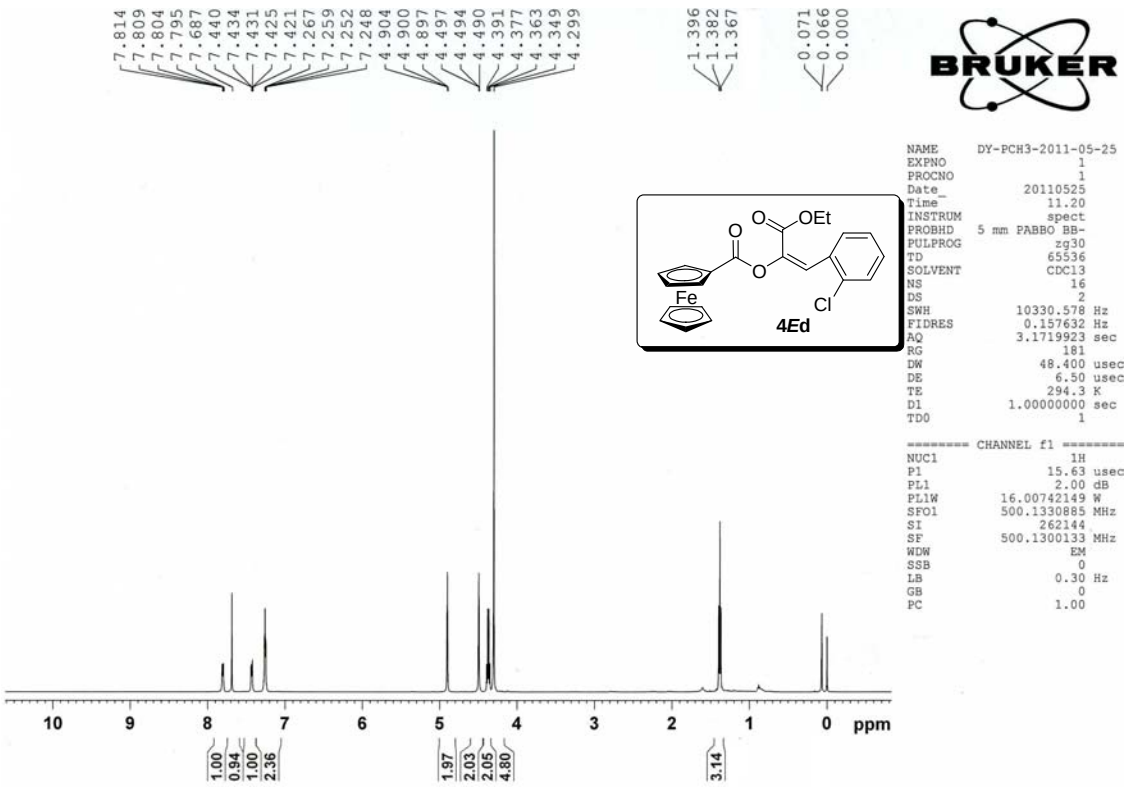
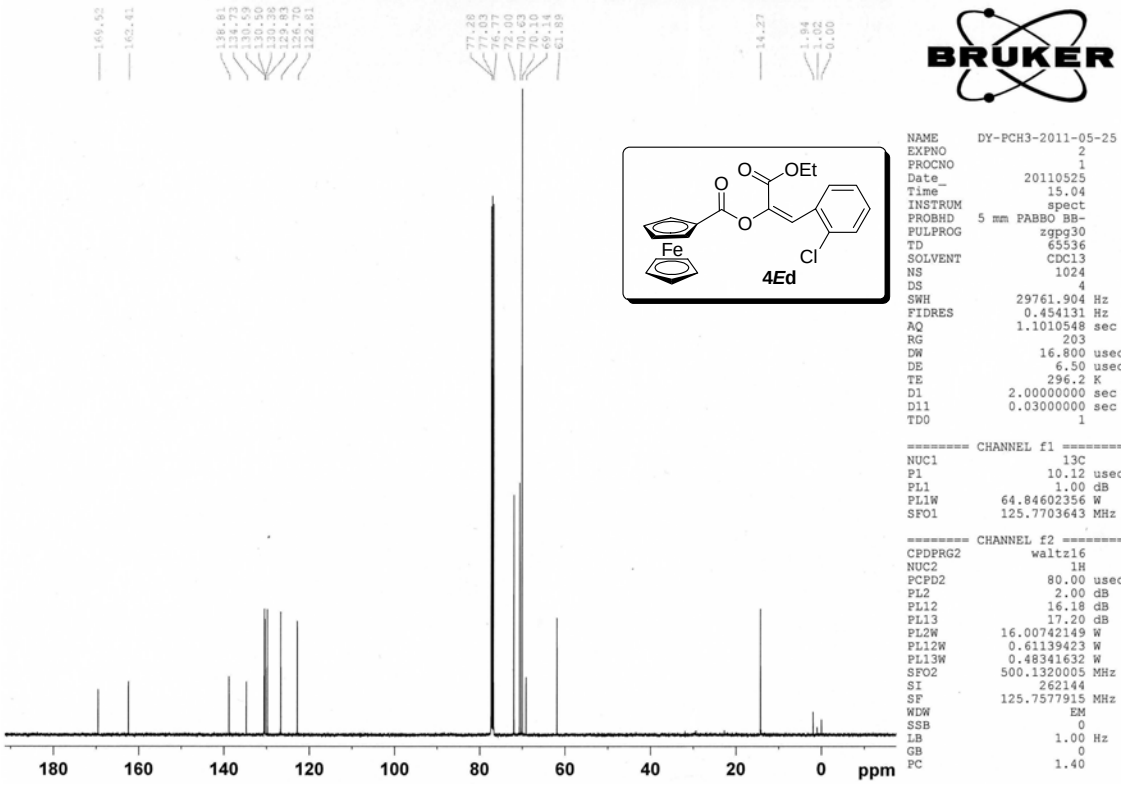
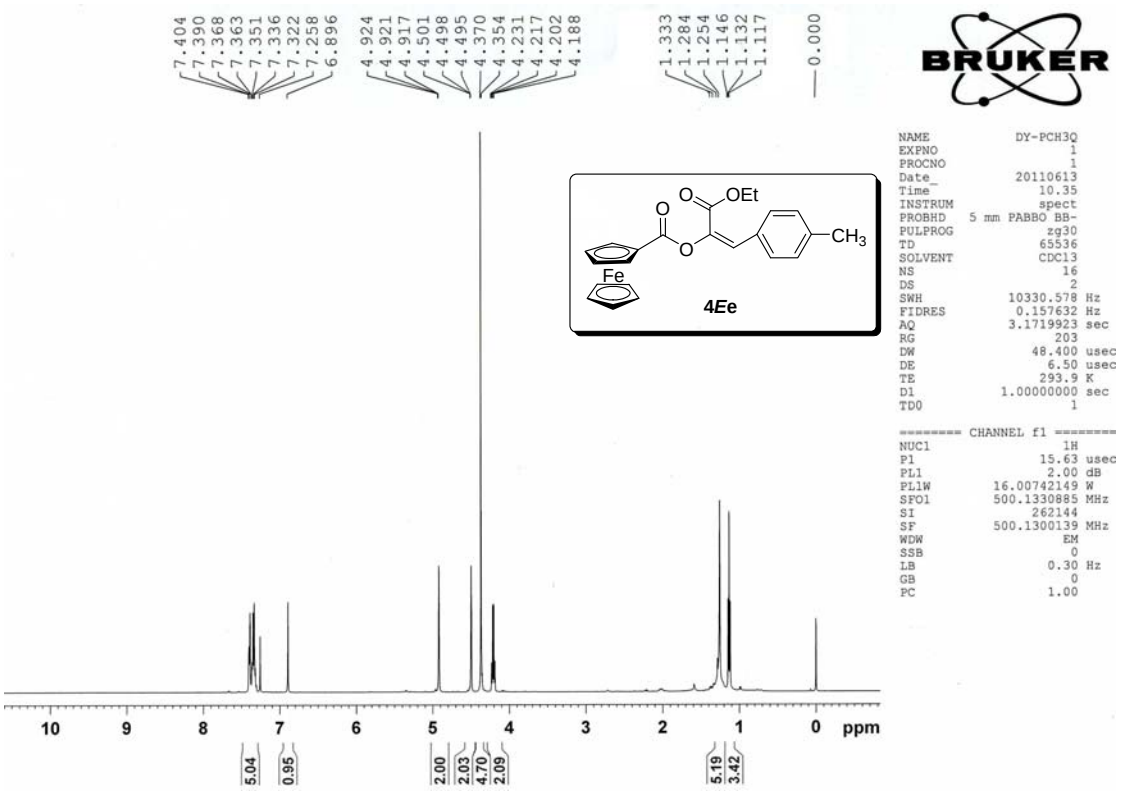
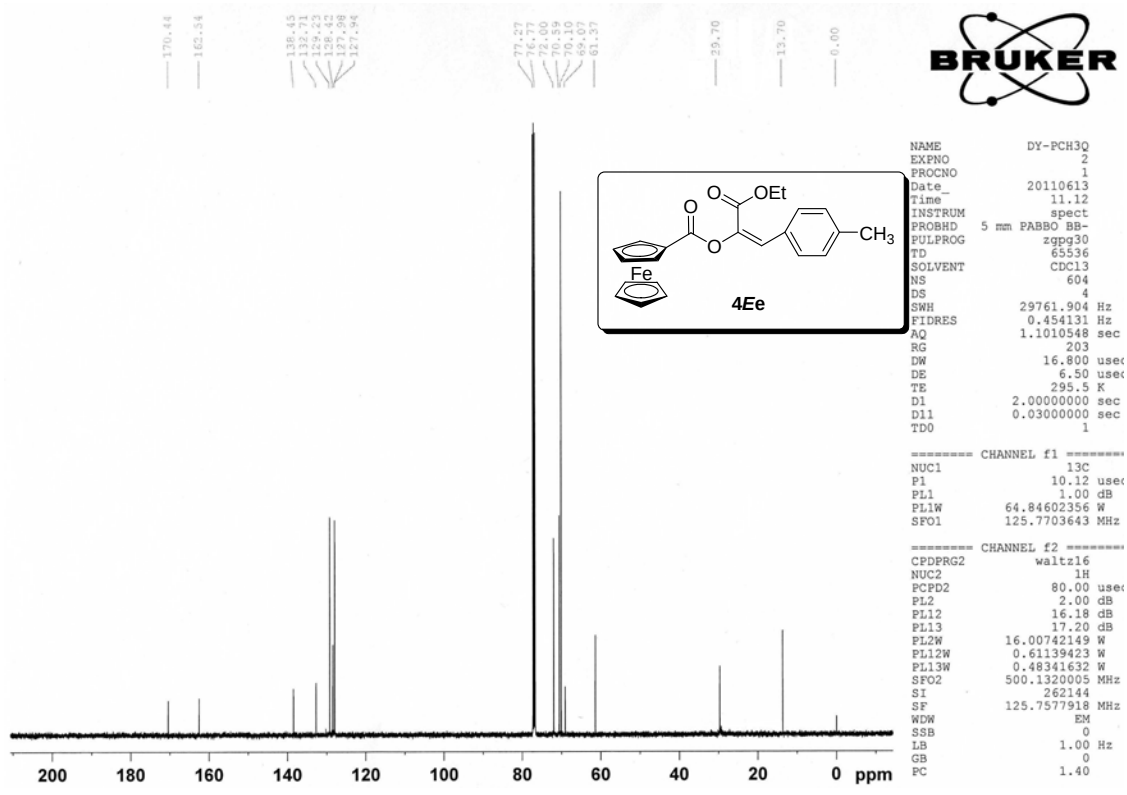
4.909
4.905
4.507
4.503
4.499
4.361
4.245
4.231
4.216
4.202
1.184
1.170
1.155
0.000
BRUKER
NAME DY-0414
EXPNO 1
PROCNO 1
Date_ 20110414
Time 15.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 114
DW 48.400 usec
DE 6.50 usec
TE 293.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 15.63 usec
PL1 2.00 dB
PL1W 16.00742149 W
SFO1 500.1330885 MHz
SI 131072
SF 500.1300123 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
OEt
O
O
Br
Fe
4Ec
10 9 8 7 6 5 4 3 2 1 0 ppm
2.15
2.02
0.98
2.00
2.08
4.83
2.15
3.48

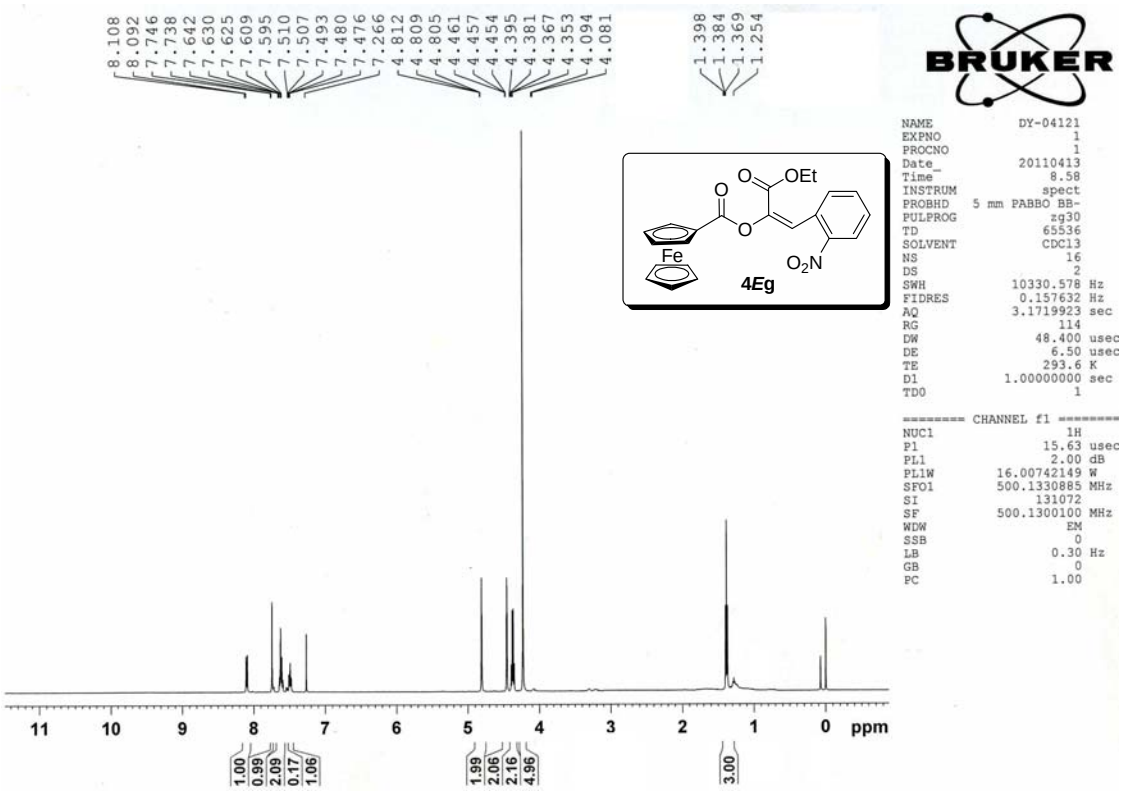

170.38
162.22
128.83
131.60
131.18
130.90
126.92
122.63
77.28
77.02
76.77
76.08
70.35
70.10
69.89
61.53
13.79
6.00
BRUKER
NAME DY-0414
EXPNO 2
PROCNO 1
Date_ 20110414
Time 16.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 295.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.12 usec
PL1 1.00 dB
PL1W 64.84602356 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 16.18 dB
PL13 17.20 dB
PL2W 16.00742149 W
PL12W 0.61139423 W
PL13W 0.48341632 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577919 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
OEt
O
O
Br
Fe
4Ec
200 180 160 140 120 100 80 60 40 20 0 ppm

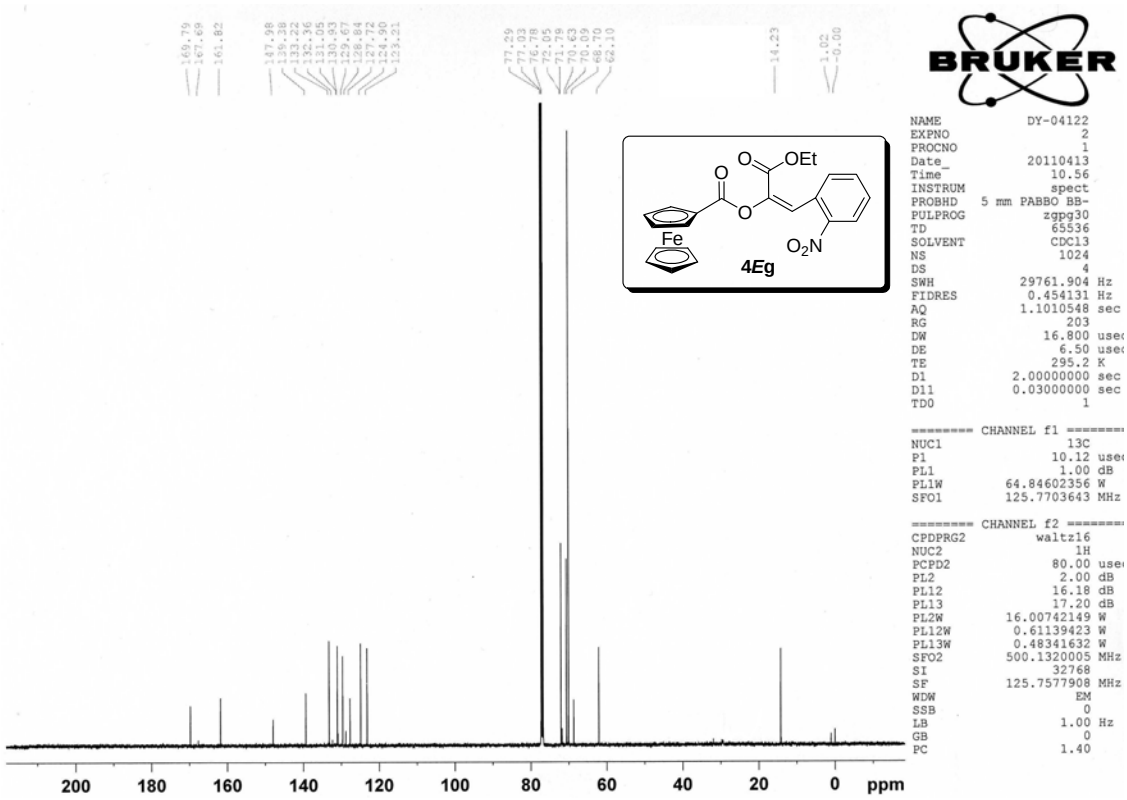

7.814
7.809
7.804
7.795
7.687
7.440
7.434
7.431
7.425
7.421
7.267
7.259
7.252
7.248
4.904
4.900
4.897
4.497
4.494
4.490
4.391
4.377
4.363
4.349
4.299
1.396
1.382
1.367
0.071
0.066
0.000
BRUKER
NAME DY-PCH3-2011-05-25
EXPNO 1
PROCNO 1
Date_ 20110525
Time 11.20
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 181
DW 48.400 usec
DE 6.50 usec
TE 294.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 15.63 usec
PL1 2.00 dB
PL1W 16.00742149 W
SFO1 500.1330885 MHz
SI 262144
SF 500.1300133 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
OEt
O
O
Fe
Cl
4Ed
10 9 8 7 6 5 4 3 2 1 0 ppm
1.00 0.94 1.00 2.36 1.97 2.03 2.05 4.80 3.14

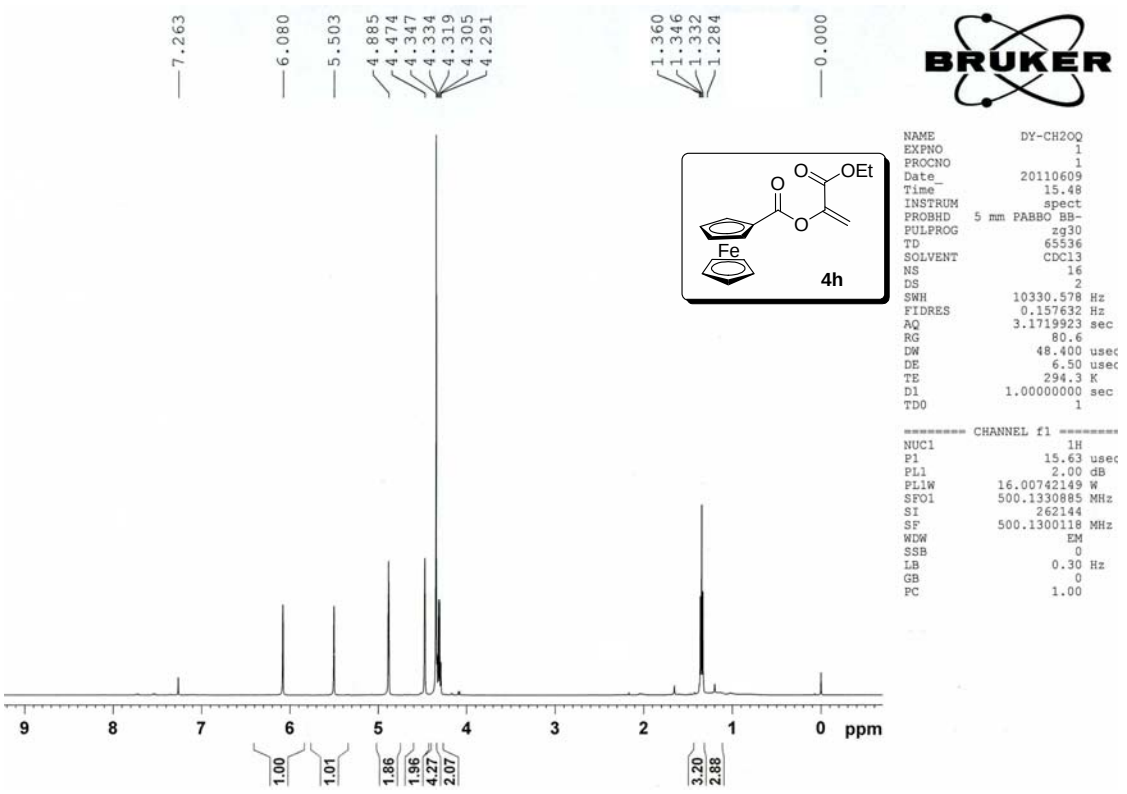

149.52
162.41
138.81
134.73
130.59
130.50
130.38
129.83
126.70
122.81
77.28
77.03
76.77
72.00
70.63
70.10
69.14
61.89
14.27
1.94
1.02
0.00
BRUKER
NAME DY-PCH3-2011-05-25
EXPNO 2
PROCNO 1
Date_ 20110525
Time 15.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 296.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.12 usec
PL1 1.00 dB
PL1W 64.84602356 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 16.18 dB
PL13 17.20 dB
PL2W 16.00742149 W
PL12W 0.61139423 W
PL13W 0.48341632 W
SFO2 500.1320005 MHz
SI 262144
SF 125.7577915 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
OEt
O
O
Fe
Cl
4Ed
180 160 140 120 100 80 60 40 20 0 ppm

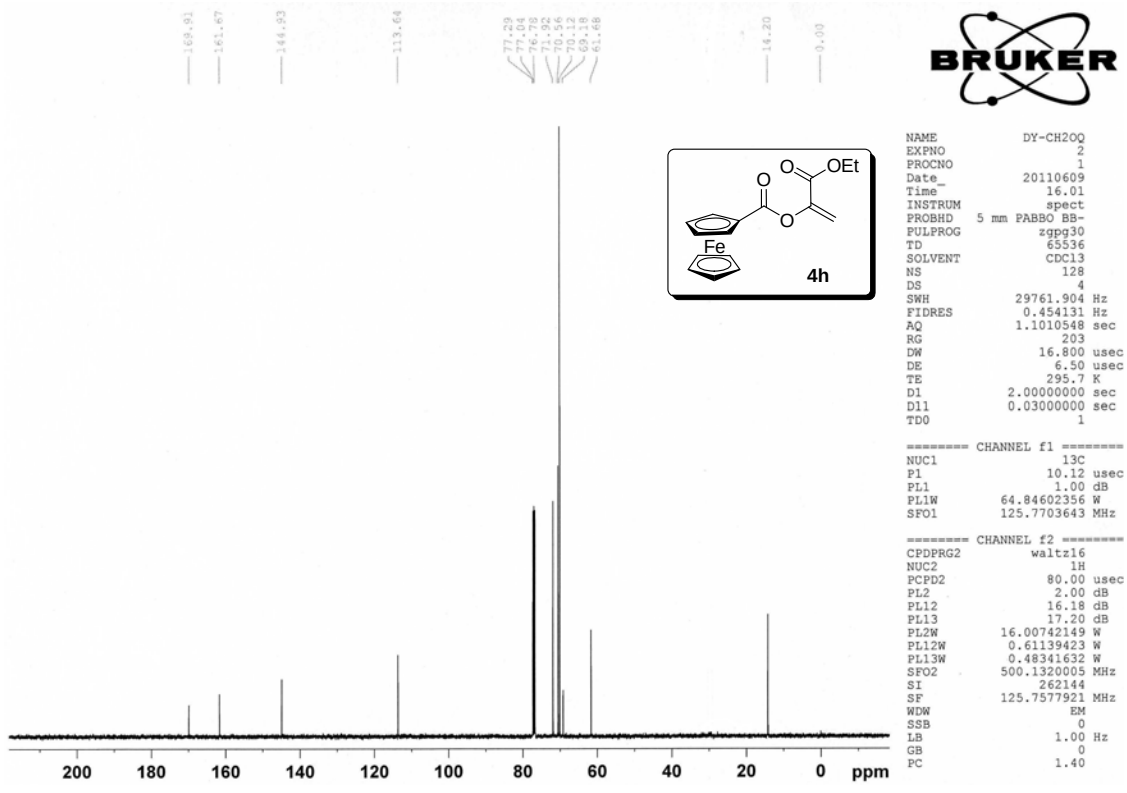

7.404
7.390
7.368
7.363
7.351
7.336
7.322
7.258
6.896
4.924
4.921
4.917
4.501
4.498
4.495
4.370
4.354
4.231
4.217
4.202
4.188
1.333
1.284
1.254
1.146
1.132
1.117
0.000
BRUKER
O
OEt
O
O
CH3
Fe
4Ee
NAME DY-PCH3Q
EXPNO 1
PROCNO 1
Date_ 20110613
Time 10.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 203
DW 48.400 usec
DE 6.50 usec
TE 293.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 15.63 usec
PL1 2.00 dB
PL1W 16.00742149 W
SFO1 500.1330885 MHz
SI 262144
SF 500.1300139 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10 9 8 7 6 5 4 3 2 1 0 ppm
5.04
0.95
2.00
2.03
4.70
2.09
5.19
3.42

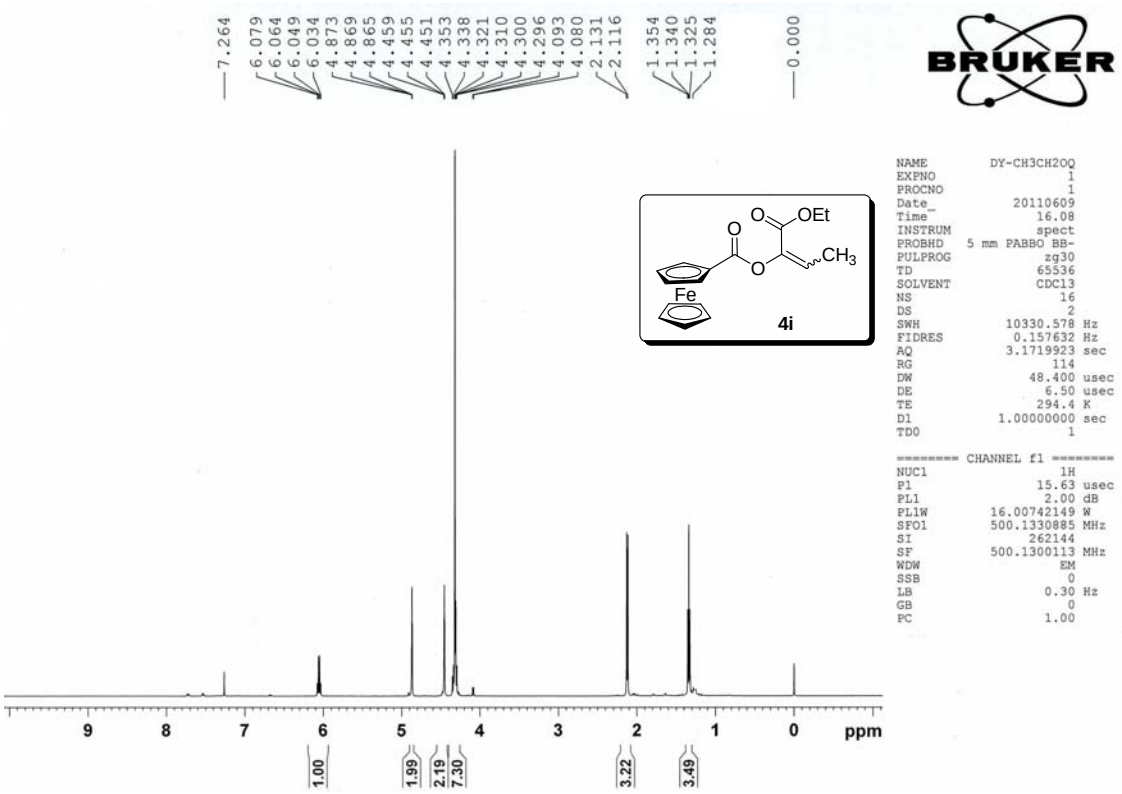

170.44
162.54
138.45
132.71
129.23
128.42
127.98
127.94
77.27
76.77
72.00
70.59
70.10
69.07
61.37
29.70
13.70
0.00
BRUKER
O
OEt
O
O
CH3
Fe
4Ee
NAME DY-PCH3Q
EXPNO 2
PROCNO 1
Date_ 20110613
Time 11.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 604
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 295.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.12 usec
PL1 1.00 dB
PL1W 64.84602356 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 16.18 dB
PL13 17.20 dB
PL2W 16.00742149 W
PL12W 0.61139423 W
PL13W 0.48341632 W
SFO2 500.1320005 MHz
SI 262144
SF 125.7577918 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 0 ppm

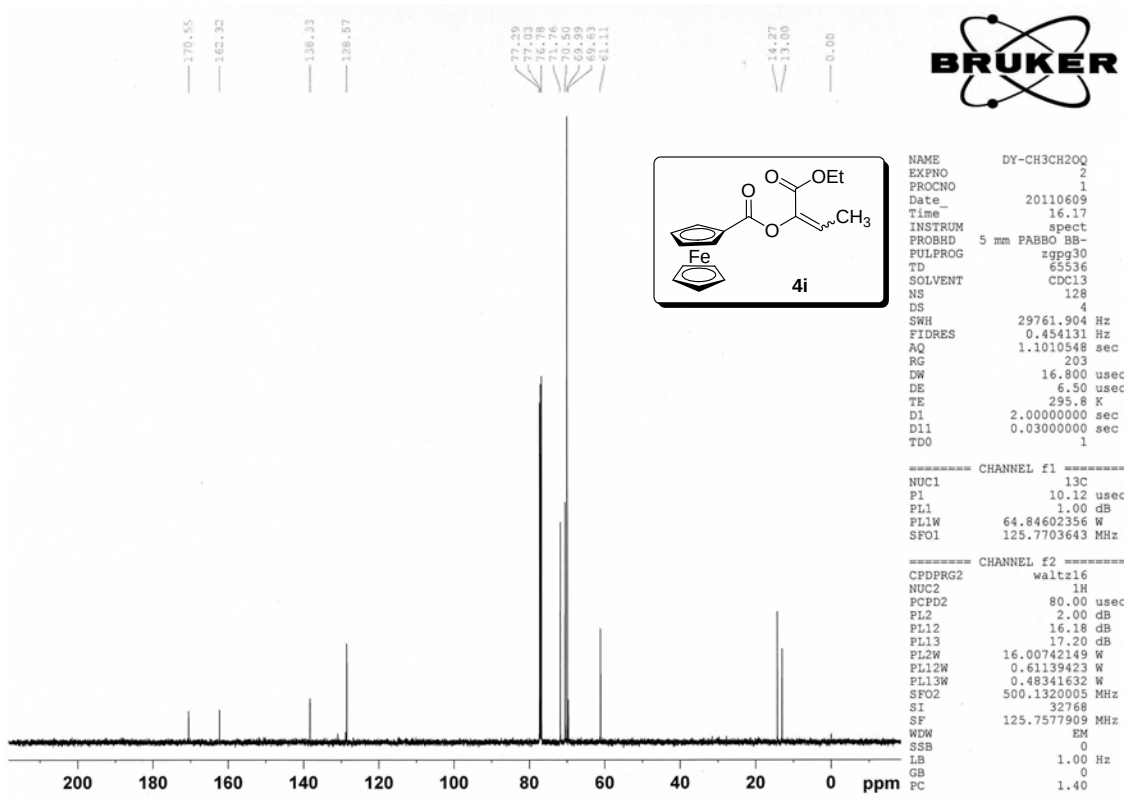

8.108
8.092
7.746
7.738
7.642
7.630
7.625
7.609
7.595
7.510
7.507
7.493
7.480
7.476
7.266
4.812
4.809
4.805
4.461
4.457
4.454
4.395
4.381
4.367
4.353
4.094
4.081
1.398
1.384
1.369
1.254
OEt
O
O
Fe
O2N
4Eg
11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.00 0.99 2.09 0.17 1.06 1.99 2.06 2.16 4.96 3.00
BRUKER
NAME DY-04121
EXPNO 1
PROCNO 1
Date_ 20110413
Time 8.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 114
DW 48.400 usec
DE 6.50 usec
TE 293.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 15.63 usec
PL1 2.00 dB
PL1W 16.00742149 W
SFO1 500.1330885 MHz
SI 131072
SF 500.1300100 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

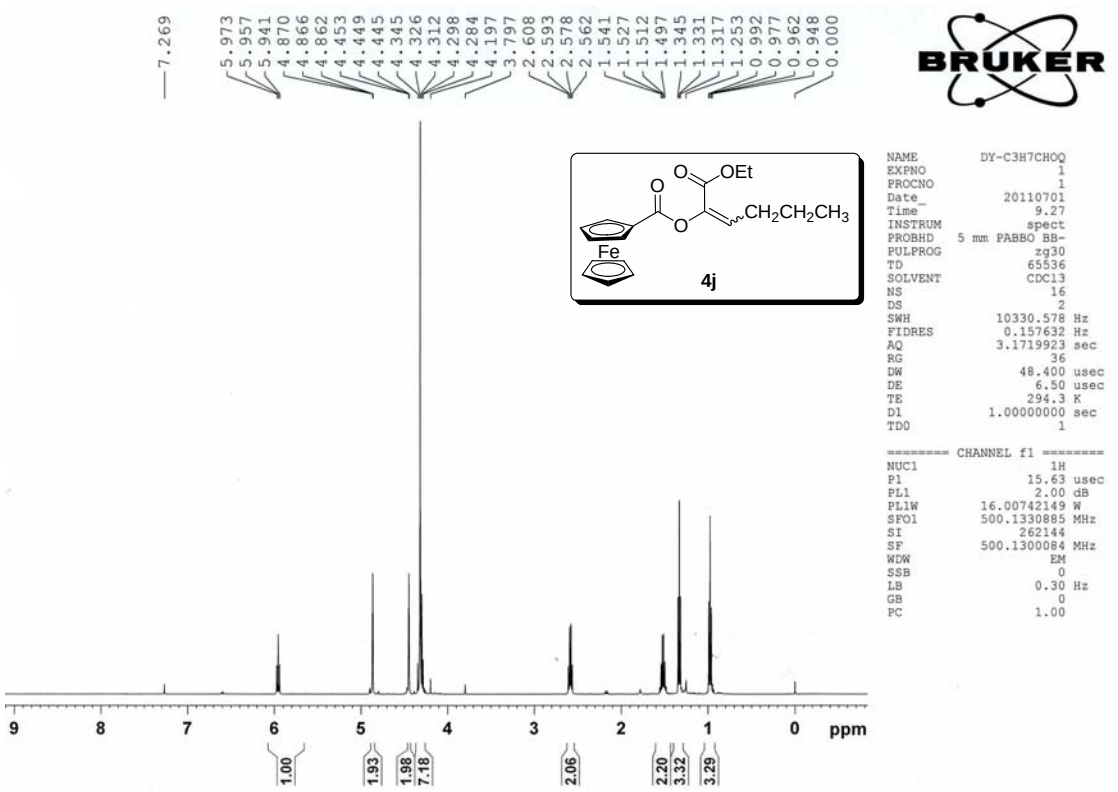

169.79
167.69
161.82
147.98
139.38
133.22
131.56
131.15
130.93
129.67
126.84
127.72
124.90
123.21
77.29
77.03
76.78
72.05
71.79
71.63
70.09
68.70
62.10
14.23
1.02
-0.00
OEt
O
O
Fe
O2N
4Eg
200 180 160 140 120 100 80 60 40 20 0 ppm
BRUKER
NAME DY-04122
EXPNO 2
PROCNO 1
Date_ 20110413
Time 10.56
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 295.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.12 usec
PL1 1.00 dB
PL1W 64.84602356 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 16.18 dB
PL13 17.20 dB
PL2W 16.00742149 W
PL12W 0.61139423 W
PL13W 0.48341632 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577908 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

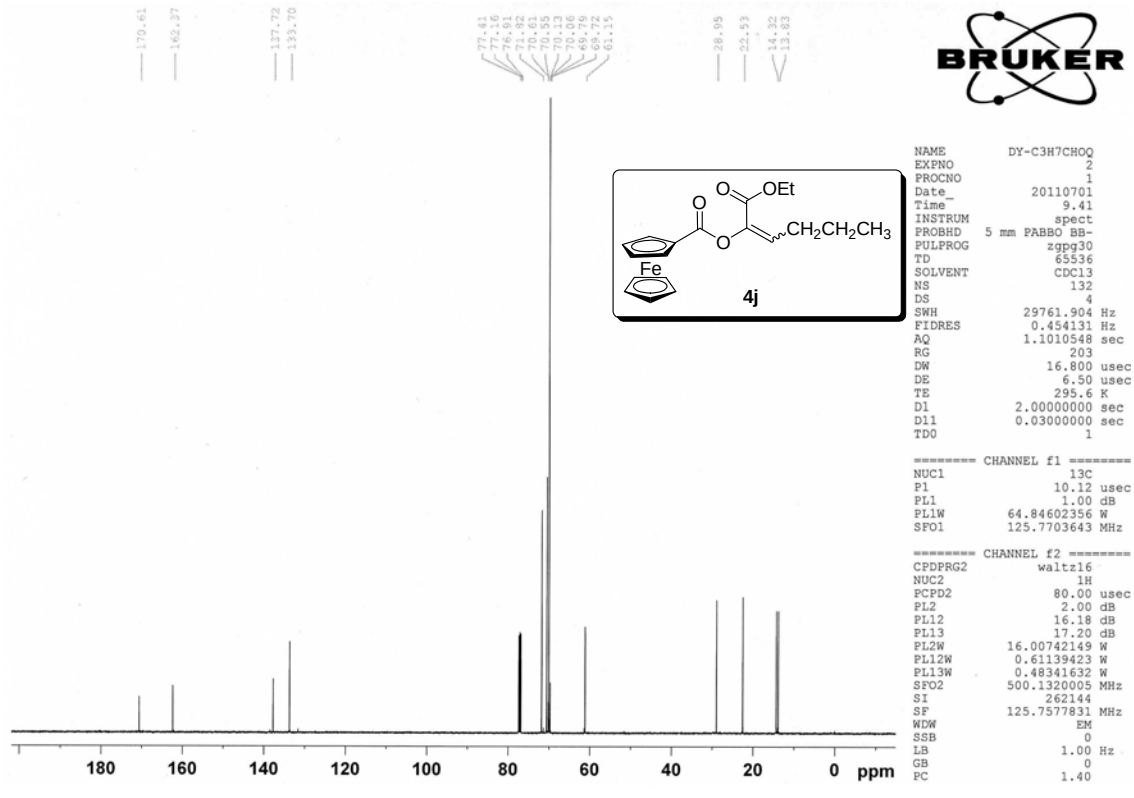

7.263
6.080
5.503
4.885
4.474
4.347
4.334
4.319
4.305
4.291
1.360
1.346
1.332
1.284
0.000
BRUKER
O
OEt
O
O
Fe
4h
NAME DY-CH2OQ
EXPNO 1
PROCNO 1
Date_ 20110609
Time 15.48
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 80.6
DW 48.400 usec
DE 6.50 usec
TE 294.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 15.63 usec
PL1 2.00 dB
PL1W 16.00742149 W
SFO1 500.1330885 MHz
SI 262144
SF 500.1300118 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9 8 7 6 5 4 3 2 1 0 ppm
1.00 1.01 1.86 1.96 4.27 2.07 3.20 2.88


169.91
161.67
144.93
113.64
77.29
77.04
76.78
72.92
70.56
70.12
69.18
61.68
14.20
0.00
BRUKER
O
OEt
O
O
Fe
4h
NAME DY-CH2OQ
EXPNO 2
PROCNO 1
Date_ 20110609
Time 16.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 295.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.12 usec
PL1 1.00 dB
PL1W 64.84602356 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 16.18 dB
PL13 17.20 dB
PL2W 16.00742149 W
PL12W 0.61139423 W
PL13W 0.48341632 W
SFO2 500.1320005 MHz
SI 262144
SF 125.7577921 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 0 ppm


7.264
6.079
6.064
6.049
6.034
4.873
4.869
4.865
4.459
4.455
4.451
4.353
4.338
4.321
4.310
4.300
4.296
4.093
4.080
2.131
2.116
1.354
1.340
1.325
1.284
0.000
BRUKER
4i
NAME DY-CH3CH2OQ
EXPNO 1
PROCNO 1
Date_ 20110609
Time 16.08
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 114
DW 48.400 usec
DE 6.50 usec
TE 294.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 15.63 usec
PL1 2.00 dB
PL1W 16.00742149 W
SFO1 500.1330885 MHz
SI 262144
SF 500.1300113 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9 8 7 6 5 4 3 2 1 0 ppm
1.00 1.99 2.19 7.30 3.22 3.49


170.55
162.32
138.33
128.57
77.29
77.03
76.78
71.76
70.50
69.39
69.63
61.11
14.27
13.00
0.00
BRUKER
4i
NAME DY-CH3CH2OQ
EXPNO 2
PROCNO 1
Date_ 20110609
Time 16.17
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 295.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.12 usec
PL1 1.00 dB
PL1W 64.84602356 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 16.18 dB
PL13 17.20 dB
PL2W 16.00742149 W
PL12W 0.61139423 W
PL13W 0.48341632 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577909 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 0 ppm


7.269
5.973
5.957
5.941
4.870
4.866
4.862
4.453
4.449
4.445
4.345
4.326
4.312
4.298
4.284
4.197
3.797
2.608
2.593
2.578
2.562
2.541
1.527
1.512
1.497
1.345
1.331
1.317
1.253
0.992
0.977
0.962
0.948
0.000
BRUKER
OEt
O
O
CH2CH2CH3
Fe
4j
NAME DY-C3H7CHOQ
EXPNO 1
PROCNO 1
Date_ 20110701
Time 9.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 36
DW 48.400 usec
DE 6.50 usec
TE 294.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 15.63 usec
PL1 2.00 dB
PL1W 16.00742149 W
SFO1 500.1330885 MHz
SI 262144
SF 500.1300084 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9 8 7 6 5 4 3 2 1 0 ppm
1.00 1.93 1.98 7.18 2.06 2.20 3.32 3.29


170.61
162.37
137.72
133.70
77.41
77.16
76.91
76.82
70.61
70.55
70.13
70.06
69.79
69.72
61.15
28.95
22.53
14.32
13.83
BRUKER
OEt
O
O
CH2CH2CH3
Fe
4j
NAME DY-C3H7CHOQ
EXPNO 2
PROCNO 1
Date_ 20110701
Time 9.41
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 132
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 295.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.12 usec
PL1 1.00 dB
PL1W 64.84602356 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 16.18 dB
PL13 17.20 dB
PL2W 16.00742149 W
PL12W 0.61139423 W
PL13W 0.48341632 W
SFO2 500.1320005 MHz
SI 262144
SF 125.7577831 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
180 160 140 120 100 80 60 40 20 0 ppm