

Supplementary Information

Ru(II)-Catalyzed C-H Alkynylation of Ferrocenes with Bromoalkynes

Directed by Carboxamide Groups

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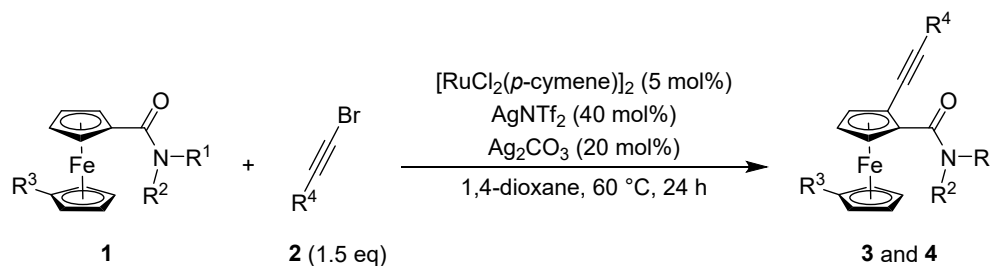
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(A) General Information

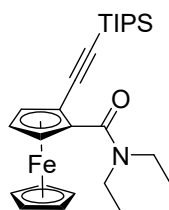
^1H NMR spectra were recorded on 400 MHz or 500 MHz, ^{13}C NMR spectra were recorded on 101 MHz or 126 MHz by using a Bruker Avance 400M spectrometer. Chemical shifts were reported in parts per million (δ) relative to tetramethylsilane (TMS). All spectra were obtained at ambient temperature. The chemical shifts (δ) were recorded in parts per million (ppm). The coupling constants (J) were shown in Hertz (Hz). Chemical shifts in CDCl_3 were reported the residual CHCl_3 (7.26 ppm for ^1H NMR, 77.16 ppm for ^{13}C NMR). ^{13}C NMR showed broad signals for most of tert-amides, we didn't make a mark (br). HRMS measurements were performed on an Ultima Global spectrometer with an ESI source. The melting points were recorded on a RY-1 microscopic melting apparatus and uncorrected. The enantiomeric ratio (er) value of the product was determined by high-performance liquid chromatography (HPLC) analysis performed on Shimadzu LC-20AT chromatography. All the reagents were obtained from commercial sources, and used without further purification. Ferrocene carboxamide derivatives **1a-1p** were known compounds in the literature,^[S1-S5] bromoalkyne compounds **2a-2p** were known compounds in the literature.^[S6-S10]

(B) General Procedure of Ru-Catalyzed C-H Alkynylation of Ferrocenes



To a dried screw-capped vial, ferrocene carboxamides **1** (0.05 mmol), bromoalkynes compounds **2** (0.075 mmol), [RuCl₂(*p*-cymene)]₂ (1.51 mg, 0.0025 mmol), AgNTf₂ (8.0 mg, 0.02 mmol), Ag₂CO₃ (2.75 mg, 0.01 mmol) and 1,4-dioxane (0.125 mL) were added under Ar atmosphere. The vial was capped, and the mixture was heated at 60 °C for 24 h with stirring. The resulting mixture was cooled to room temperature, and directly purified by silica gel column chromatography to give the alkynylated ferrocenecarboxamide products **3** and **4**.

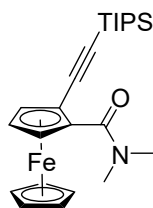
2-Triisopropylsilylethynyl-(diethyl-1-carbonyl)ferrocene (**3a**):



3a

Compound **3a** was prepared according to the general procedure. Yellow solid; **m.p.**: 62-64 °C; ¹H NMR (400 MHz, CDCl₃) δ 4.44-4.40 (m, 2H), 4.35 (s, 5H), 4.20 (s, 1H), 3.60-3.59 (m, 1H), 3.33-3.32 (m, 2H), 3.07-3.06 (m, 1H), 1.20-1.18 (m, 27H); ¹³C NMR (101 MHz, CDCl₃) δ 167.3, 104.2, 89.2, 72.1, 71.5, 71.2, 70.5, 67.6, 64.3, 43.4, 40.3, 18.8, 14.4, 13.3, 11.4; HRMS (ESI): *m/z* calculated for C₂₆H₄₀FeNOSi⁺ [M+H]⁺: 466.2223, found: 466.2172.

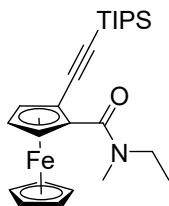
2-Triisopropylsilylethynyl-(dimethyl-1-carbonyl)ferrocene (**3b**):



3b

Compound **3b** was prepared according to the general procedure. Yellow solid; **m.p.**: 60-62 °C; **¹H NMR (400 MHz, CDCl₃)** δ 4.55 (s, 1H), 4.47 (s, 1H), 4.33 (s, 5H), 4.24 (s, 1H), 3.00-2.91 (m, 6H), 1.12 (s, 21H); **¹³C NMR (101 MHz, CDCl₃)** δ 168.6, 104.3, 89.2, 87.3, 72.1, 71.5, 71.4, 68.0, 63.8, 38.7, 35.4, 18.7, 18.6, 11.2; **HRMS (ESI)**: m/z calculated for C₂₄H₃₆FeNOSi⁺ [M+H]⁺: 438.1910, found: 438.1860.

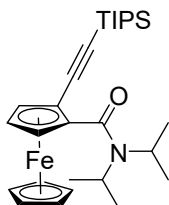
2-Triisopropylsilylethynyl-(methyl-ethyl-1-carbonyl)ferrocene (3c):



3c

Compound **3c** was prepared according to the general procedure. Yellow solid; **m.p.**: 60-62 °C; **¹H NMR (400 MHz, CDCl₃)** δ 4.54-4.45 (m, 2H), 4.33 (s, 5H), 4.22 (s, 1H), 3.53-3.41 (m, 2H), 2.96-2.87 (m, 3H), 1.10 (s, 24H); **¹³C NMR (101 MHz, CDCl₃)** δ 167.9, 104.1, 89.1, 87.7, 72.0, 71.4, 70.6, 67.9, 67.6, 45.6, 42.6, 35.9, 18.7, 13.5, 11.2; **HRMS (ESI)**: m/z calculated for C₂₅H₃₈FeNOSi⁺ [M+H]⁺: 452.2067, found: 452.2008.

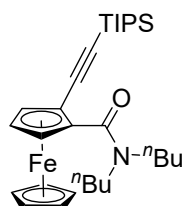
2-Triisopropylsilylethynyl-(diisopropyl-1-carbonyl)ferrocene (3d):



3d

Compound **3d** was prepared according to the general procedure. Yellow solid; **m.p.**: 73-75 °C; **¹H NMR (400 MHz, CDCl₃)** δ 4.43 (s, 1H), 4.36 (s, 5H), 4.30 (s, 1H), 4.16 (s, 1H), 3.72-3.59 (m, 1H), 3.42-3.35 (m, 1H), 1.50-1.47 (m, 6H), 1.11-1.05 (m, 27H); **¹³C NMR (101 MHz, CDCl₃)** δ 166.2, 104.1, 92.2, 88.8, 71.8, 70.9, 68.7, 67.0, 64.1, 50.8, 45.7, 20.3, 18.7, 18.7, 11.3; **HRMS (ESI)**: m/z calculated for C₂₈H₄₄FeNOSi⁺ [M+H]⁺: 494.2536, found: 494.2708.

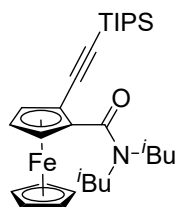
2-Triisopropylsilylethynyl-(dibutyl-1-carbonyl)ferrocene (**3e**):



3e

Compound **3e** was prepared according to the general procedure. Yellow solid; **m.p.**: 77-79 °C; **¹H NMR (400 MHz, CDCl₃)** δ 4.45-4.44 (m, 2H), 4.34 (s, 5H), 4.19 (s, 1H), 3.62-2.95 (m, 4H), 1.64-1.36 (m, 8H), 1.12-1.11(m, 21H), 0.96-0.93 (m, 3H), 0.74-0.70 (m, 3H); **¹³C NMR (101 MHz, CDCl₃)** δ 167.5, 104.2, 89.1, 88.9, 72.0, 71.2, 70.8, 67.5, 64.2, 48.7, 45.8, 30.8, 30.1, 20.5, 19.7, 18.7, 18.7, 14.0, 13.6, 11.2; **HRMS (ESI)**: m/z calculated for C₃₀H₄₈FeNOSi⁺ [M+H]⁺: 522.2849, found: 522.2851.

2-Triisopropylsilylethynyl-(diisobutyl-1-carbonyl)ferrocene (**3f**):

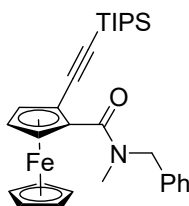


3f

Compound **3f** was prepared according to the general procedure. Yellow solid; **m.p.**: 77-79 °C; **¹H NMR (400 MHz, CDCl₃)** δ 4.51-4.46 (m, 2H), 4.30 (s, 5H), 4.22 (s, 1H), 3.76-3.71 (m, 1H), 3.33-3.27 (m, 1H), 2.99-2.95 (m, 1H), 2.82-2.77 (m, 1H),

2.07-2.04 (m, 1H), 1.77-1.70 (m, 1H), 1.11 (s, 21H), 0.97 (s, 6H), 0.71-0.57 (m, 6H); ^{13}C NMR (101 MHz, CDCl_3) δ 168.6, 104.7, 89.5, 87.1, 72.4, 72.2, 67.9, 64.0, 56.6, 52.5, 27.1, 26.5, 20.6, 20.4, 20.1, 19.7, 18.7, 18.7, 11.2; HRMS (ESI): m/z calculated for $\text{C}_{30}\text{H}_{48}\text{FeNOSi}^+ [\text{M}+\text{H}]^+$: 522.2849, found: 522.2850.

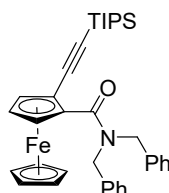
2-Triisopropylsilylethynyl-(methyl-benzyl-1-carbonyl)ferrocene (3g):



3g

Compound **3g** was prepared according to the general procedure. Yellow solid; **m.p.**: 68-70 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.32-7.26 (m, 5H), 5.01-4.75 (m, 1H), 4.58-4.56 (m, 1H), 4.49 (s, 1H), 4.36 (s, 5H), 4.26-4.22 (m, 2H), 2.86 (s, 3H), 1.14 (s, 21H); ^{13}C NMR (101 MHz, CDCl_3) δ 168.7, 137.2, 128.8, 128.5, 128.2, 127.2, 104.1, 89.5, 86.7, 72.1, 71.8, 71.3, 68.1, 55.0, 51.2, 36.1, 33.2, 18.7, 11.2; HRMS (ESI): m/z calculated for $\text{C}_{30}\text{H}_{40}\text{FeNOSi}^+ [\text{M}+\text{H}]^+$: 514.2223, found: 514.2206.

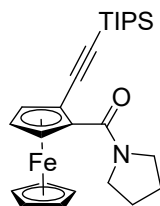
2-Triisopropylsilylethynyl-(dibenzyl-1-carbonyl)ferrocene (3h):



3h

Compound **3h** was prepared according to the general procedure. Yellow solid; **m.p.**: 75-77 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.29-7.26 (m, 8H), 7.04-7.03 (m, 2H), 5.05 (d, $J = 14.7$ Hz, 1H), 4.73 (d, $J = 15.9$ Hz, 1H), 4.52-4.51 (m, 2H), 4.37 (s, 5H), 4.28 (d, $J = 16.0$ Hz, 1H), 4.21 (t, $J = 2.3$ Hz, 1H), 4.16 (d, $J = 14.5$ Hz, 1H), 1.14-1.12 (m, 21H); ^{13}C NMR (101 MHz, CDCl_3) δ 168.8, 137.2, 128.6, 128.3, 127.3, 104.1, 89.9, 85.5, 72.5, 72.2, 70.9, 68.2, 65.6, 51.7, 47.7, 18.8, 18.7, 11.3; HRMS (ESI): m/z calculated for $\text{C}_{36}\text{H}_{44}\text{FeNOSi}^+ [\text{M}+\text{H}]^+$: 590.2536, found: 590.2532.

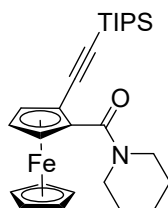
2-Triisopropylsilylethynyl-(pyrrolidine-1-carbonyl)ferrocene (**3i**):



3i

Compound **3i** was prepared according to the general procedure. Yellow solid; **m.p.**: 59-61 °C; **¹H NMR (400 MHz, CDCl₃)** δ 4.55 (s, 1H), 4.47 (s, 1H), 4.33 (s, 5H), 4.22 (t, *J* = 2.3 Hz, 1H), 3.73-3.46 (m, 3H), 3.14-3.08 (m, 1H), 1.89-1.74 (m, 4H), 1.12-1.11 (m, 21H); **¹³C NMR (101 MHz, CDCl₃)** δ 167.4, 104.9, 89.4, 88.5, 72.3, 72.0, 71.4, 68.3, 63.6, 48.1, 46.3, 26.2, 24.8, 18.9, 18.9, 11.5; **HRMS (ESI)**: *m/z* calculated for C₂₆H₃₈FeNOSi⁺ [M+H]⁺: 464.2067, found: 464.2069.

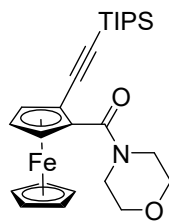
2-Triisopropylsilylethynyl-(piperidine-1-carbonyl)ferrocene (**3j**):



3j

Compound **3j** was prepared according to the general procedure. Yellow solid; **m.p.**: 60-62 °C; **¹H NMR (400 MHz, CDCl₃)** δ 4.49-4.46 (m, 2H), 4.33 (s, 5H), 4.23 (t, *J* = 2.0 Hz, 1H), 3.87-3.84 (m, 1H), 3.32-3.28 (m, 3H), 1.63-1.56 (m, 6H), 1.13-1.12 (m, 21H); **¹³C NMR (101 MHz, CDCl₃)** δ 166.8, 104.2, 89.2, 87.7, 72.0, 71.4, 71.2, 67.8, 64.0, 24.6, 18.7, 11.2; **HRMS (ESI)**: *m/z* calculated for C₂₇H₄₀FeNOSi⁺ [M+H]⁺: 478.2223, found: 478.2183.

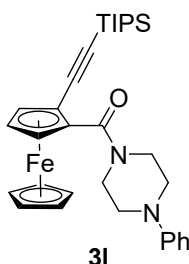
2-Triisopropylsilylethynyl-(morpholine-1-carbonyl)ferrocene (**3k**):



3k

Compound **3k** was prepared according to the general procedure. Yellow solid; **m.p.**: 95-97 °C; **¹H NMR (400 MHz, CDCl₃)** δ 4.54 (s, 1H), 4.49 (s, 1H), 4.33 (s, 5H), 4.26 (s, 1H), 3.74-3.31 (m, 8H), 1.12 (s, 21H); **¹³C NMR (101 MHz, CDCl₃)** δ 167.4, 104.0, 89.7, 85.9, 72.1, 71.9, 71.7, 68.2, 63.9, 18.7, 11.2; **HRMS (ESI):** m/z calculated for C₂₆H₃₈FeNO₂Si⁺ [M+H]⁺: 480.2016, found: 480.2011.

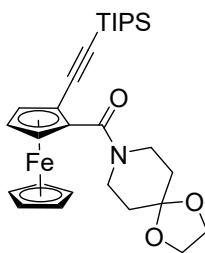
2-Triisopropylsilylethynyl-(N-phenylpiperazine-1-carbonyl)ferrocene (3l):



3l

Compound **3l** was prepared according to the general procedure. Yellow solid; **m.p.**: 108-110 °C; **¹H NMR (400 MHz, CDCl₃)** δ 7.30-7.26 (m, 2H), 6.92-6.90 (m, 3H), 4.58 (s, 1H), 4.53 (s, 1H), 4.38 (s, 5H), 4.30 (t, *J* = 2.4 Hz, 1H), 3.62-3.58 (m, 4H), 3.23-3.20 (m, 4H), 1.28-1.13 (m, 21H); **¹³C NMR (101 MHz, CDCl₃)** δ 167.2, 151.0, 129.1, 120.2, 116.5, 104.0, 89.7, 86.3, 72.1, 71.8, 71.6, 68.2, 64.0, 18.7, 11.2; **HRMS (ESI):** m/z calculated for C₃₂H₄₃FeN₂OSi⁺ [M+H]⁺: 555.2489, found: 555.2495.

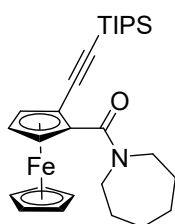
2-Triisopropylsilylethynyl-((4-piperidine-1-carbonyl)ferrocene (3m):



3m

Compound **3m** was prepared according to the general procedure. Yellow solid; **m.p.**: 81-83 °C; **¹H NMR (400 MHz, CDCl₃)** δ 4.51-4.47 (m, 2H), 4.33 (s, 5H), 4.24 (t, *J* = 2.2 Hz, 1H), 3.93 (s, 4H), 3.37-3.51 (m, 4H), 1.77-1.58 (m, 4H), 1.12 (s, 21H); **¹³C NMR (101 MHz, CDCl₃)** δ 167.1, 107.1, 104.0, 89.5, 86.8, 72.1, 71.6, 71.3, 68.0, 64.3, 64.1, 40.4, 34.5, 18.7, 11.2; **HRMS (ESI)**: *m/z* calculated for C₂₉H₄₂FeNO₃Si⁺ [M+H]⁺: 536.2278, found: 536.2272.

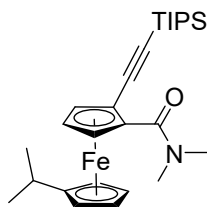
2-Triisopropylsilylethynyl-(azepane-1-carbonyl)ferrocene (**3n**):



3n

Compound **3n** was prepared according to the general procedure. Yellow solid; **m.p.**: 79-81 °C; **¹H NMR (400 MHz, CDCl₃)** δ 4.46-4.44 (m, 2H), 4.34 (s, 5H), 4.20 (s, 1H), 3.90-3.87 (m, 1H), 3.43-3.39 (m, 1H), 3.24-3.19 (m, 2H), 1.83-1.72 (m, 3H), 1.61-1.52 (m, 3H), 1.42-1.34 (m, 2H), 1.10 (s, 21H); **¹³C NMR (101 MHz, CDCl₃)** δ 167.9, 104.2, 89.1, 72.0, 70.9, 70.6, 67.5, 64.1, 49.3, 46.5, 29.1, 27.8, 27.1, 26.3, 18.7, 11.2; **HRMS (ESI)**: *m/z* calculated for C₂₈H₄₂FeNOSi⁺ [M+H]⁺: 492.2380, found: 492.2382.

2-Triisopropylsilylethynyl-(dimethyl-1-carbonyl)-1'-isopropyl-ferrocene (**3o**):

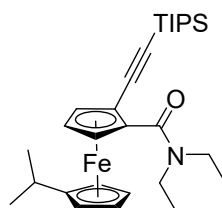


3o

Compound **3o** was prepared according to the general procedure. Yellow oil; **¹H NMR (400 MHz, CDCl₃)** δ 4.49 (s, 1H), 4.37 (s, 1H), 4.30 (s, 1H), 4.25 (s, 1H), 4.23-4.18

(m, 2H), 4.16 (s, 1H), 2.98-2.90 (m, 6H), 2.77-2.70 (m, 1H), 1.17-1.16 (m, 6H), 1.10 (s, 21H); ^{13}C NMR (101 MHz, CDCl_3) δ 168.9, 104.3, 98.7, 89.4, 87.0, 72.6, 72.2, 71.9, 71.7, 70.8, 68.9, 68.5, 64.1, 38.8, 35.5, 26.6, 23.6, 23.5, 18.7, 11.9. **HRMS (ESI)**: m/z calculated for $\text{C}_{27}\text{H}_{42}\text{FeNOSi}^+ [\text{M}+\text{H}]^+$: 480.2380, found: 480.2382.

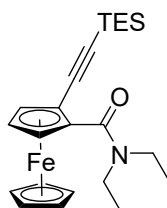
2-Triisopropylsilylethynyl-(diethyl-1-carbonyl)-1'-ispropyl-ferrocene (3p):



3p

Compound **3p** was prepared according to the general procedure. Yellow oil; ^1H NMR (400 MHz, CDCl_3) δ 4.40 (s, 1H), 4.38-4.35 (s, 2H), 4.28 (s, 1H), 4.23-4.21 (m, 2H), 4.17-4.16 (m, 1H), 3.64-3.04 (m, 4H), 2.74 (dt, $J = 13.7, 6.8$ Hz, 1H), 1.18-1.16 (m, 12H), 1.11-1.10 (m, 21H); ^{13}C NMR (101 MHz, CDCl_3) δ 167.3, 104.0, 98.6, 89.3, 88.6, 72.5, 71.9, 71.4, 70.9, 70.6, 68.5, 68.0, 64.6, 43.2, 40.1, 29.7, 26.6, 23.6, 18.7, 14.3, 13.2, 11.3; **HRMS (ESI)**: m/z calculated for $\text{C}_{29}\text{H}_{46}\text{FeNOSi}^+ [\text{M}+\text{H}]^+$: 508.2693, found: 508.2689.

2-Triethylsilylethynyl-(diethyl-1-carbonyl)ferrocene (4a):

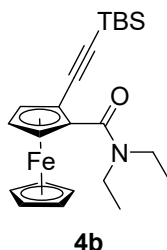


4a

Compound **4a** was prepared according to the general procedure. Yellow solid; **m.p.**: 60-62 °C; ^1H NMR (400 MHz, CDCl_3) δ 4.45-4.43 (m, 2H), 4.33 (s, 5H), 4.20 (t, $J = 2.3$ Hz, 1H), 3.68-3.65 (m, 1H), 3.29-3.07 (m, 3H), 1.04-1.00 (m, 9H), 0.65-0.59 (m, 6H); ^{13}C NMR (101 MHz, CDCl_3) δ 167.2, 103.5, 90.4, 89.0, 72.1, 70.9, 70.5, 67.6,

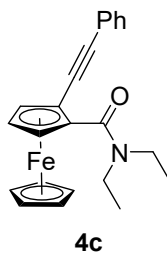
64.0, 43.1, 39.8, 14.2, 13.0, 7.6, 4.5; **HRMS (ESI):** m/z calculated for $C_{23}H_{34}FeNOSi^+$ $[M+H]^+$: 424.1754, found: 424.1750.

2-tert-butylsilyl-ethynyl-(diethyl-1-carbonyl)ferrocene (4b):



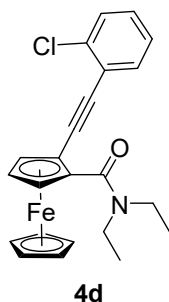
Compound **4b** was prepared according to the general procedure. Yellow solid; **m.p.:** 60-62 °C; **1H NMR (400 MHz, $CDCl_3$)** δ 4.45-4.43 (m, 2H), 4.34 (s, 5H), 4.20 (s, 1H), 3.65-3.08 (m, 4H), 1.25-1.10 (m, 6H), 0.97 (s, 9H), 0.14-0.12 (m, 6H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 167.1, 102.9, 91.3, 89.0, 72.0, 70.9, 70.4, 67.5, 63.9, 43.1, 39.8, 26.1, 18.7, 16.5, 14.2, 13.1; **HRMS (ESI):** m/z calculated for $C_{23}H_{34}FeNOSi^+$ $[M+H]^+$: 424.1754, found: 424.1748.

2-phenylethynyl-(diethyl-1-carbonyl)ferrocene (4c):



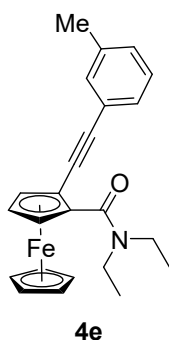
Compound **4c** was prepared according to the general procedure. Yellow solid; **m.p.:** 104-106 °C; **1H NMR (400 MHz, $CDCl_3$)** δ 7.46-7.44 (m, 2H), 7.32-7.31 (m, 3H), 4.52 (s, 2H), 4.39 (s, 5H), 4.28 (s, 1H), 3.76-3.72 (m, 1H), 3.30-3.19 (m, 3H), 1.25 (s, 6H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 167.3, 131.3, 128.3, 127.8, 123.7, 88.2, 88.0, 86.7, 71.9, 70.5, 70.3, 67.7, 64.6, 42.9, 39.6, 14.2, 13.0; **HRMS (ESI):** m/z calculated for $C_{23}H_{24}FeNO^+$ $[M+H]^+$: 386.1202, found: 386.1208.

2-(2-chlorophenyl)ethynyl-(diethyl-1-carbonyl)ferrocene (4d):



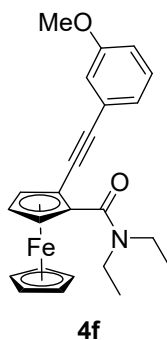
Compound **4d** was prepared according to the general procedure. Yellow solid; **m.p.**: 115-117 °C; **¹H NMR (400 MHz, CDCl₃)** δ 7.48 (d, *J* = 6.3 Hz, 1H), 7.40 (d, *J* = 7.0 Hz, 1H), 7.39-7.20 (m, 2H), 4.55 (s, 2H), 4.41 (s, 5H), 4.30 (s, 1H), 3.67-3.65 (m, 1H), 3.34-3.20 (m, 3H), 1.25-1.20 (m, 6H); **¹³C NMR (101 MHz, CDCl₃)** δ 167.2, 135.4, 1330, 129.2, 128.7, 126.4, 123.6, 92.3, 88.4, 84.5, 72.0, 70.9, 70.6, 68.0, 63.9, 39.8, 29.7, 14.2, 13.0; **HRMS (ESI)**: *m/z* calculated for C₂₃H₂₃ClFeNO⁺ [M+H]⁺: 420.0812, found: 420.0805.

2-(*m*-tolylethynyl)ethynyl-(diethyl-1-carbonyl)ferrocene (4e):



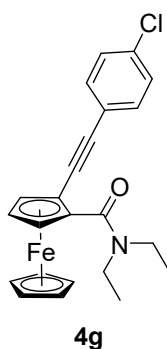
Compound **4e** was prepared according to the general procedure. Yellow solid; **m.p.**: 109-111 °C; **¹H NMR (400 MHz, CDCl₃)** δ 7.30-7.28 (m, 2H), 7.22 (t, *J* = 7.5 Hz, 1H), 7.13 (d, *J* = 7.3 Hz, 1H), 4.52 (s, 2H), 4.41 (s, 5H), 4.29 (s, 1H), 3.77-3.75 (m, 1H), 3.31-3.21 (m, 3H), 2.36 (s, 3H), 1.24-1.03 (m, 6H); **¹³C NMR (101 MHz, CDCl₃)** δ 167.4, 138.0, 131.9, 128.7, 128.3, 128.2, 123.5, 88.2, 88.1, 86.3, 71.9, 70.5, 70.2, 67.7, 64.7, 39.6, 29.7, 21.2, 14.1, 13.0; **HRMS (ESI)**: *m/z* calculated for C₂₄H₂₆FeNO⁺ [M+H]⁺: 400.1358, found: 400.1350.

2-(3-methoxyphenyl)ethynyl-(diethyl-1-carbonyl)ferrocene (4f):



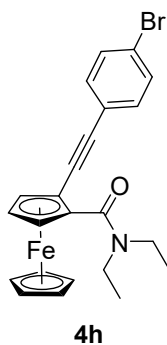
Compound **4f** was prepared according to the general procedure. Yellow solid; **m.p.**: 108-110 °C; **¹H NMR (400 MHz, CDCl₃)** δ 7.22-7.20 (m, 1H), 7.05-6.97 (m, 2H), 6.87 (d, *J* = 6.6 Hz, 1H), 4.52-4.28 (m, 8H), 3.81-3.70 (m, 4H), 3.28-3.19 (m, 3H), 1.25-1.23 (m, 6H); **¹³C NMR (101 MHz, CDCl₃)** δ 167.4, 159.3, 129.3, 124.7, 123.9, 116.0, 114.4, 88.2, 87.9, 86.6, 71.9, 70.5, 70.3, 67.7, 64.5, 55.3, 43.0, 39.6, 14.1, 13.1; **HRMS (ESI)**: *m/z* calculated for C₂₄H₂₆FeNO₂⁺ [M+H]⁺: 416.1307, found: 416.1301.

2-(4-chlorophenyl)ethynyl-(diethyl-1-carbonyl)ferrocene (4g):



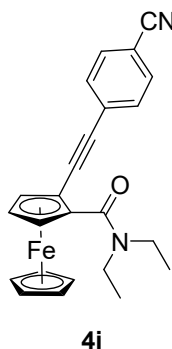
Compound **4g** was prepared according to the general procedure. Yellow solid; **m.p.**: 117-119 °C; **¹H NMR (400 MHz, CDCl₃)** δ 7.38-7.36 (m, 2H), 7.29-7.27 (m, 2H), 4.51-4.50 (m, 2H), 4.39 (s, 5H), 4.28 (t, *J* = 2.4 Hz, 1H), 3.73-3.69 (m, 1H), 3.28-3.17 (m, 3H), 1.25-1.20 (m, 6H); **¹³C NMR (101 MHz, CDCl₃)** δ 167.2, 133.7, 132.5, 128.6, 122.2, 88.2, 87.9, 86.8, 71.9, 70.6, 70.1, 67.8, 64.4, 39.6, 14.1; **HRMS (ESI)**: *m/z* calculated for C₂₃H₂₃ClFeNO⁺ [M+H]⁺: 420.0812, found: 420.0808.

2-(4-bromophenyl)ethynyl-(diethyl-1-carbonyl)ferrocene (4h):



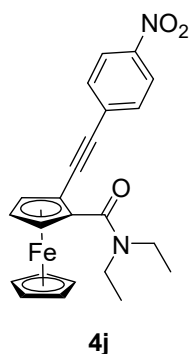
Compound **4h** was prepared according to the general procedure. Yellow solid; **m.p.:** 115-117 °C; **¹H NMR (400 MHz, CDCl₃)** δ 7.45-7.43 (m, 2H), 7.31-7.29 (m, 2H), 4.51-4.50 (m, 2H), 4.38 (s, 5H), 4.28 (s, 1H), 3.73-3.71 (m, 1H), 3.28-3.18 (m, 3H), 1.25-1.20 (m, 6H); **¹³C NMR (101 MHz, CDCl₃)** δ 167.2, 132.7, 131.5, 122.7, 121.8, 88.2, 88.1, 86.9, 71.9, 70.6, 70.1, 67.8, 64.4, 39.6, 29.7, 14.2, 13.0; **HRMS (ESI):** m/z calculated for C₂₃H₂₃BrFeNO⁺ [M+H]⁺: 464.0307, found: 464.0301.

2-(4-cyanophenyl)ethynyl-(diethyl-1-carbonyl)ferrocene (4i):



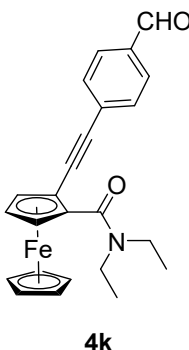
Compound **4i** was prepared according to the general procedure. Yellow solid; **m.p.:** 110-112 °C; **¹H NMR (400 MHz, CDCl₃)** δ 7.60-7.58 (m, 2H), 7.51-7.49 (m, 2H), 4.54 (s, 2H), 4.39 (s, 5H), 4.33 (s, 1H), 3.73-3.70 (m, 1H), 3.29-3.17 (m, 3H), 1.25-1.21 (m, 6H); **¹³C NMR (101 MHz, CDCl₃)** δ 167.0, 132.0, 131.6, 128.7, 118.7, 110.7, 92.3, 88.3, 86.5, 72.0, 70.9, 70.3, 69.7, 68.3, 63.7, 43.0, 39.7, 14.3, 13.0; **HRMS (ESI):** m/z calculated for C₂₄H₂₃FeN₂O⁺ [M+H]⁺: 411.1154, found: 411.1142.

2-(4-nitrophenyl)ethynyl-(diethyl-1-carbonyl)ferrocene (4j):



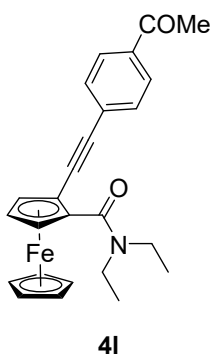
Compound **4j** was prepared according to the general procedure. Yellow solid; **m.p.:** 107-109 °C; **¹H NMR (400 MHz, CDCl₃)** δ 8.28-8.27 (m, 1H), 8.16-8.13 (m, 1H), 7.76 (d, *J* = 7.7 Hz, 1H), 7.51 (t, *J* = 8.0 Hz, 1H), 4.57-4.54 (m, 2H), 4.41 (s, 5H), 4.35 (t, *J* = 2.5 Hz, 1H), 3.73-3.71 (m, 1H), 3.30-3.21 (m, 3H), 1.25-1.23 (m, 6H); **¹³C NMR (101 MHz, CDCl₃)** δ 167.0, 148.1, 136.9, 129.3, 126.0, 125.6, 122.3, 90.1, 88.7, 85.6, 72.0, 70.9, 70.2, 68.2, 63.7, 43.0, 39.1, 14.2, 13.1; **HRMS (ESI):** *m/z* calculated for C₂₃H₂₃FeN₂O₃⁺ [M+H]⁺: 431.1053, found: 431.1059.

2-(4-formylphenyl)ethynyl-(diethyl-1-carbonyl)ferrocene (4k):



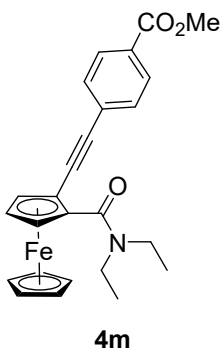
Compound **4k** was prepared according to the general procedure. Yellow solid; **m.p.:** 97-99 °C; **¹H NMR (400 MHz, CDCl₃)** δ 10.00 (s, 1H), 7.84-7.82 (m, 2H), 7.59-7.57 (m, 2H), 4.55-4.54 (m, 2H), 4.40 (s, 5H), 4.33 (s, 1H), 3.76-3.71 (m, 1H), 3.29-3.20 (m, 3H), 1.25-1.23 (m, 6H); **¹³C NMR (101 MHz, CDCl₃)** δ 191.4, 167.1, 134.9, 131.7, 130.1, 129.6, 91.9, 88.4, 87.4, 72.0, 70.9, 70.4, 68.2, 63.9, 43.1, 39.7, 14.2, 13.1; **HRMS (ESI):** *m/z* calculated for C₂₄H₂₄FeNO₂⁺ [M+H]⁺: 414.1151, found: 414.1144.

2-(4-acetylphenyl)ethynyl-(diethyl-1-carbonyl)ferrocene (4l):



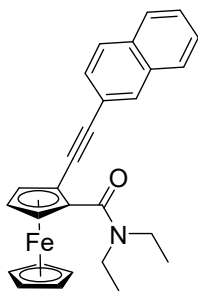
Compound **4l** was prepared according to the general procedure. Yellow solid; **m.p.**: 98-100 °C; **¹H NMR (400 MHz, CDCl₃)** δ 7.91-7.89 (m, 2H), 7.52-7.50 (m, 2H), 4.54-4.53 (m, 2H), 4.40 (s, 5H), 4.32 (t, *J* = 2.4 Hz, 1H), 3.75-3.73 (m, 1H), 3.29-3.19 (m, 3H), 2.60 (s, 3H), 1.25-1.21 (m, 6H); **¹³C NMR (101 MHz, CDCl₃)** δ 197.3, 167.1, 135.6, 131.3, 128.7, 128.3, 90.9, 88.4, 87.4, 72.0, 70.8, 70.3, 68.1, 64.0, 43.0, 39.6, 26.6, 14.2, 13.0; **HRMS (ESI)**: *m/z* calculated for C₂₅H₂₆FeNO₂⁺ [M+H]⁺: 428.1307, found: 428.1295.

2-(4-methyl benzoate)ethynyl-(diethyl-1-carbonyl)ferrocene (4m):



Compound **4m** was prepared according to the general procedure. Yellow solid; **m.p.**: 103-105 °C; **¹H NMR (400 MHz, CDCl₃)** δ 7.99-7.97 (m, 2H), 7.50-7.48 (m, 2H), 4.54-4.53 (m, 2H), 4.40 (s, 5H), 4.31 (t, *J* = 2.3 Hz, 1H), 3.92 (s, 3H), 3.75-3.72 (m, 1H), 3.28-3.18 (m, 3H), 1.25-1.22 (m, 6H); **¹³C NMR (101 MHz, CDCl₃)** δ 167.1, 166.6, 131.1, 129.5, 128.9, 128.5, 90.4, 88.4, 87.4, 72.0, 70.8, 70.3, 68.1, 68.0, 64.1, 52.2, 39.7, 38.7, 14.0, 13.1; **HRMS (ESI)**: *m/z* calculated for C₂₅H₂₆FeNO₃⁺ [M+H]⁺: 444.1257, found: 444.1249.

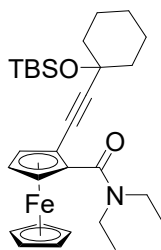
2-(naphthalen-2-ylethynyl)-(diethyl-1-carbonyl)ferrocene (4n):



4n

Compound **4n** was prepared according to the general procedure. Yellow solid; **m.p.:** 94-96 °C; **¹H NMR (400 MHz, CDCl₃)** δ 7.97 (s, 1H), 7.82-7.77 (m, 3H), 7.51-7.47 (m, 3H), 4.56-4.54 (m, 2H), 4.42 (s, 5H), 4.30 (t, *J* = 2.4 Hz, 1H), 3.81-3.75 (m, 1H), 3.32-3.22 (m, 3H), 1.25 (s, 6H); **¹³C NMR (101 MHz, CDCl₃)** δ 167.4, 133.0, 132.5, 130.9, 128.3, 128.0, 127.8, 127.6, 126.5, 126.4, 121.0, 88.4, 88.3, 87.2, 71.9, 70.6, 70.2, 67.7, 64.7, 43.1, 39.6, 14.1, 13.1; **HRMS (ESI):** *m/z* calculated for C₂₇H₂₆FeNO⁺ [M+H]⁺: 436.1358, found: 436.1351.

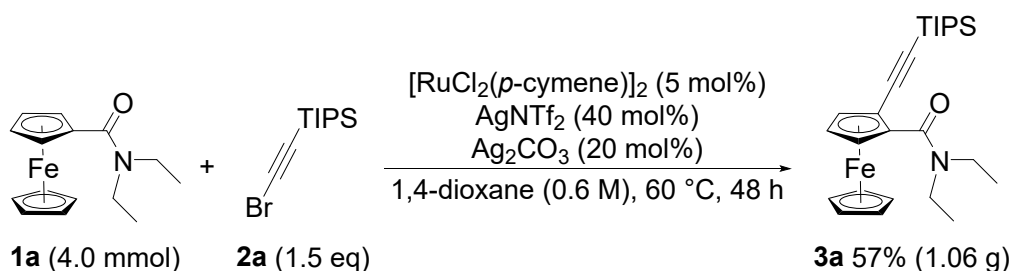
2-((1-((tert-butyldimethylsilyl)oxy)cyclohexyl)ethynyl)-(diethyl-1-carbonyl)ferrocene (4o):



4o

Compound **4o** was prepared according to the general procedure. Yellow oil; **¹H NMR (500 MHz, CDCl₃)** δ 4.45 (s, 1H), 4.39 (s, 1H), 4.34 (s, 5H), 4.20 (s, 1H), 3.71-3.70 (m, 1H), 3.26-3.13 (m, 3H), 2.16-2.01 (m, 5H), 1.65-1.59 (m, 7H), 1.45-1.19 (m, 12H), 1.04-0.98 (m, 4H), 0.93-0.91 (m, 3H); **¹³C NMR (126 MHz, CDCl₃)** δ 167.8, 89.9, 88.1, 83.6, 71.8, 70.4, 70.0, 68.2, 67.4, 65.5, 43.0, 39.5, 38.8, 30.4, 29.4, 29.0, 25.7, 23.8, 23.0, 22.4, 21.6, 14.1, 13.0; **HRMS (ESI):** *m/z* calculated for C₂₉H₄₃FeNNaO₂Si [M+Na]⁺: 544.2305, found: 544.2304.

(C) Gram-Scale Reaction



To a dried screw-capped vial, **1a** (4.0 mmol), **2a** (6.0 mmol), $[\text{RuCl}_2(p\text{-cymene})]_2$ (120.8 mg, 0.2 mmol), AgNTf_2 (640.0 mg, 1.6 mmol), Ag_2CO_3 (220.0 mg, 0.8 mmol) and 1,4-dioxane (6.7 mL) were added under Ar atmosphere. The vial was capped, and the mixture was heated at 60 °C for 48 h with stirring. The resulting mixture was cooled to room temperature, and directly purified by silica gel column chromatography to give the desired products **3a** in 57% yield (1.06 g).

(D) Synthetic Utilizations

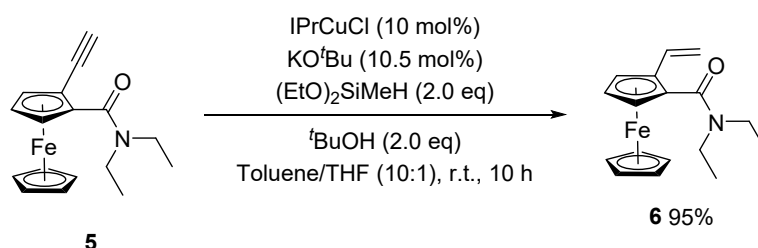
(a) 2-Ethynyl-(diethyl-1-carbonyl)ferrocene (**5**):



Reaction was carried out in an oven-dried flask under an argon atmosphere. To a solution of **3a** (93.1 mg, 0.2 mmol, 1.0 eq) in THF (6 mL) was added TBAF (1 M in THF, 200 μL , 0.20 mmol, 1.0 eq) dropwise at r.t., and the reaction was stirred for 30 min. Saturated NH_4Cl (10 mL) was then added, and the mixture was extracted with EA (10 mL \times 2). The combined organic layer was washed with brine, dried over anhydrous Na_2SO_4 , and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (hexane/ethyl acetate, 10:1) to afford **5** as a yellow solid (60.6 mg, 98% yield); **m.p.**: 97-99 °C; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 4.48-4.43 (m, 2H), 4.35 (s, 5H), 4.22 (s, 1H), 3.62-3.61 (m, 1H), 3.33-3.19 (m, 3H), 2.81 (s, 1H), 1.18-1.01 (m, 6H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 167.1, 88.0,

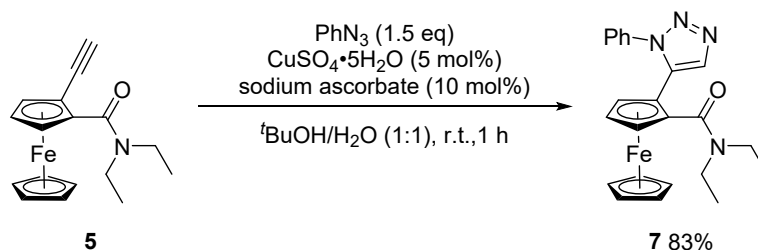
80.8, 75.9, 71.9, 71.2, 69.6, 67.6, 64.0, 42.9, 39.6, 14.2, 12.9; **HRMS (ESI):** m/z calculated for $C_{17}H_{20}FeNO^+$ $[M+H]^+$: 310.0889, found: 310.0883.

(b) 2-vinyl-(diethyl-1-carbonyl)ferrocene (6):



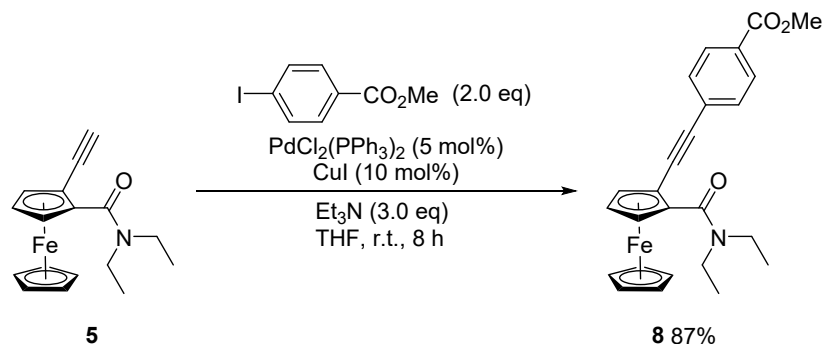
IPrCuCl (5.0 mg, 0.01 mmol) and aqueous potassium *tert*-butoxide (1.2 mg, 0.0105 mmol) were dissolved in THF (0.1 mL), and the mixture was stirred using a magnetic stirrer at room temperature under argon atmosphere for 15 min before adding a solution of **5** (31.0 mg, 0.1 mmol), *tert*-butanol (18.6 μ L, 0.2 mmol) and (EtO)₂MeSiH (22.4 μ L, 0.2 mmol) in toluene (1 mL). The reaction mixture was allowed to stir at ambient temperature for 10 h. The mixture was concentrate under vacuo and purified by flash column chromatography (hexane/ethyl acetate, 10:1) to afford **6** as a yellow solid (29.6 mg, 95% yield); **m.p.**: 99-101 °C; **¹H NMR (400 MHz, CDCl₃)** δ 6.58 (dd, $J = 17.3, 11.0$ Hz, 1H), 5.36 (d, $J = 17.5$ Hz, 1H), 5.07 (d, $J = 10.7$ Hz, 1H), 4.48 (s, 1H), 4.37 (s, 1H), 4.23 (s, 6H), 3.60-3.58 (m, 1H), 3.29-3.15 (m, 3H), 1.24-1.17 (m, 6H). **¹³C NMR (101 MHz, CDCl₃)** δ 168.4, 133.1, 112.1, 84.7, 83.1, 71.0, 68.8, 67.2, 64.4, 42.9, 39.6, 23.8, 23.6, 14.1, 12.9; **HRMS (ESI):** m/z calculated for $C_{17}H_{22}FeNO^+$ $[M+H]^+$: 312.1045, found: 312.1031.

(c) 2-(1-phenyl-1H-1,2,3-triazol-5-yl)-(diethyl-1-carbonyl)ferrocene (7):



5 (31.0 mg, 0.1 mmol) was dissolved in *tert*-butanol (0.5 mL) and H₂O (0.5 mL) 1:1. Add CuSO₄·5H₂O (0.8 mg, 0.005 mmol) and sodium ascorbate (1.98 mg, 0.01 mmol) to the solution. Stir the solution for 10 min and add PhN₃ (18 μL, 0.15 mmol), stir the react for 1 h at room temperature. At the end of reaction, added water and extracted with EA. The extract was washed with saturated sodium chloride solution, dried over anhydrous Na₂SO₄, and separated by column chromatography (hexane/ethyl acetate, 2:1) to afford **7** as a yellow solid (35.6 mg, 83% yield); **m.p.**: 119-121 °C; **¹H NMR (400 MHz, CDCl₃)** δ 8.28 (s, 1H), 7.78-7.76 (m, 2H), 7.54-7.51 (m, 2H), 7.43 (t, *J* = 7.3 Hz, 1H), 5.12 (s, 1H), 4.46 (s, 1H), 4.36 (s, 1H), 4.23 (s, 5H), 3.66-3.65 (m, 1H), 3.31-3.10 (m, 3H), 1.25-1.20 (m, 6H). **¹³C NMR (101 MHz, CDCl₃)** δ 168.6, 145.9, 137.1, 129.7, 128.5, 120.3, 118.6, 83.7, 76.0, 71.5, 67.9, 67.5, 67.3, 43.2, 40.0, 14.0, 13.1; **HRMS (ESI)**: *m/z* calculated for C₂₃H₂₅FeN₄O⁺ [M+H]⁺: 429.1372, found: 429.1333.

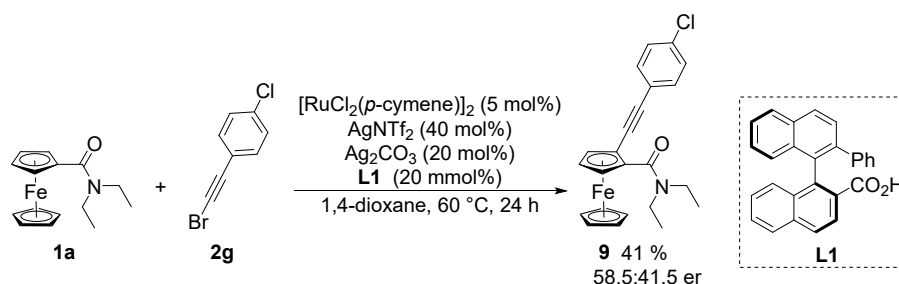
(d) 2-(4-methyl benzoate)ethynyl-(diethyl-1-carbonyl)ferrocene (8**):**



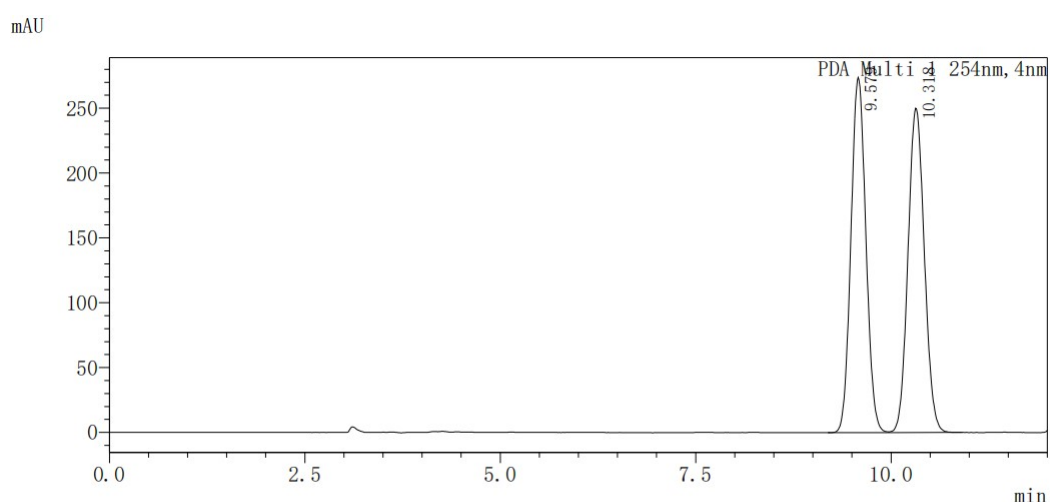
4-Iodobenzoic acid methyl ester (52.4 mg, 0.2 mmol) and **5** (31.0 mg, 0.1 mmol) were dissolved in THF (1.0 mL), and Et₃N (21.0 μL, 0.3 mmol), Pd(PPh₃)₂Cl₂ (3.6 mg, 0.005 mmol) and CuI (2.0 mg, 0.01 mmol) were added. The mixture was stirred at room temperature for 8 h. At the end of reaction, added water and extracted with EA. The extract was washed with saturated sodium chloride solution, dried over anhydrous Na₂SO₄, and separated by column chromatography (hexane/ethyl acetate, 5:1) to afford **8** as a yellow solid (38.6 mg, 87% yield); **m.p.**: 103-105 °C; **¹H NMR (400 MHz, CDCl₃)** δ 7.99-7.97 (m, 2H), 7.50-7.48 (m, 2H), 4.54-4.53 (m, 2H), 4.40 (s, 5H), 4.31 (t, *J* = 2.3 Hz, 1H), 3.92 (s, 3H), 3.75-3.72 (m, 1H), 3.28-3.18 (m, 3H),

1.25-1.22 (m, 6H); ^{13}C NMR (101 MHz, CDCl_3) δ 167.1, 166.6, 131.1, 129.5, 128.9, 128.5, 90.4, 88.4, 87.4, 72.0, 70.8, 70.3, 68.1, 68.0, 64.1, 52.2, 39.7, 38.7, 14.0, 13.1; HRMS (ESI): m/z calculated for $\text{C}_{25}\text{H}_{26}\text{FeNO}_3^+ [\text{M}+\text{H}]^+$: 444.1257, found: 444.1249.

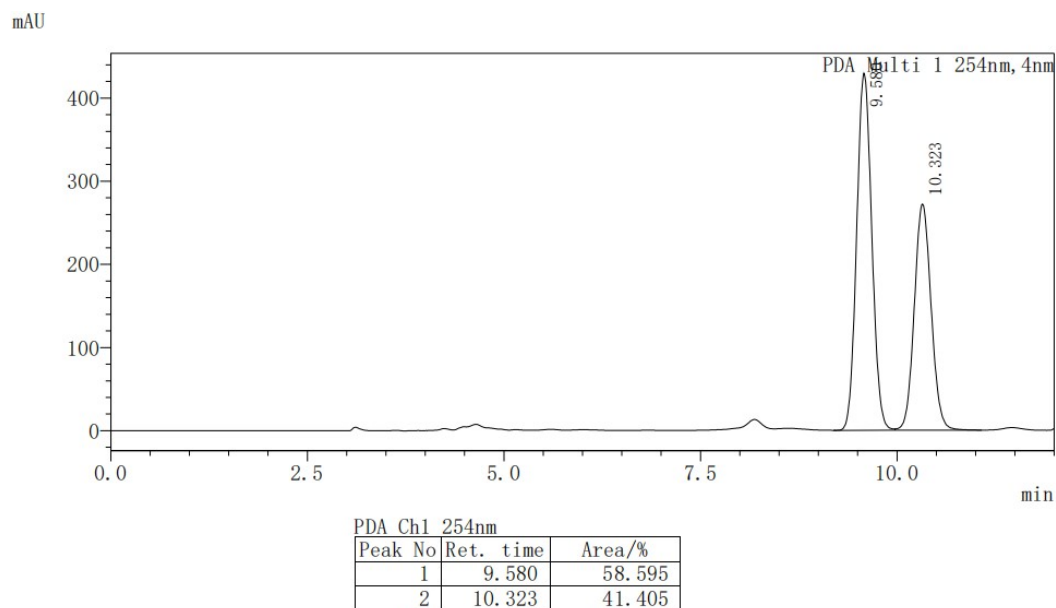
(E) Enantioselective C-H Alkynylation of Ferrocene



To a dried screw-capped vial, **1a** (14.2 mg, 0.05 mmol), **2g** (16.2 mg, 0.075 mmol), $[\text{RuCl}_2(p\text{-cymene})]_2$ (1.51 mg, 0.0025 mmol), AgNTf_2 (8.0 mg, 0.02 mmol), Ag_2CO_3 (2.75 mg, 0.01 mmol), **L1** (3.74 mg, 0.01 mmol) and 1,4-dioxane (0.125 mL) were added under Ar atmosphere. The vial was capped, and the mixture was heated at 60 °C for 24 h with stirring. The resulting mixture was cooled to room temperature, and directly purified by silica gel column chromatography to give the alkynylated ferrocenecarboxamide product **9** (21.0 mg, 41% yield). HPLC separation (DAICEL CHIRALPAK AD-H, hexane:2-propanol = 95:5, flow rate: 1.0 mL/min, detection at 254nm): $t_{\text{R}}(\text{major}) = 9.6$ min, $t_{\text{R}}(\text{minor}) = 10.3$ min, 58.5:41.5 er.



PDA Ch1 254nm		
Peak No	Ret. time	Area/%
1	9.579	49.947
2	10.318	50.053

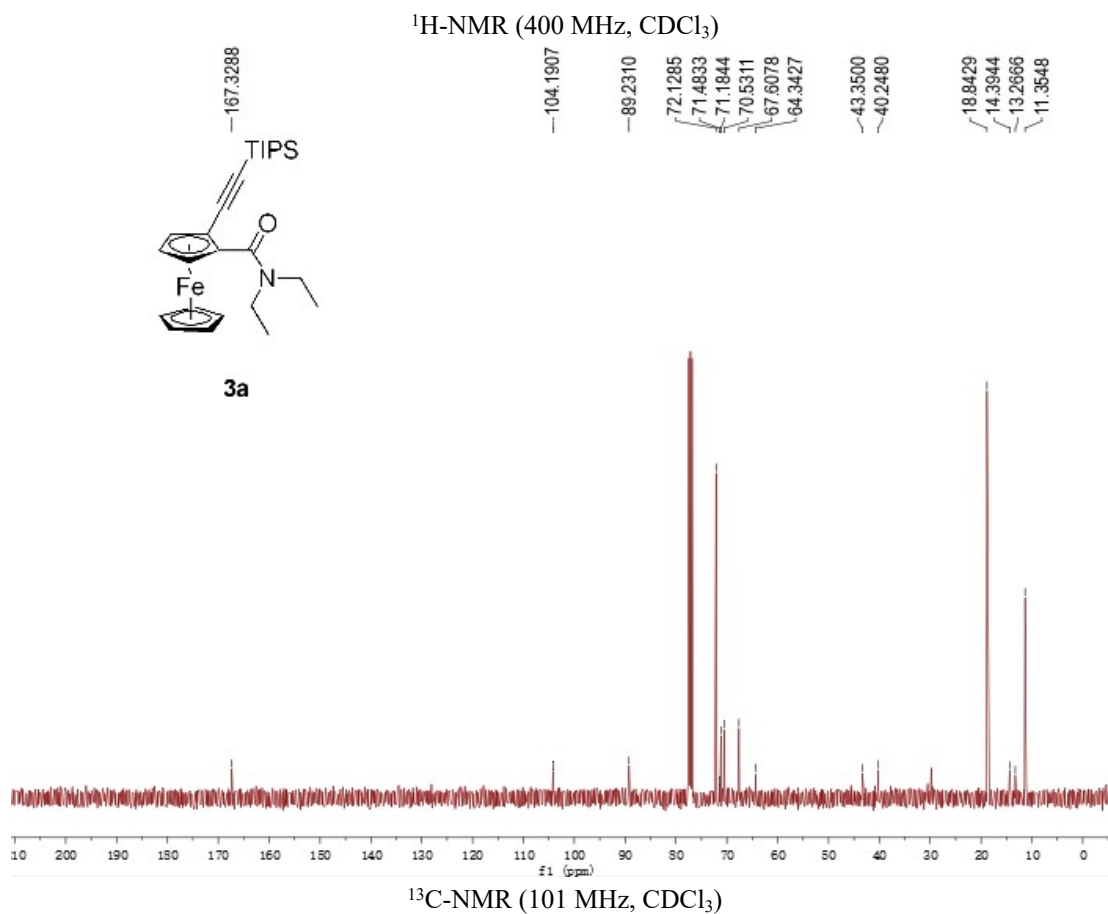
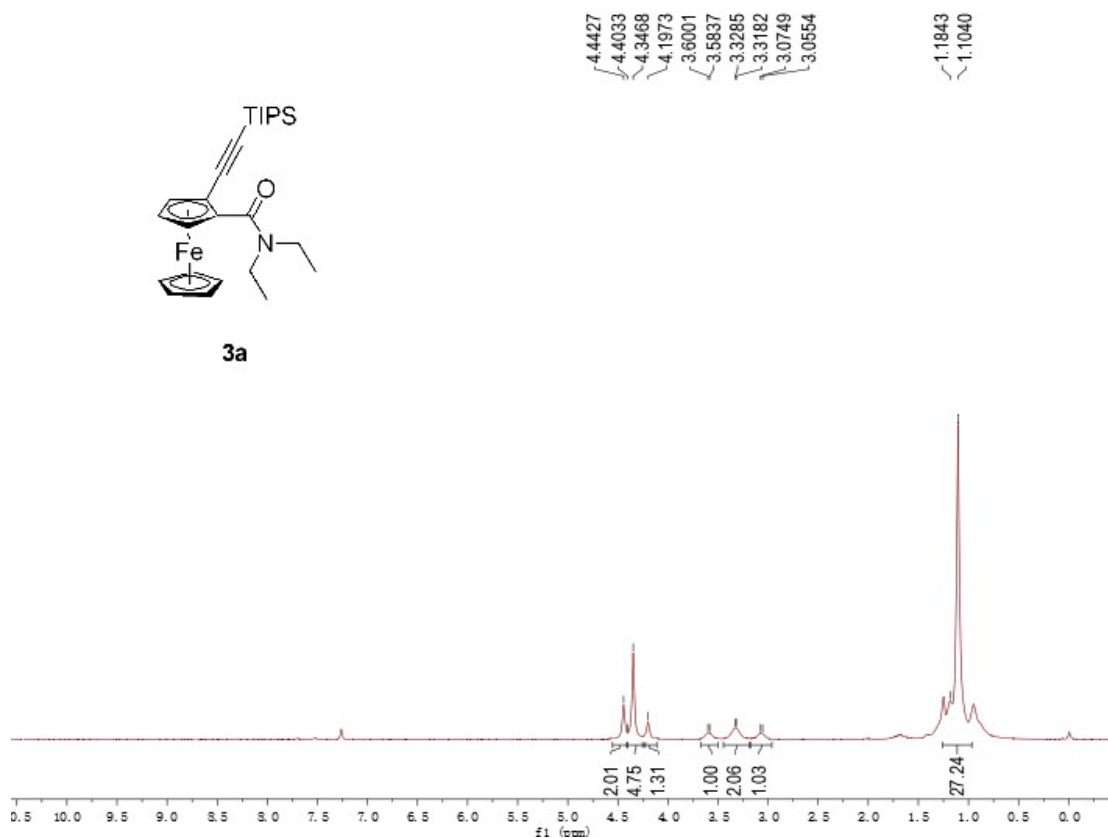


(F) References

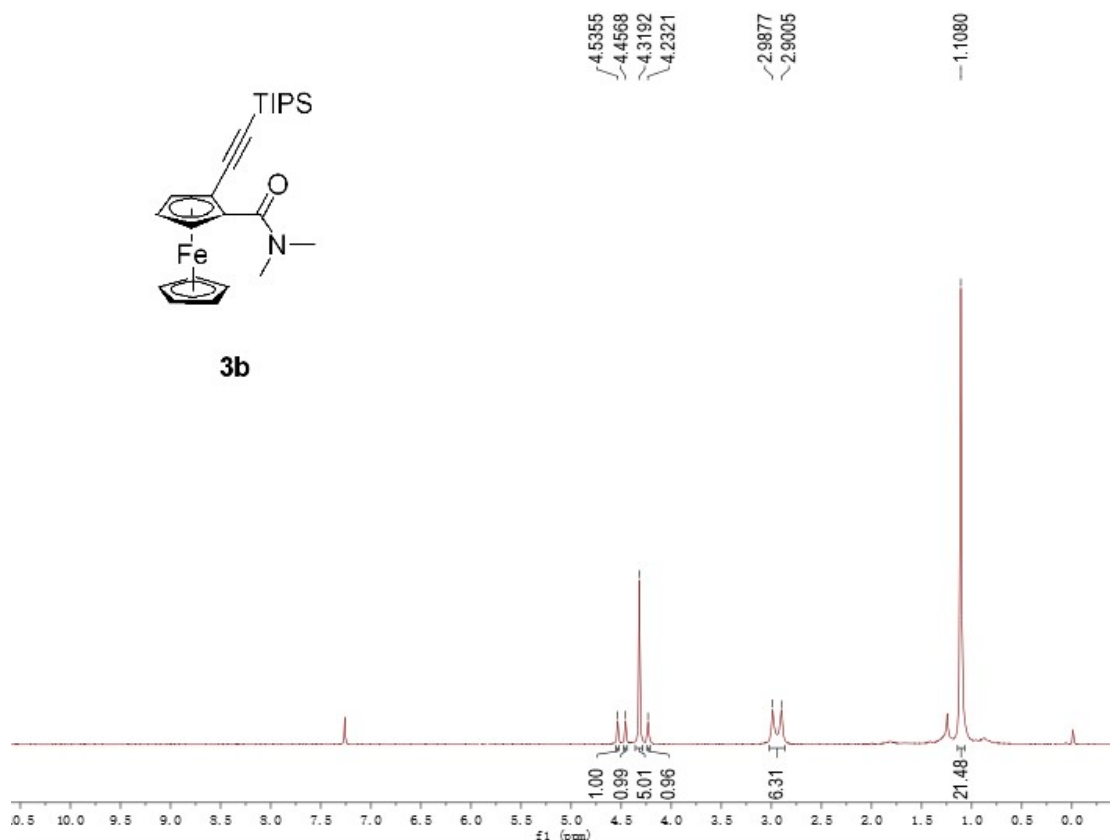
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- [S7] S. R. Mudshinge, Y.-H. Yang, B. Xu, G. B. Hammond, Z.-C. Lu, *Angew. Chem. Int. Ed.*, 2022, **61**, e202115687.
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(G) NMR Spectra

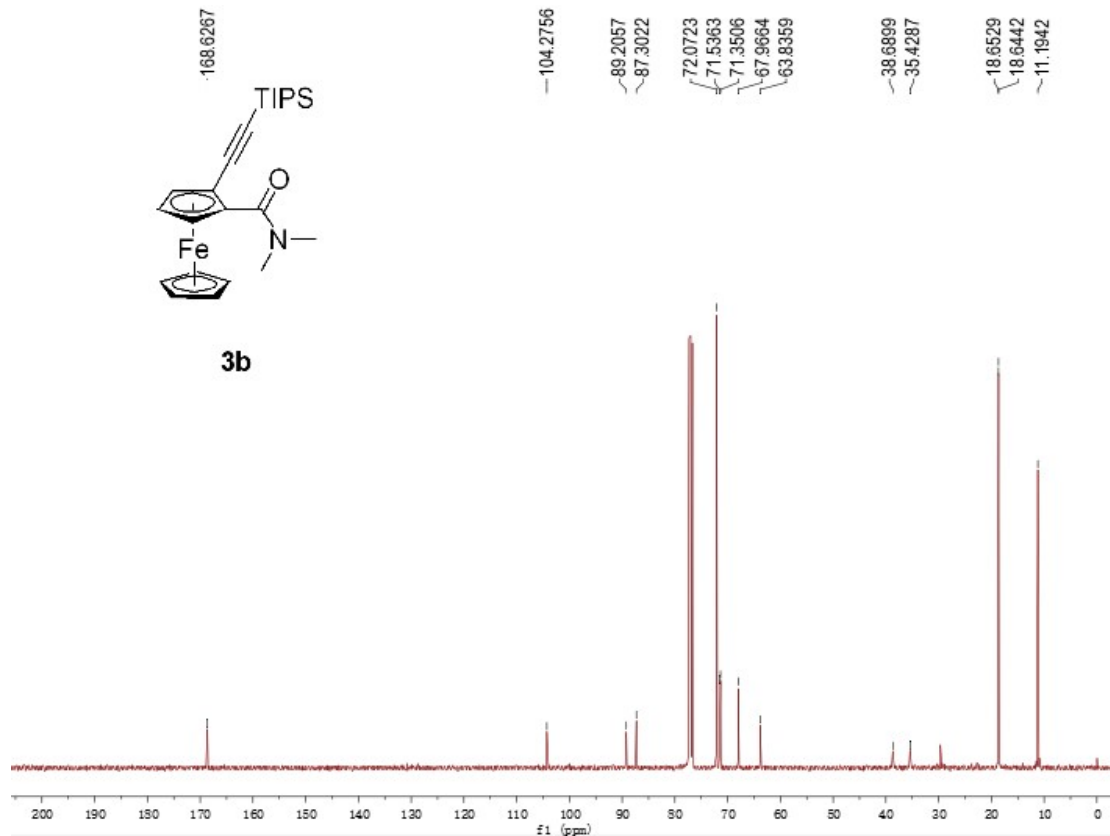
2-Triisopropylsilyl ethynyl-(diethyl-1-carbonyl)ferrocene (**3a**):



2-Triisopropylsilylethynyl-(dimethyl-1-carbonyl)ferrocene (3b):

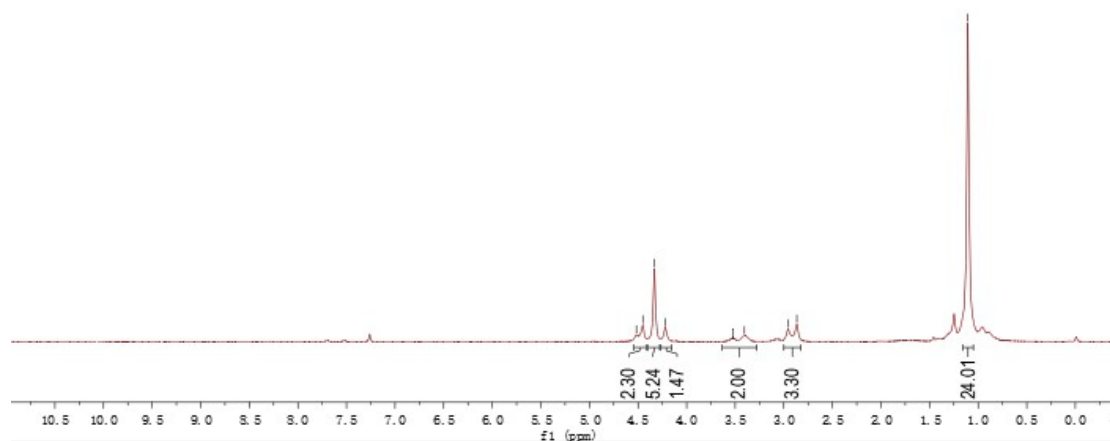


¹H-NMR (400 MHz, CDCl₃)

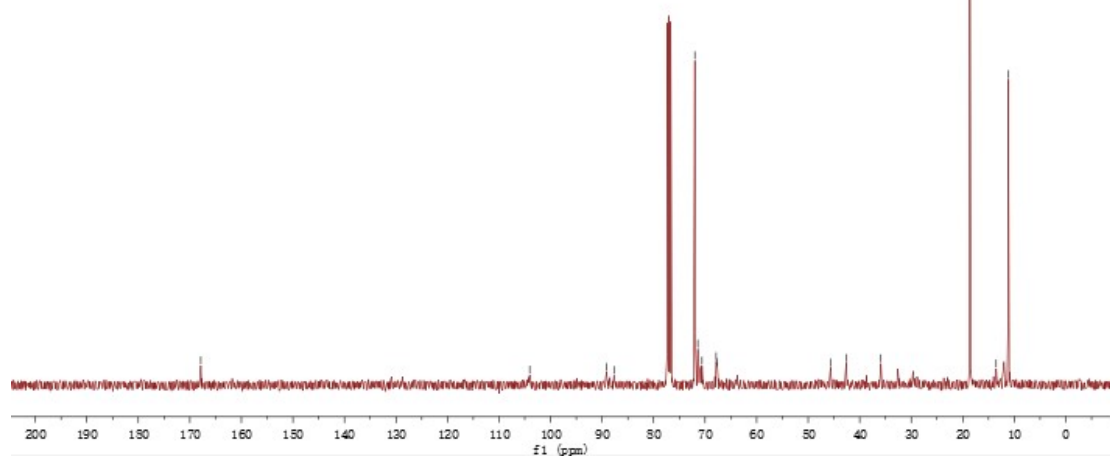


¹³C-NMR (101 MHz, CDCl₃)

2-Triisopropylsilylethynyl-(methyl-ethyl-1-carbonyl)ferrocene (3c):

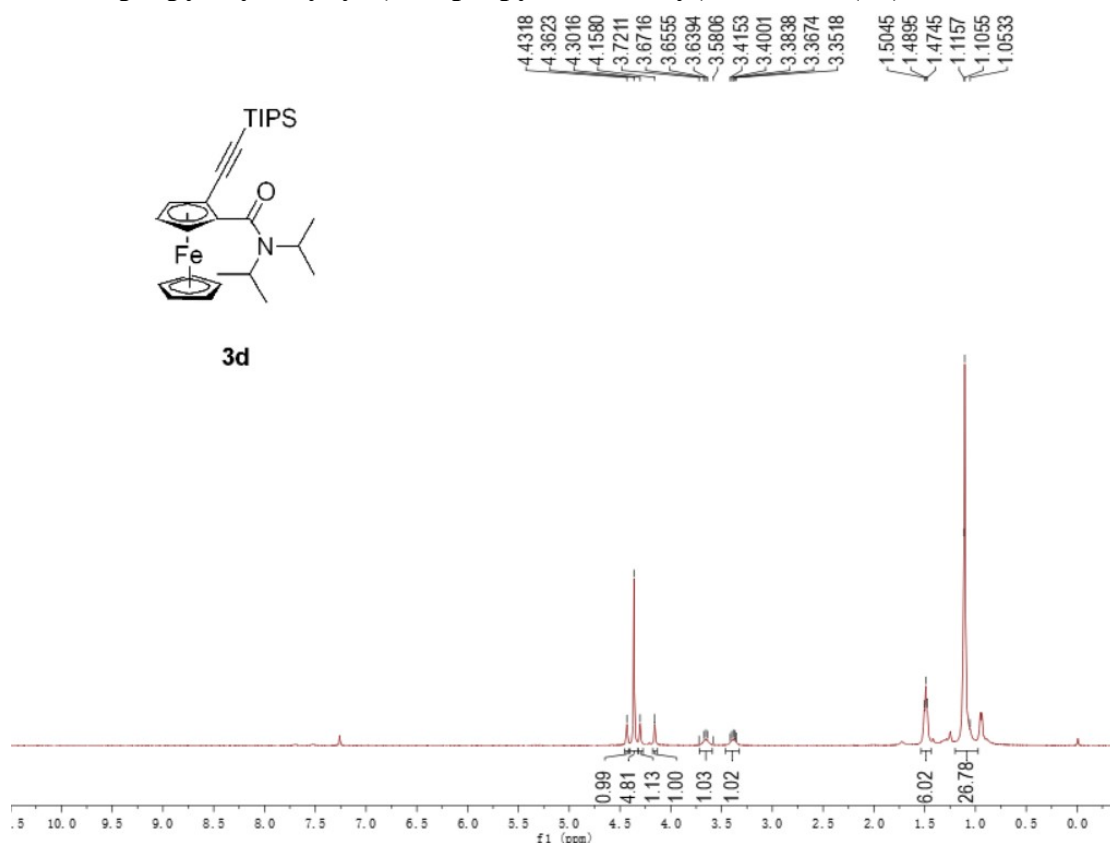


¹H-NMR (400 MHz, CDCl₃)

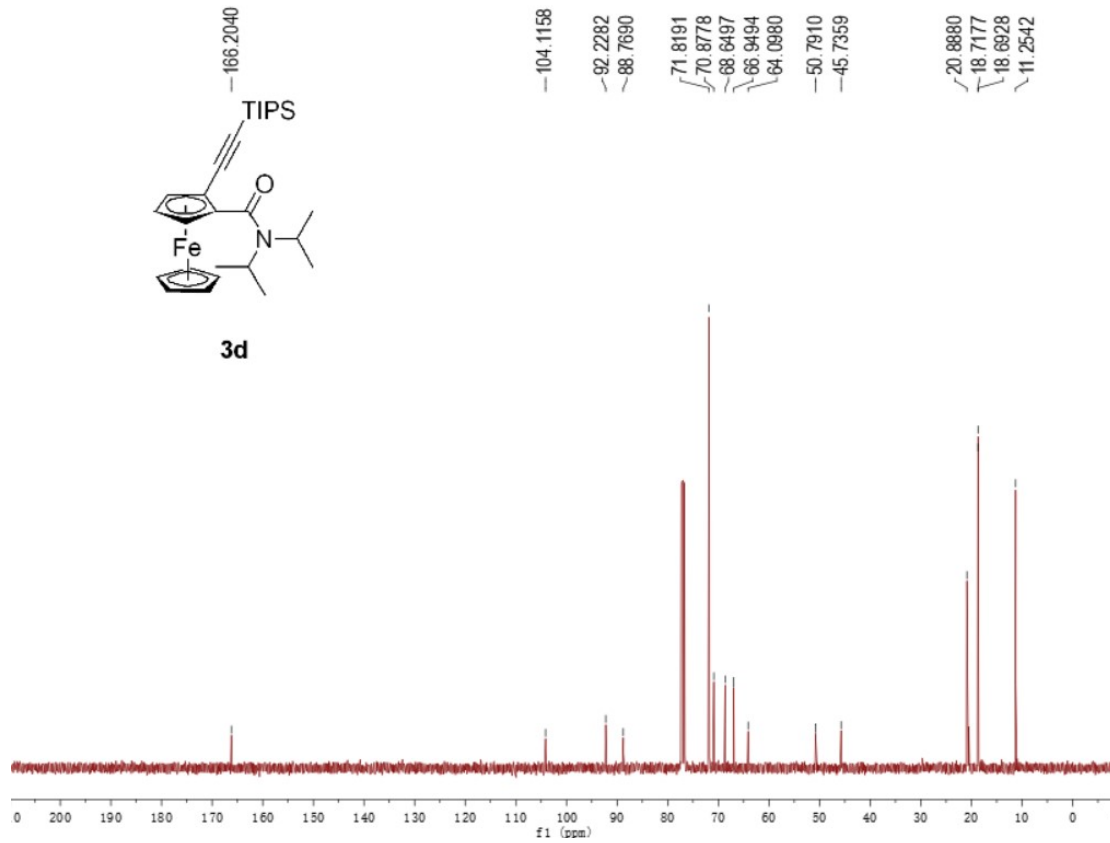


¹³C-NMR (101 MHz, CDCl₃)

2-Triisopropylsilylethynyl-(diisopropyl-1-carbonyl)ferrocene (3d):

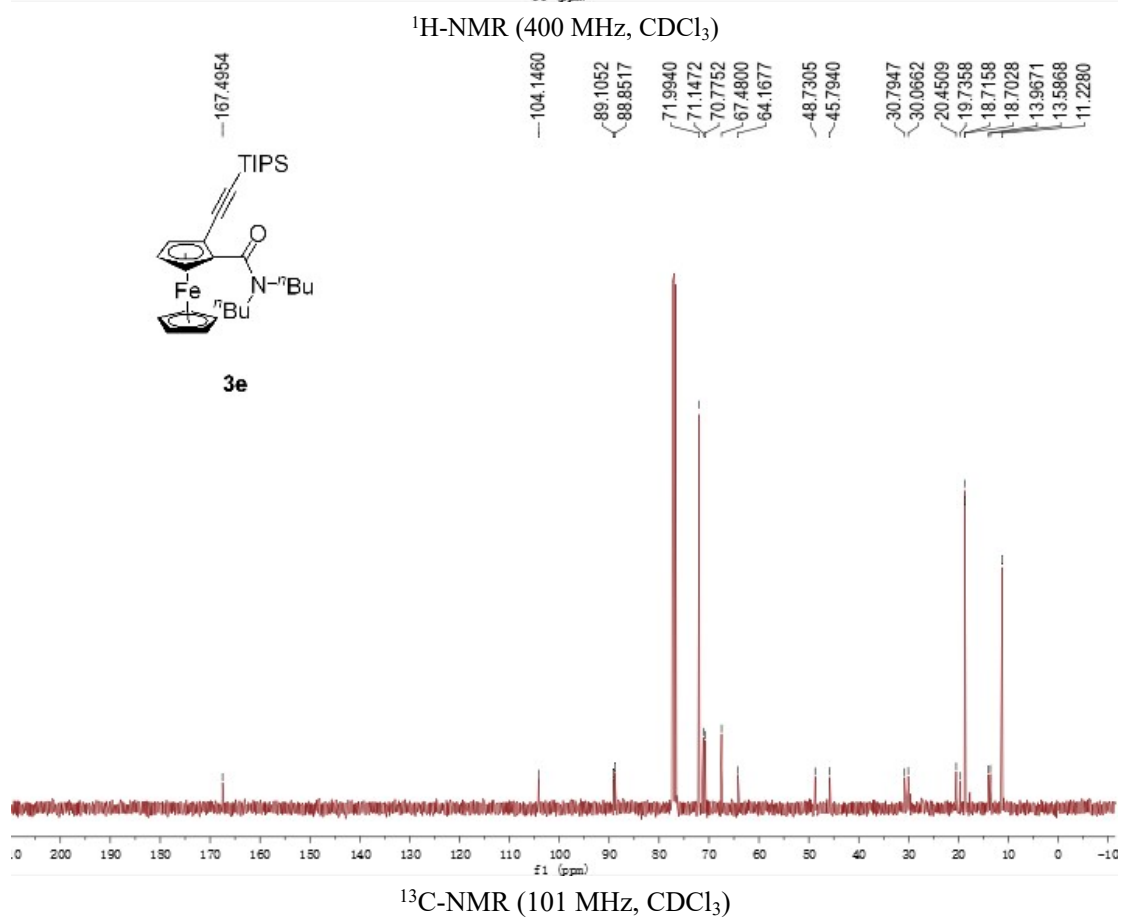
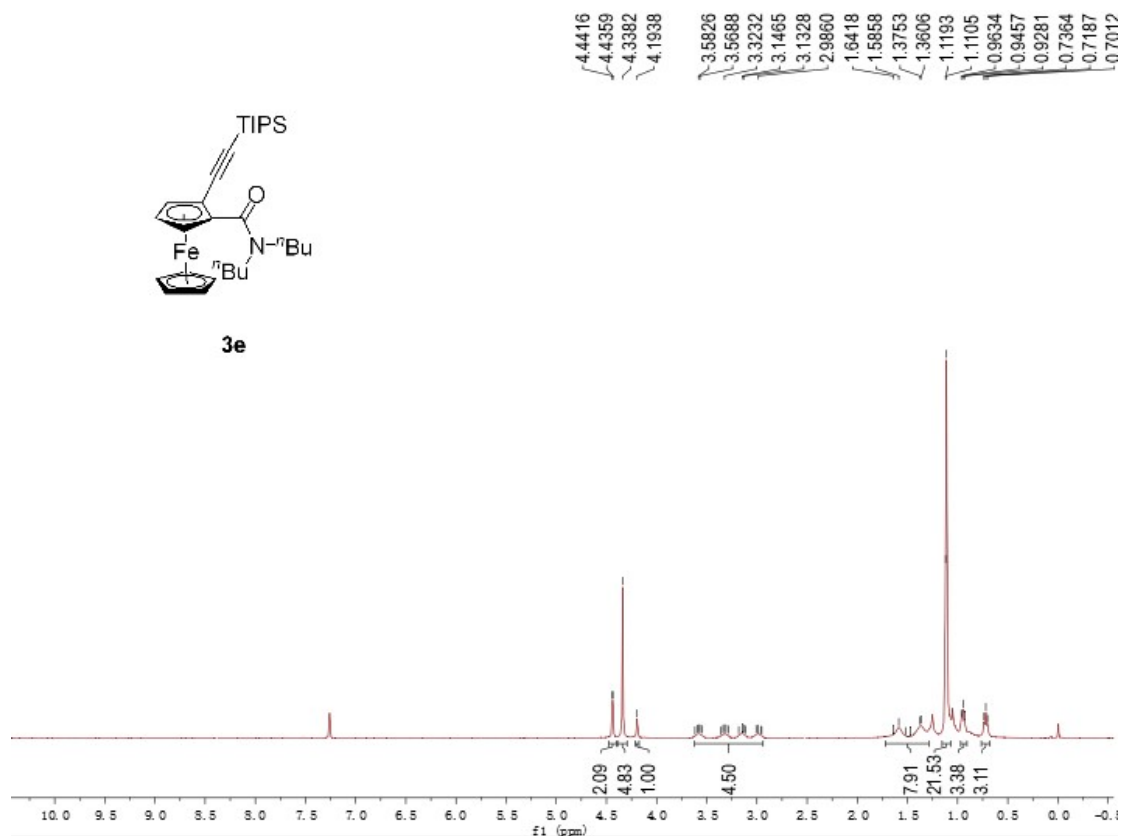


¹H-NMR (400 MHz, CDCl₃)

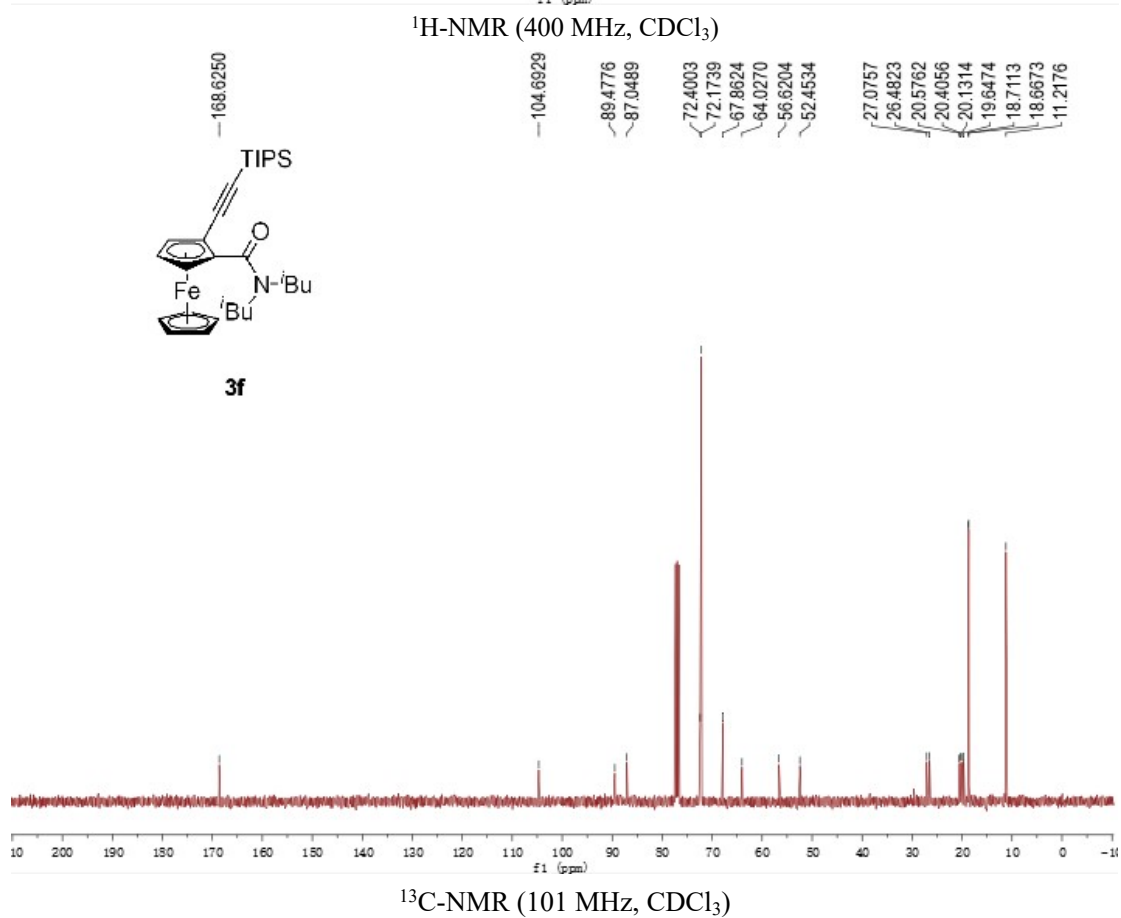
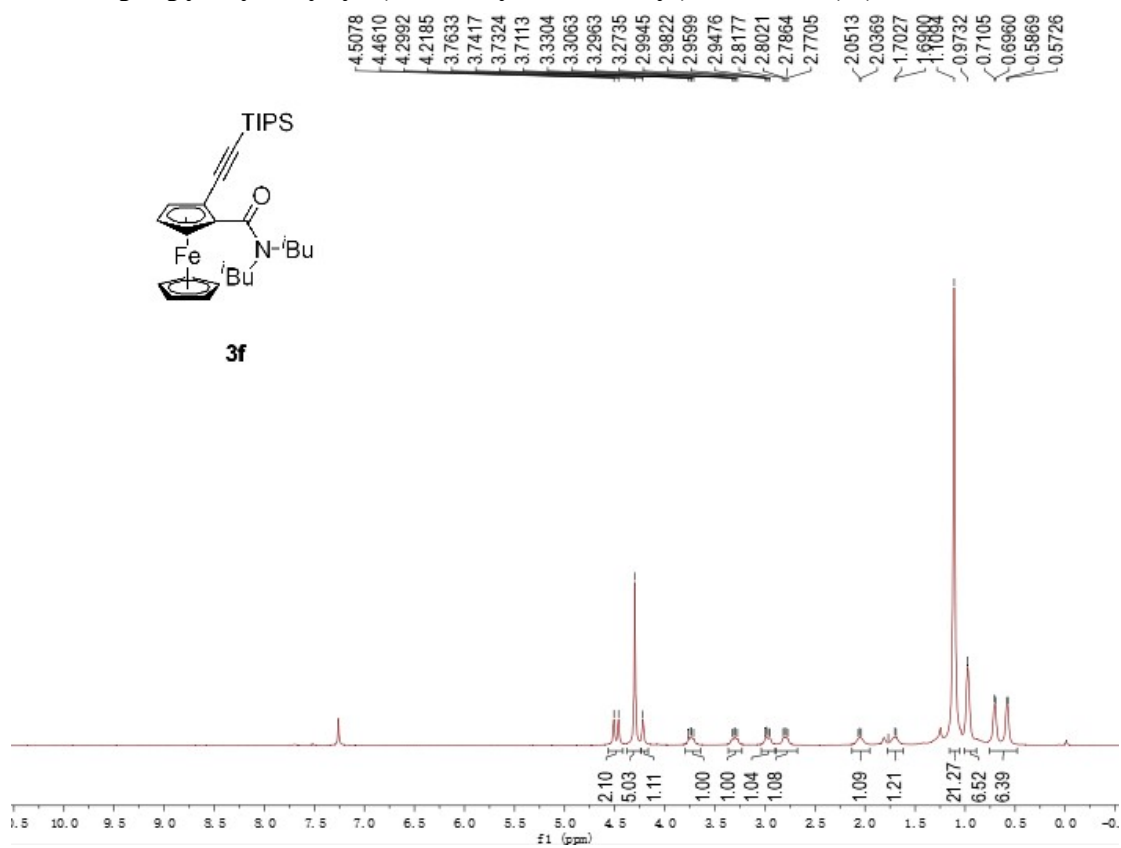


¹³C-NMR (101 MHz, CDCl₃)

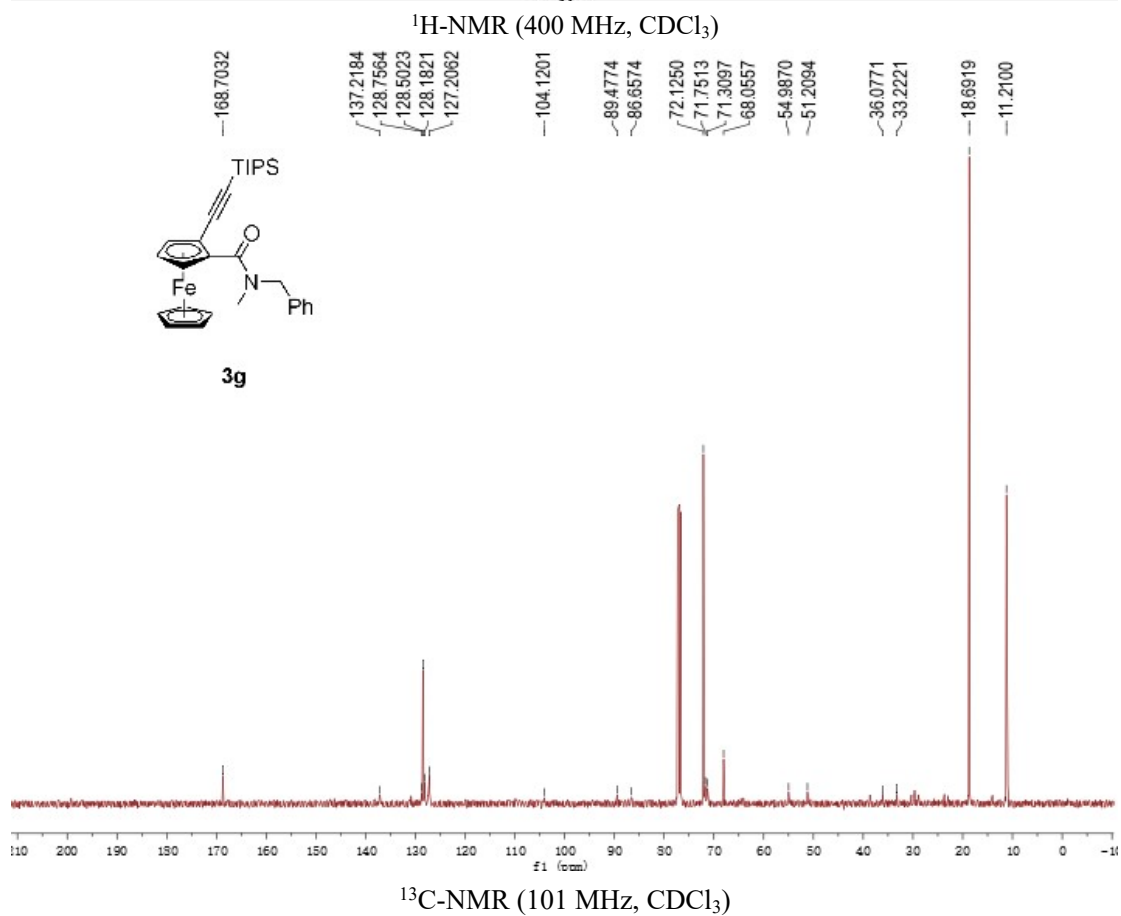
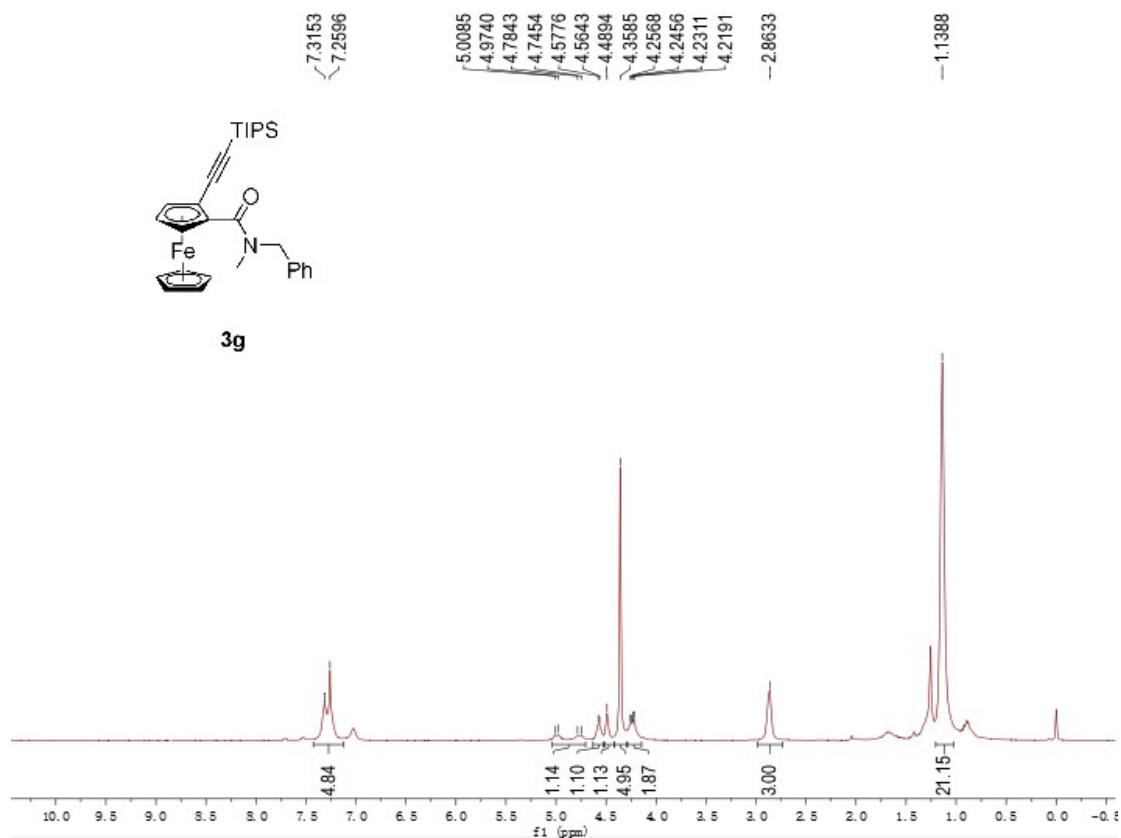
2-Triisopropylsilylethynyl-(dibutyl-1-carbonyl)ferrocene (3e):



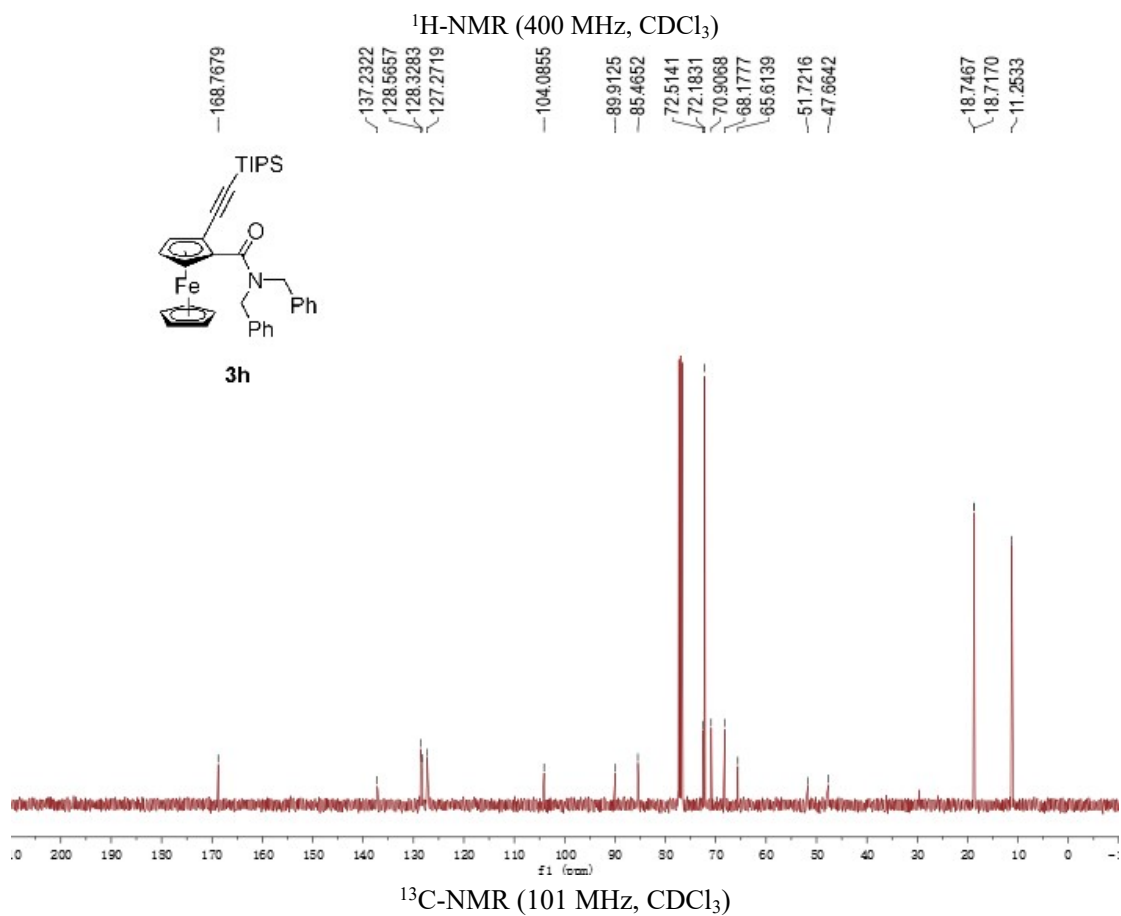
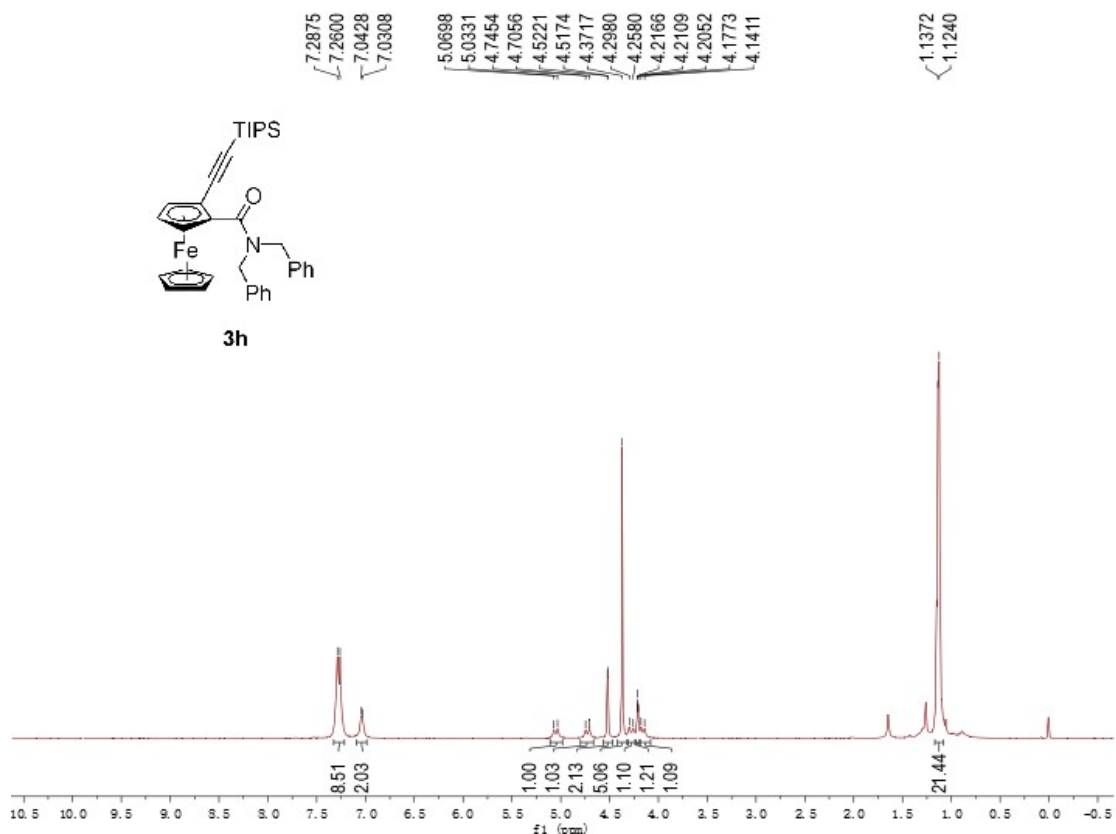
2-Triisopropylsilylethynyl-(diisobutyl-1-carbonyl)ferrocene (**3f**):



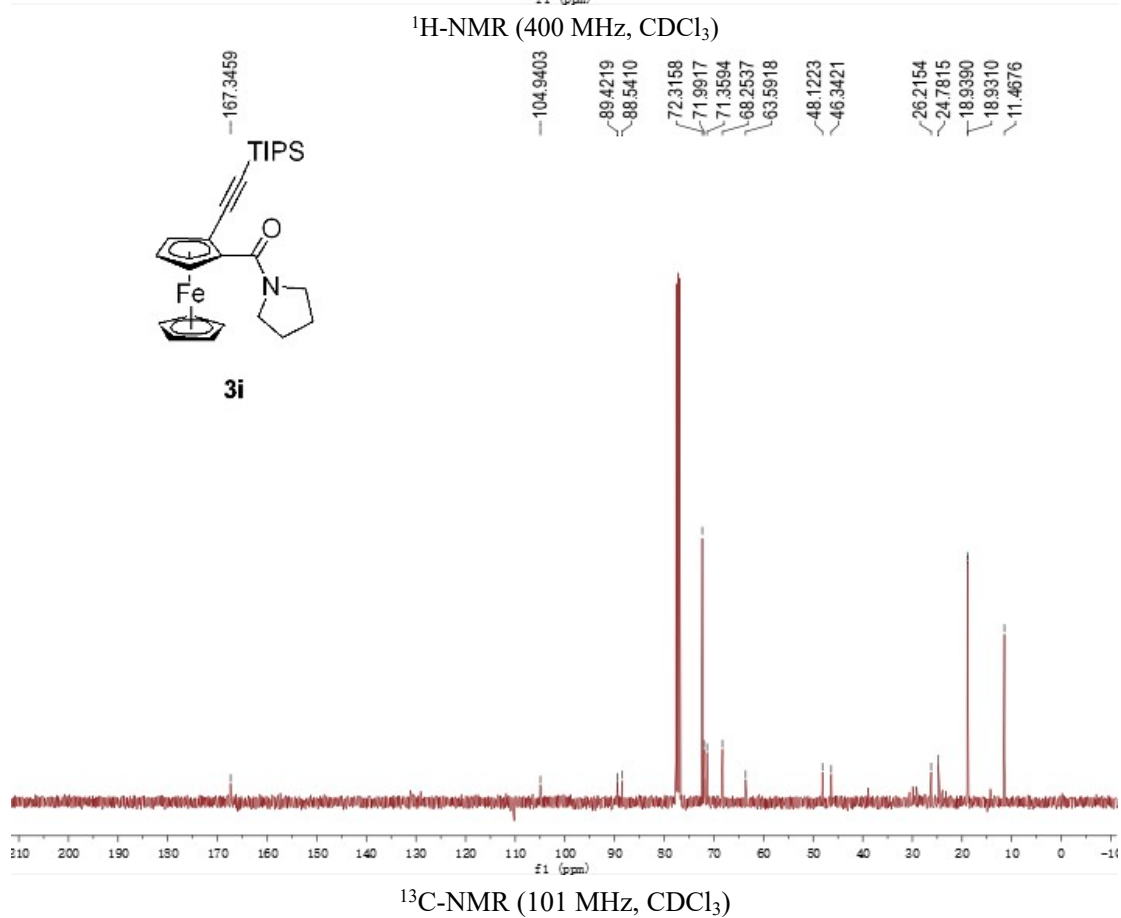
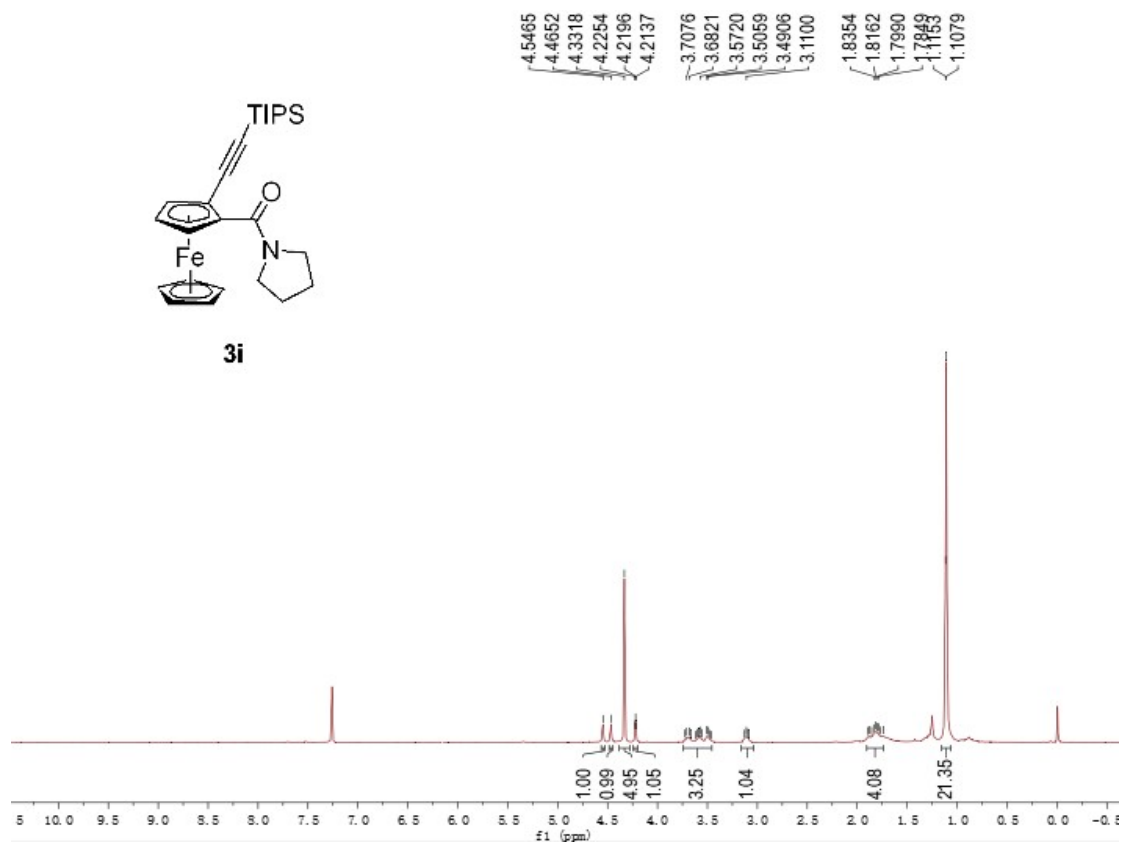
2-Triisopropylsilylethynyl-(methyl-benzyl-1-carbonyl)ferrocene (3g):



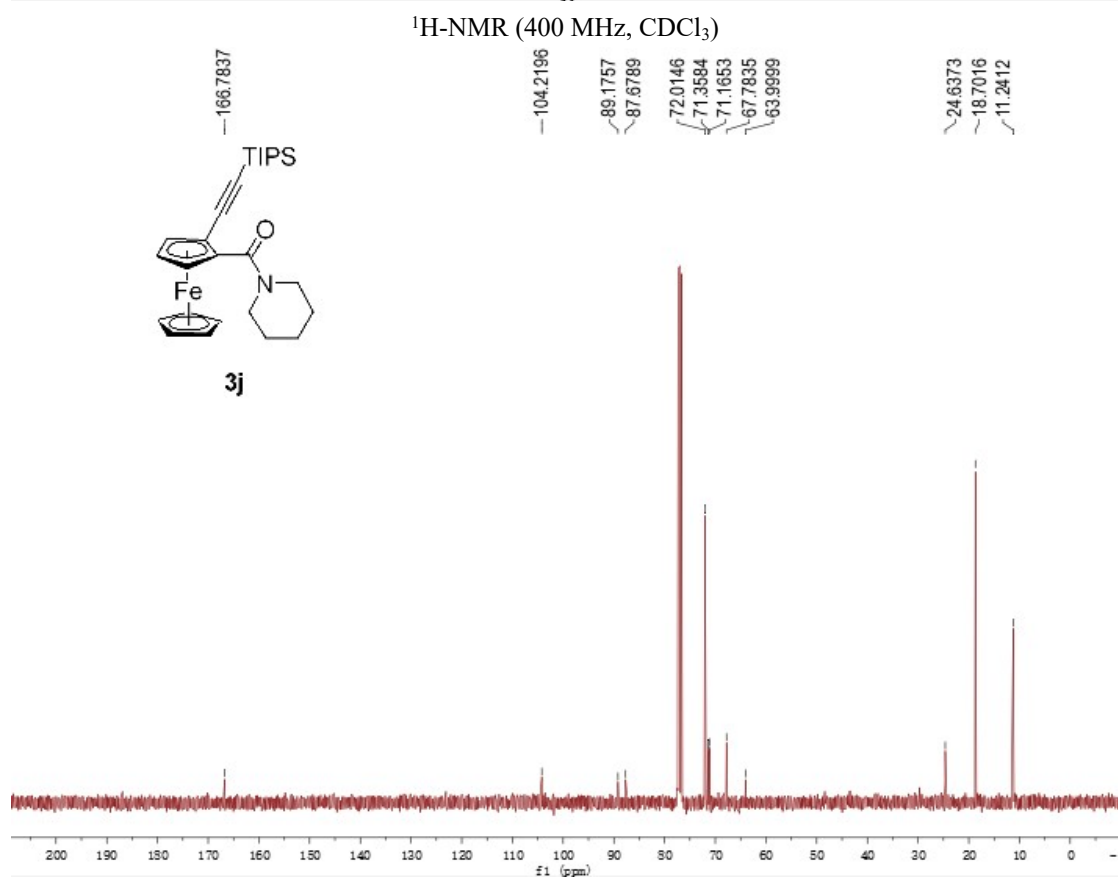
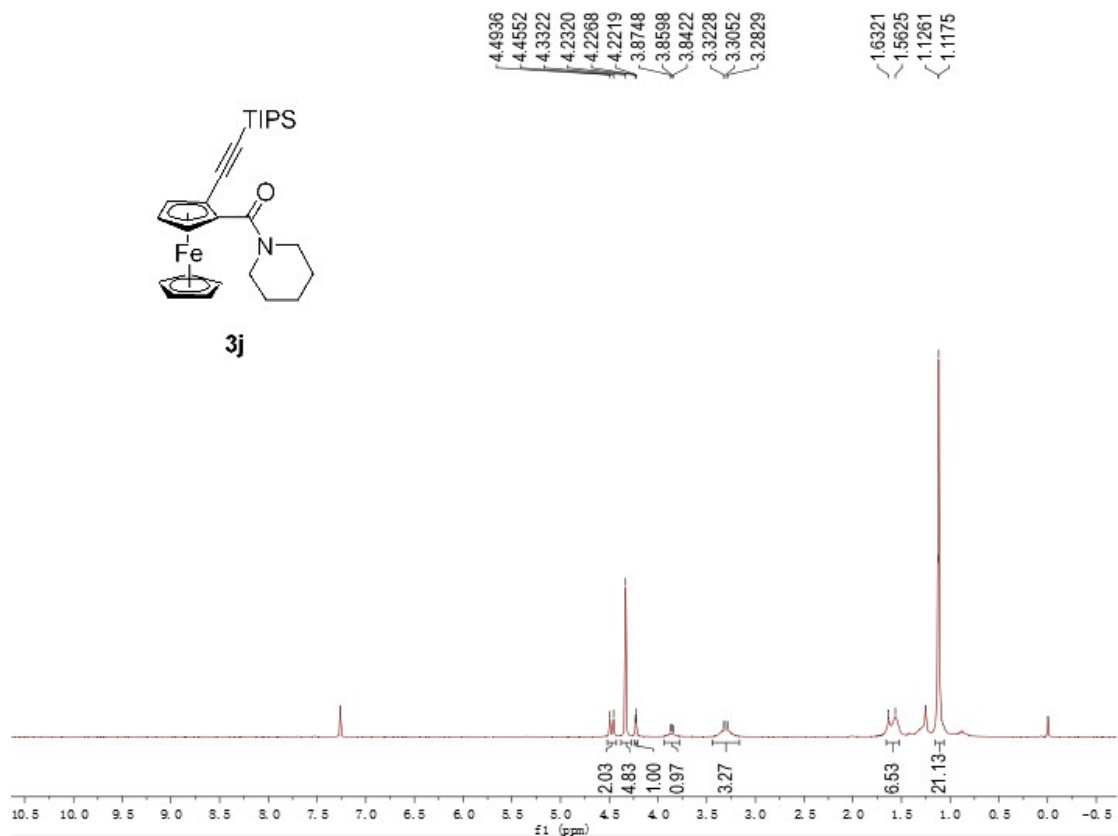
2-Triisopropylsilylethynyl-(dibenzyl-1-carbonyl)ferrocene (3h):



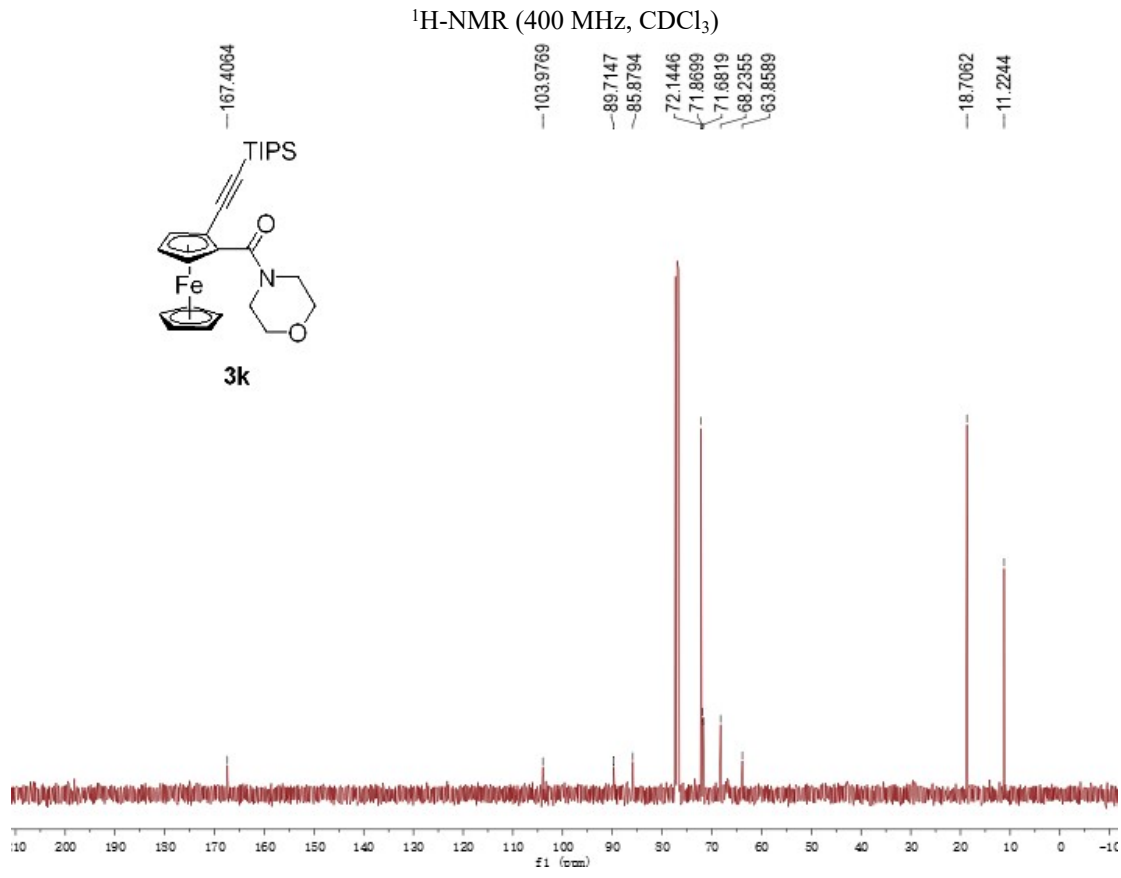
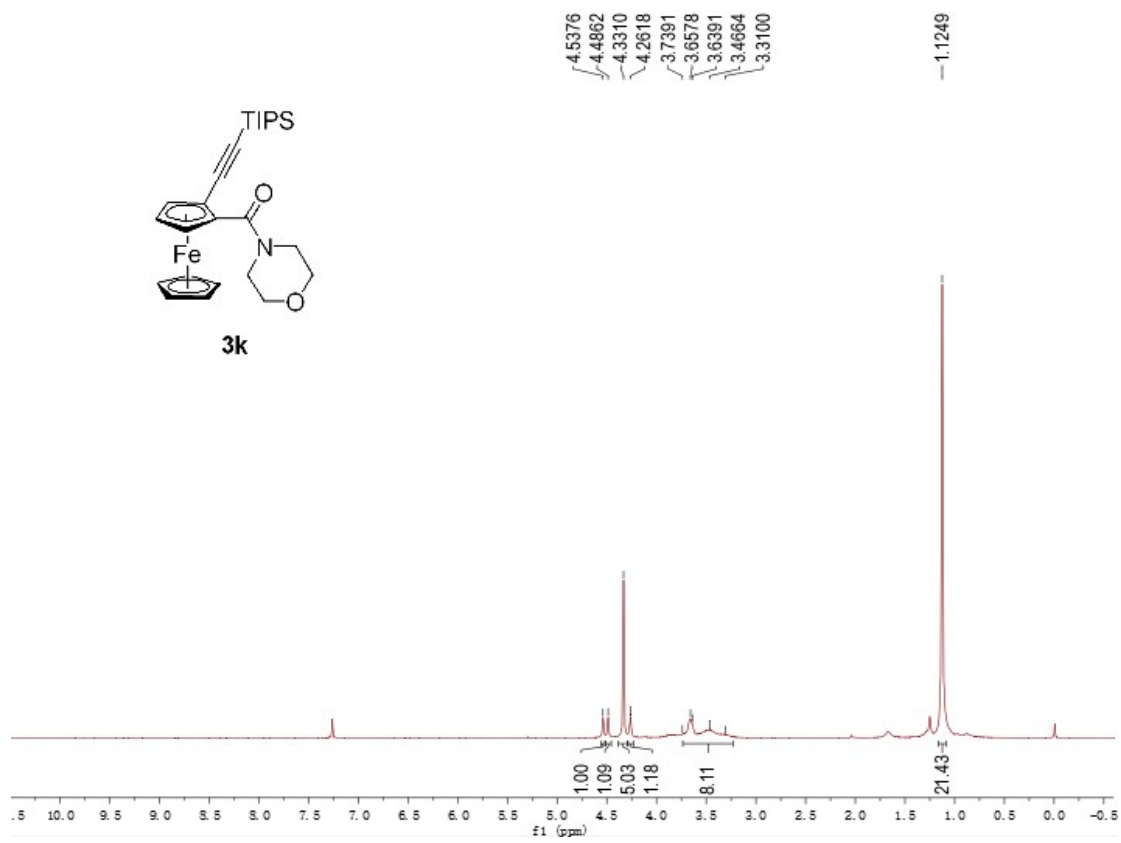
2-Triisopropylsilylethynyl-(pyrrolidine-1-carbonyl)ferrocene (**3i**):



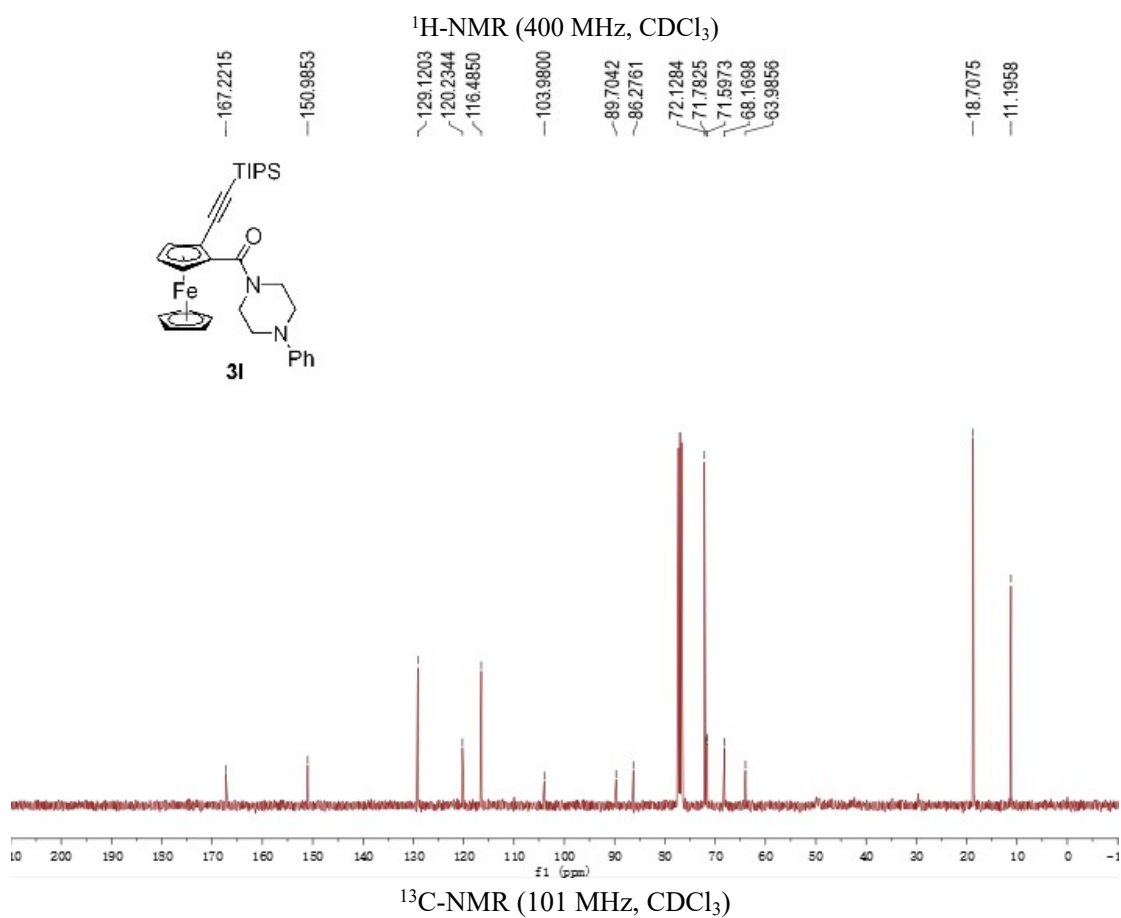
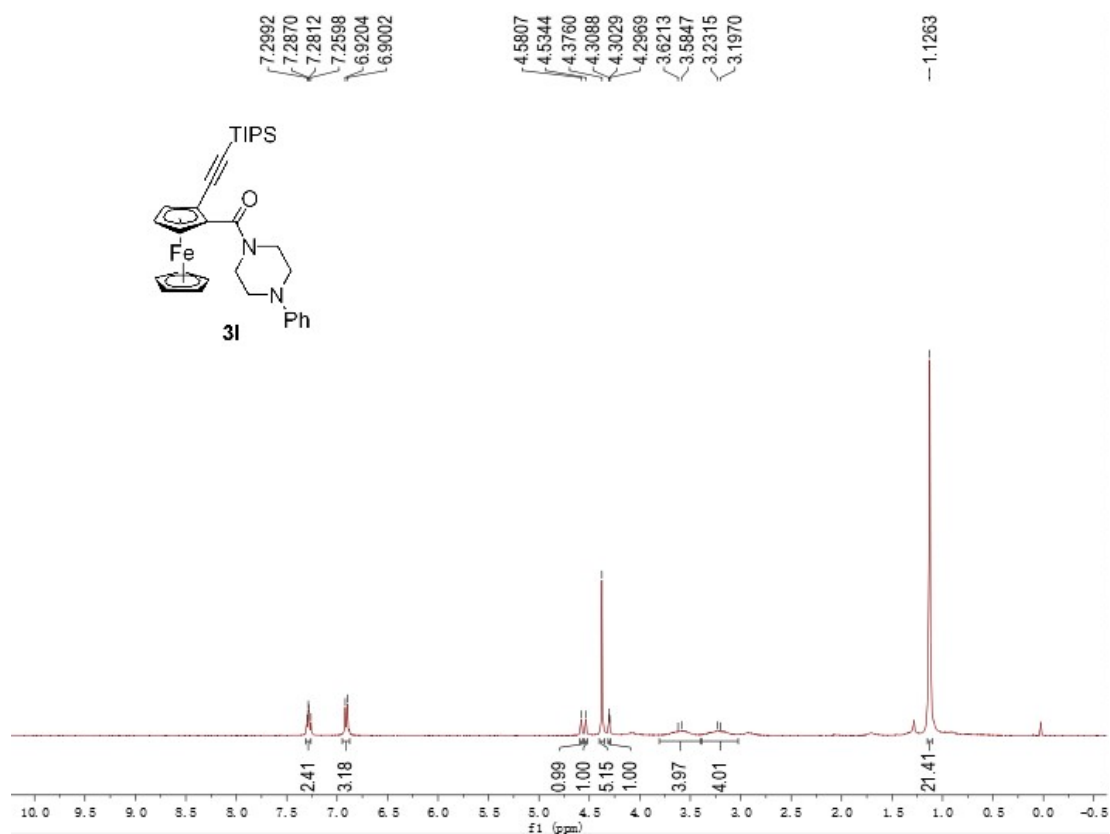
2-Triisopropylsilylethynyl-(piperidine-1-carbonyl)ferrocene (3j):



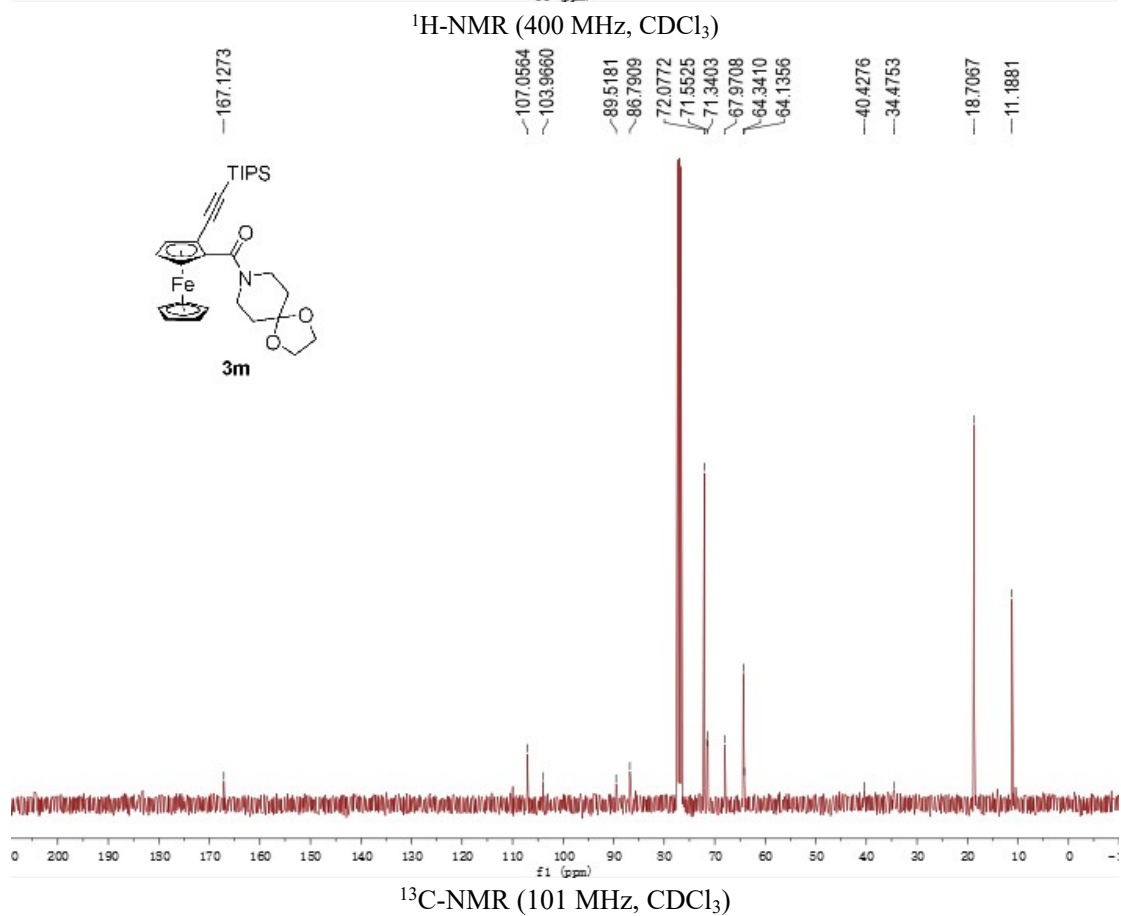
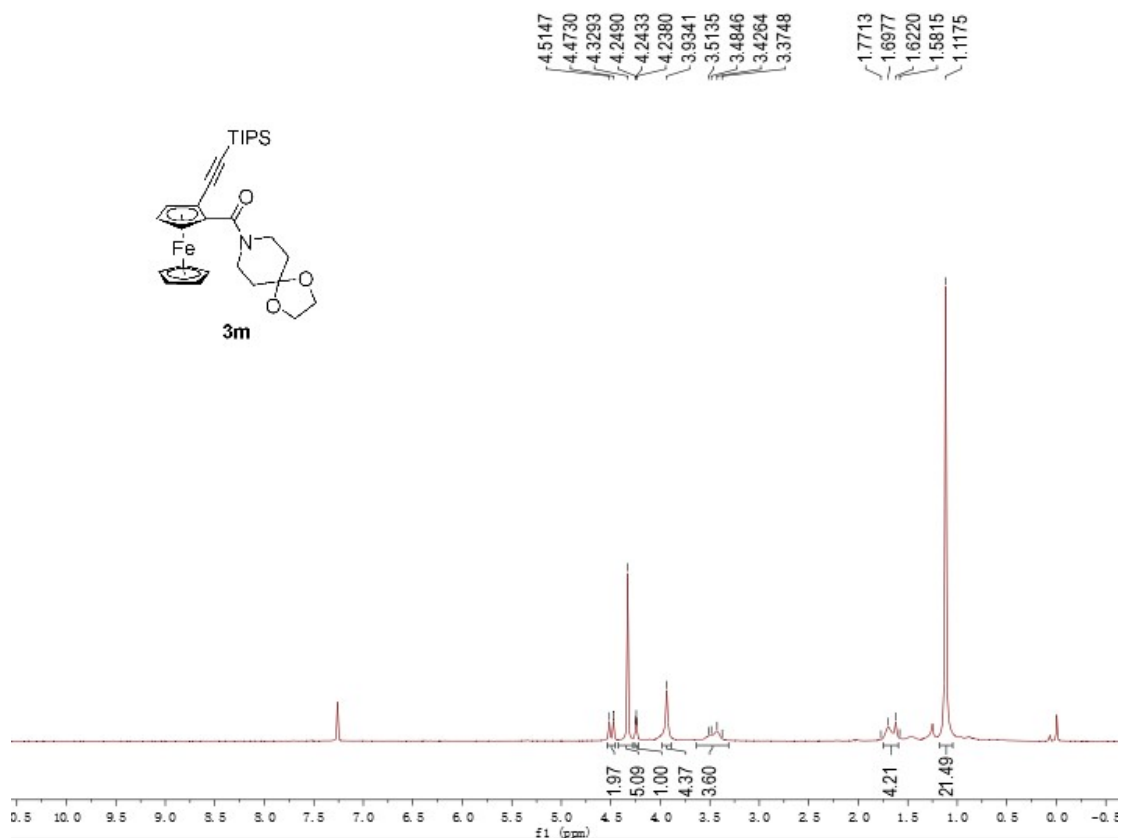
2-Triisopropylsilylethynyl-(morpholine-1-carbonyl)ferrocene (3k):



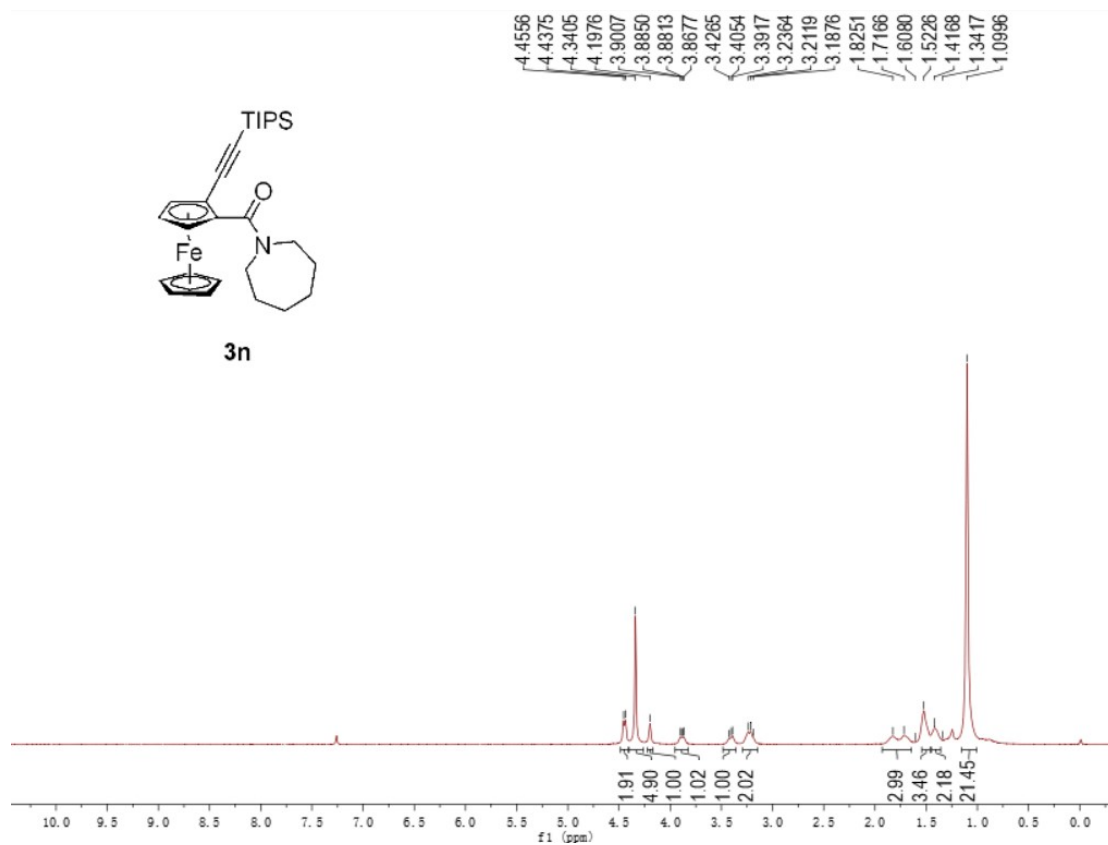
2-Triisopropylsilylethynyl-(N-phenylpiperazine-1-carbonyl)ferrocene (3I):



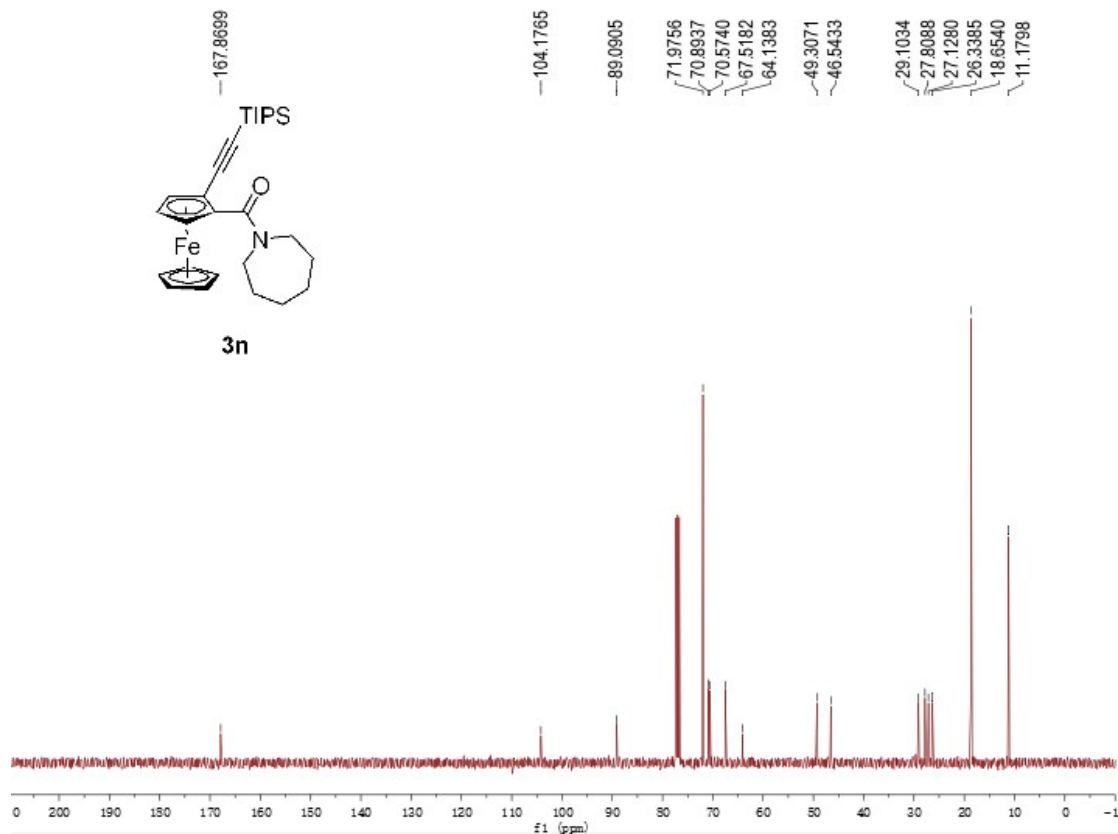
2-Triisopropylsilylethynyl-((4-piperidine-1-carbonyl)ferrocene (3m):



2-Triisopropylsilylethynyl-(azepane-1-carbonyl)ferrocene (**3n**):

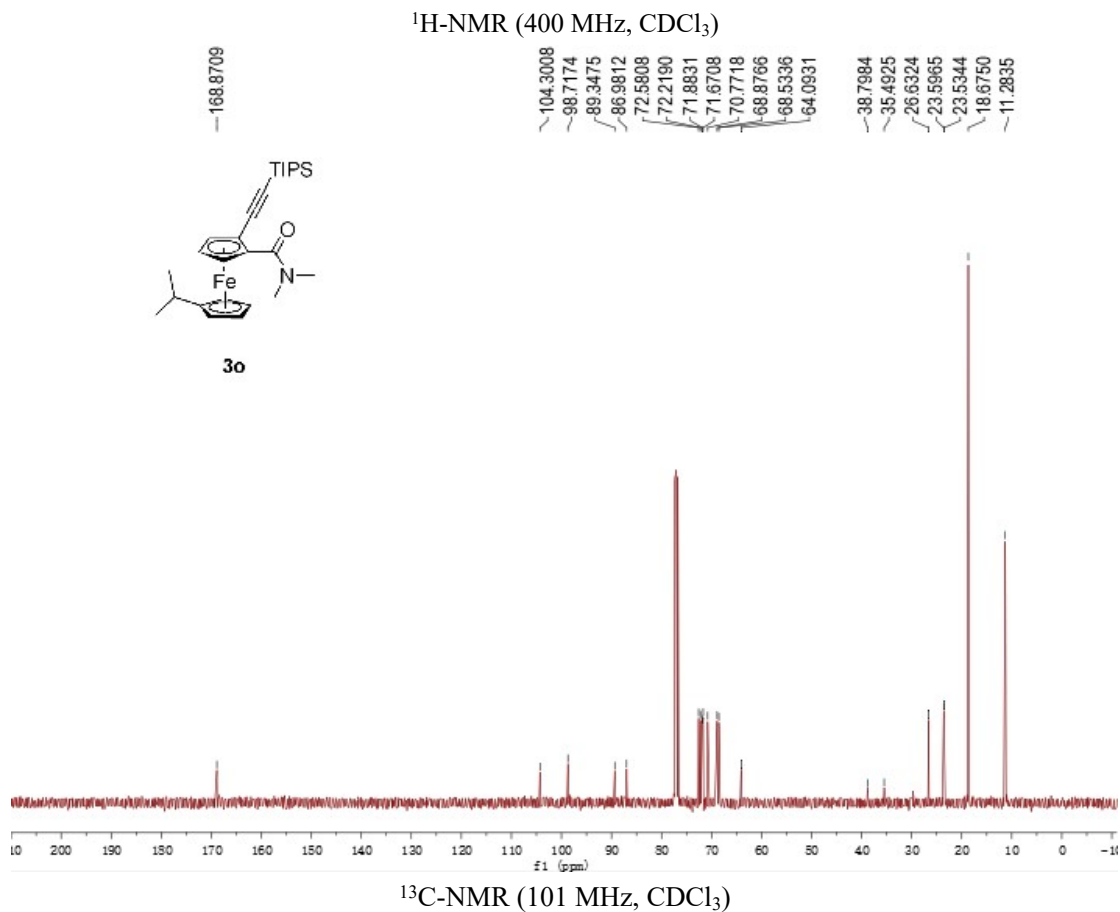
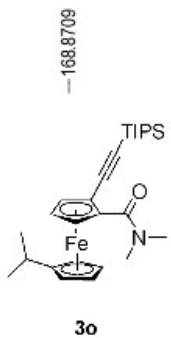
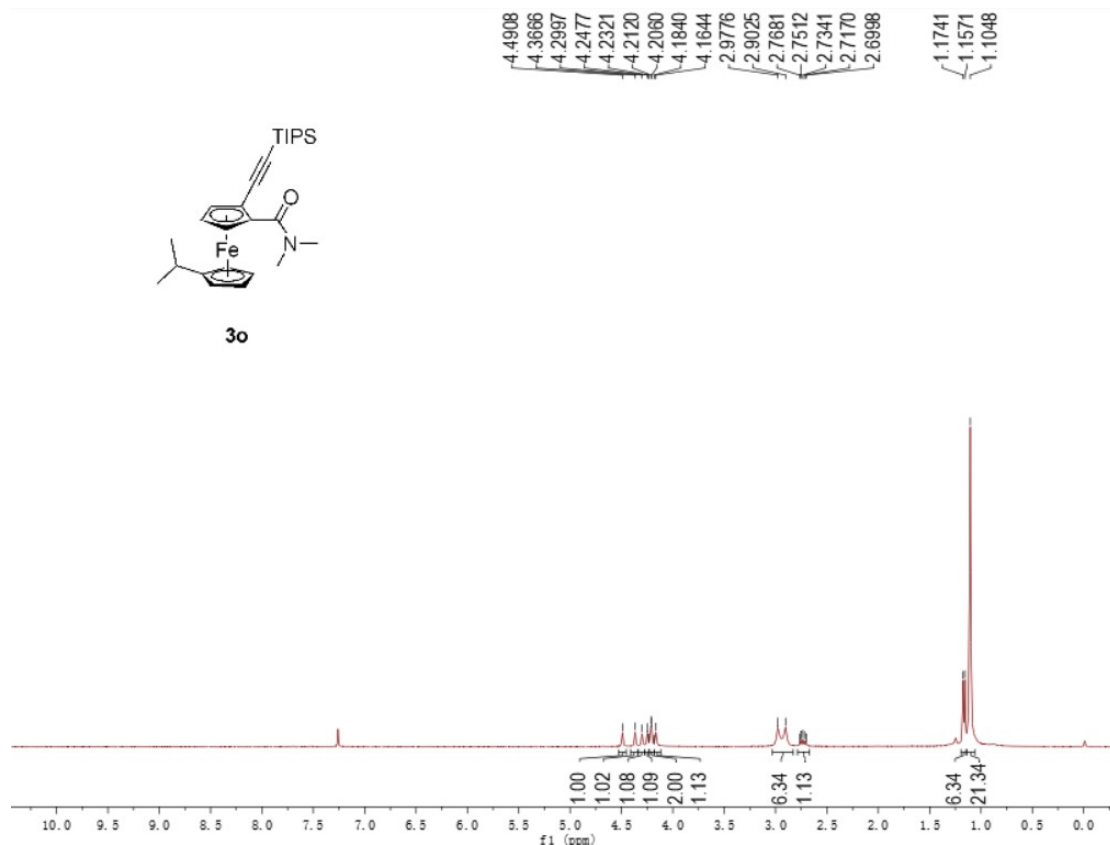
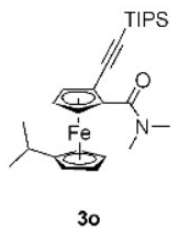


¹H-NMR (400 MHz, CDCl₃)

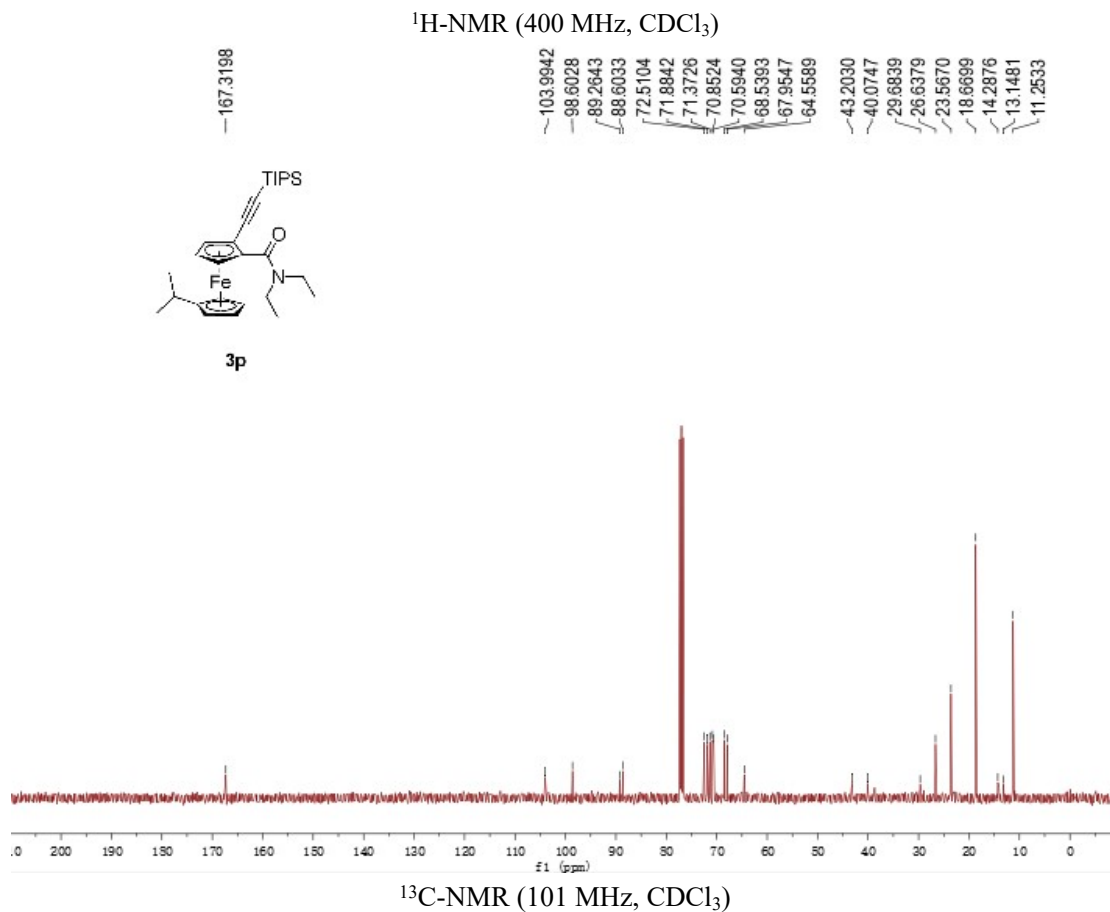
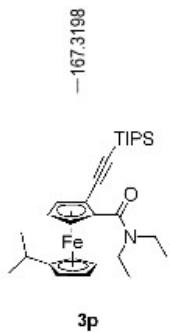
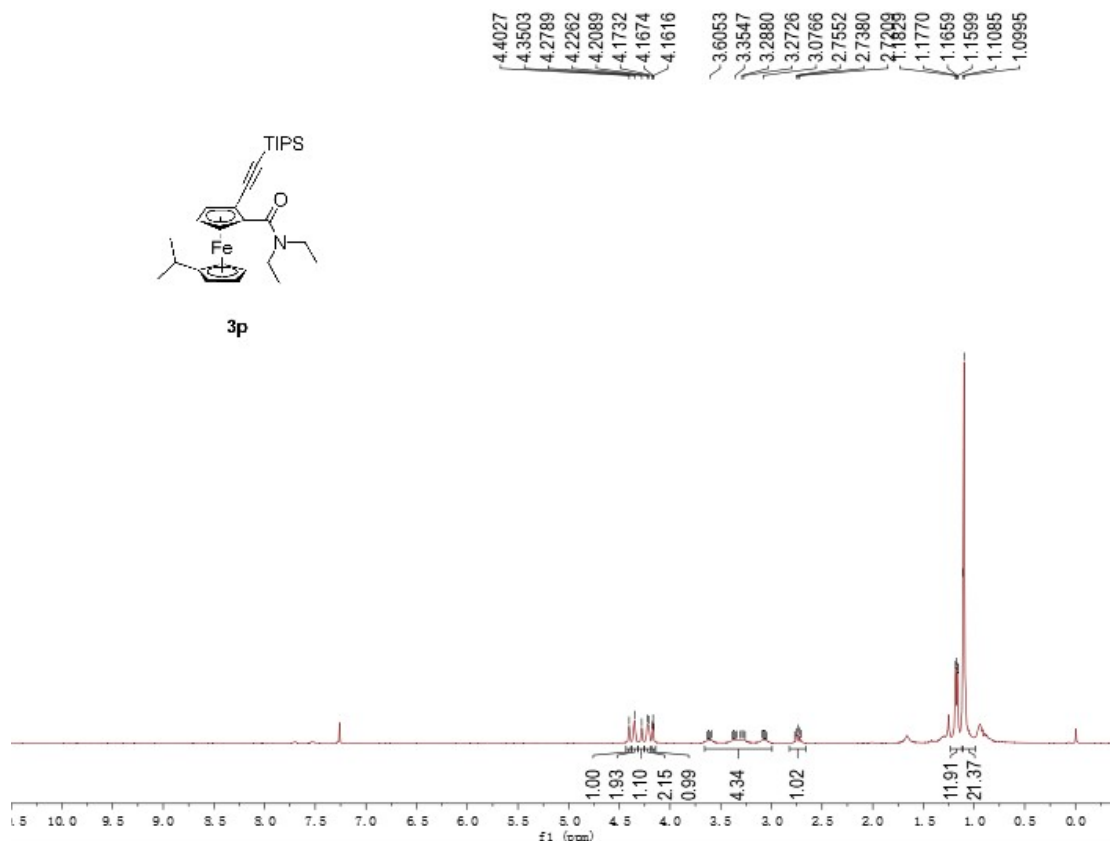
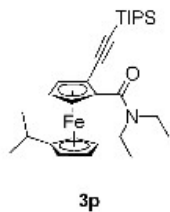


¹³C-NMR (101 MHz, CDCl₃)

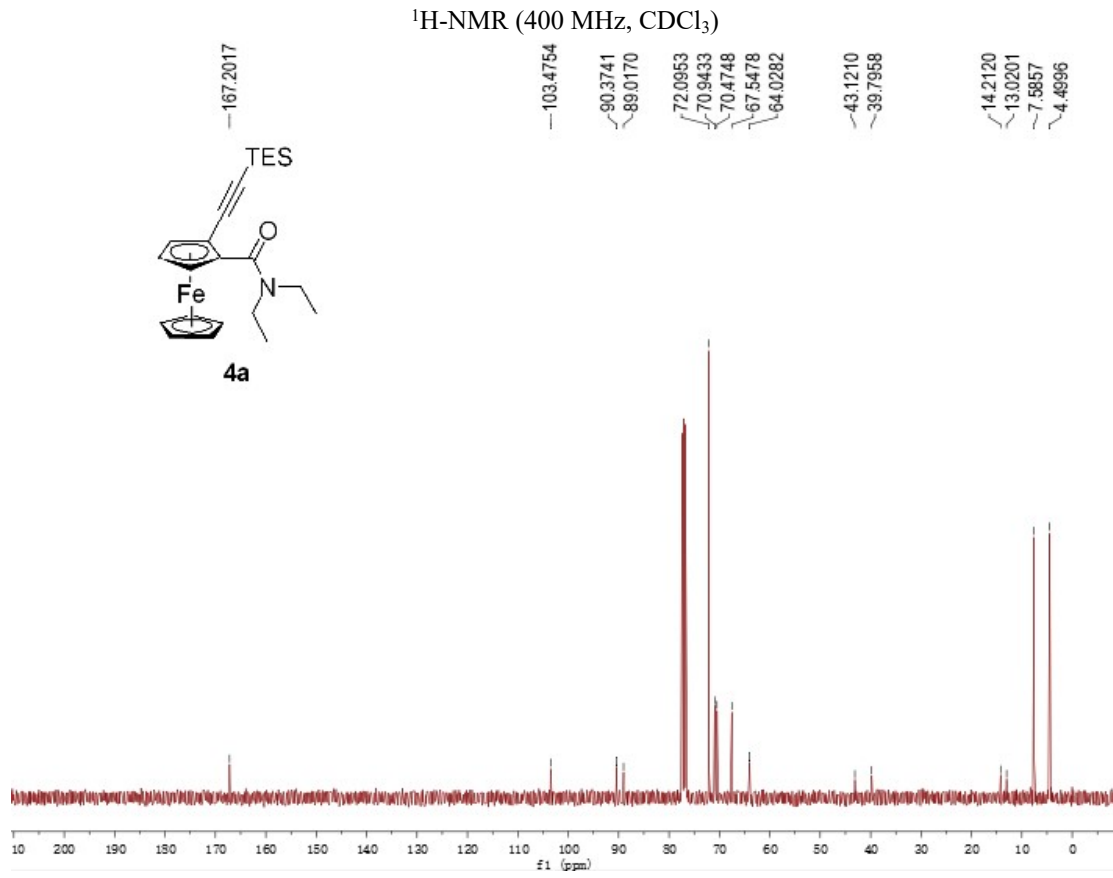
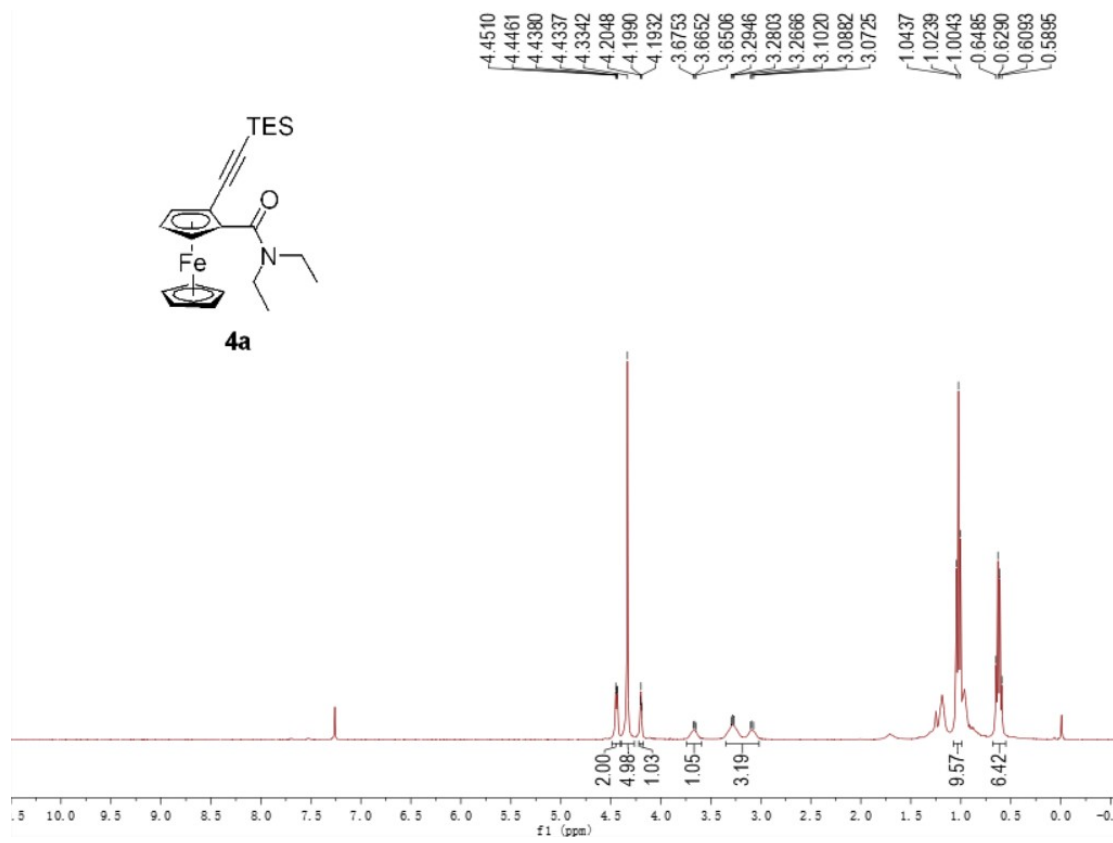
2-Triisopropylsilylethynyl-(dimethyl-1-carbonyl)-1'-isopropyl-ferrocene (3o):



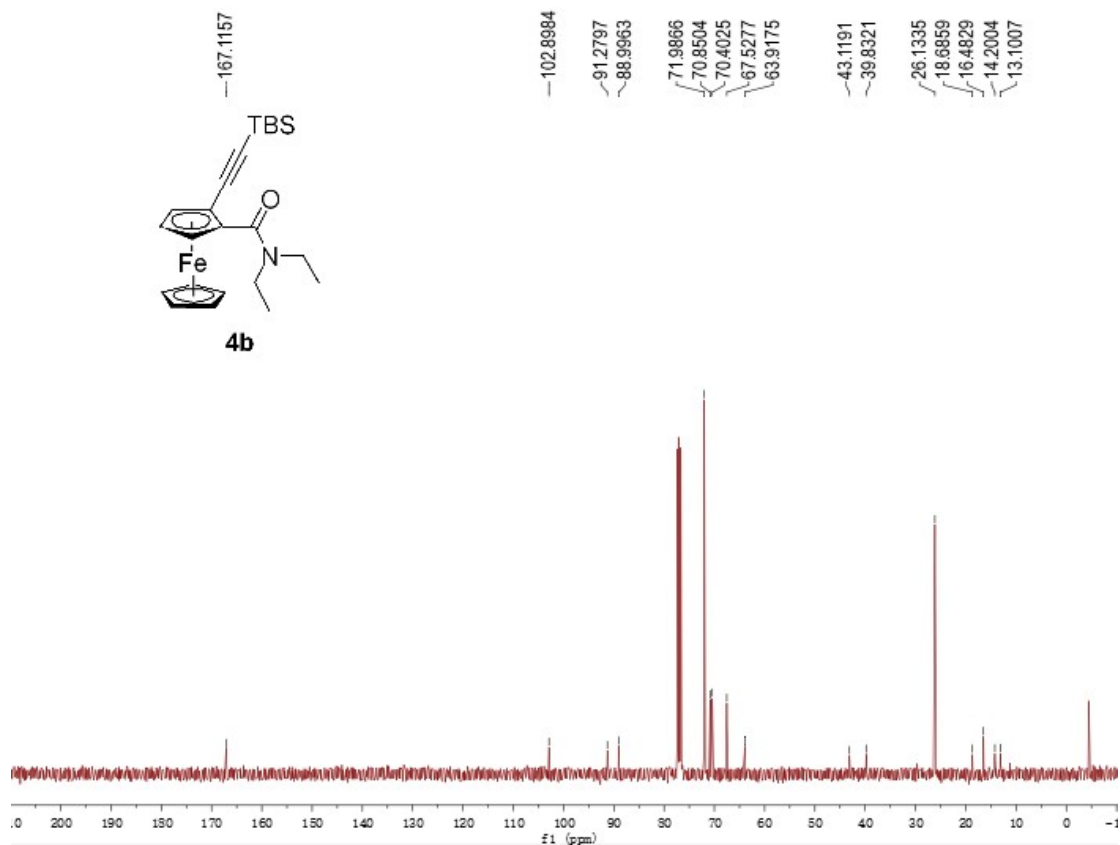
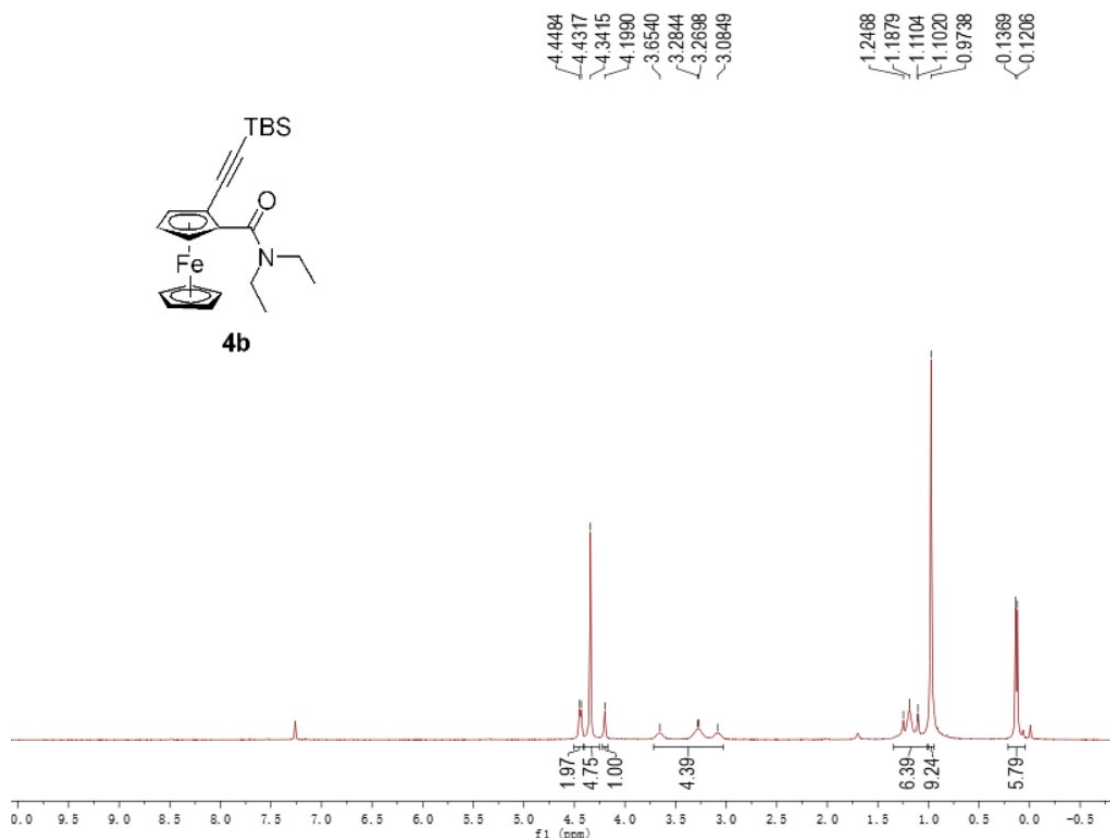
2-Triisopropylsilylethynyl-(diethyl-1-carbonyl)-1'-ispropyl-ferrocene (3p):



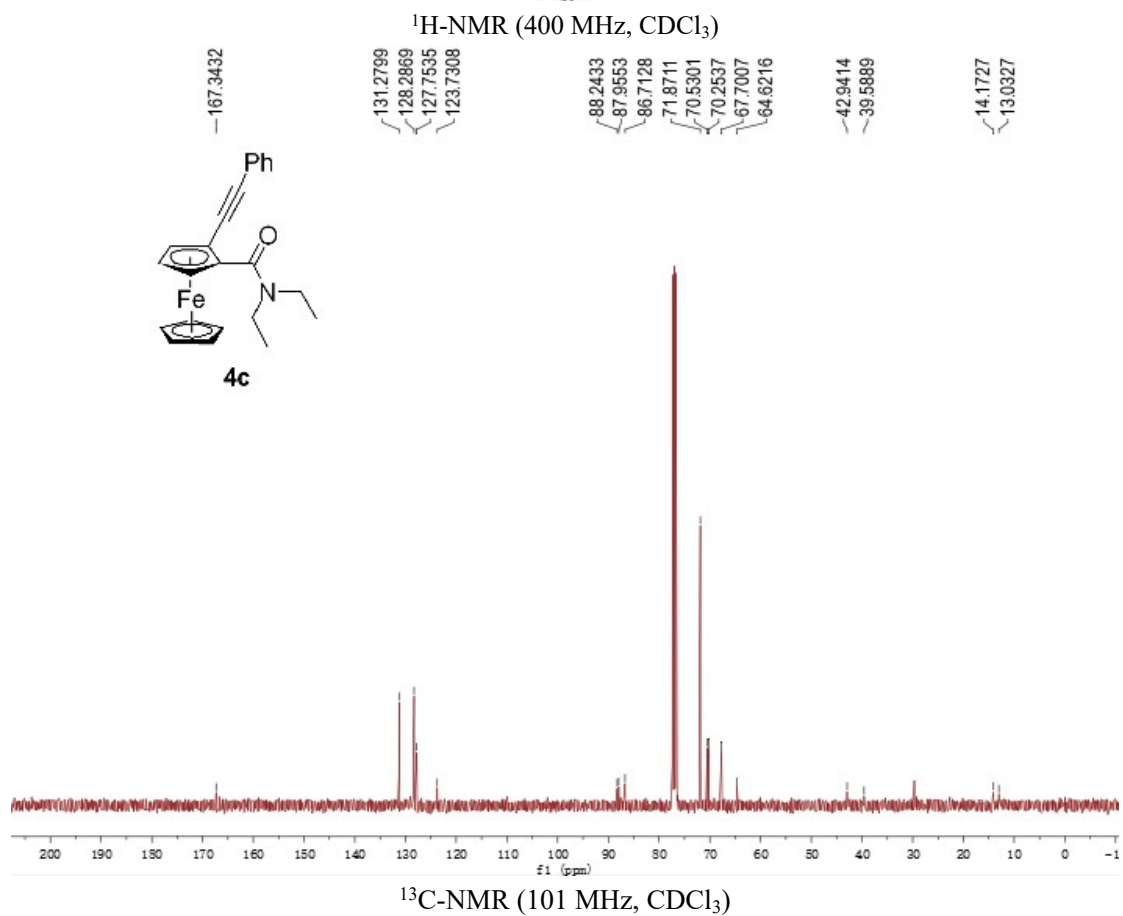
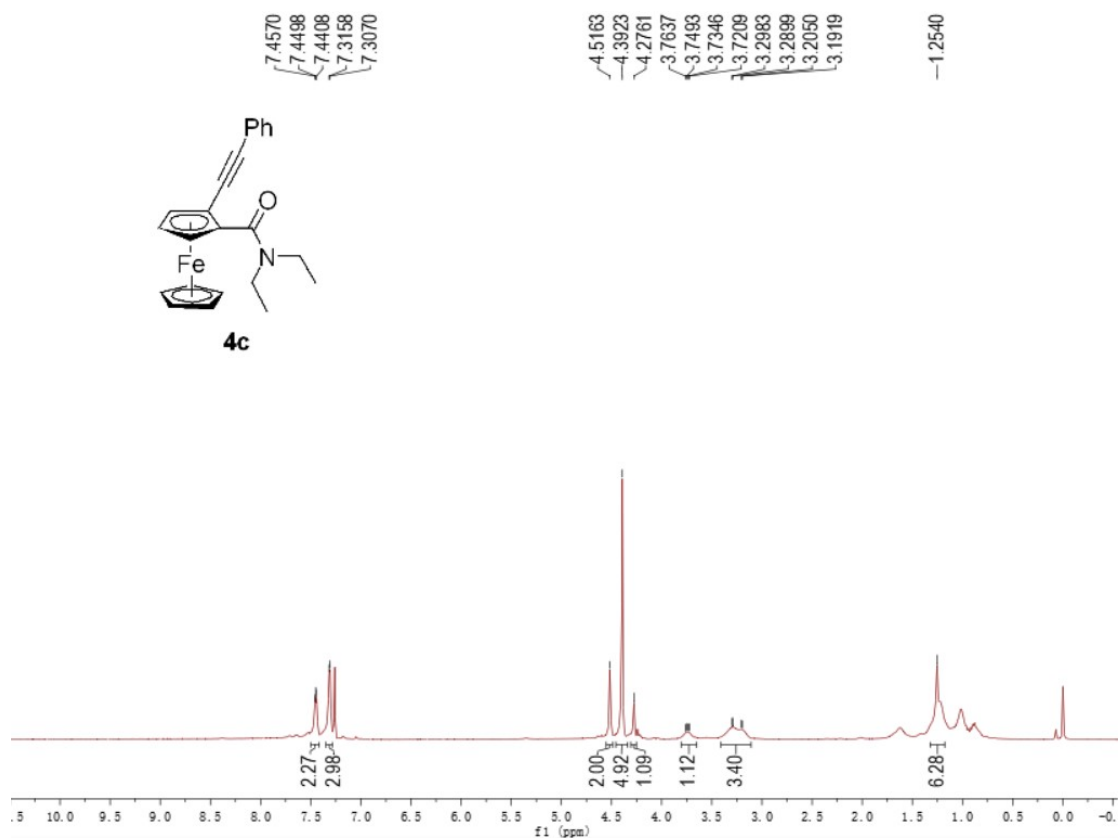
2-Triethylsilyylethynyl-(diethyl-1-carbonyl)ferrocene (4a):



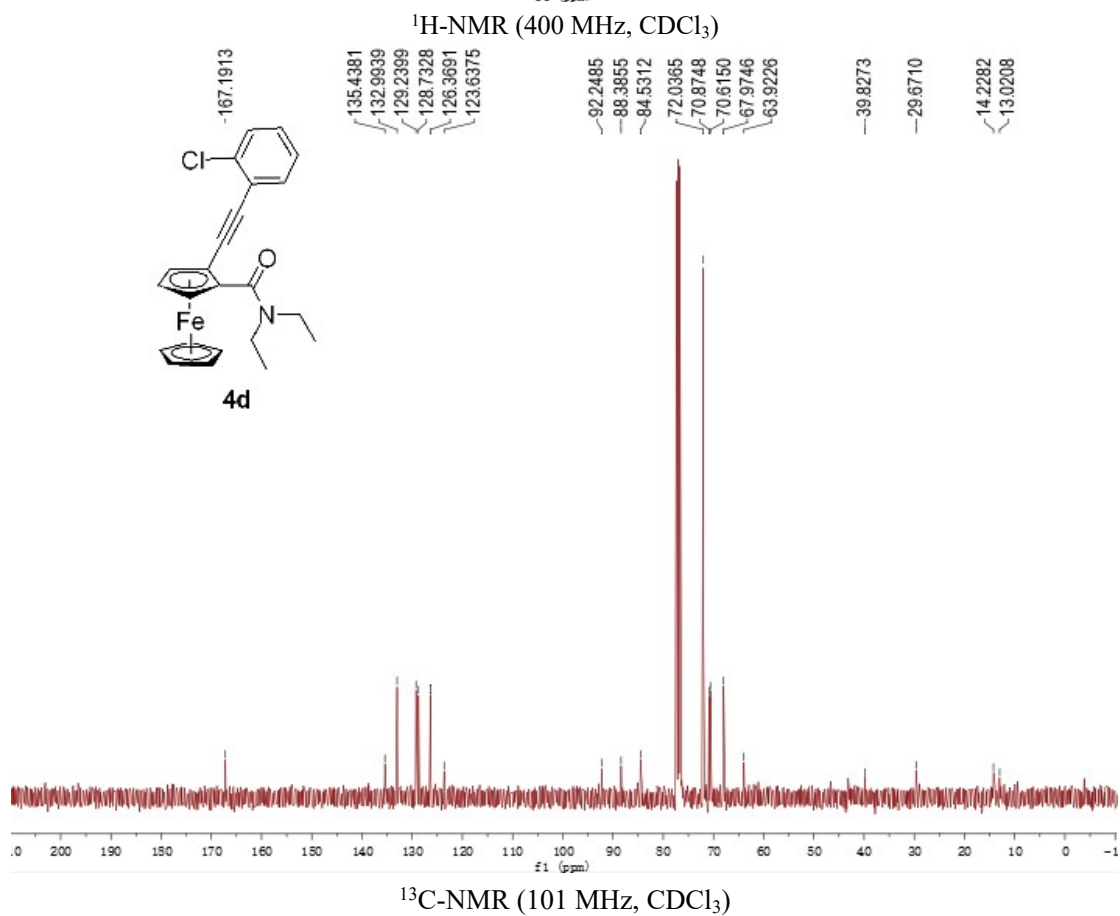
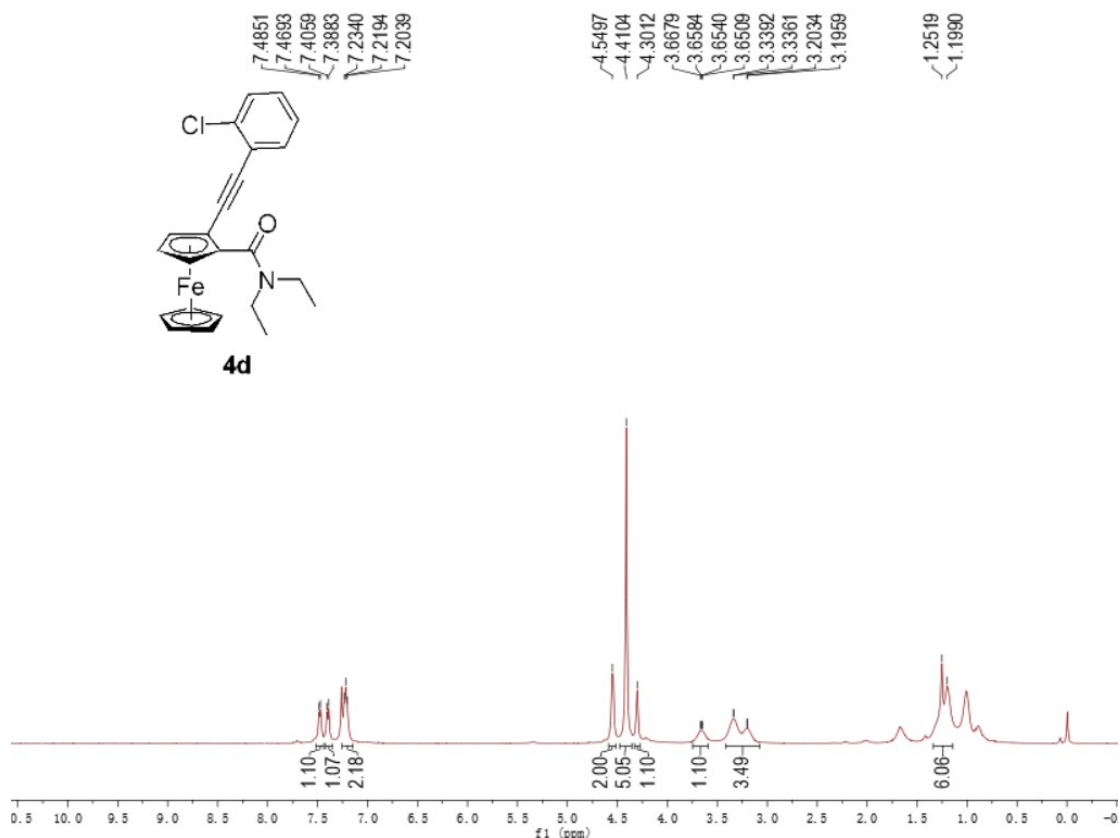
2-tert-butylsilyl ethynyl-(diethyl-1-carbonyl)ferrocene (4b):



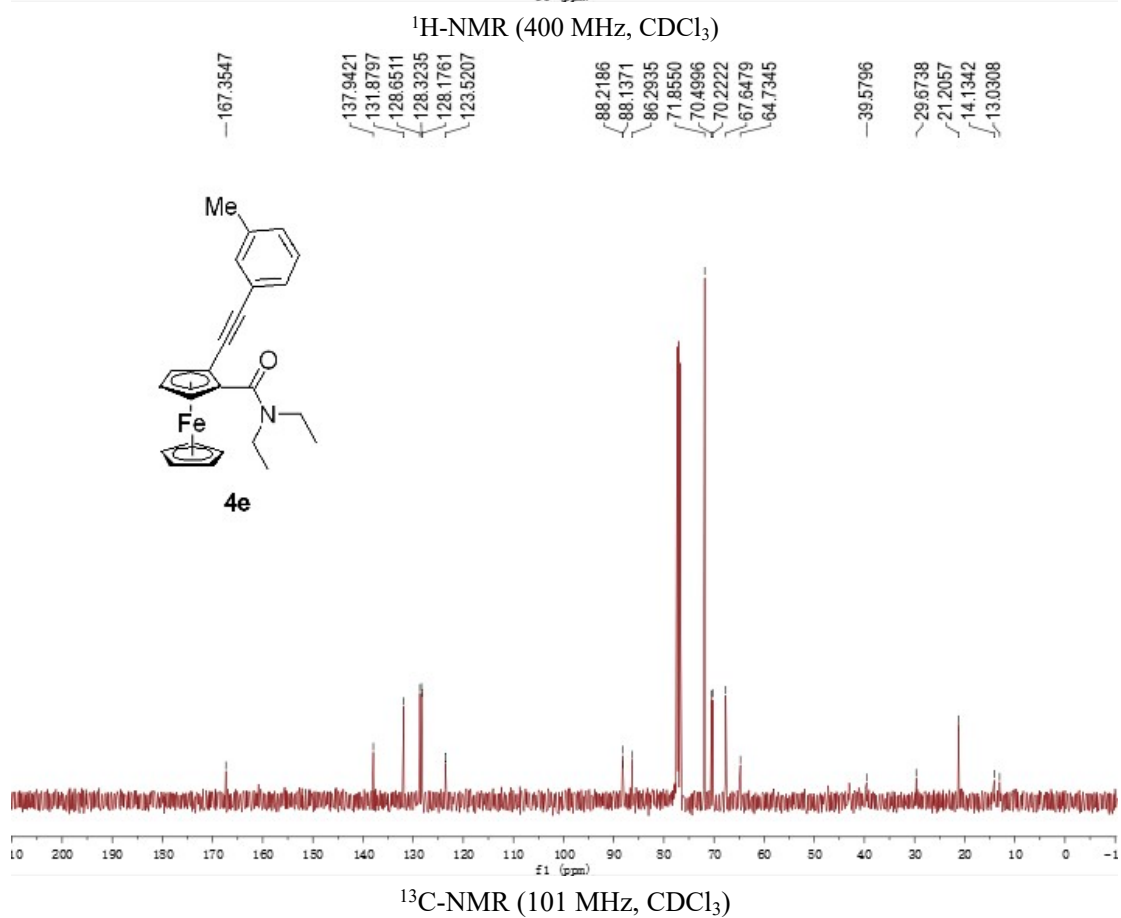
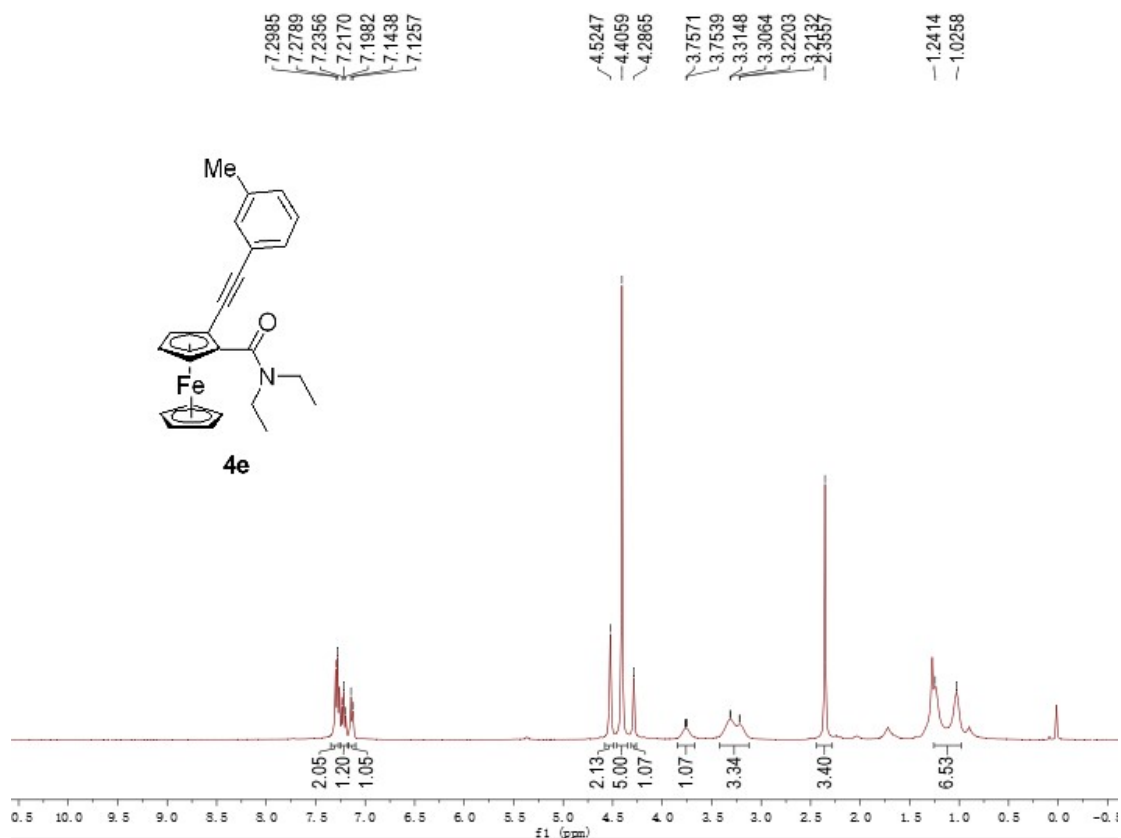
2-phenylethynyl-(diethyl-1-carbonyl)ferrocene (4c):



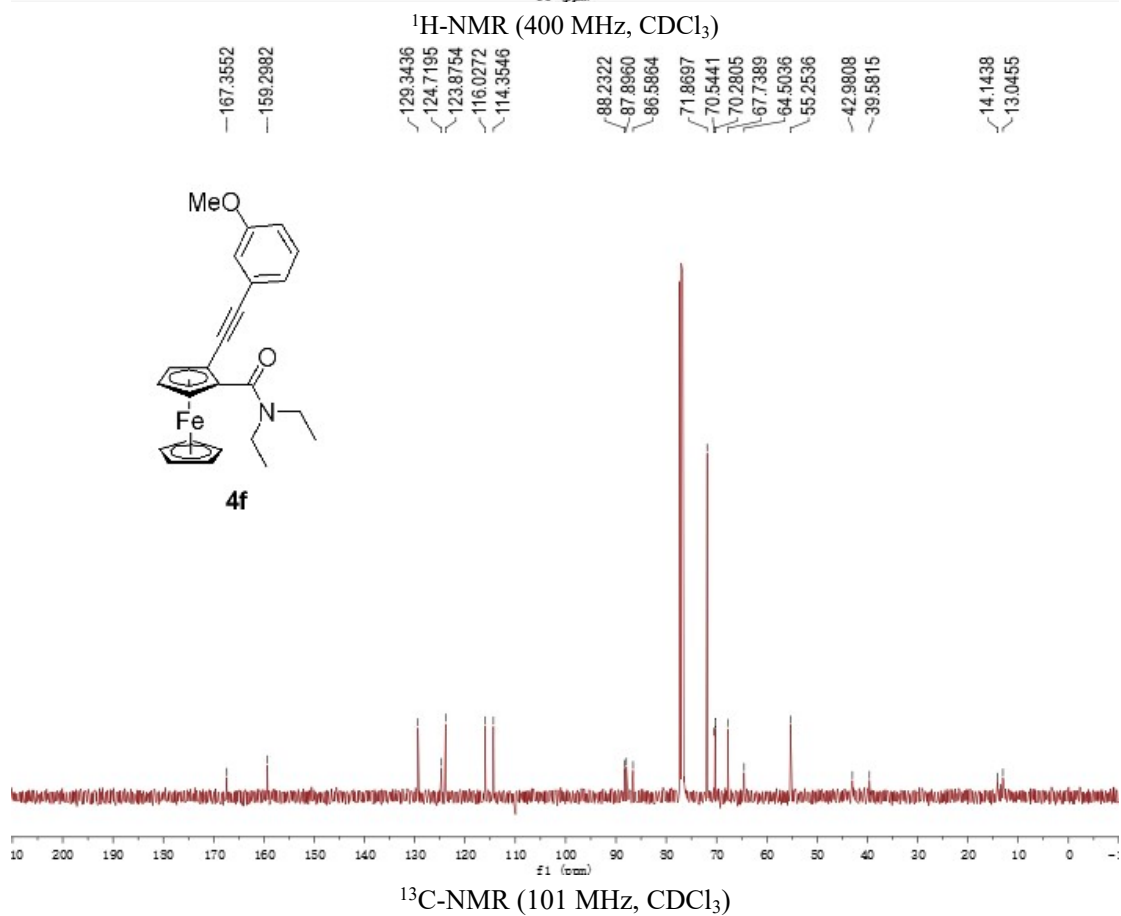
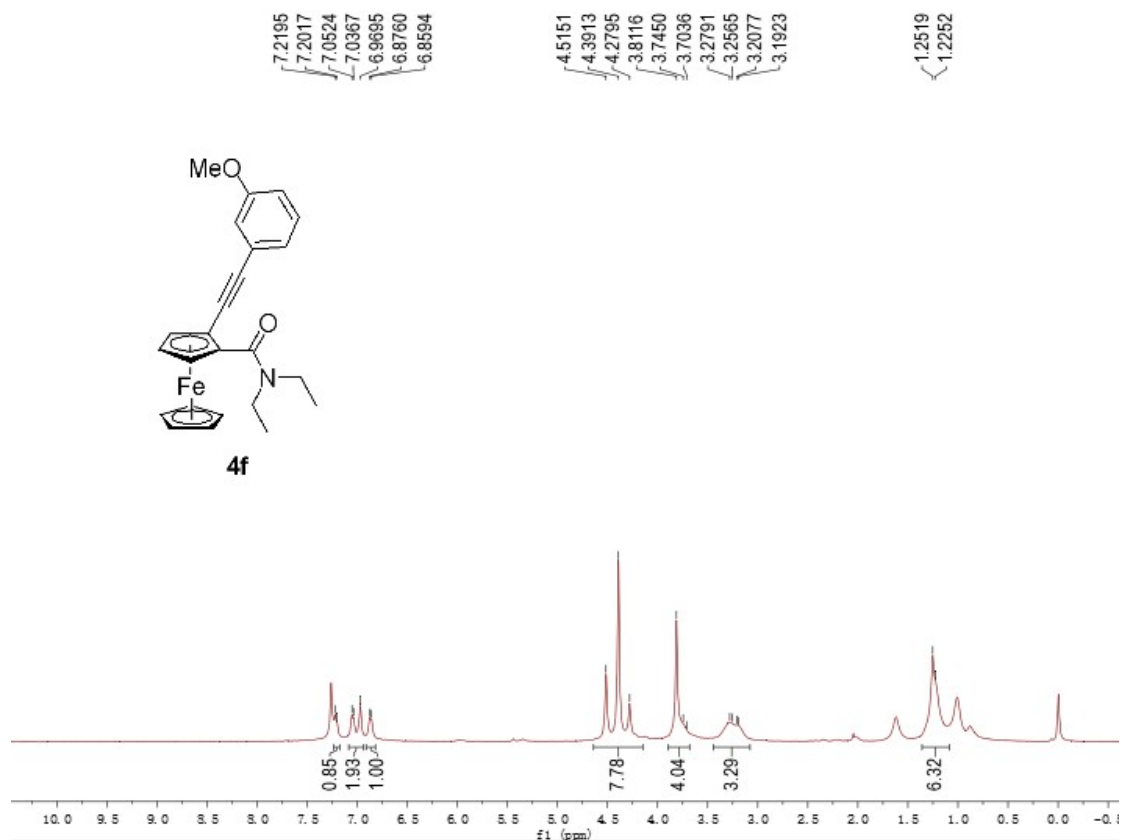
2-(2-chlorophenyl)ethynyl-(diethyl-1-carbonyl)ferrocene (4d):



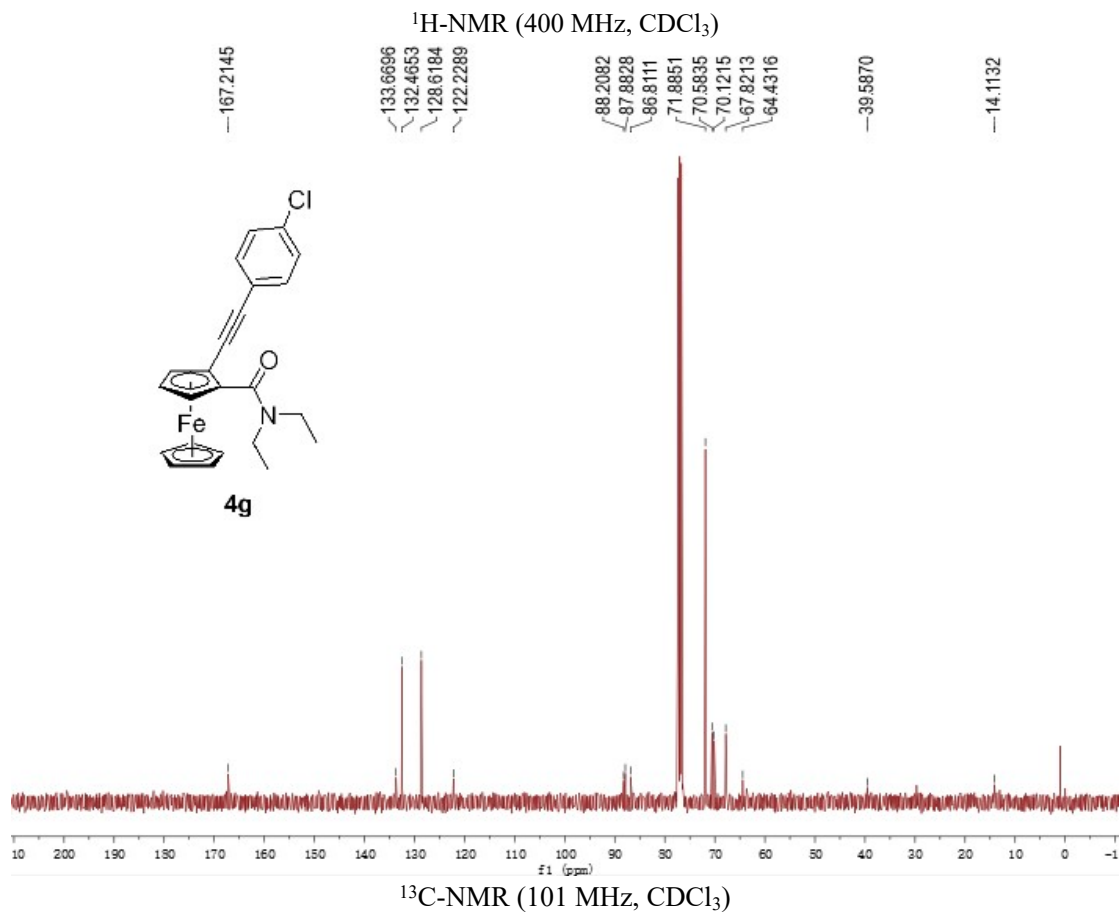
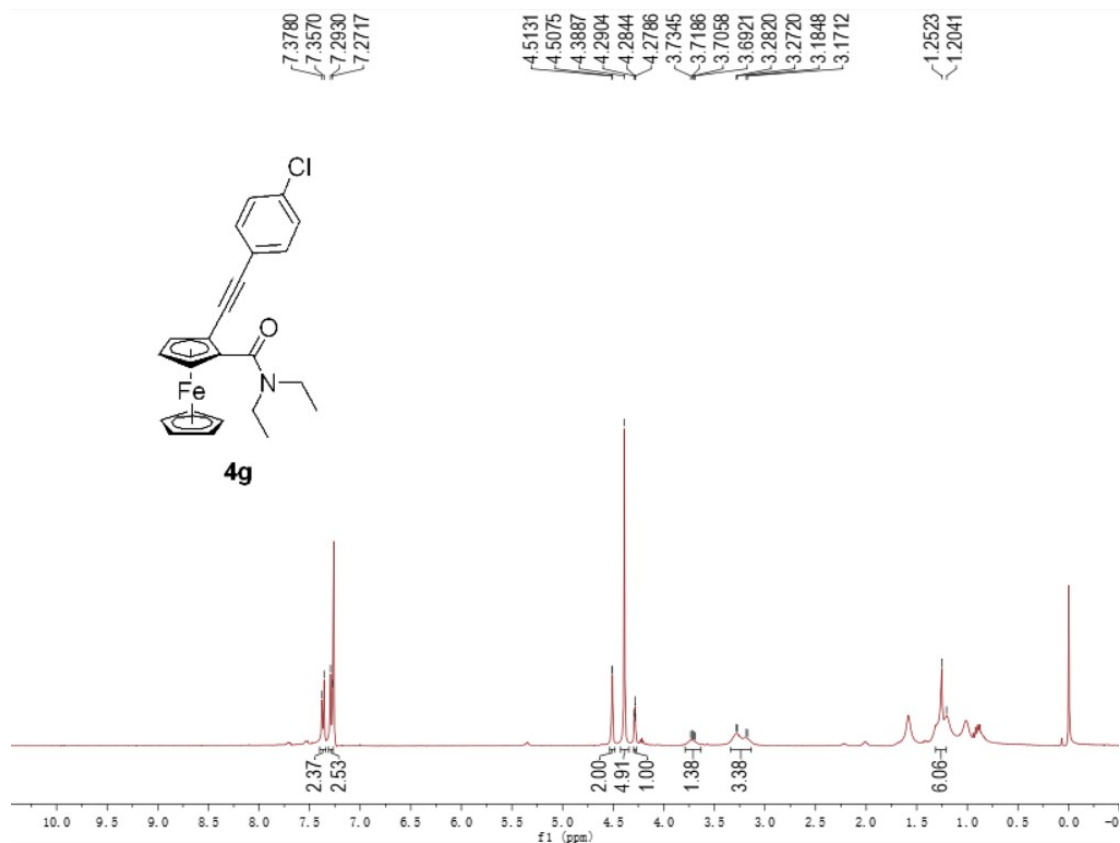
2-(m-tolylethynyl)ethynyl-(diethyl-1-carbonyl)ferrocene (4e):



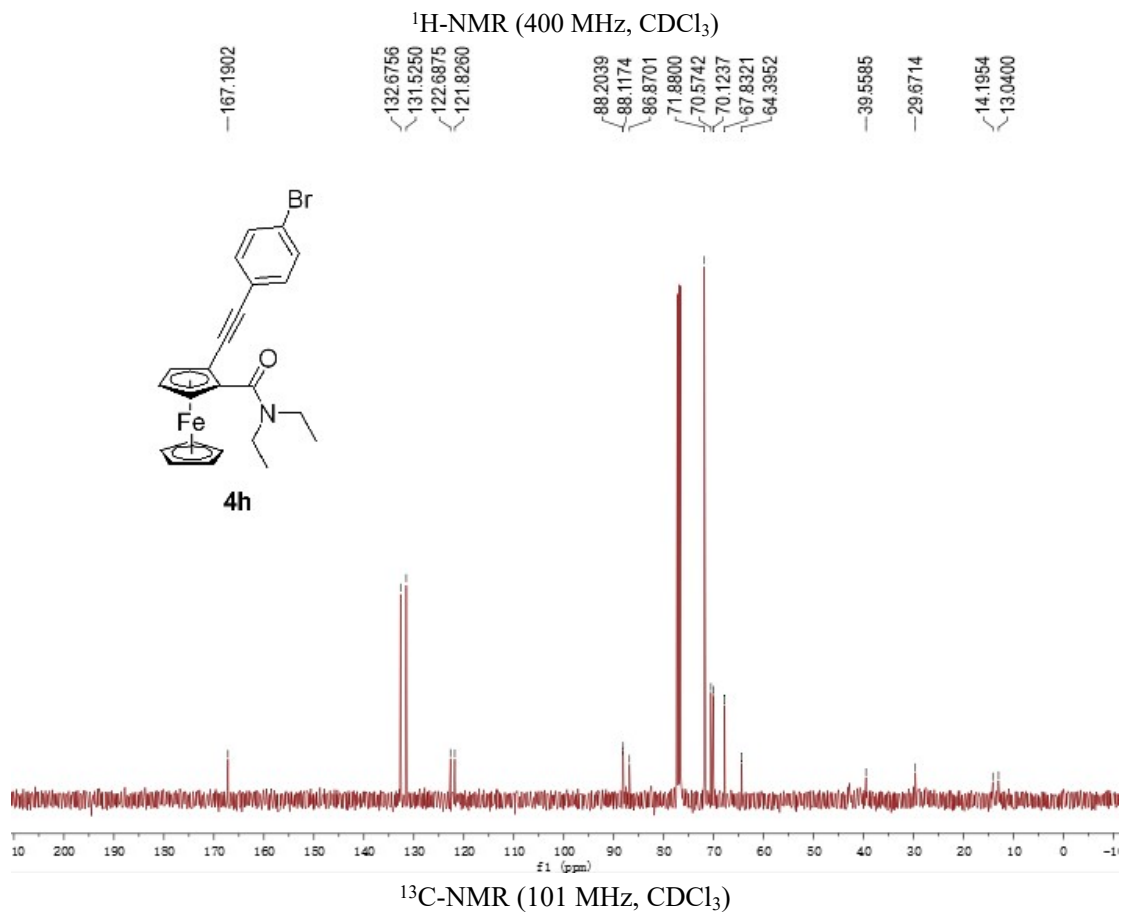
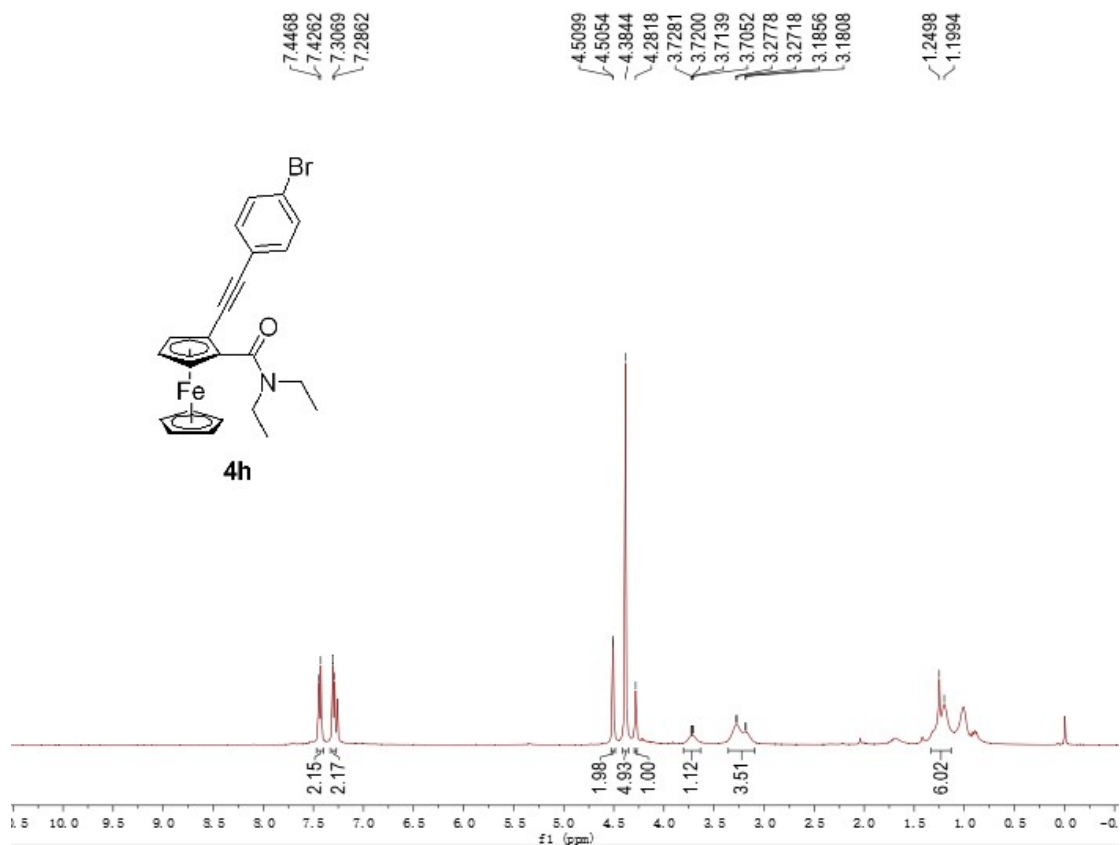
2-(3-methoxyphenyl)ethynyl-(diethyl-1-carbonyl)ferrocene (4f):



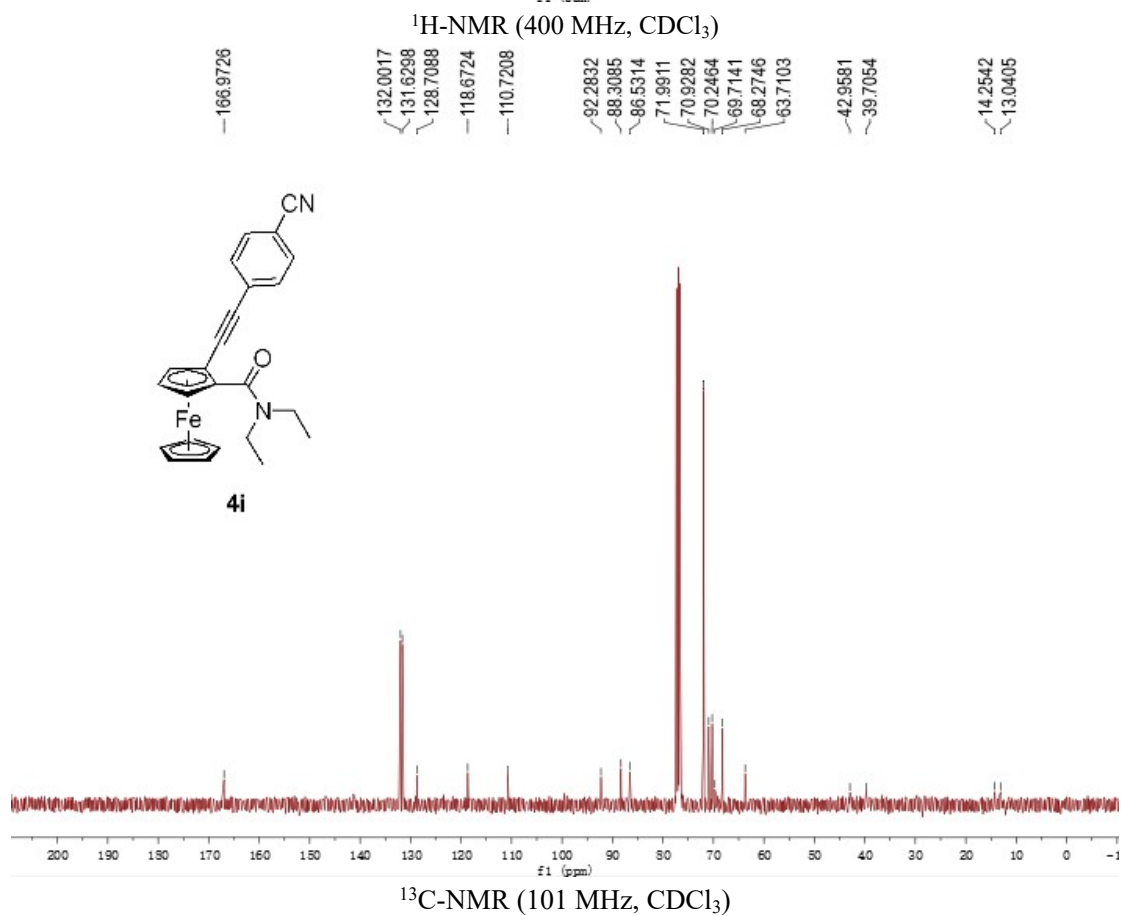
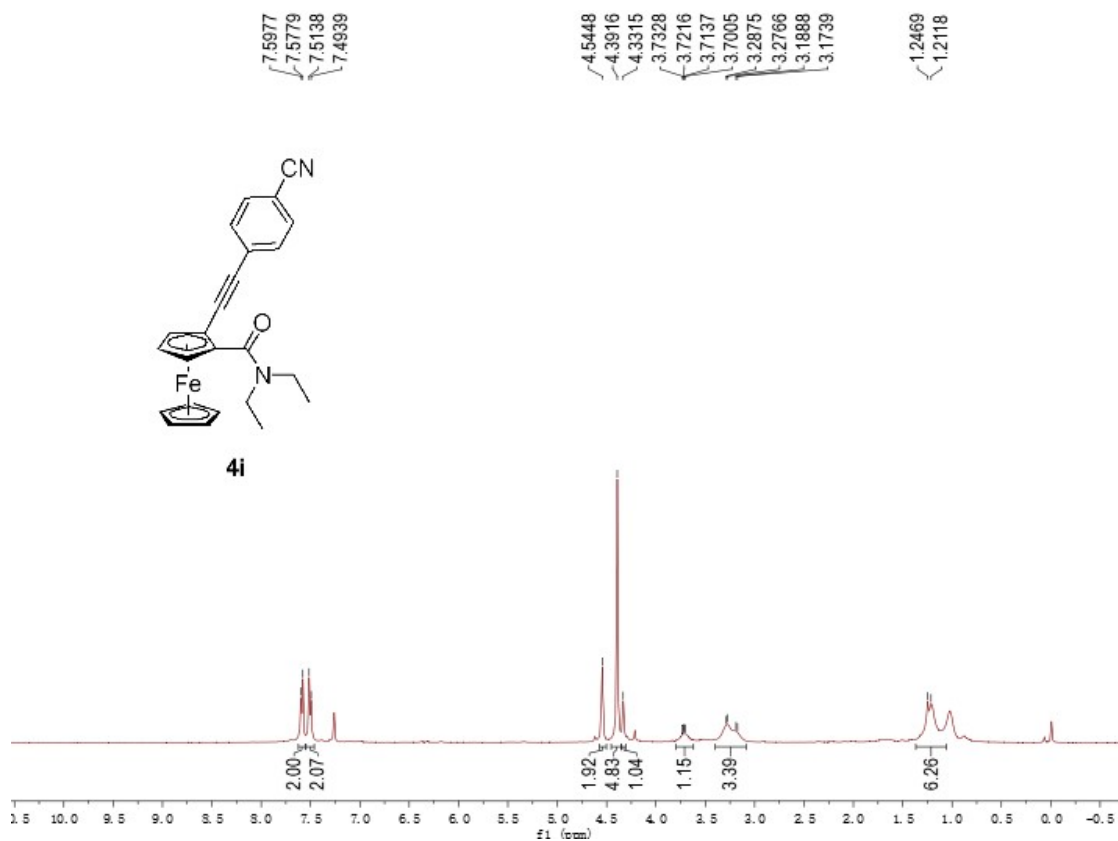
2-(4-chlorophenyl)ethynyl-(diethyl-1-carbonyl)ferrocene (4g):



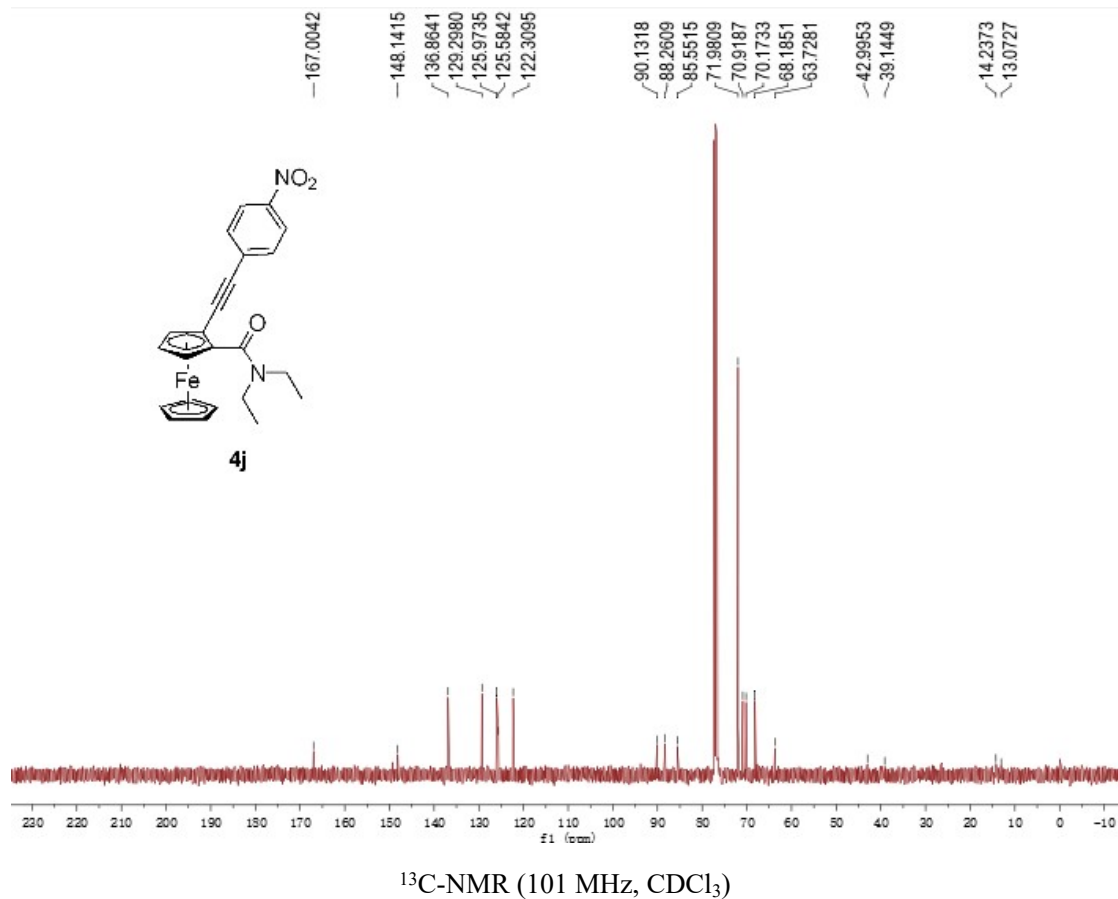
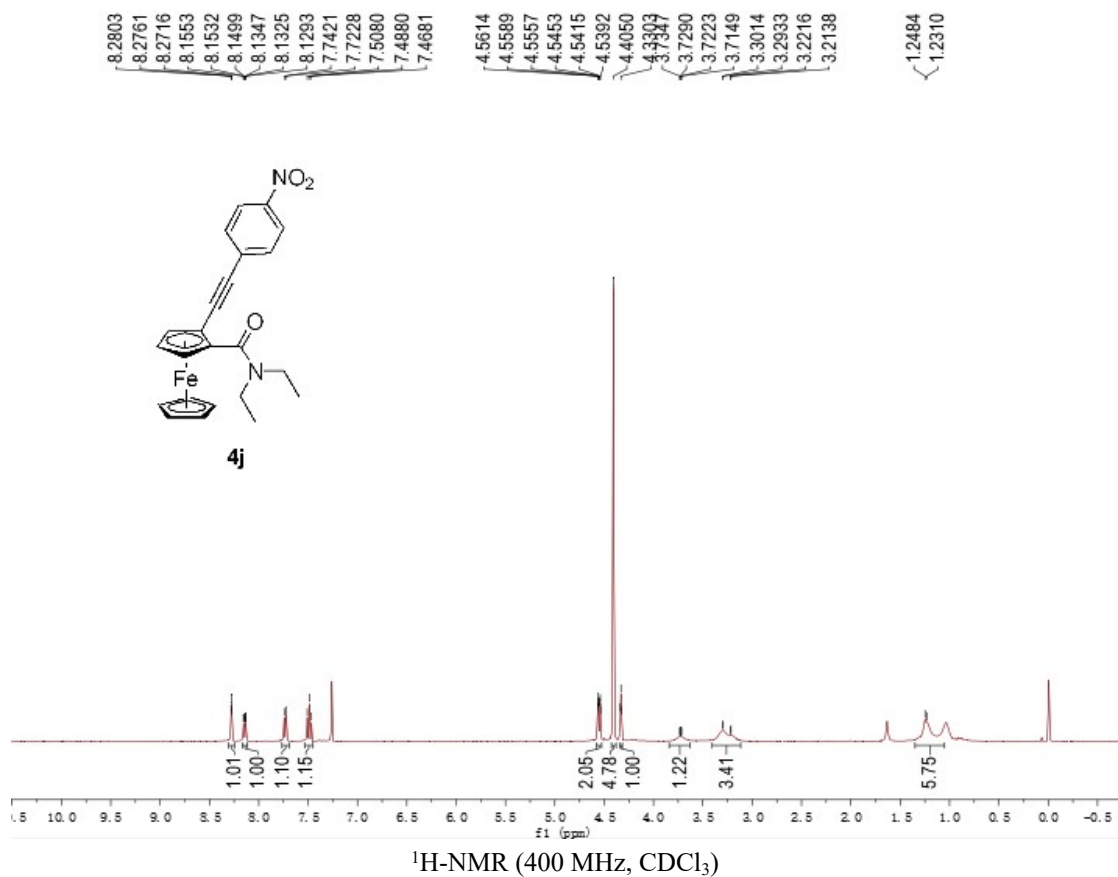
2-(4-bromophenyl)ethynyl-(diethyl-1-carbonyl)ferrocene (4h):



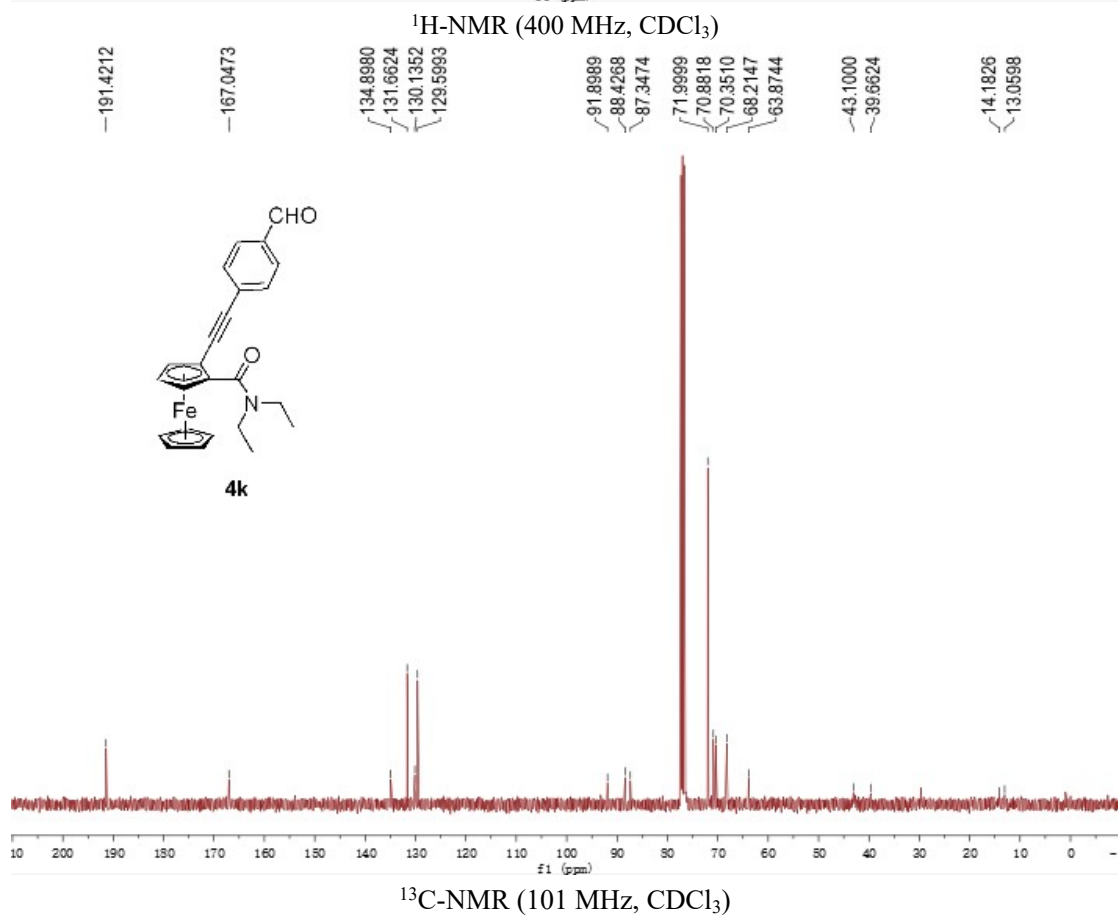
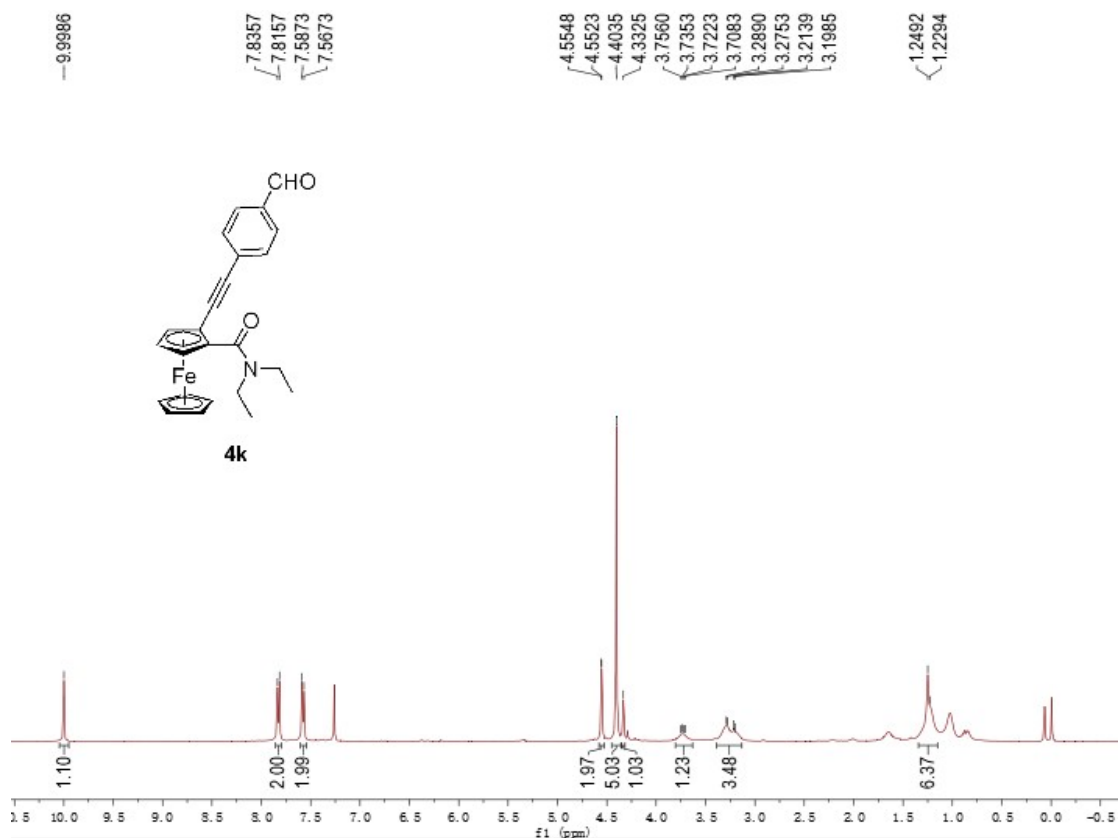
2-(4-cyanophenyl)ethynyl-(diethyl-1-carbonyl)ferrocene (**4i**):



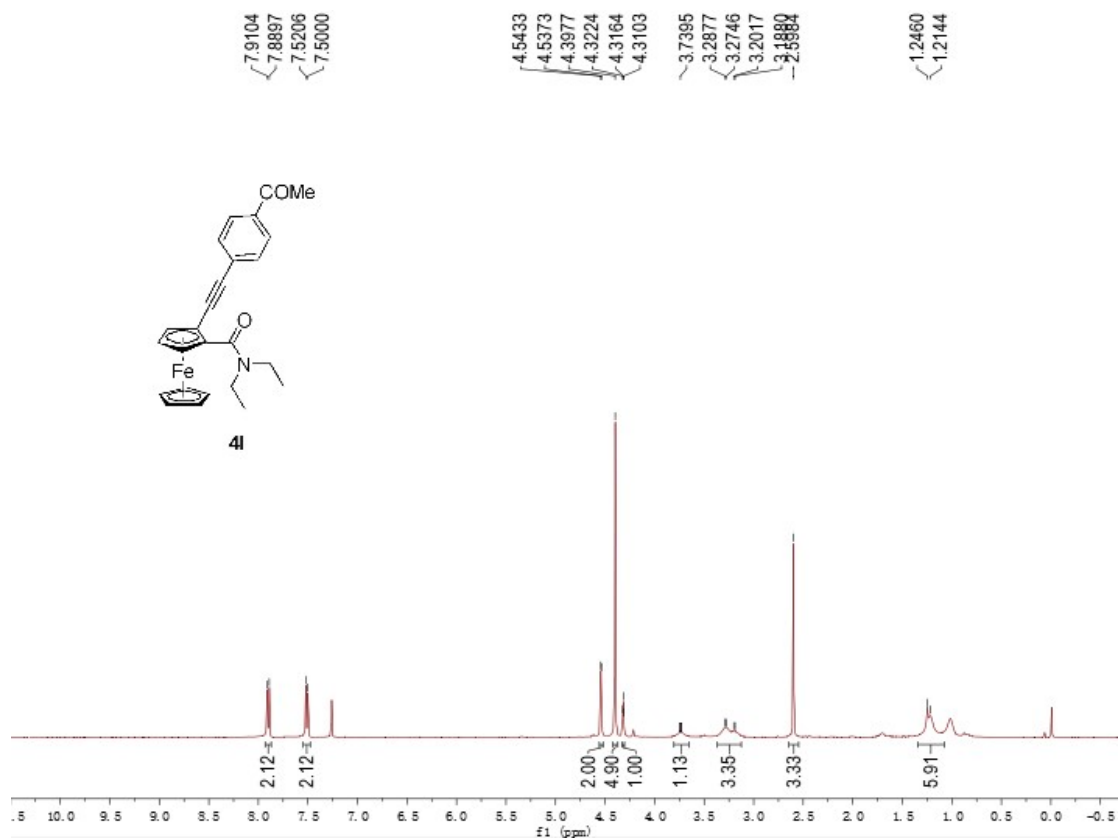
2-(4-nitrophenyl)ethynyl-(diethyl-1-carbonyl)ferrocene (4j):



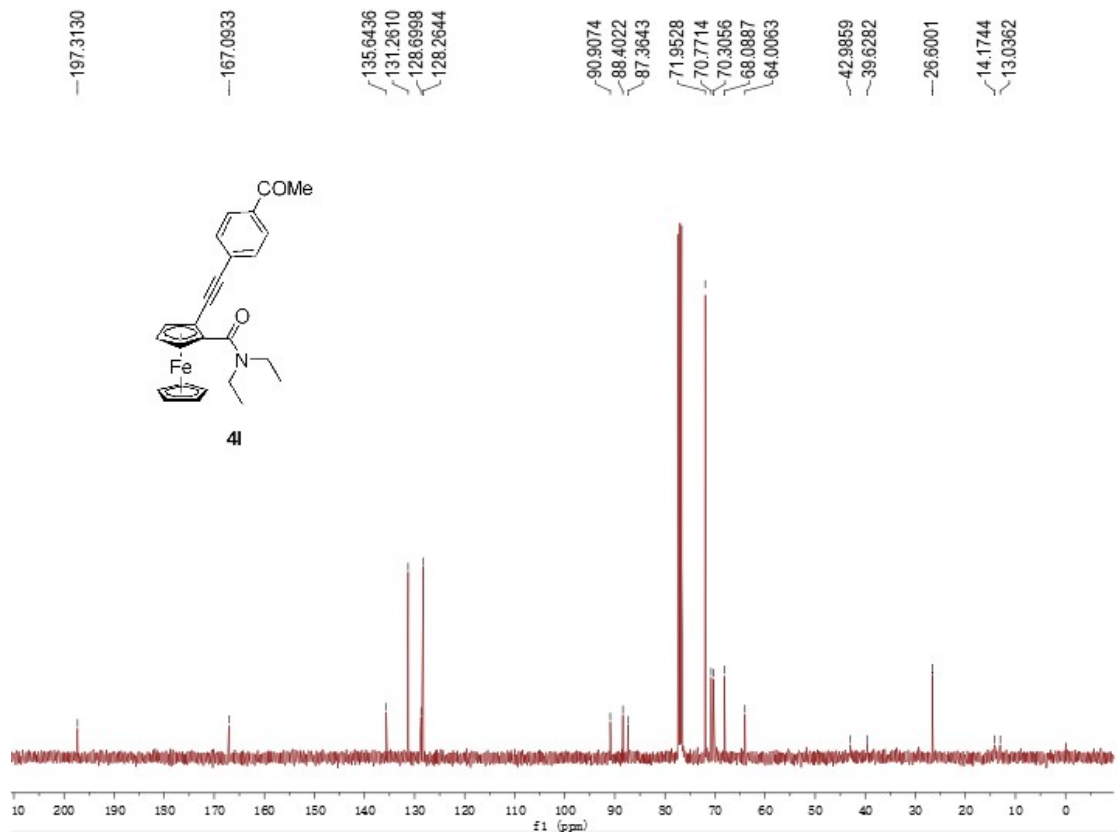
2-(4-formylphenyl)ethynyl-(diethyl-1-carbonyl)ferrocene (4k):



2-(4-acetylphenyl)ethynyl-(diethyl-1-carbonyl)ferrocene (**4**):

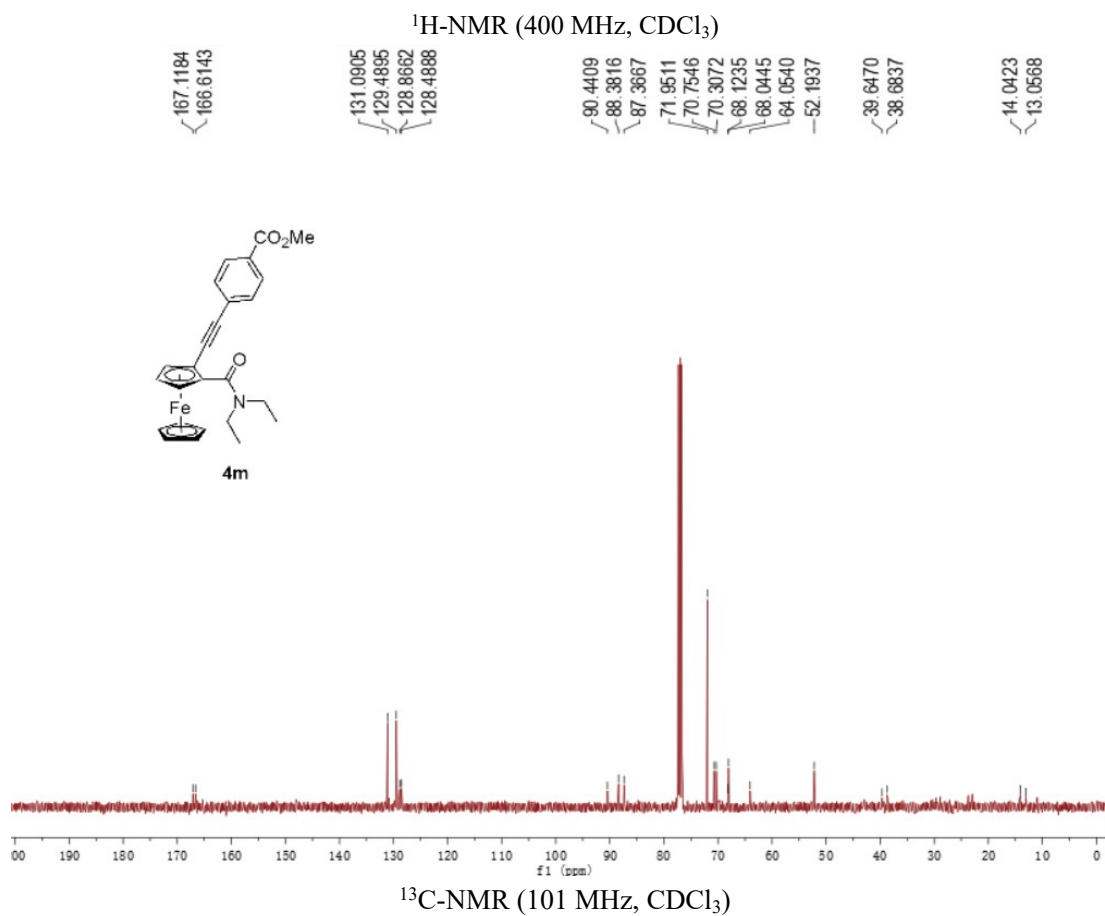
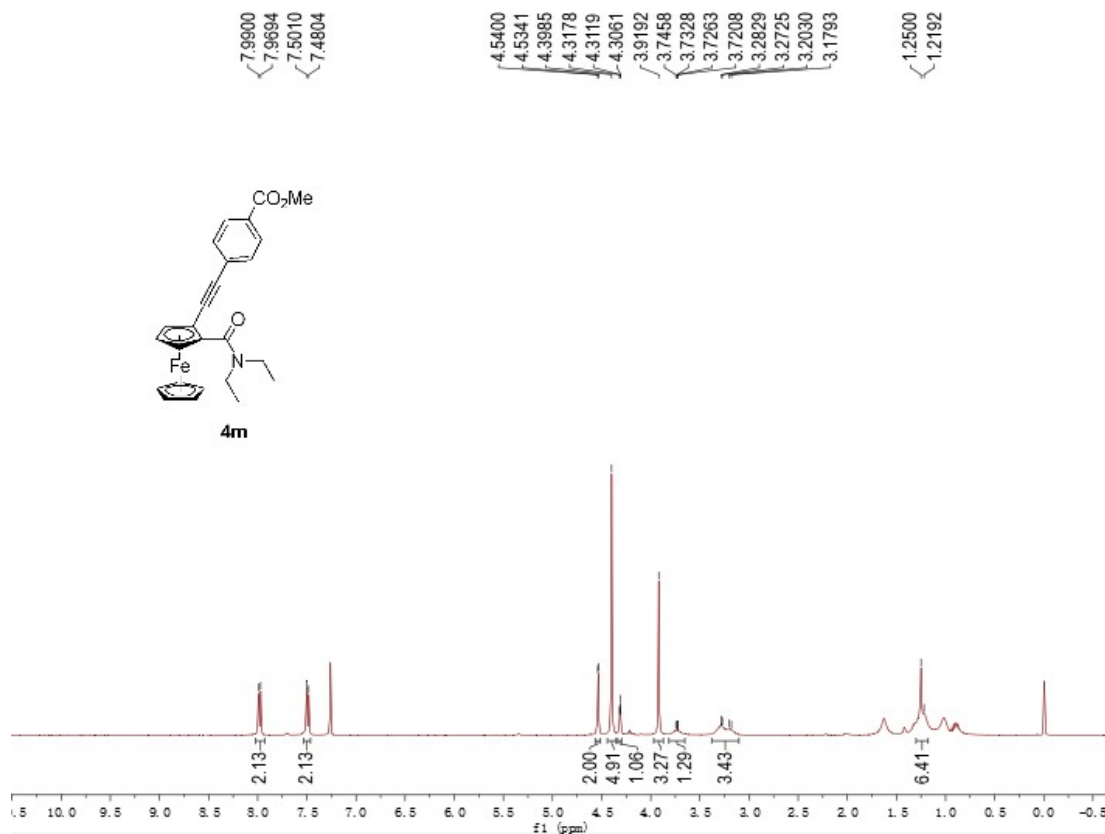


¹H-NMR (400 MHz, CDCl₃)

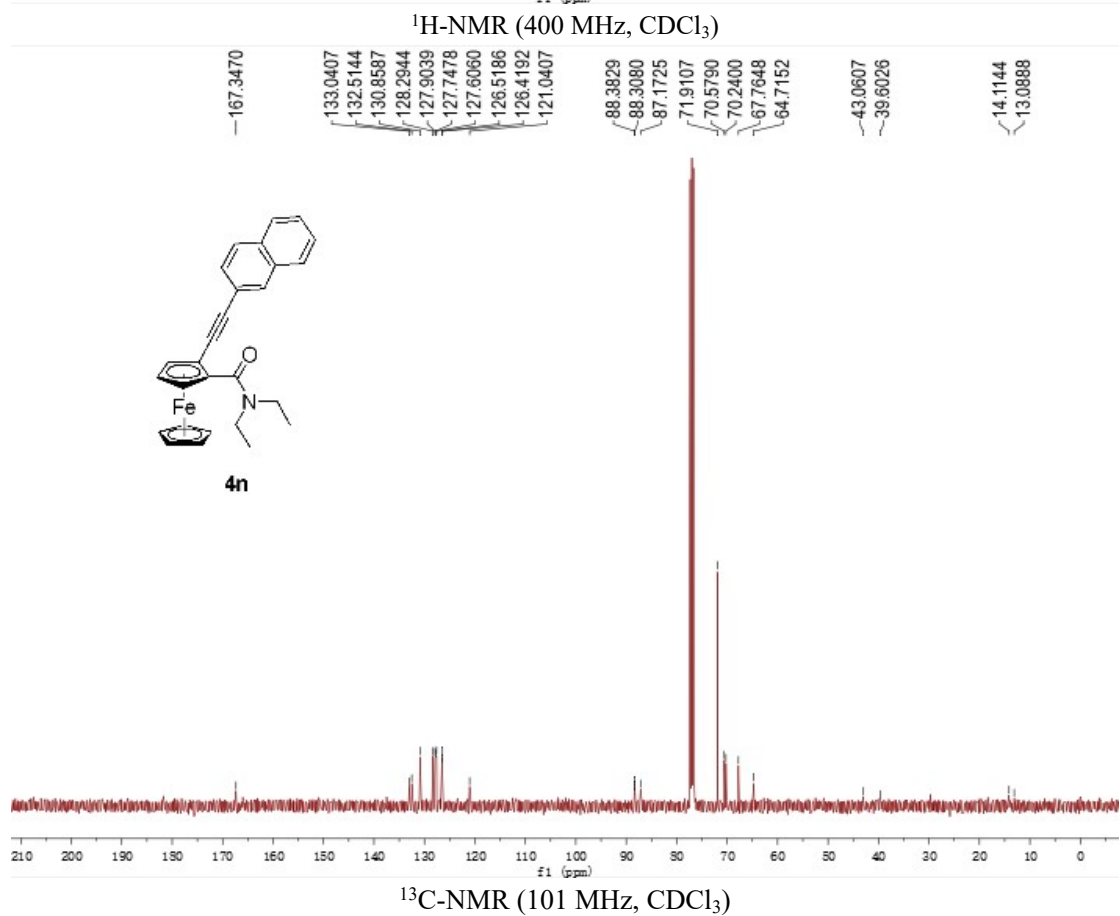
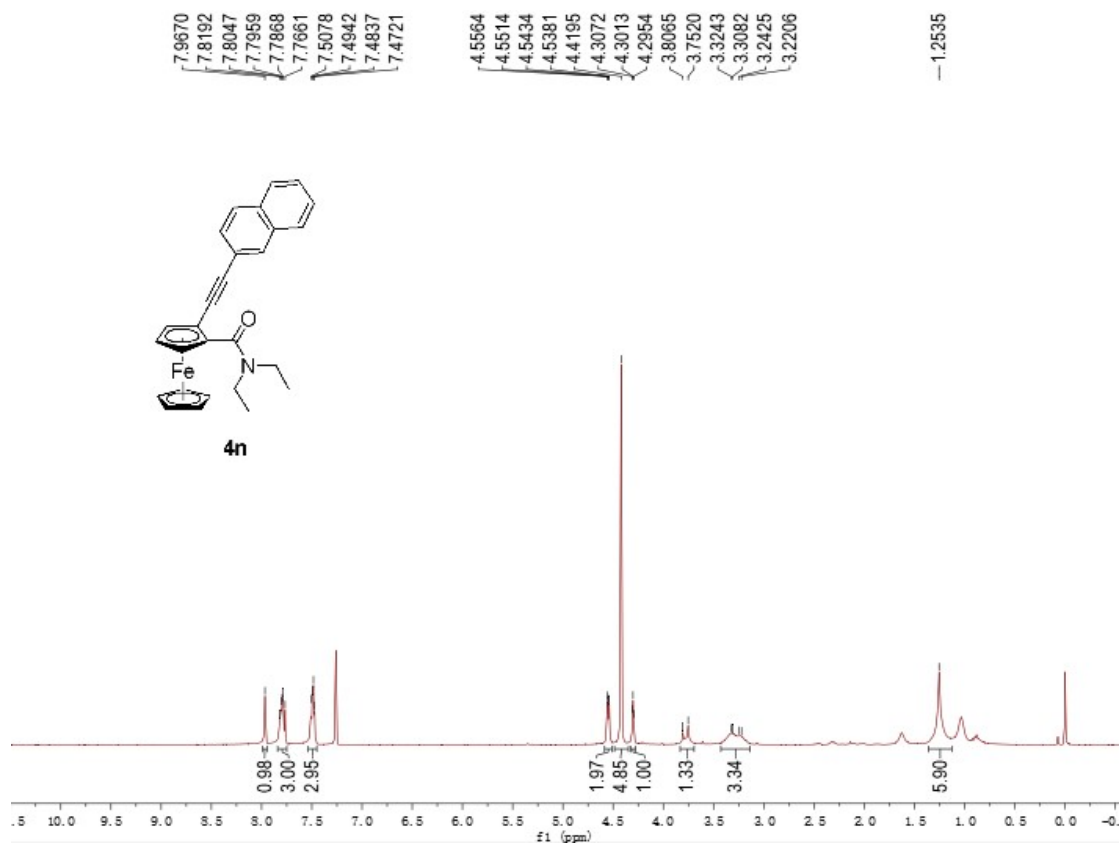


¹³C-NMR (101 MHz, CDCl₃)

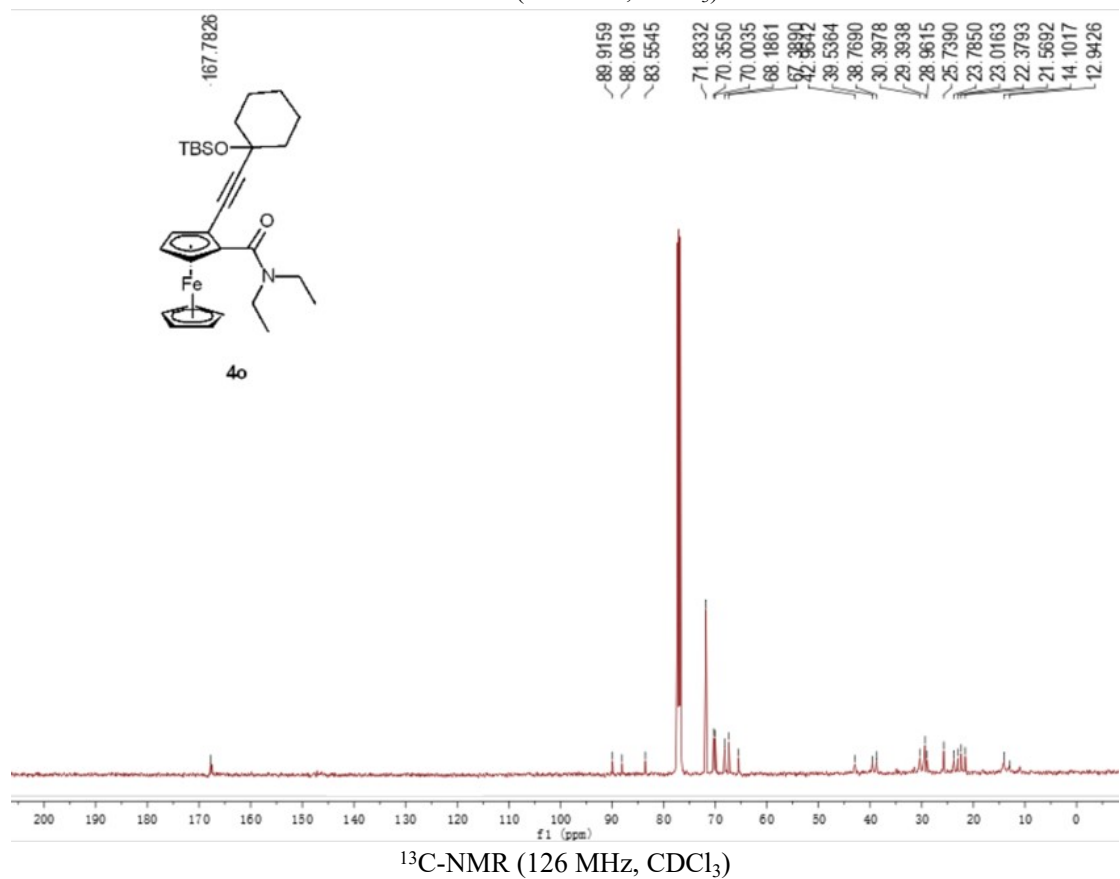
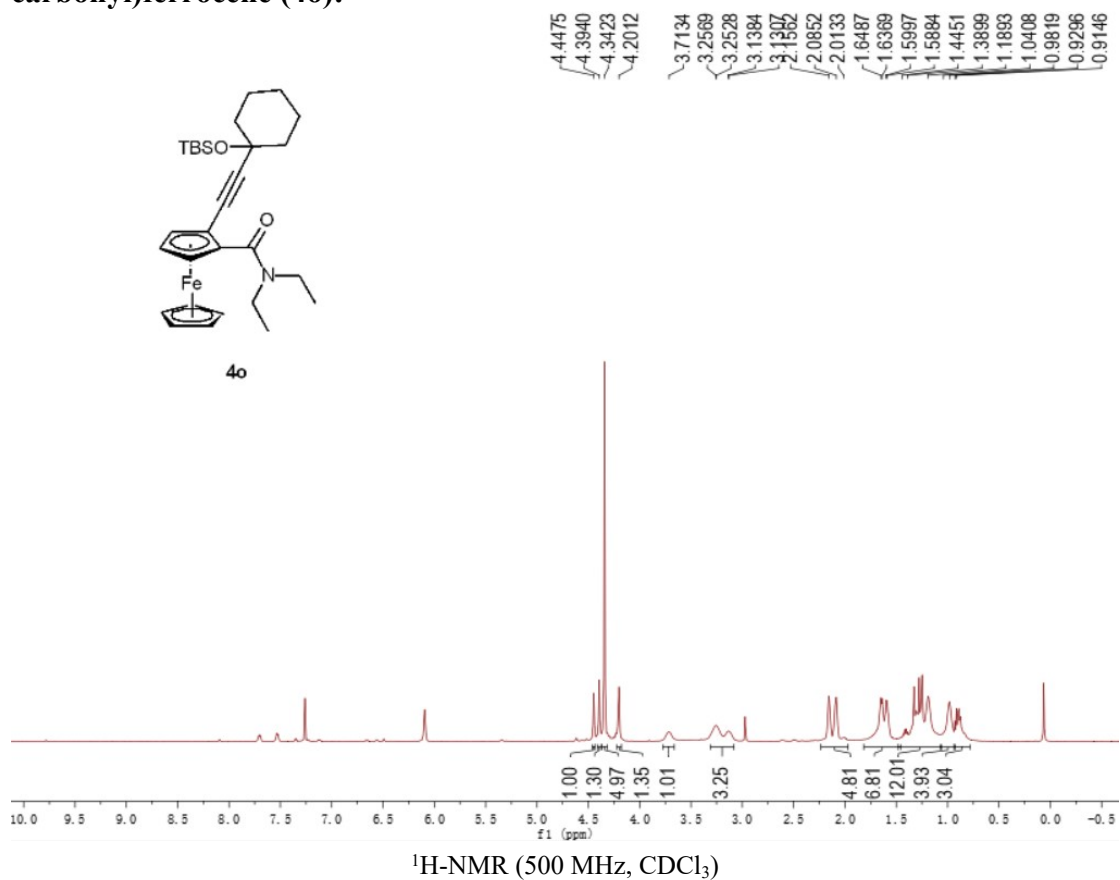
2-(4-methyl benzoate)ethynyl-(diethyl-1-carbonyl)ferrocene (4m):



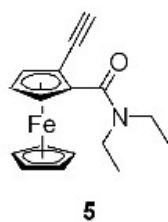
2-(naphthalen-2-ylethynyl)-(diethyl-1-carbonyl)ferrocene (4n):



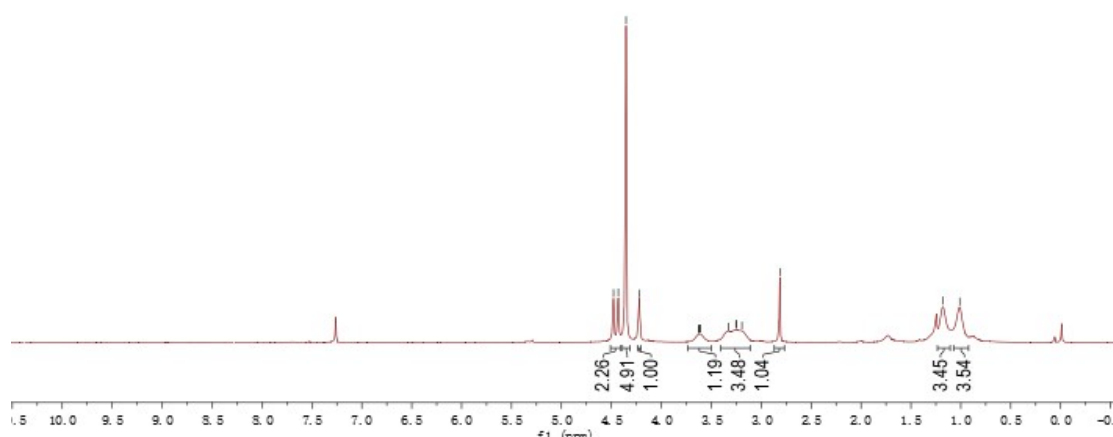
2-((1-((tert-butyldimethylsilyloxy)cyclohexyl)ethynyl)-(diethyl-1-carbonyl)ferrocene (4o):



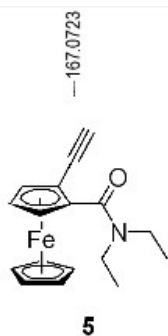
2-Ethynyl-(diethyl-1-carbonyl)ferrocene (5):



4.4786
4.4306
4.3533
4.2208
3.6236
3.6212
3.6160
3.6125
3.3272
3.2532
3.2448
3.1926
2.8134
1.1805
1.0117

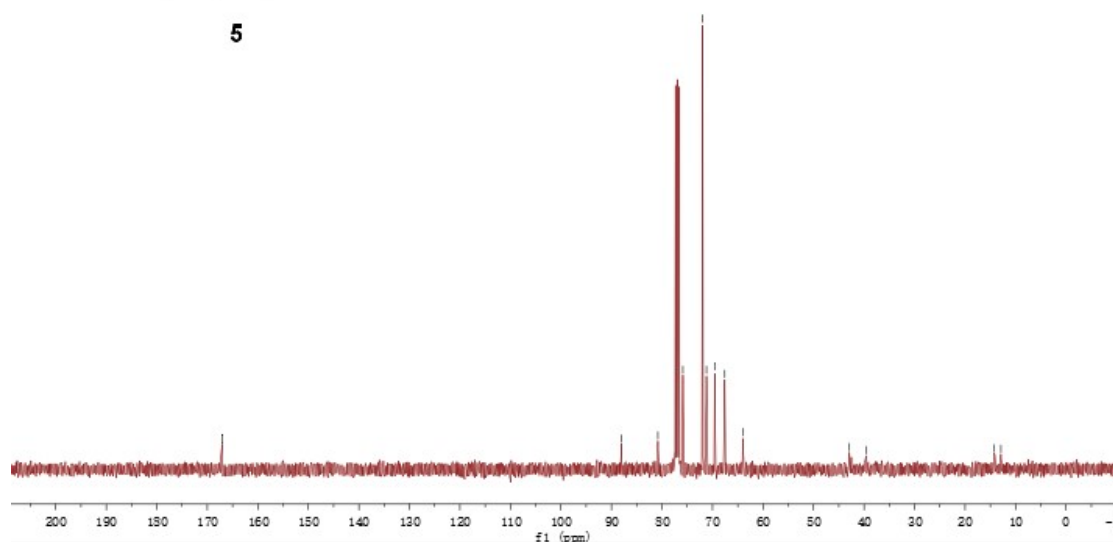


¹H-NMR (400 MHz, CDCl₃)



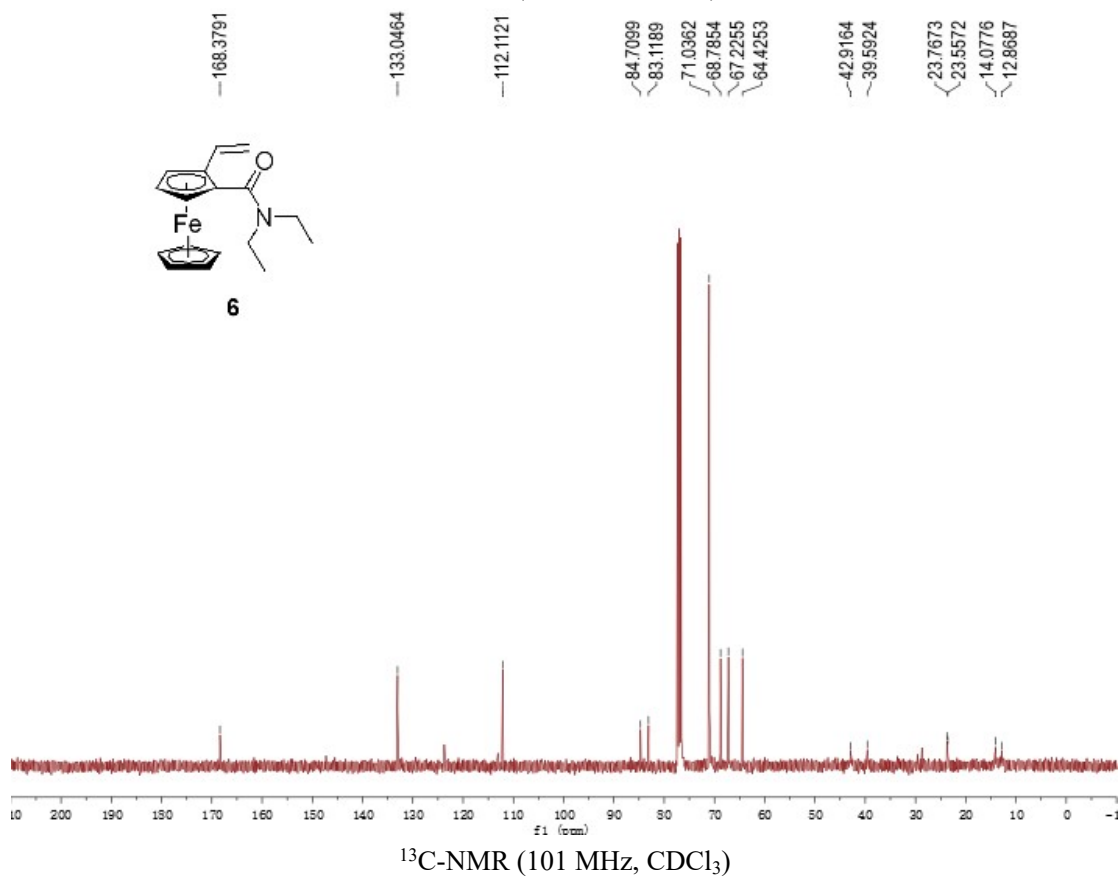
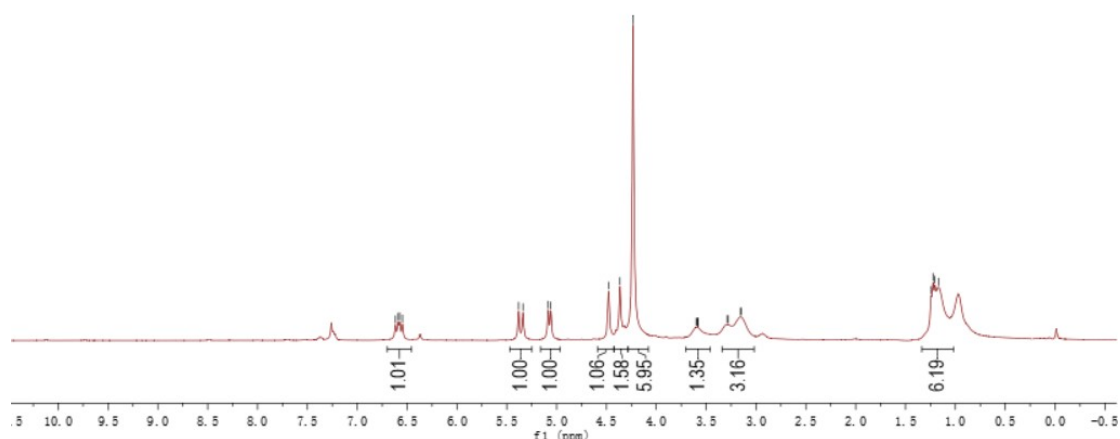
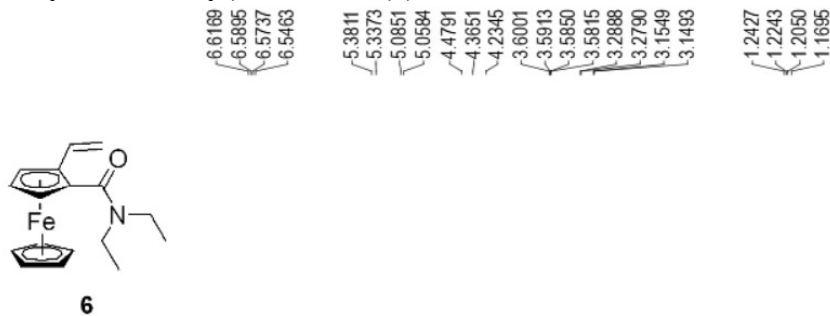
167.0723

88.0083
80.7989
75.8557
71.9283
71.1929
69.5521
67.5797
63.9924
42.9004
39.5897
14.2203
12.9040

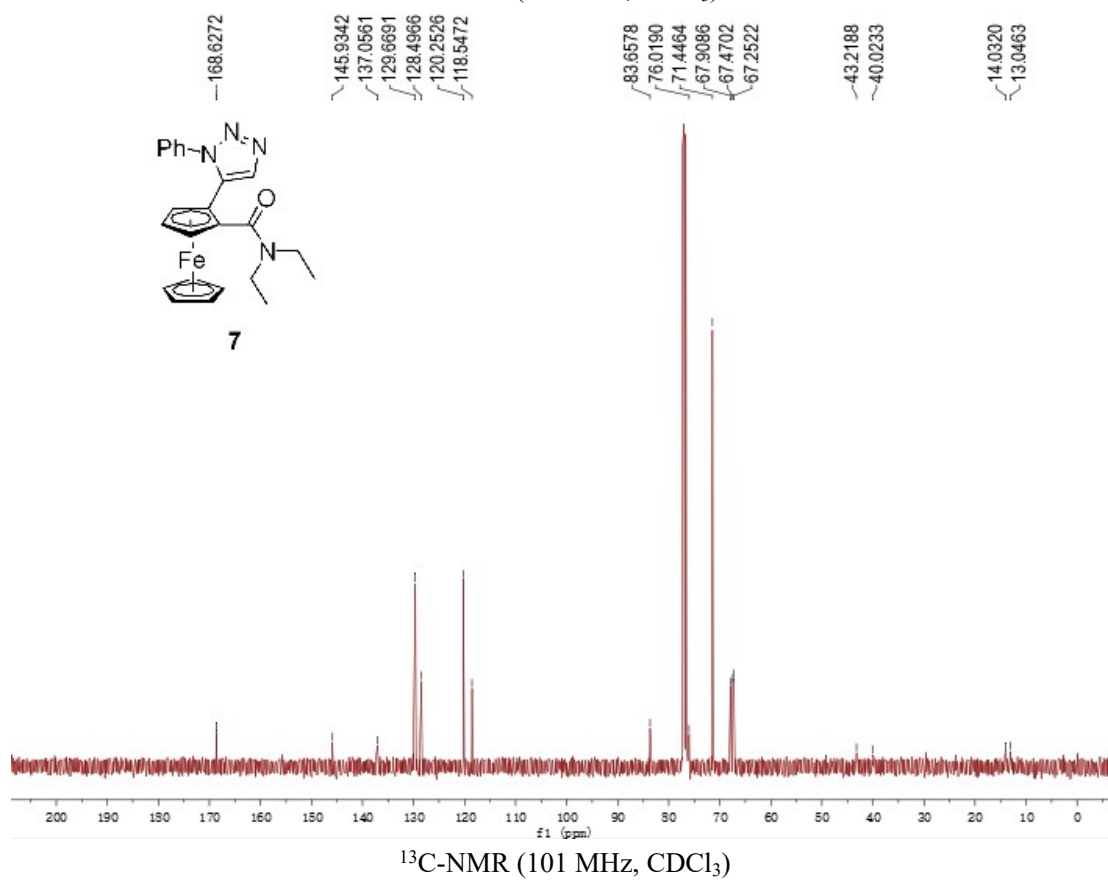
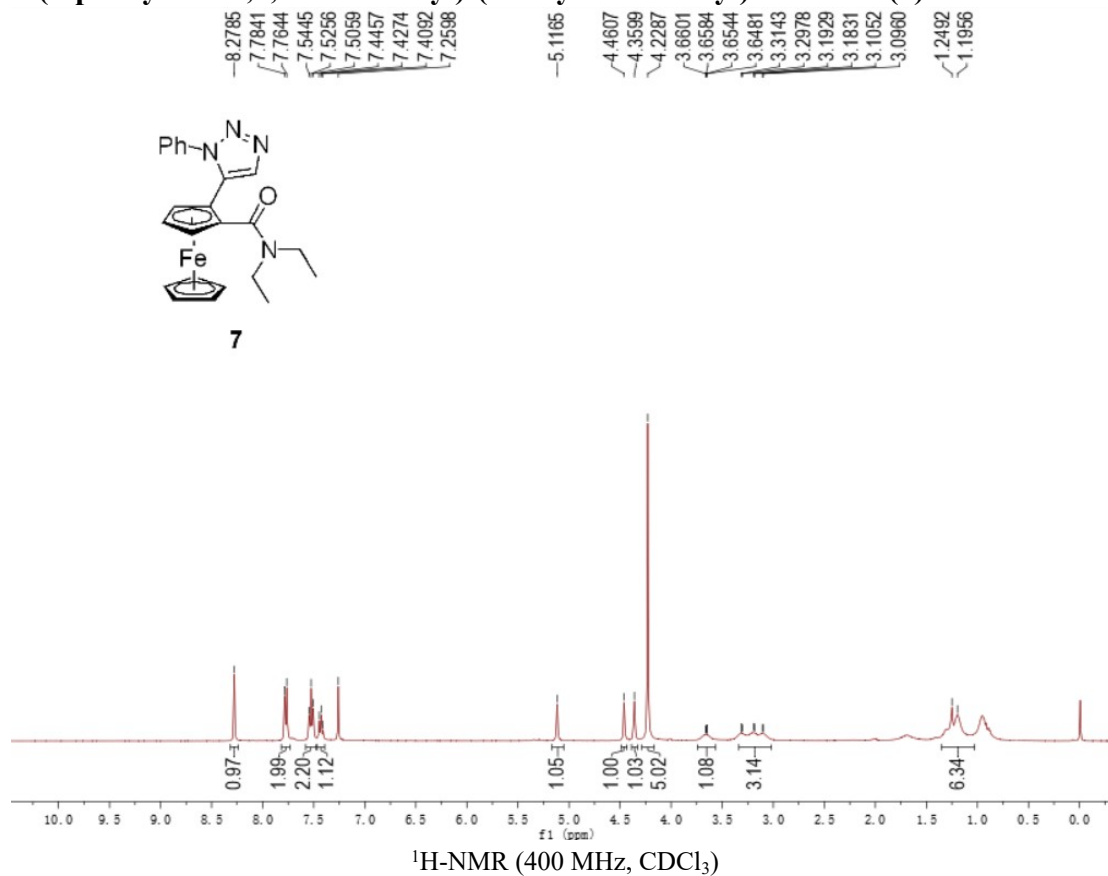


¹³C-NMR (101 MHz, CDCl₃)

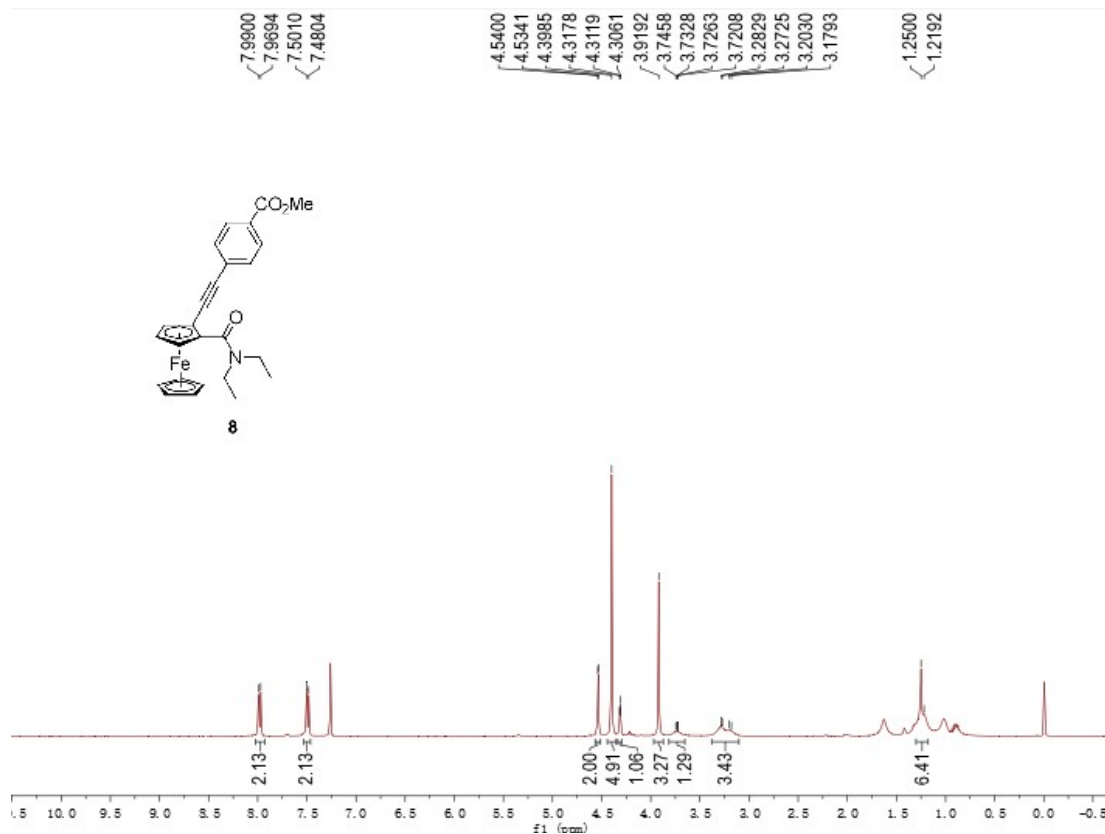
2-vinyl-(diethyl-1-carbonyl)ferrocene (6):



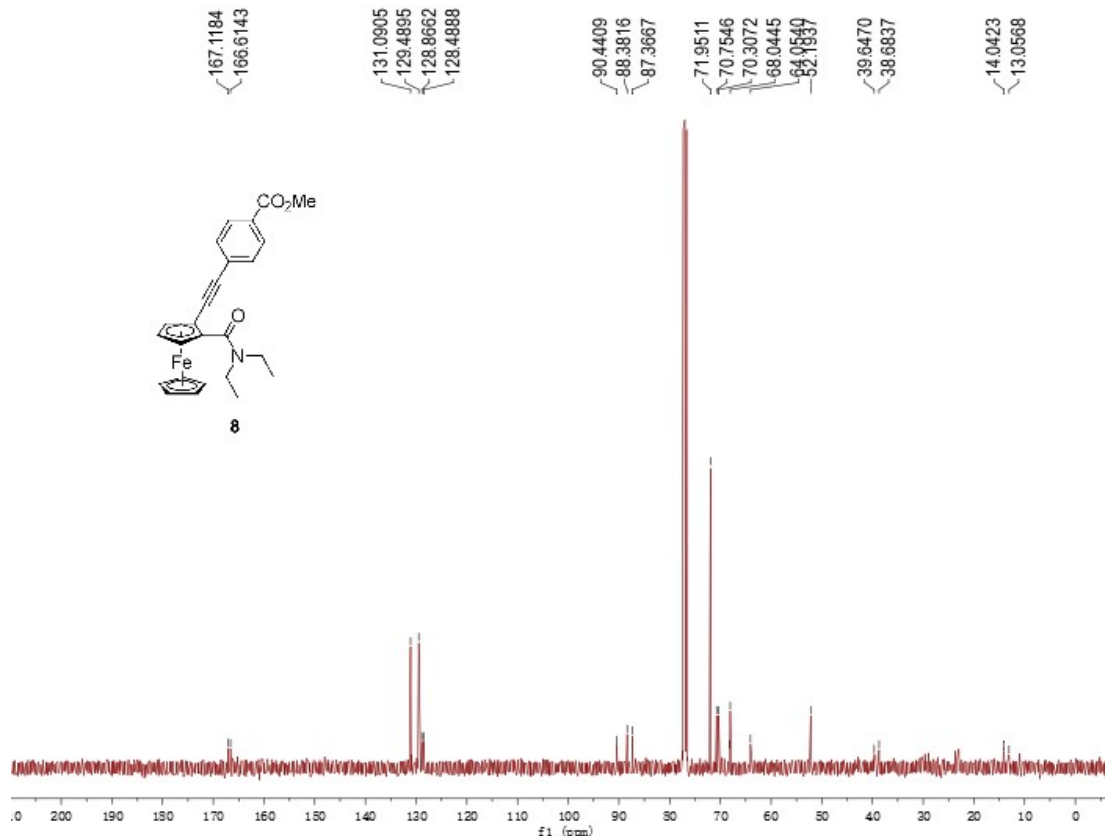
2-(1-phenyl-1H-1,2,3-triazol-5-yl)-(diethyl-1-carbonyl)ferrocene (7):



2-(4-methyl benzoate)ethynyl-(diethyl-1-carbonyl)ferrocene (8):



¹H-NMR (400 MHz, CDCl₃)



¹³C-NMR (101 MHz, CDCl₃)