Direct enantiospecific substitution of primary α-aminoalkylferrocenes via Lewis acid-catalyzed C-N bond cleavage

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Supporting information

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General information

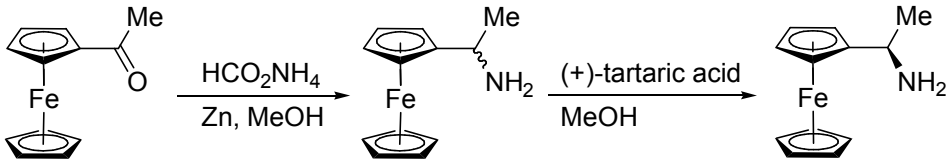
^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker AC-400 FT (400 MHz and 100 MHz, respectively) using tetramethylsilane as an internal reference. Chemical shifts (δ) and coupling constants (J) were expressed in ppm and Hz, respectively. The following abbreviations are used in reporting NMR data: s, singlet; br, broad; d, doublet; t, triplet; q, quartet; m, multiplet. High resolution mass spectra (HRMS) were recorded on a LC-TOF spectrometer (Micromass). High pressure liquid chromatography (HPLC) analyses were performed on a Hewlett-Packard 1200 Series instrument equipped with an isostatic pump, using a Daicel Chiralpak column (IC, AD, AD-H, OD, AS, AS-H, 250 x 4.6 mm) with *n*-hexane/isopropanol as mobile phase, and the UV detection was monitored at 254 nm. Optical rotations were measured on a Perkin-Elmer 343 polarimeter with a sodium lamp at λ = 589 nm and reported as $[\alpha]_D^{T\,^\circ C}$ (c =g/100 mL, solvent). Melting points are uncorrected.

Malononitrile **2m**[1a] and amine **1j**[1b] were prepared according to the literature. The chemicals were purchased from the Sinopharm Chemical Reagent Co., Meryer, Acros, Alfa Aesar, and TCI, and used as received.

Abbreviations: Bn = benzyl. Tf = trifluoromethanesulfonyl. THF = tetrahydrofuran. Ts = *p*-toluenesulfonyl.

Preparation of enantioenriched primary α-aminoalkylferrocenes

(1) Preparation of amine 1a[2]



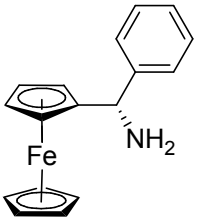
rac-1a **1a**

A mixture of acetylferrocene (22.8 g, 100 mmol), HCO_2NH_4 (37.9 g, 600 mmol), and Zn powder (19.6 g, 300 mmol) in methanol (300 mL) was stirred under reflux for 8 h. The mixture was cooled to room temperature, filtered, and concentrated under reduced pressure. The residue was treated with water (200 mL) and aqueous HCl (6 M, 20 mL), and then extracted with diethyl ether (2 x 100 mL). The aqueous phase was alkalized with aqueous ammonia (25% wt) to pH = 10 and extracted with dichloromethane (3 x 100 mL). The organic phase was washed with brine, dried over sodium sulfate, and concentrated under reduced pressure to give amine **rac-1a** (6.84 g, 30% yield) as an orange oil.

To a stirred solution of (+)-tartaric acid (15.0 g, 100 mmol) in methanol (300 mL) was added a solution of amine **rac-1a** (22.9 g, 100 mmol) in methanol (100 mL). The solution stood at room temperature for 24 h. The resulting crystals were filtered and washed with a small portion of cold methanol (3 x 5 mL). Three further crystallizations from hot methanol gave the (+)-tartrate salt of the chiral amine. The salt was dissolved in water (100 mL) and treated with aqueous sodium hydroxide (10.0 g in 50 mL). The mixture was extracted with ether (3 x 100 mL) and the organic phase was washed with brine, dried over sodium sulfate, and concentrated under reduced pressure to give amine **1a** (6.85 g, 30% yield, 96% ee) as an orange oil.[3] The ee of amine **1a** was determined by converting it to amide **1a-Bz** (see below). $[\alpha]_D^{20}$ = -25.8 (c = 1.0, EtOH); Lit.:[3] $[\alpha]_D^{20}$ = -22.1 (c

= 3.3, EtOH); ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.16–4.09 (m, 9H), 3.78 (q, J = 6.4 Hz, 1H), 1.71 (s, br, 2H), 1.33 (d, J = 6.4Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 96.5, 68.3, 67.4, 65.7, 46.0, 24.8.

(2) Preparation of amine ent-1g

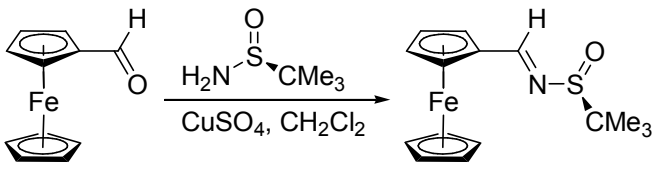


ent-1g

According to known procedures, amine **ent-1g** was prepared by resolution of the racemic mixture[4a] with (-)-dibenzoyl-*L*-tartaric acid monohydrate.[4b] The absolute configuration of amine **ent-1g** was confirmed to be *S* by single-crystal X-ray analysis (see below). The ee of amine **ent-1g** was determined to be 94% by converting it to amide **ent-1g-Bz** (see below). $[\alpha]_D^{20}$ = +12.5 (c = 1.3, C_6H_6); Lit.:[5] $[\alpha]_D^{25}$ = +15.4 (c = 1.13, C_6H_6, 98% ee); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36–7.18 (m, 5H), 4.88 (s, 1H), 4.31–4.29 (m, 1H), 4.18–4.08 (m, 8H), 1.87 (s, br, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.7, 128.4, 127.1, 126.9, 94.8, 68.6, 68.0, 67.6, 67.3, 65.8, 55.5.

(3) Preparation of amines 1b-f and 1h

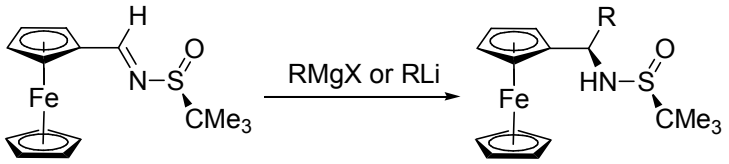
(3a) Preparation of *N*-*tert*-butanesulfinyl imines[6]



S-1

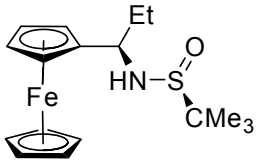
To a solution of (*S*)-*tert*-butanesulfinamide (1.21 g, 10 mmol) in dichloromethane (20 mL) was added $CuSO_4$ (3.51 g, 22 mmol) followed by ferrocenecarboxaldehyde (2.35 g, 11 mmol). The mixture was stirred at room temperature for 24 h and then filtered. The filter cake was washed well with dichloromethane (3 x 5 mL). The filtrate was concentrated under reduced pressure and the residue was purified by silica gel chromatography (petroleum/ethyl acetate = 5/1) to give imine **S-1** (2.85 g, 90% yield) as a red solid. m.p. 115–116 ^{o}C; $[\alpha]_D^{20}$ = -34.9 (c = 0.9, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (s, 1H), 4.77–4.73 (m, 2H), 4.54–4.51 (m, 2H), 4.22 (s, 5H), 1.25 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.2, 78.6, 72.0, 69.9, 69.6, 69.1, 56.8, 22.6; HRMS (EI) calcd for $C_{15}H_{19}NOSFe$ (M) 317.0537, found 317.0530.

(3b) Addition of organometallic reagents to imine **S-1**[7]



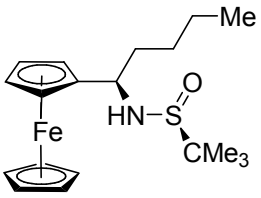
S-1 **5**

To a solution of imine **S-1** (1.59 g, 5.0 mmol) in dichloromethane (20 mL) under nitrogen at -78 °C was added dropwise a solution of RMgX or RLi (10 mmol). The mixture was stirred at -78 °C for 5 h, slowly warmed to room temperature, and stirred for 8 h. Saturated aqueous ammonium chloride (10 mL) was added, and the resulting mixture was extracted with dichloromethane (3 x 10 mL). The organic phases were combined, washed with brine, dried over sodium sulfate, filtered, and concentrated under reduced pressure. The residue was purified by silica gel chromatography (petroleum/ethyl acetate = 10:1 to 4:1) to give sulfinamide **5**.



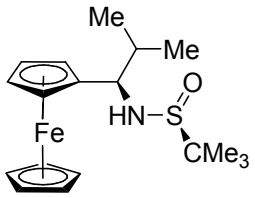
5b

Sulfinamide **5b** was obtained in 99% yield with 99% de (inseparable diastereomers) from the reaction of imine **S-1** with EtMgBr (3.0 M in ether). The de of sulfinamide **5b** was determined by converting it to amine **1b** (see below). Yellow solid; m.p. 43–44 °C; $[\alpha]_D^{20}$ = -10.7 (c = 0.6, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.22–4.05 (m, 10H), 3.42 (d, J = 6.0 Hz, 1H), 2.04–1.90 (m, 1H), 1.88–1.75 (m, 1H), 1.26 (s, 9H), 1.04 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 91.9, 68.7, 67.9, 67.6, 66.4, 57.5, 56.0, 30.4, 22.9, 10.8; HRMS (EI) calcd for $C_{17}H_{25}NOSFe$ (M) 347.1006, found 347.0999.



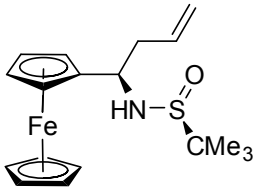
5c

Sulfinamide **5c** was obtained in 95% yield with 75% de (separable diastereomers) from the reaction of imine **S-1** with *n*-BuLi (2.5 M in hexane). Yellow solid; m.p. 56–57 °C; $[\alpha]_D^{20}$ = +6.9 (c = 0.6, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.22–4.06 (m, 10H), 3.40 (d, J = 6.4 Hz, 1H), 1.98–1.88 (m, 1H), 1.84–1.72 (m, 1H), 1.52–1.30 (m, 4H), 1.25 (s, 9H), 0.93 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 92.2, 68.7, 67.8, 67.6, 66.3, 56.0, 37.3, 28.4, 22.9, 22.8, 14.2; HRMS (EI) calcd for $C_{19}H_{29}NOSFe$ (M) 375.1319, found 375.1327.



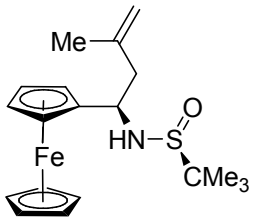
5d

Sulfinamide **5d** was obtained in 99% yield with 99% de (inseparable diastereomers**)** from the reaction of imine **S-1** with *i*-PrMgBr (1.0 M in THF). The de of sulfinamide **5d** was determined by converting it to amine **1d** (see below). Yellow solid; m.p. 107–108 ^{o}C; $[\alpha]_D^{20}$ = -35.3 (c = 0.6, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.19–4.13 (m, 8H), 4.11–4.08 (m, 2H), 3.50 (d, J = 6.0 Hz, 1H), 2.15–2.06 (m, 1H), 1.34 (s, 9H), 0.90 (d, J = 6.8 Hz, 3H), 0.82 (d, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 90.4, 68.8, 67.7, 67.5, 67.0, 66.7, 61.1, 56.2, 34.7, 23.1, 18.7, 18.2; HRMS (EI) calcd for $C_{18}H_{27}NOSFe$ (M) 361.1163, found 361.1159.



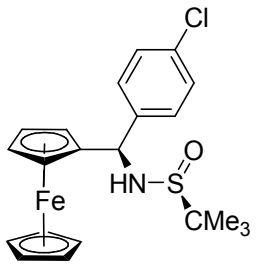
5e

Sulfinamide **5e** was obtained in 99% yield with 97% de (inseparable diastereomers**)** from the reaction of imine **S-1** with allylmagnesium bromide (1.0 M in ether). The de of sulfinamide **5e** was determined by converting it to amine **1e** (see below). Yellow solid; m.p. 40–42 ^{o}C; $[\alpha]_D^{20}$ = +33.1 (c = 0.8, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.89–5.78 (m, 1H), 5.23–5.17 (m, 2H), 4.35–4.29 (m, 1H), 4.24–4.21 (m, 1H), 4.17–4.11 (m, 8H), 3.64 (d, J = 5.6 Hz, 1H), 2.82–2.74 (m, 1H), 2.58–2.50 (m, 1H), 1.23 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 134.6, 119.2, 90.9, 68.8, 68.2, 68.0, 67.5, 66.0, 56.0, 53.9, 42.2, 22.9; HRMS (EI) calcd for $C_{18}H_{25}NOSFe$ (M) 359.1006, found 359.1005.



5f

Sulfinamide **5f** was obtained in 96% yield with 75% de (separable diastereomers) from the reaction of imine **S-1** with (2-methylallyl)magnesium chloride (0.50 M in THF). Yellow solid; m.p. 80–81 ^{o}C; $[\alpha]_D^{20}$ = +58.6 (c = 0.3, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.95 (s, 1H), 4.86 (s, 1H), 4.38–4.27 (m, 2H), 4.21–4.10 (m, 8H), 3.65 (s, br, 1H), 2.75 (dd, J = 13.6, 3.2 Hz, 1H), 2.45 (dd, J = 13.6, 10.0 Hz, 1H), 1.80 (s, 3H), 1.18 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.5, 114.9, 90.8, 68.8, 68.7, 68.0, 67.5, 65.8, 55.7, 50.1, 46.1, 22.8, 22.1; HRMS (EI) calcd for $C_{19}H_{27}NOSFe$ (M) 373.1163, found 373.1166.



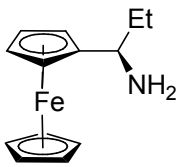
5h

Sulfinamide **5h** was obtained in 95% yield with 96% de (inseparable diastereomers**)** from the reaction of imine **S-1** with (4-chlorophenyl)magnesium bromide (1.0 M in THF). The de of sulfinamide **5h** was determined by converting it to amine **1h** (see below). Yellow solid; m.p. 145–147 ^{o}C; $[\alpha]_D^{20}$ = +45.0 (c = 0.3, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36–7.30 (m, 4H), 5.30 (d, J = 5.2 Hz, 1H), 4.19–4.09 (m, 8H), 4.01–3.98 (m, 1H), 3.87 (d, J = 5.2 Hz, 1H), 1.23 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.0, 133.6, 129.3, 128.7, 90.7, 68.9, 68.8, 68.7, 67.9, 66.8, 57.7, 56.2, 22.9; HRMS (EI) calcd for $C_{21}H_{24}NOSClFe$ (M) 429.0617, found 429.0609.

(3c) Acid hydrolysis[8]

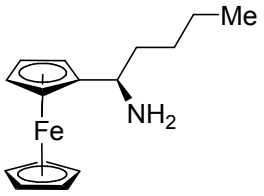
5 **1**

Sulfinamide **5** (2.0 mmol) was dissolved in a solution of HCl in methanol (1.5 M, 8 mL; prepared by dropwise addition of $SOCl_2$ to methanol at 0 ^{o}C). The mixture was stirred at room temperature for 1 h and concentrated under reduced pressure. To the residue was added aqueous HCl (2 M, 10 mL) and the mixture was extracted with ethyl acetate (3 x 10 mL). The aqueous layer was basified with aqueous buffer solution of NH_3 (1 M)/NH_4Cl (1 M) and extracted with dichloromethane (3 x 10 mL). The combined organic phases were dried over sodium sulfate, filtered, and concentrated to give amine **1**.



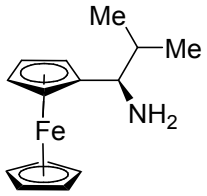
1b

Amine **1b**[9] was obtained in 80% yield. The ee of amine **1b** was determined to be 99% by converting it to amide **1b-Bz** (see below). Orange oil; $[\alpha]_D^{20}$ = -57.2 (c = 1.0, C_6H_6); For (*S*)-isomer, lit.:[9] $[\alpha]_D^{20}$ = +58.0 (c = 1.0, C_6H_6); ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.13–4.03 (m, 9H), 3.49–3.44 (m, 1H), 1.78 (s, br, 2H), 1.58–1.39 (m, 2H), 0.85 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 95.5, 68.4, 67.4, 67.3, 67.0, 65.1, 52.3, 32.2, 11.1.



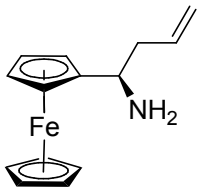
1c

Amine **1c**[5] was obtained in 46% yield. The ee of amine **1c** was determined to be 96% by converting it to amide **1c-Bz** (see below). Orange oil; $[\alpha]_D^{20}$ = -30.8 (c = 0.8, C_6H_6); For (*S*)-isomer, >99% ee, lit.:[5] $[\alpha]_D^{26}$ = +41.2 (c = 1.13, C_6H_6); ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.20–4.10 (m, 9H), 3.62–3.58 (m, 1H), 1.77 (s, br, 2H), 1.60–1.46(m, 2H), 1.41–1.24 (m, 4H), 0.89 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 95.9, 68.4, 67.4, 67.0, 65.1, 50.8, 39.3, 28.9, 22.9, 14.2.



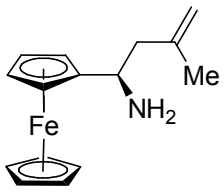
1d

Amine **1d**[10] was obtained in 85% yield. The ee of amine **1d** was determined to be 99% by converting it to amide **1d-Bz** (see below). Orange oil; $[\alpha]_D^{20}$ = -79.1 (c = 0.5, C_6H_6); For (*S*)-isomer, lit.:[10] $[\alpha]_D^{28}$ = +43.3 (c = 0.53, C_6H_6); ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.21–4.09 (m, 9H), 3.47 (d, *J* = 5.6 Hz, 1H), 1.72 (s, br, 2H), 1.68–1.57 (m, 1H), 0.85 (d, *J* = 6.8 Hz, 3H), 0.79 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 94.0, 68.4, 67.2, 65.3, 56.7, 35.4, 19.1, 18.8.



1e

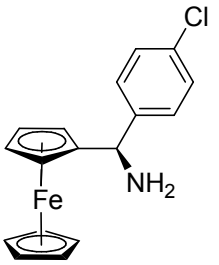
Amine **1e** was obtained in 70% yield. The ee of amine **1e** was determined to be 97% by converting it to amide **1e-Bz** (see below). Orange oil; $[\alpha]_D^{20}$ = -32.4 (c = 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.86–5.76 (m, 1H), 5.15–5.08 (m, 2H), 4.24–4.11 (m, 9H), 3.77–3.72 (m, 1H), 2.52–2.18 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 135.6, 117.7, 94.1, 68.8, 68.5, 67.6, 67.5, 66.7, 65.7, 50.3, 43.6; HRMS (EI) calcd for $C_{14}H_{17}NFe$ (M) 255.0710, found 255.0702.



1f

Amine **1f** was obtained in 55% yield. The ee of amine **1f** was determined to be 99% by converting it to amide **1f-Bz** (see below). Orange solid; m.p. 61–62 ^{o}C; $[\alpha]_D^{20}$ = -43.4 (c = 0.7,

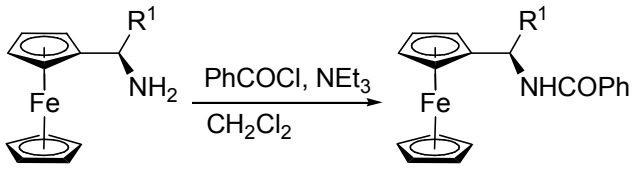
$CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 4.87 (s, 1H), 4.80 (s, 1H), 4.28–4.26 (m, 1H), 4.19–4.12 (m, 8H), 3.84 (dd, J = 9.6, 4.0 Hz, 1H), 2.60 (s, br, 2H), 2.42 (dd, J = 13.2, 4.0 Hz, 1H), 2.24 (dd, J = 13.2, 9.6 Hz, 1H), 1.77 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.8, 113.5, 93.9, 68.7, 68.5, 67.6, 66.6, 65.9, 48.3, 47.7, 22.5; HRMS (EI) calcd for $C_{15}H_{19}NFe$ (M) 269.0867, found 269.0862.



1h

Amine **1h** was obtained in 50% yield. The ee of amine **1h** was determined to be 96% by converting it to amide **1h-Bz** (see below). Yellow solid; m.p. 118-119 °C; $[\alpha]_D^{20}$ = -10.8 (c = 0.7, C_6H_6); ^1H NMR (400 MHz, $CDCl_3$) δ 7.30–7.23 (m, 4H), 4.86 (s, 1H), 4.29–4.26 (m, 1H), 4.19–4.11 (m, 7H), 4.07–4.05 (m, 1H), 1.83 (s, br, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.2, 132.7, 128.5, 128.3, 94.5, 68.6, 68.1, 67.7, 67.2, 65.6, 54.9; HRMS (EI) calcd for $C_{17}H_{16}NClFe$ (M) 325.0321, found 325.0320.

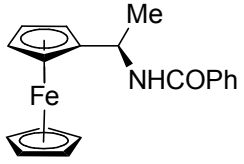
(4) Determination of the ee[11]



1 **1-Bz**

To a solution of amine **1** (0.20 mmol) and triethylamine (30.4 mg, 0.042 mL, 0.30 mmol) in dichloromethane (0.80 mL) at 0 °C was added dropwise a solution of benzoyl chloride (33.7 mg, 0.24 mmol) in dichloromethane (0.20 mL). The mixture was allowed to warm to room temperature and stirred for 1 hour. The mixture was quenched with water (1.0 mL) and extracted with dichloromethane (5.0 mL), and the aqueous layer was washed with dichloromethane (3.0 mL). The organic layers were combined, dried over sodium sulfate, and concentrated. The residue was purified by silica gel chromatography (petroleum/ethyl acetate = 10:1) to give amide **1-Bz**.

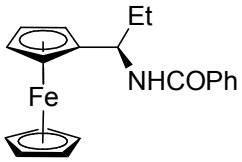
According to the literature, the corresponding racemic amides were prepared by the acid-catalyzed alkylation of benzamide with the corresponding alcohols.[12]



1a-Bz

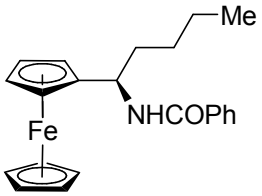
Amide **1a-Bz** was obtained in 96% yield. Orange solid; m.p. 133–134 °C; $[\alpha]_D^{20}$ = -4.3 (c = 0.3, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.80–7.77 (m, 2H), 7.53–7.42 (m, 3H), 6.38 (d, J = 7.2 Hz,

1H), 5.12–5.02 (m, 1H), 4.28–4.25 (m, 1H), 4.22–4.15 (m, 8H), 1.57 (d, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.2, 134.9, 131.6, 128.8, 126.9, 91.6, 68.7, 68.3, 68.0, 67.7, 66.0, 44.2, 20.9; HRMS (EI) calcd for $C_{19}H_{19}NOFe$ (M) 333.0816, found 333.0810. The ee was determined to be 96% by HPLC analysis (Chiralpak AD column, λ = 254 nm, *n*-hexane/isopropanol = 90/10, flow rate = 1.0 mL/min): t_R(minor) = 22.3 min, t_R(major) = 24.9 min.



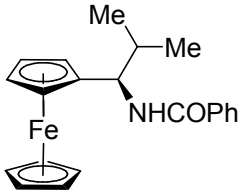
1b-Bz

Amide **1b-Bz** was obtained in 95% yield. Orange solid; m.p. 154–155 °C; $[\alpha]_D^{20}$ = -43.3 (c = 0.2, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84–7.80 (m, 2H), 7.53–7.44 (m, 3H), 6.27 (d, J = 8.4 Hz, 1H), 5.00–4.93 (m, 1H), 4.23–4.14 (m, 9H), 2.05–1.92 (m, 1H), 1.81–1.70 (m, 1H), 1.03 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.7, 135.1, 131.6, 128.8, 126.9, 91.3, 68.9, 68.1, 67.9, 67.0, 66.7, 49.8, 29.3, 11.0; HRMS (EI) calcd for $C_{20}H_{21}NOFe$ (M) 347.0973, found 347.0974. The ee was determined to be 99% by HPLC analysis (Chiralpak AD column, λ = 254 nm, *n*-hexane/isopropanol = 90/10, flow rate = 1.0 mL/min): t_R(minor) = 18.9 min, t_R(major) = 23.3 min.



1c-Bz

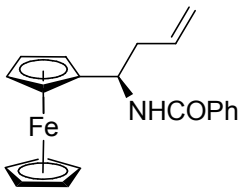
Amide **1c-Bz** was obtained in 90% yield. Orange solid; m.p. 159–160 °C; $[\alpha]_D^{20}$ = -40.2 (c = 0.6, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83–7.81 (m, 2H), 7.53–7.44 (m, 3H), 6.26 (d, J = 8.8 Hz, 1H), 5.06–5.00 (m, 1H), 4.23–4.21 (m, 1H), 4.18–4.14 (m, 8H), 1.96–1.86 (m, 1H), 1.80–1.67 (m, 1H), 1.46–1.24 (m, 4H), 0.91 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.5, 135.1, 131.5, 128.8, 126.9, 91.5, 68.7, 68.0, 67.7, 66.8, 66.5, 48.3, 36.2, 28.6, 22.8, 14.2; HRMS (EI) calcd for $C_{22}H_{25}NOFe$ (M) 375.1286, found 375.1290. The ee was determined to be 96% by HPLC analysis (Chiralpak AD column, λ = 254 nm, *n*-hexane/isopropanol = 90/10, flow rate = 1.0 mL/min): t_R(minor) = 14.0 min, t_R(major) = 21.6 min.



1d-Bz

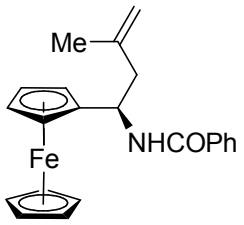
Amide **1d-Bz** was obtained in 99% yield. Orange solid; m.p. 178–180 °C; $[\alpha]_D^{20}$ = -66.7 (c = 0.4, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89–7.85 (m, 2H), 7.56–7.47 (m, 3H), 6.39 (d, J = 9.2 Hz, 1H), 4.97 (dd, J = 9.2, 4.8 Hz, 1H), 4.23–4.20 (m, 1H), 4.16–4.11 (m, 7H), 4.08–4.06 (m, 1H),

2.04–1.94 (m, 1H), 0.92–0.86 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.7, 135.3, 131.6, 128.9, 126.9, 89.5, 68.9, 68.7, 67.5, 65.1, 54.0, 34.4, 19.3, 18.3; HRMS (EI) calcd for $C_{21}H_{23}NOFe$ (M) 361.1129, found 361.1137. The ee was determined to be 99% by HPLC analysis (Chiralpak AD column, λ = 254 nm, *n*-hexane/isopropanol = 90/10, flow rate = 1.0 mL/min): t_R(minor) = 11.3 min, t_R(major) = 15.2 min.



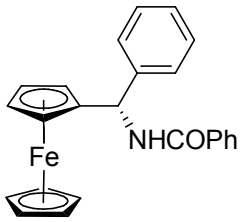
1e-Bz

Amide **1e-Bz** was obtained in 91% yield. Orange solid; m.p. 138–139 °C; $[\alpha]_D^{20}$ = -40.5 (c = 0.2, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81–7.77 (m, 2H), 7.53–7.43 (m, 3H), 6.32 (d, *J* = 8.4 Hz, 1H), 5.96–5.83 (m, 1H), 5.19–5.08 (m, 3H), 4.25–4.15 (m, 9H), 2.77–2.69 (m, 1H), 2.58–2.49 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.5, 135.0, 134.7, 131.6, 128.8, 126.9, 117.9, 90.7, 68.9, 68.1, 68.0, 67.0, 66.9, 47.8, 40.6; HRMS (EI) calcd for $C_{21}H_{21}NOFe$ (M) 359.0973, found 359.0981. The ee was determined to be 97% by HPLC analysis (Chiralpak AD column, λ = 254 nm, *n*-hexane/isopropanol = 90/10, flow rate = 1.0 mL/min): t_R(minor) = 19.8 min, t_R(major) = 23.9 min.



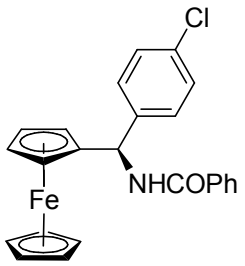
1f-Bz

Amide **1f-Bz** was obtained in 95% yield. Orange solid; m.p. 136–137 °C; $[\alpha]_D^{20}$ = -52.1 (c = 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79–7.76 (m, 2H), 7.52–7.41 (m, 3H), 6.21 (d, *J* = 8.8 Hz, 1H), 5.31–5.23 (m, 1H), 4.82 (s, 1H), 4.78 (s, 1H), 4.29–4.27 (m, 1H), 4.20–4.13 (m, 8H), 2.69 (dd, *J* = 14.0, 4.8 Hz, 1H), 2.50 (dd, *J* = 14.0, 9.6 Hz, 1H), 1.82 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.6, 142.6, 135.1, 131.5, 128.8, 126.9, 113.5, 91.2, 68.8, 68.0, 67.8, 67.0, 66.6, 46.2, 45.0, 22.4; HRMS (EI) calcd for $C_{22}H_{23}NOFe$ (M) 373.1129, found 373.1125. The ee was determined to be 99% by HPLC analysis (Chiralpak AD column, λ = 254 nm, *n*-hexane/isopropanol = 80/20, flow rate = 1.0 mL/min): t_R(minor) = 9.6 min, t_R(major) = 11.1 min.



ent-1g-Bz

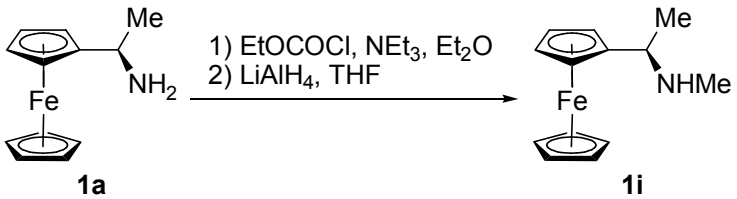
Amide **ent-1g-Bz** was obtained in 92% yield. Orange solid; m.p. 194–195 °C; $[\alpha]_D^{20}$ = +20.0 (c = 0.3, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.87–7.83 (m, 2H), 7.55–7.44 (m, 3H), 7.41–7.26 (m, 5H), 6.91 (d, J = 8.0 Hz, 1H), 6.11 (d, J = 8.0 Hz, 1H), 4.28–4.10 (m, 7H), 4.14–4.12 (m, 1H), 4.09–4.07 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.1, 141.9, 134.7, 131.8, 128.9, 128.5, 127.5, 127.2, 127.0, 91.0, 68.9, 68.3, 68.2, 67.7, 67.4, 52.6; HRMS (EI) calcd for $C_{24}H_{21}NOFe$ (M) 395.0973, found 395.0982. The ee was determined to be 94% by HPLC analysis (Chiralpak OD column, λ = 254 nm, *n*-hexane/isopropanol = 85/15, flow rate = 1.0 mL/min): t_R(major) = 8.4 min, t_R(minor) = 10.9 min.



1h-Bz

Amide **1h-Bz** was obtained in 96% yield. Orange solid; m.p. 217–218 °C; $[\alpha]_D^{20}$ = -20.0 (c = 0.2, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, J = 7.2 Hz, 2H), 7.57–7.45 (m, 3H), 7.35–7.29 (m, 4H), 6.92 (d, J = 7.6 Hz, 1H), 6.03 (d, J = 7.6 Hz, 1H), 4.22–4.18 (m, 7H), 4.13–4.10 (m, 1H), 4.05–4.03 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.1, 140.5, 134.4, 133.3, 131.9, 128.9, 128.7, 128.5, 127.0, 90.5, 69.0, 68.5, 68.4, 67.6, 67.3, 52.2; HRMS (EI) calcd for $C_{24}H_{20}NOClFe$ (M) 429.0583, found 429.0586. The ee was determined to be 96% by HPLC analysis (Chiralpak AD column, λ = 254 nm, *n*-hexane/isopropanol = 70/30, flow rate = 1.0 mL/min): t_R(minor) = 9.2 min, t_R(major) = 17.6 min.

Preparation of amine 1i[13]

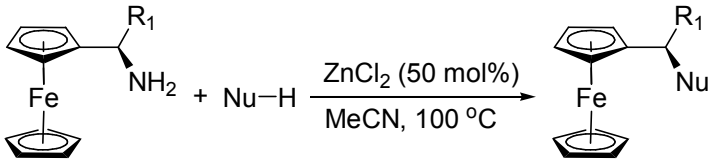


1a **1i**

To a solution of amine **1a** (96% ee, 0.23 g, 1.0 mmol) and triethylamine (0.11 g, 0.15 mL, 1.1 mmol) in dry ether (2.0 mL) at 0 °C was added dropwise ethyl chloroformate (0.12 g, 0.11 mL, 1.1 mmol). The mixture was stirred at room temperature for 10 min and then filtered. The precipitate was washed with ether (2 x 1.0 mL). The filtrate was washed successively with aqueous HCl (0.5 M, 2.0 mL) and saturated aqueous sodium bicarbonate (2.0 mL), dried over sodium sulfate, and concentrated under reduced pressure. The residue was dissolved in dry tetrahydrofuran (2.0 mL) and the resulting solution was added dropwise to a suspension of lithium aluminium hydride (0.19 g, 5.0 mmol) in dry tetrahydrofuran (1.0 mL). The mixture was heated at 80 °C for 1 h, cooled with ice-water, and slowly added aqueous potassium hydroxide (2.5 M, 2.0 mL). The mixture was filtered and the precipitate was washed with hot tetrahydrofuran (2 x 1.0 mL). The filtrate was separated and the organic layer was dried over sodium sulfate and concentrated under reduced

pressure. The residue was purified by silica gel chromatography (ethyl acetate/methanol = 10:1) to give amine **1i** (0.15 g, 60% yield, 96% ee) as an orange oil. $[\alpha]_D^{20}$ = -8.5 (c = 2.4, $CHCl_3$); For (+)-isomer, lit.:[14] $[\alpha]_D$ = +7.9 (c = 7.18, $CHCl_3$, 87.4% ee); ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.20–4.10 (m, 9H), 3.49 (q, J = 6.4 Hz, 1H), 2.61 (s, br, 1H), 2.40 (s, 3H), 1.41 (d, J = 6.4Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 92.4, 68.6, 67.6, 67.5, 66.0, 54.1, 33.7, 20.7.

General procedure for the substitution of enantioenriched primary α-aminoalkylferrocenes with nucleophiles

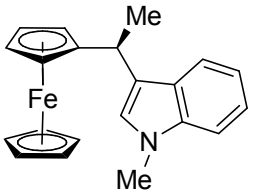


1 **2** **3**

A mixture of amine **1** (0.20 mmol), nucleophile **2** (0.24 mmol), and $ZnCl_2$ (13.6 mg, 0.10 mmol, 50 mol%) in acetonitrile (1.0 mL) was heated at 100 °C (oil bath) in sealed tube for 1-9 h. The mixture was cooled to room temperature and purified by silica gel chromatography (petroleum/ethyl acetate = 20:1 to 5:1) to give compound **3**.

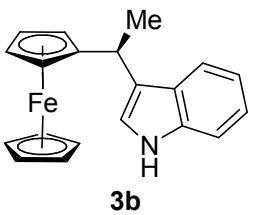
The absolute configuration of compounds **3d**, **ent-3q**, and **3s** was assigned by single-crystal X-ray analysis (see below) and that of the rest of new products shown in Tables 2 and 3 was assigned by analogy.

Analytical data for the products



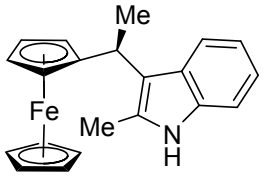
3a

Compound **3a**,[15] yellow solid; m.p. 105–106 °C; $[\alpha]_D^{20}$ = -90.7 (c = 1.2, $CHCl_3$); Lit.:[15] $[\alpha]_D$ = -94 (c = 0.38, $CHCl_3$, 99% ee); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, J = 8.0 Hz, 1H), 7.24–7.15 (m, 2H), 7.10– 7.05 (m, 1H), 6.55 (s, 1H), 4.24–4.05 (m, 10H), 3.63 (s, 3H), 1.69 (d, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.1, 126.9, 125.6, 121.9, 121.4, 119.4, 118.6, 109.3, 95.0, 68.7, 68.3, 67.4, 66.9, 66.4, 32.7, 30.7, 22.0. The ee was determined to be 96% by HPLC analysis (Chiralpak AD column, λ = 254 nm, *n*-hexane/isopropanol = 85/15, flow rate = 0.7 mL/min): t_R(major) = 6.3 min, t_R(minor) = 7.4 min.



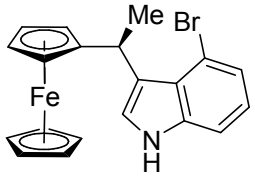
3b

Compound **3b**,[15] yellow solid; m.p. 133–134 °C; $[\alpha]_D^{20}$ = -67.2 (c = 0.6, $CHCl_3$); Lit.:[15] $[\alpha]_D$ = -53 (c = 0.6, $CHCl_3$, 99% ee); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (s, br, 1H), 7.65 (d, *J* = 8.0 Hz, 1H), 7.31 (d, *J* = 8.0 Hz, 1H), 7.19–7.05 (m, 2H), 6.75 (s, 1H), 4.25–4.24 (m, 1H), 4.19–4.06 (m, 9H), 1.70 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.5, 126.6, 123.4, 121.9, 120.8, 119.5, 119.2, 111.3, 95.0, 68.8, 68.3, 67.5, 66.9, 66.6, 30.8, 21.9. The ee was determined to be 96% by HPLC analysis (Chiralpak AD column, λ = 254 nm, *n*-hexane/isopropanol = 85/15, flow rate = 0.8 mL/min): t_R(major) = 12.3 min, t_R(minor) = 14.3 min.



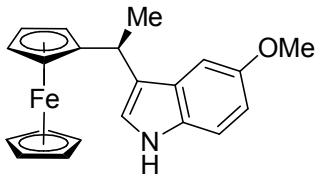
3c

Compound **3c**, orange oil; $[\alpha]_D^{20}$ = -126.8 (c = 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (s, br, 1H), 7.43 (d, *J* = 8.0 Hz, 1H), 7.19 (d, *J* = 8.0 Hz, 1H), 7.06–7.00 (m, 1H), 6.99–6.94 (m, 1H), 4.41–4.38 (m, 1H), 4.22 (q, *J* = 7.2 Hz, 1H), 4.14–4.07 (m, 6H), 4.02–4.01 (m, 2H), 2.30 (s, 3H), 1.65 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 135.2, 129.6, 127.5, 120.7, 119.3, 118.9, 117.2, 110.2, 94.6, 68.8, 68.7, 67.6, 67.0, 66.6, 30.9, 20.9, 12.4; HRMS (EI) calcd for $C_{21}H_{21}NFe$ (M) 343.1023, found 343.1015. The ee was determined to be 96% by HPLC analysis (Chiralpak AS column, λ = 254 nm, *n*-hexane/isopropanol = 95/5, flow rate = 0.5 mL/min): t_R(minor) = 21.9 min, t_R(major) = 23.2 min.



3d

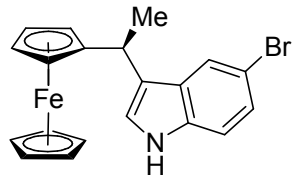
Compound **3d**, yellow solid; m.p. 178–179 °C; $[\alpha]_D^{20}$ = -93.2 (c = 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (s, br, 1H), 7.29 (d, *J* = 7.6 Hz, 1H), 7.24 (d, *J* = 8.0 Hz, 1H), 7.00–6.95 (m, 1H), 6.65 (s, 1H), 4.82 (q, *J* = 6.8 Hz, 1H), 4.27–4.11 (m, 9H), 1.69 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.5, 125.3, 124.5, 124.4, 123.0, 122.7, 114.3, 110.6, 95.6, 69.2, 68.6, 68.0, 67.0, 29.9, 23.5; HRMS (EI) calcd for $C_{20}H_{18}NFeBr$ (M) 406.9972, found 406.9965. The ee was determined to be 96% by HPLC analysis (Chiralpak AS column, λ = 254 nm, *n*-hexane/isopropanol = 92/8, flow rate = 0.5 mL/min): t_R(minor) = 19.3 min, t_R(major) = 20.8 min.



3e

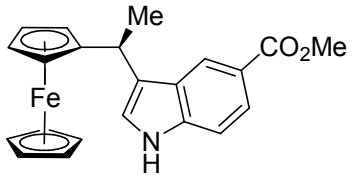
Compound **3e**,[15] orange solid; m.p. 38–39 °C; $[\alpha]_D^{20}$ = -63.6 (c = 0.8, $CHCl_3$); Lit.:[15] $[\alpha]_D$ = -57

(c = 0.35, $CHCl_3$, 99% ee); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (s, br, 1H), 7.18 (d, J = 8.4 Hz, 1H), 7.07 (d, J = 2.4 Hz, 1H), 6.82 (dd, J = 8.4, 2.4 Hz, 1H), 6.71 (s, 1H), 4.24–4.21 (m, 1H), 4.16–4.05 (m, 9H), 3.85 (s, 3H), 1.68 (d, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.8, 131.6, 126.9, 123.0, 121.7, 111.9, 101.4, 94.8, 68.7, 68.1, 67.4, 66.9, 66.5, 56.1, 30.7, 21.8. The ee was determined to be 96% by HPLC analysis (Chiralpak AD column, λ = 254 nm, *n*-hexane/isopropanol = 85/15, flow rate = 0.8 mL/min): t_R(major) = 18.2 min, t_R(minor) = 23.1 min.



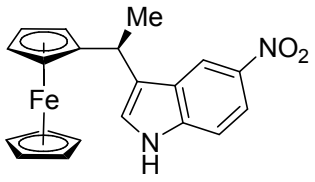
3f

Compound **3f**,[15] yellow solid; m.p. 163–164 °C; $[\alpha]_D^{20}$ = -64.9 (c = 1.0, $CHCl_3$); Lit.:[15] $[\alpha]_D$ = -58 (c = 0.45, $CHCl_3$, 99% ee); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (s, br, 1H), 7.76 (s, 1H), 7.26–7.16 (m, 2H), 6.74 (s, 1H), 4.27–4.04 (m, 10H), 1.67 (d, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 135.0, 128.3, 124.8, 123.2, 122.1, 122.0, 112.7, 112.6, 95.1, 69.3, 68.5, 68.0, 67.4, 66.8, 30.7, 21.8. The ee was determined to be 96% by HPLC analysis (Chiralpak AD column, λ = 254 nm, *n*-hexane/isopropanol = 85/15, flow rate = 0.7 mL/min): t_R(major) = 12.1 min, t_R(minor) = 13.8 min.



3g

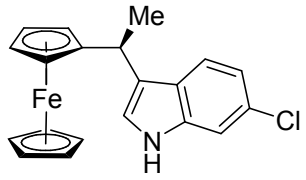
Compound **3g**, yellow solid; m.p. 135–136 °C; $[\alpha]_D^{20}$ = -66.4 (c = 1.1, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (s, 1H), 8.09 (s, br, 1H), 7.87 (d, J = 8.8 Hz, 1H), 7.31 (d, J = 8.8 Hz, 1H), 6.78 (s, 1H), 4.26–4.08 (m, 10H), 3.94 (s, 3H), 1.71 (d, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.5, 138.9, 126.2, 124.8, 123.3, 122.3, 122.1, 121.2, 111.0, 95.9, 69.8, 68.8, 68.3, 67.7, 67.2, 52.0, 30.5, 21.9; HRMS (EI) calcd for $C_{22}H_{21}NO_2Fe$ (M) 387.0922, found 387.0919. The ee was determined to be 96% by HPLC analysis (Chiralpak AD column, λ = 254 nm, *n*-hexane/isopropanol = 85/15, flow rate = 1.0 mL/min): t_R(major) = 11.0 min, t_R(minor) = 14.4 min.



3h

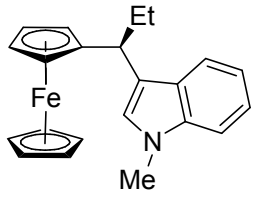
Compound **3h**,[16] yellow solid; m.p. 172–174 °C; $[\alpha]_D^{20}$ = -72.5 (c = 0.7, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.63 (s, 1H), 8.26 (s, br, 1H), 8.08 (d, J = 9.2 Hz, 1H), 7.34 (d, J = 9.2 Hz, 1H),

6.90 (s, 1H), 4.30–4.12 (m, 10H), 1.72 (d, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.4, 139.4, 126.0, 123.8, 117.7, 116.8, 111.2, 94.4, 69.1, 68.3, 67.9, 67.4, 66.5, 30.7, 21.9. The ee was determined to be 96% by HPLC analysis (Chiralpak AD column, λ = 254 nm, *n*-hexane/isopropanol = 85/15, flow rate = 1.0 mL/min): t_R(major) = 11.0 min, t_R(minor) = 13.0 min.



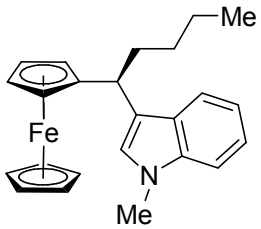
3i

Compound **3i**, yellow solid; m.p. 123–124 °C; $[\alpha]_D^{20}$ = -79.3 (c = 0.9, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (s, br, 1H), 7.52 (d, J = 8.4 Hz, 1H), 7.28 (d, J = 1.6 Hz, 1H), 7.05 (dd, J = 8.4, 1.6 Hz, 1H), 6.73 (s, 1H), 4.25–4.07 (m, 10H), 1.67 (d, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.7, 127.7, 125.2, 123.4, 121.4, 120.3, 119.9, 111.1, 94.7, 68.8, 68.2, 67.6, 67.0, 66.5, 30.7, 21.8; HRMS (EI) calcd for $C_{20}H_{18}NClFe$ (M) 363.0477, found 363.0470. The ee was determined to be 95% by HPLC analysis (Chiralpak AD column, λ = 254 nm, *n*-hexane/isopropanol = 85/15, flow rate = 0.7 mL/min): t_R(major) = 17.1 min, t_R(minor) = 22.3 min.



3j

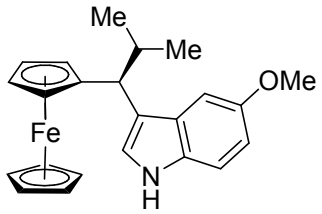
Compound **3j**, yellow solid; m.p. 80–81 °C; $[\alpha]_D^{20}$ = -103.0 (c = 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, J = 7.6 Hz, 1H), 7.26 (d, J = 8.4 Hz, 1H), 7.20–7.15 (m, 1H), 7.07–7.02 (m, 1H), 6.79 (s, 1H), 4.30–4.27 (m, 1H), 4.10–4.00 (m, 8H), 3.82 (dd, J = 10.4, 4.0 Hz, 1H), 3.73 (s, 3H), 2.26–2.14 (m, 1H), 2.03–1.90 (m, 1H), 0.90 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.0, 127.6, 126.2, 121.3, 119.8, 119.1, 118.5, 109.2, 95.6, 69.0, 68.3, 67.5, 67.2, 66.9, 38.6, 32.8, 29.6, 13.3; HRMS (EI) calcd for $C_{22}H_{23}NFe$ (M) 357.1180, found 357.1172. The ee was determined to be 99% by HPLC analysis (Chiralpak OD column, λ = 254 nm, *n*-hexane/isopropanol = 90/10, flow rate = 1.0 mL/min): t_R(minor) = 5.6 min, t_R(major) = 6.6 min.



3k

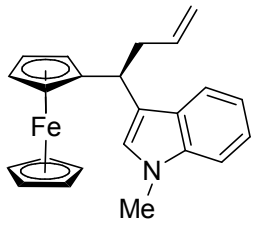
Compound **3k**, orange oil; $[\alpha]_D^{20}$ = -71.4 (c = 1.1, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, J = 8.0 Hz, 1H), 7.25 (d, J = 8.0 Hz, 1H), 7.20–7.14 (m, 1H), 7.07–7.02 (m, 1H), 6.77 (s, 1H), 4.30–4.27 (m, 1H), 4.11–4.00 (m, 8H), 3.90 (dd, J = 10.8, 4.0 Hz, 1H), 3.71 (s, 3H), 2.19–2.08 (m,

1H), 2.02–1.91 (m, 1H), 1.40–1.22 (m, 4H), 0.86 (t, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.0, 127.5, 126.1, 121.3, 119.8, 119.4, 118.5, 109.2, 95.8, 68.9, 68.2, 67.4, 67.1, 66.9, 36.7, 36.5, 32.8, 30.6, 23.0, 14.3; HRMS (EI) calcd for $C_{24}H_{27}NFe$ (M) 385.1493, found 385.1483. The ee was determined to be 96% by HPLC analysis (Chiralpak OD column, λ = 254 nm, *n*-hexane/isopropanol = 98/2, flow rate = 0.8 mL/min): t_R(minor) = 8.2 min, t_R(major) = 10.1 min.



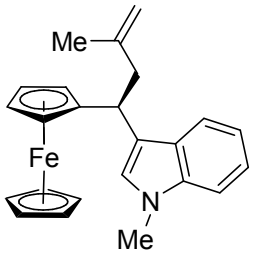
3l

Compound **3l**, orange oil; $[\alpha]_D^{20}$ = +38.6 (c = 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (s, br, 1H), 7.27 (d, J = 8.8 Hz, 1H), 7.12 (d, J = 2.0 Hz, 1H), 7.08 (s, 1H), 6.86 (dd, J = 8.8, 2.0 Hz, 1H), 4.26–4.24 (m, 1H), 4.14–4.05 (m, 3H), 3.88 (s, 3H), 3.81 (s, 5H), 3.69 (d, J = 7.2 Hz, 1H), 2.16–2.06 (m, 1H), 0.88 (d, J = 6.8 Hz, 3H), 0.80 (d, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.8, 131.1, 128.7, 122.7, 119.3, 111.7, 102.1, 93.8, 69.6, 68.7, 68.2, 67.5, 66.5, 56.2, 44.1, 35.2, 22.0, 21.0; HRMS (EI) calcd for $C_{23}H_{25}NOFe$ (M) 387.1286, found 387.1280. The ee was determined to be 96% by HPLC analysis (Chiralpak IC column, λ = 254 nm, *n*-hexane/isopropanol = 90/10, flow rate = 1.0 mL/min): t_R(major) = 5.1 min, t_R(minor) = 6.0 min.



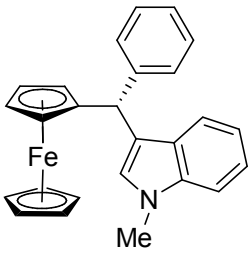
3m

Compound **3m**, orange oil; $[\alpha]_D^{20}$ = -56.8 (c = 1.1, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, J = 8.0 Hz, 1H), 7.27–7.15 (m, 2H), 7.08–7.03 (m, 1H), 6.77 (s, 1H), 5.85–5.73 (m, 1H), 5.07–5.01 (m, 1H), 4.94–4.89 (m, 1H), 4.28–4.26 (m, 1H), 4.10–4.01 (m, 9H), 3.70 (s, 3H), 2.97–2.88 (m, 1H), 2.82–2.72 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.1, 137.0, 127.4, 126.3, 121.4, 119.8, 118.8, 118.6, 115.5, 109.3, 94.5, 68.7, 68.2, 67.3, 67.0, 66.9, 41.1, 37.1, 32.8; HRMS (EI) calcd for $C_{23}H_{23}NFe$ (M) 369.1180, found 369.1175. The ee was determined to be 97% by HPLC analysis (Chiralpak AD column, λ = 254 nm, *n*-hexane/isopropanol = 98/2, flow rate = 0.8 mL/min): t_R(major) = 6.4 min, t_R(minor) = 7.1 min.



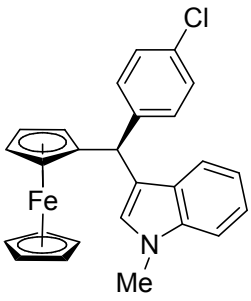
3n

Compound **3n**, yellow solid; m.p. 114–115 °C; $[\alpha]_D^{20}$ = -50.0 (c = 1.1, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, J = 8.0 Hz, 1H), 7.24 (d, J = 8.0 Hz, 1H), 7.19–7.14 (m, 1H), 7.07–7.02 (m, 1H), 6.81 (s, 1H), 4.64 (s, 1H), 4.59 (s, 1H), 4.24– 4.00 (m, 10H), 3.71 (s, 3H), 2.92 (dd, J = 13.6, 4.0 Hz, 1H), 2.76 (dd, J = 13.6, 10.8 Hz, 1H), 1.70 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.4, 137.0, 127.5, 126.1, 121.2, 119.7, 118.7, 118.5, 112.2, 109.2, 95.5, 68.8, 68.2, 67.4, 67.0, 44.9, 35.2, 32.8, 22.7; HRMS (EI) calcd for $C_{24}H_{25}NFe$ (M) 383.1336, found 383.1342. The ee was determined to be 96% by HPLC analysis (Chiralpak AD column, λ = 254 nm, *n*-hexane/isopropanol = 98/2, flow rate = 1.0 mL/min): t_R(major) = 5.2 min, t_R(minor) = 6.0 min.



ent-3o

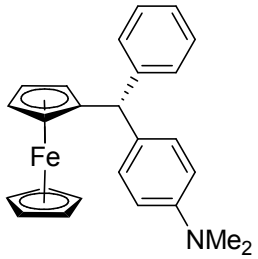
Compound **ent-3o**, yellow solid; m.p. 160–161 °C; $[\alpha]_D^{20}$ = -74.4 (c = 1.3, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.38–7.34 (m, 2H), 7.30–7.16 (m, 5H), 7.15–7.10 (m, 1H), 6.96–6.91 (m, 1H), 6.62 (s, 1H), 5.31 (s, 1H), 4.21–4.19 (m, 1H), 4.15–4.10 (m, 2H), 4.00–3.93 (m, 6H), 3.67 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.6, 137.2, 128.8, 128.0, 127.4, 127.1, 126.1, 121.4, 119.9, 119.8, 118.7, 109.1, 92.7, 68.9, 68.4, 67.5, 67.3, 43.6, 32.7; HRMS (EI) calcd for $C_{26}H_{23}NFe$ (M) 405.1180, found 405.1172. The ee was determined to be 94% by HPLC analysis (Chiralpak AD column, λ = 254 nm, *n*-hexane/isopropanol = 95/5, flow rate = 0.8 mL/min): t_R(minor) = 6.4 min, t_R(major) = 6.8 min.



3p

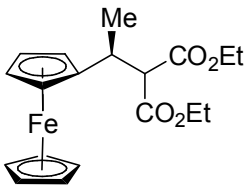
Compound **3p**, yellow solid; m.p. 160–161 °C; $[\alpha]_D^{20}$ = +96.1 (c = 1.2, $CHCl_3$); ^1H NMR (400

MHz, $CDCl_3$) δ 7.31–7.12 (m, 7H), 6.98–6.92 (m, 1H), 6.62 (s, 1H), 5.27 (s, 1H), 4.28–3.93 (m, 9H), 3.70 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.2, 137.3, 131.8, 130.2, 128.2, 127.5, 126.9, 121.6, 119.6, 119.5, 118.9, 109.3, 92.1, 68.8, 68.2, 67.7, 67.4, 43.0, 32.8; HRMS (EI) calcd for $C_{26}H_{22}NClFe$ (M) 439.0790, found 439.0782. The ee was determined to be 96% by HPLC analysis (Chiralpak AD column, λ = 254 nm, *n*-hexane/isopropanol = 90/10, flow rate = 0.5 mL/min): t_R(major) = 10.2 min, t_R(minor) = 10.9 min.



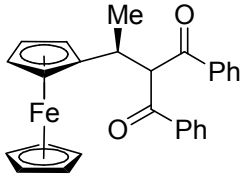
ent-3q

Compound **ent-3q**, yellow solid; m.p. 109–110 °C; $[\alpha]_D^{20}$ = +70.3 (c = 0.7, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.27–7.22 (m, 2H), 7.18–7.14 (m, 3H), 7.03 (d, *J* = 8.4 Hz, 2H), 6.66 (d, *J* = 8.4 Hz, 2H), 5.06 (s, 1H), 4.14–4.11 (m, 2H), 4.02–3.96 (m, 7H), 2.90 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.8, 145.8, 133.8, 129.4, 128.8, 128.0, 125.9, 112.6, 92.5, 69.0, 68.8, 67.6, 67.5, 50.9, 41.0; HRMS (EI) calcd for $C_{25}H_{25}NFe$ (M) 395.1336, found 395.1319. The ee was determined to be 92% by HPLC analysis (Chiralpak AD-H column, λ = 254 nm, *n*-hexane/isopropanol = 99/1, flow rate = 0.5 mL/min): t_R(minor) = 18.7 min, t_R(major) = 21.4 min.



3r

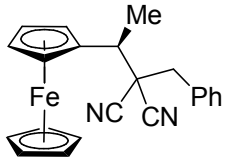
Compound **3r**,[17] orange oil; $[\alpha]_D^{20}$ = +18.7 (c = 1.2, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 4.20–4.01 (m, 13H), 3.36–3.24 (m, 2H), 1.42 (d, *J* = 6.4 Hz, 3H), 1.24 (t, *J* = 7.2 Hz, 3H), 1.15 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.7, 168.4, 91.3, 68.7, 68.4, 67.5, 67.4, 66.0, 61.3, 60.4, 34.0, 18.1, 14.2, 14.1. The ee was determined to be 92% by HPLC analysis (Chiralpak AD column, λ = 254 nm, *n*-hexane/isopropanol = 95/5, flow rate = 0.5 mL/min): t_R(minor) = 16.9 min, t_R(major) = 18.3 min.



3s

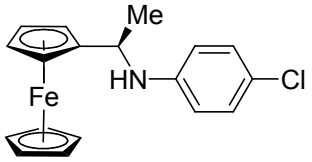
Compound **3s**,[18] yellow solid; m.p. 151–153 °C; $[\alpha]_D^{20}$ = -23.6 (c = 0.5, $CHCl_3$); Lit.:[18] $[\alpha]_D^{25.5}$ = -25.9 (c = 1.690, $CHCl_3$, 95% ee); ^1H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, *J* = 7.6 Hz, 2H), 7.70 (d,

J = 7.6 Hz, 2H), 7.51–7.41 (m, 2H), 7.38–7.27 (m, 4H), 5.30 (d, *J* = 8.8 Hz, 1H), 4.15–4.05 (m, 6H), 3.99–3.95 (m, 2H), 3.88–3.77 (m, 2H), 1.42 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.7, 194.5, 137.2, 137.0, 133.4, 133.1, 128.8, 128.7, 128.5, 92.5, 69.6, 69.1, 67.8, 67.7, 66.2, 64.9, 35.3, 18.6. The ee was determined to be 94% by HPLC analysis (Chiralpak OD column, λ = 254 nm, *n*-hexane/isopropanol = 90/10, flow rate = 0.5 mL/min): t_R(major) = 14.7 min, t_R(minor) = 17.3 min.



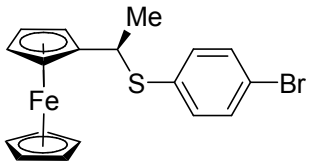
3t

Compound **3t**, yellow solid; m.p. 180–181 °C; $[\alpha]_D^{20}$ = +16.4 (c = 0.9, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37–7.28 (m, 5H), 4.37–4.18 (m, 9H), 3.16 (q, *J* = 6.8 Hz, 1H), 3.00–2.89 (m, 2H), 1.83 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 132.8, 130.2, 128.9, 128.7, 115.4, 114.7, 85.7, 70.1, 69.2, 69.0, 68.4, 67.0, 46.6, 42.4, 41.4, 17.8; HRMS (EI) calcd for $C_{22}H_{20}N_2Fe$ (M) 368.0976, found 368.0971. The ee was determined to be 96% by HPLC analysis (Chiralpak AD column, λ = 254 nm, *n*-hexane/isopropanol = 85/15, flow rate = 1.0 mL/min): t_R(minor) = 9.4 min, t_R(major) = 11.8 min.



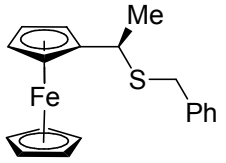
3u

Compound **3u**,[19] yellow solid; m.p. 94–96 °C; $[\alpha]_D^{20}$ = +5.6 (c = 0.9, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.12 (d, *J* = 8.8 Hz, 2H), 6.55 (d, *J* = 8.8 Hz, 2H), 4.26 (q, *J* = 6.4 Hz, 1H), 4.19–4.11 (m, 9H), 1.48 (d, *J* = 6.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.9, 129.2, 121.8, 114.5, 93.0, 68.6, 68.0, 67.7, 67.2, 66.2, 47.6, 20.8. The ee was determined to be 96% by HPLC analysis (Chiralpak AD column, λ = 254 nm, *n*-hexane/isopropanol = 99/1, flow rate = 1.0 mL/min): t_R(major) = 13.4 min, t_R(minor) = 15.6 min.



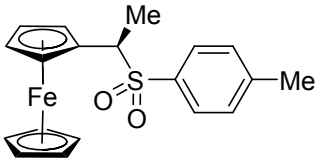
3v

Compound **3v**, yellow solid; m.p. 105–106 °C; $[\alpha]_D^{20}$ = -55.5 (c = 0.9, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (d, *J* = 8.4 Hz, 2H), 7.19 (d, *J* = 8.4 Hz, 2H), 4.17–4.06 (m, 9H), 4.03–4.01 (m, 1H), 1.61 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 135.0, 134.3, 131.9, 121.6, 91.0, 69.2, 68.4, 68.2, 68.1, 66.4, 44.0, 21.2; HRMS (EI) calcd for $C_{18}H_{17}SFeBr$ (M) 399.9584, found 399.9567. The ee was determined to be 96% by HPLC analysis (Chiralpak AS-H column, λ = 254 nm, *n*-hexane/isopropanol = 99/1, flow rate = 0.8 mL/min): t_R(minor) = 7.8 min, t_R(major) = 8.8 min.



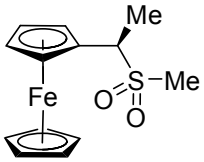
3w

Compound **3w**, yellow solid; m.p. 50–51 °C; $[\alpha]_D^{20}$ = -58.4 (c = 1.2, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.34–7.19 (m, 5H), 4.20–4.11 (m, 9H), 3.72–3.58 (m, 3H), 1.64 (d, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.7, 129.0, 128.5, 126.9, 91.7, 68.8, 68.0, 67.8, 67.6, 66.1, 38.8, 35.7, 21.5; HRMS (EI) calcd for $C_{19}H_{20}SFe$ (M) 336.0635, found 336.0612. The ee was determined to be 96% by HPLC analysis (Chiralpak AD column, λ = 254 nm, *n*-hexane/isopropanol = 95/5, flow rate = 1.0 mL/min): t_R(major) = 5.0 min, t_R(minor) = 5.8 min.



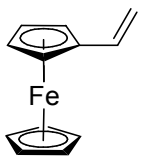
3x

Compound **3x**, yellow solid; m.p. 134–135 °C; $[\alpha]_D^{20}$ = -7.3 (c = 1.0, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.38 (d, J = 8.0 Hz, 2H), 7.18 (d, J = 8.0 Hz, 2H), 4.15–4.09 (m, 8H), 4.02–3.93 (m, 2H), 2.39 (s, 3H), 1.69 (d, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.4, 133.2, 129.8, 129.2, 81.5, 70.9, 68.9, 68.8, 68.6, 67.1, 62.5, 21.7, 14.1; HRMS (EI) calcd for $C_{19}H_{20}O_2SFe$ (M) 368.0533, found 368.0506. The ee was determined to be 96% by HPLC analysis (Chiralpak OD column, λ = 254 nm, *n*-hexane/isopropanol = 90/10, flow rate = 1.0 mL/min): t_R(minor) = 15.2 min, t_R(major) = 16.6 min.



3y

Compound **3y**, yellow solid; m.p. 119–120 °C; $[\alpha]_D^{20}$ = +23.0 (c = 1.0, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 4.42–4.40 (m, 1H), 4.29–4.26 (m, 3H), 4.20 (s, 5H), 3.91 (q, J = 7.2 Hz, 1H), 2.55 (s, 3H), 1.82 (d, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 81.8, 70.4, 69.2, 66.7, 61.3, 36.1, 13.8; HRMS (EI) calcd for $C_{13}H_{16}O_2SFe$ (M) 292.0220, found 292.0219. The ee was determined to be 96% by HPLC analysis (Chiralpak AD column, λ = 254 nm, *n*-hexane/isopropanol = 70/30, flow rate = 1.0 mL/min): t_R(major) = 7.6 min, t_R(minor) = 16.2 min.



4

Alkene **4**[20] was obtained in 30% yield as a minor product from the reaction of tertiary amine **1j**

with indole **2a**. Orange solid; m.p. 51-53 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.45 (dd, J = 17.6, 10.4 Hz, 1H), 5.33 (d, J = 17.6 Hz, 1H), 5.02 (d, J = 10.4 Hz, 1H), 4.37–4.33 (m, 2H), 4.21–4.06 (m, 7H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 134.8, 111.2, 83.7, 69.3, 68.8, 66.8.

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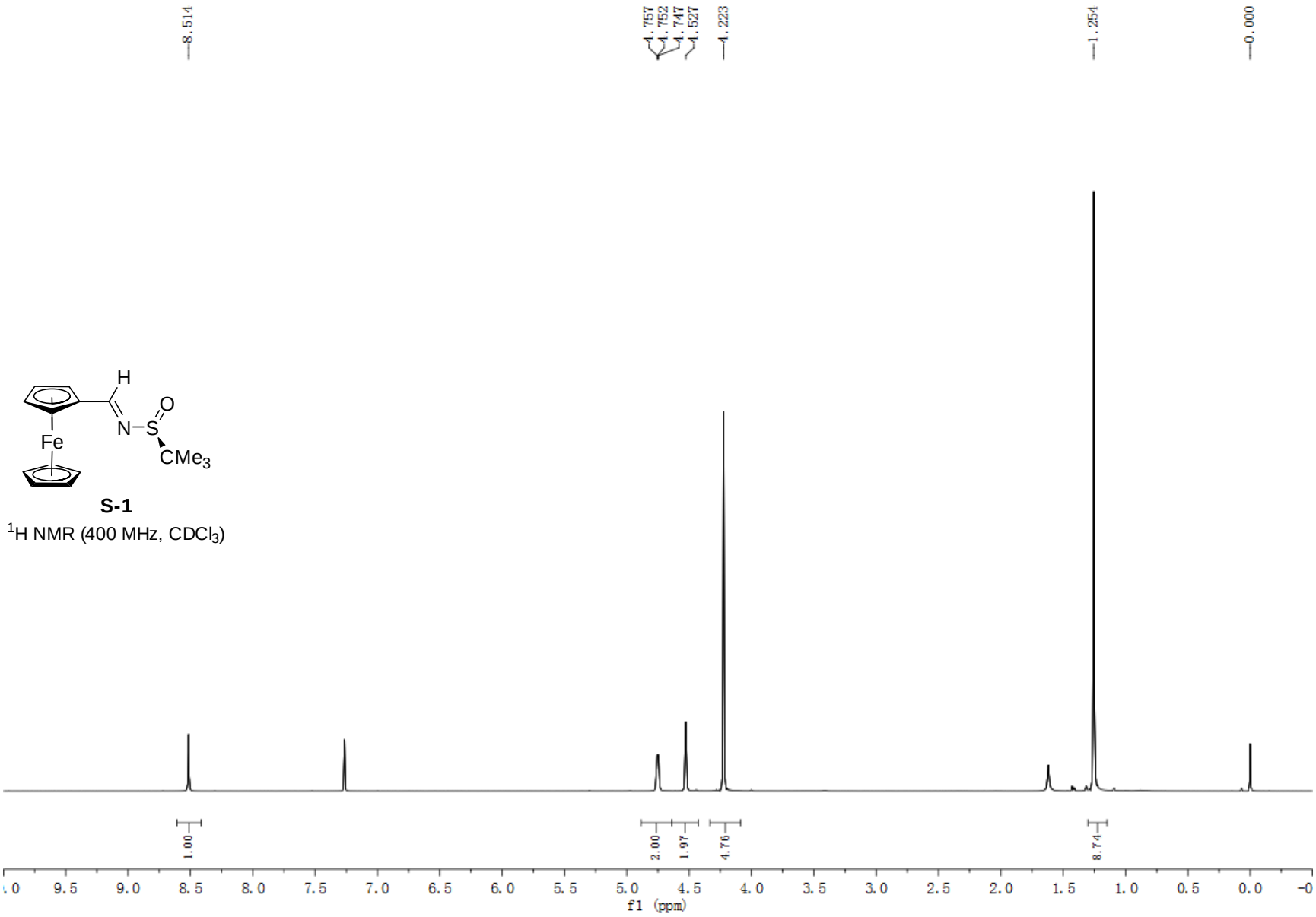
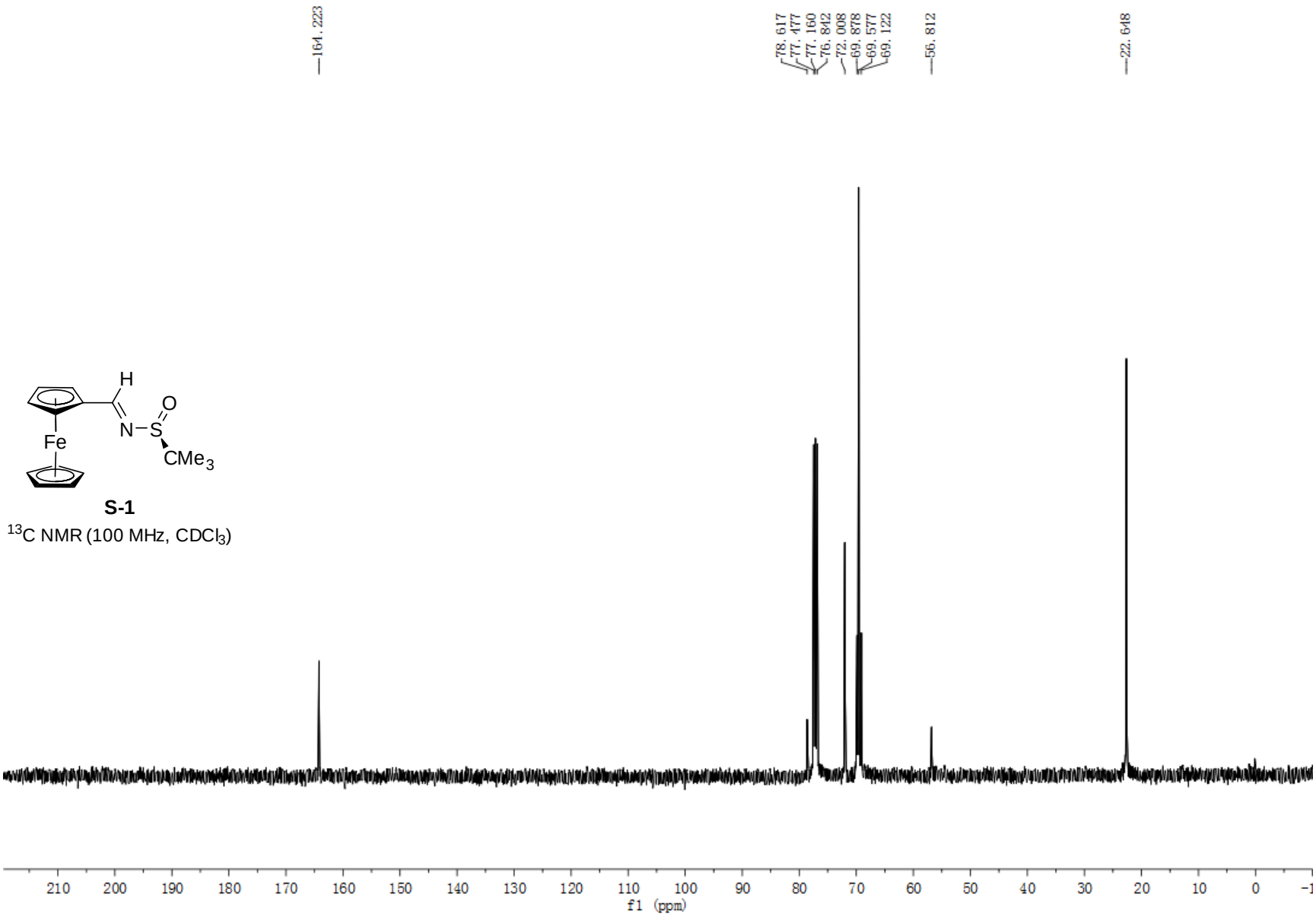


S-1

^{1}H NMR (400 MHz, $CDCl_3$)



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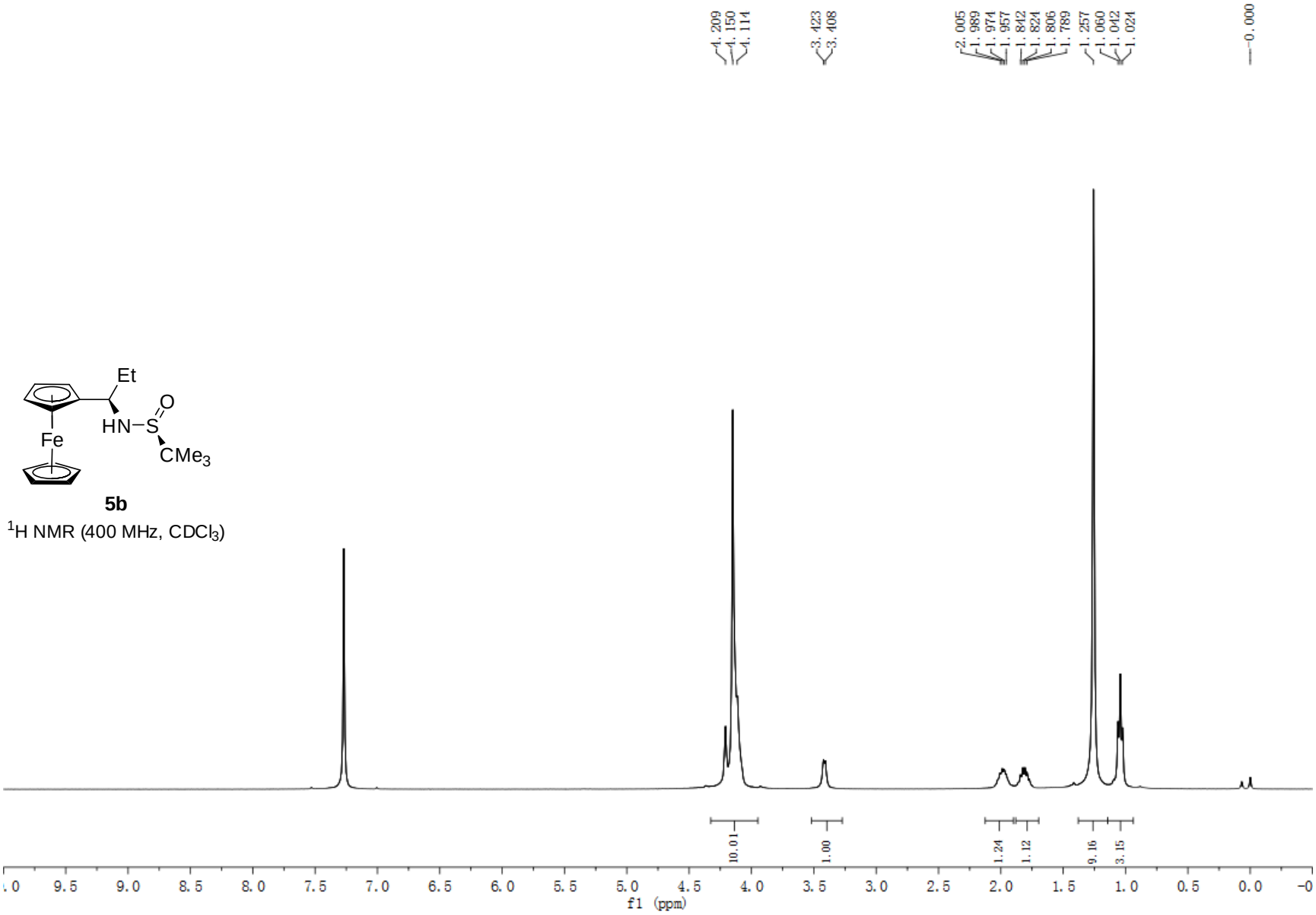

5b

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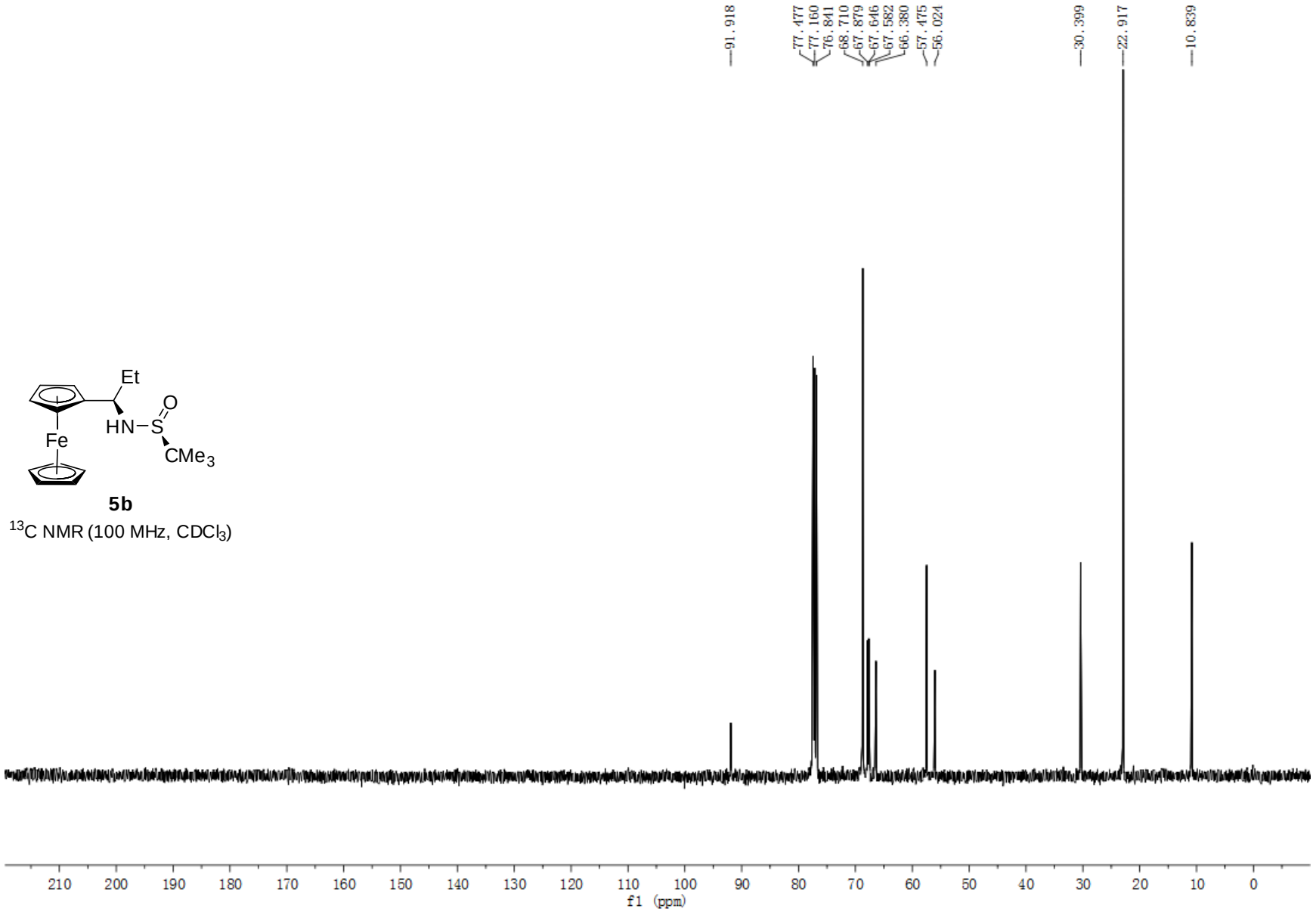

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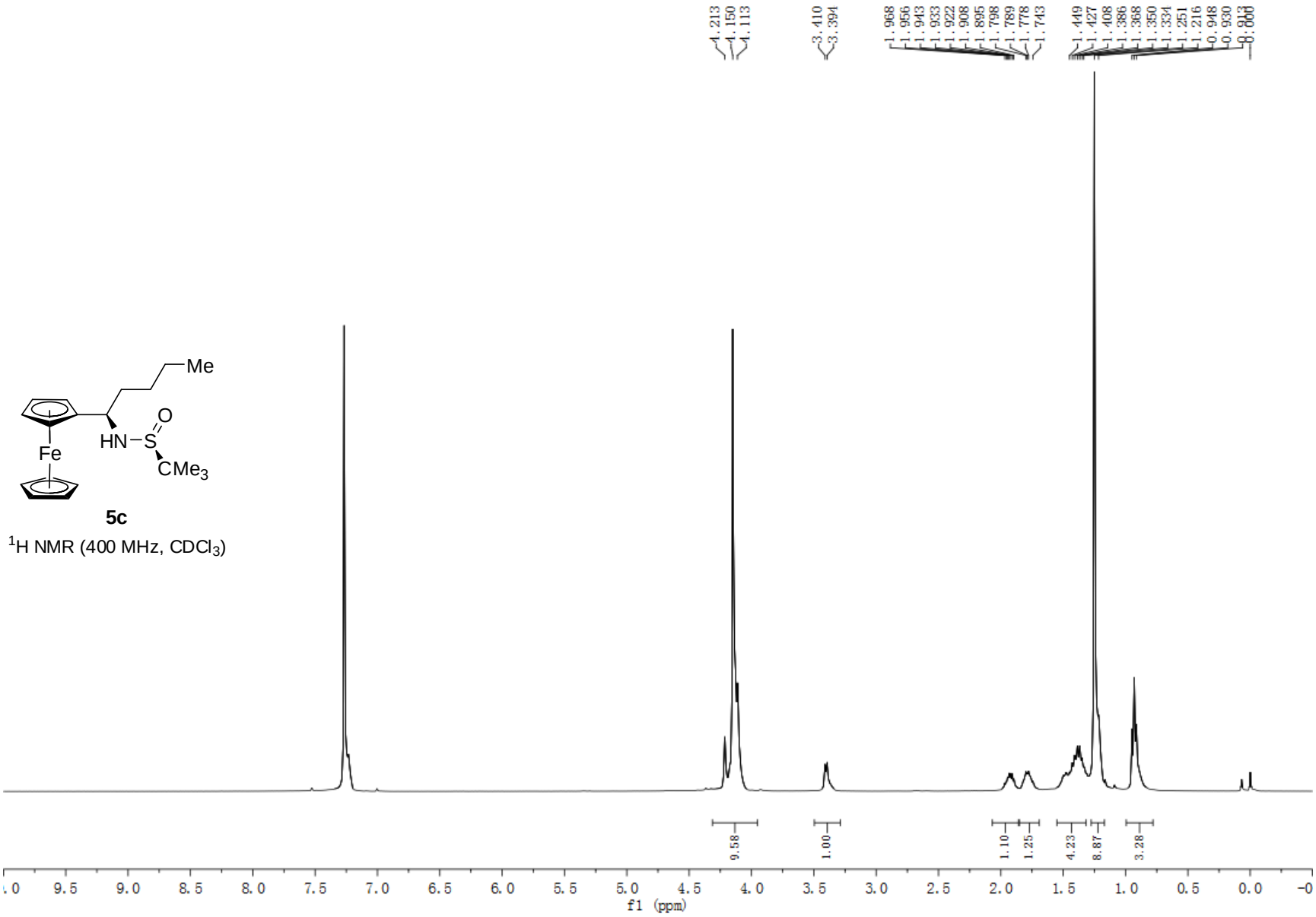

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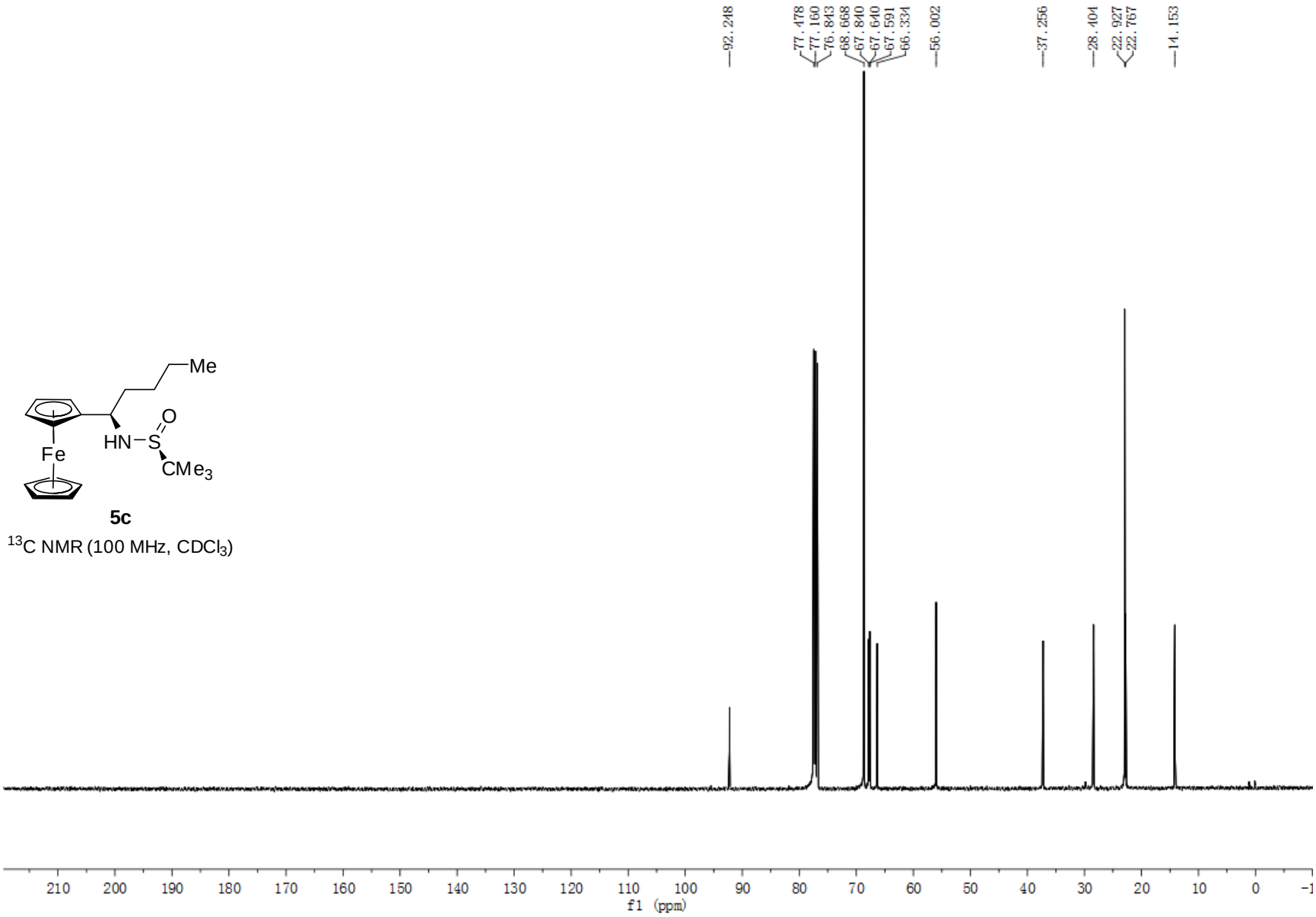

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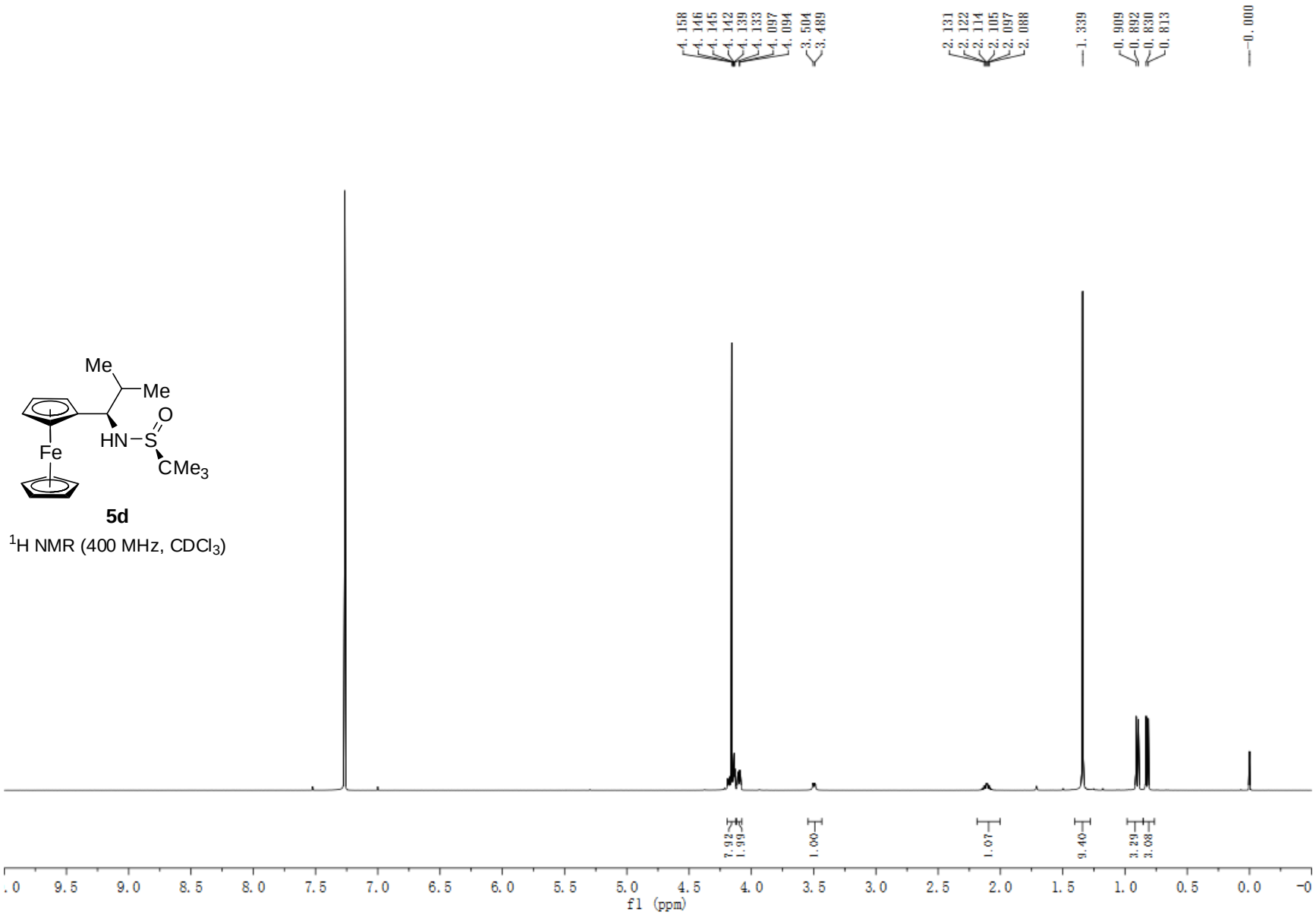

5d

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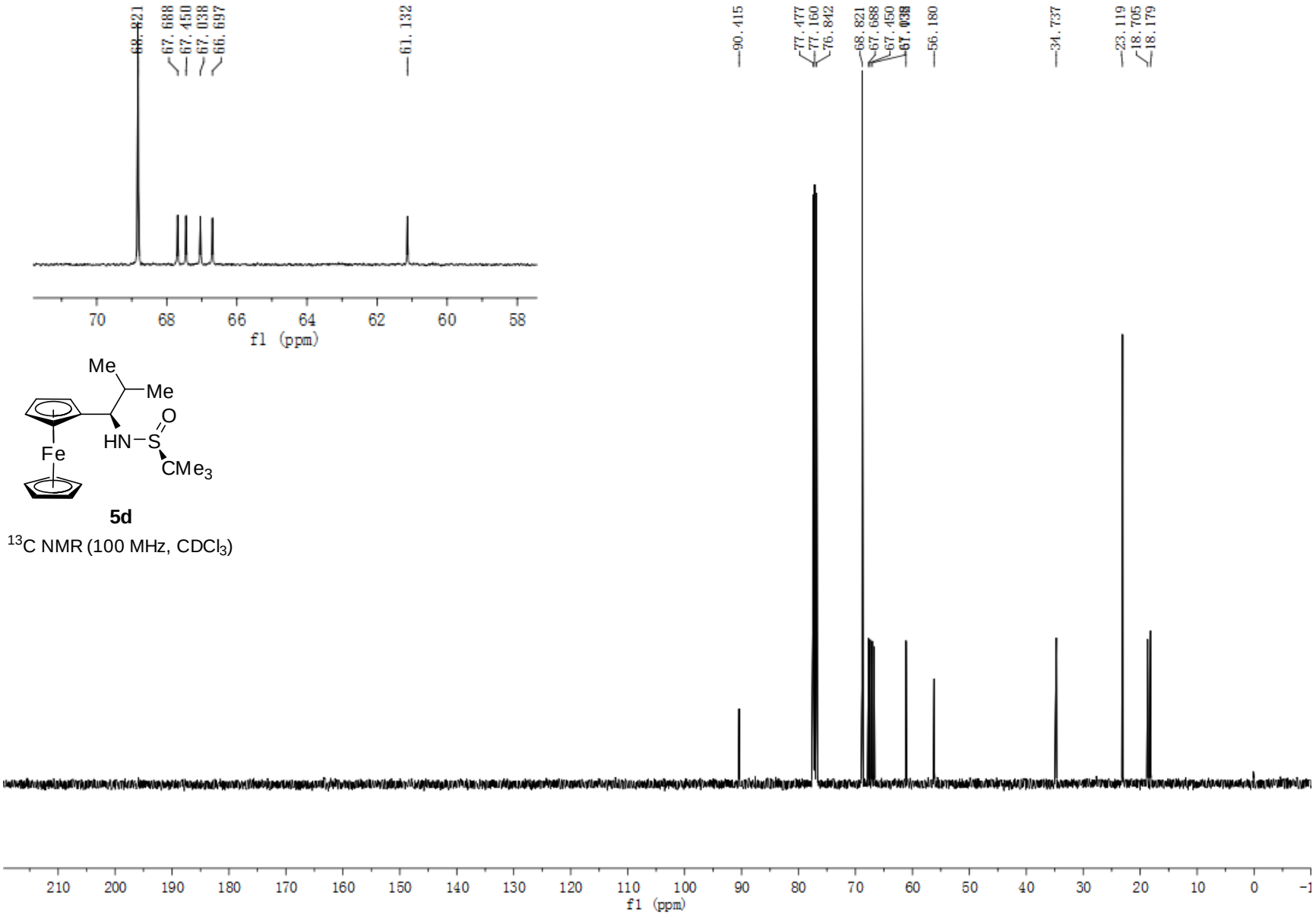

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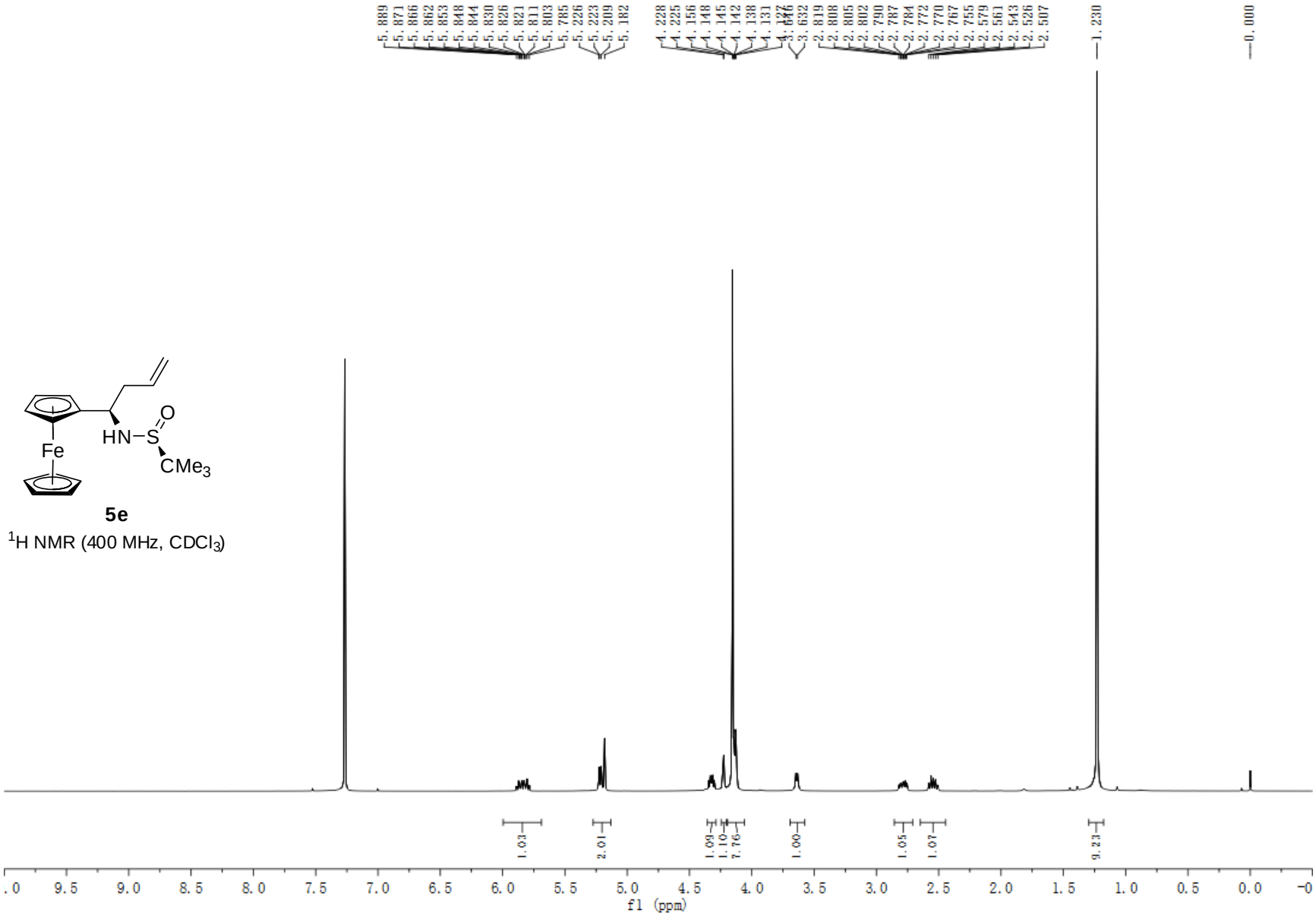
Fe
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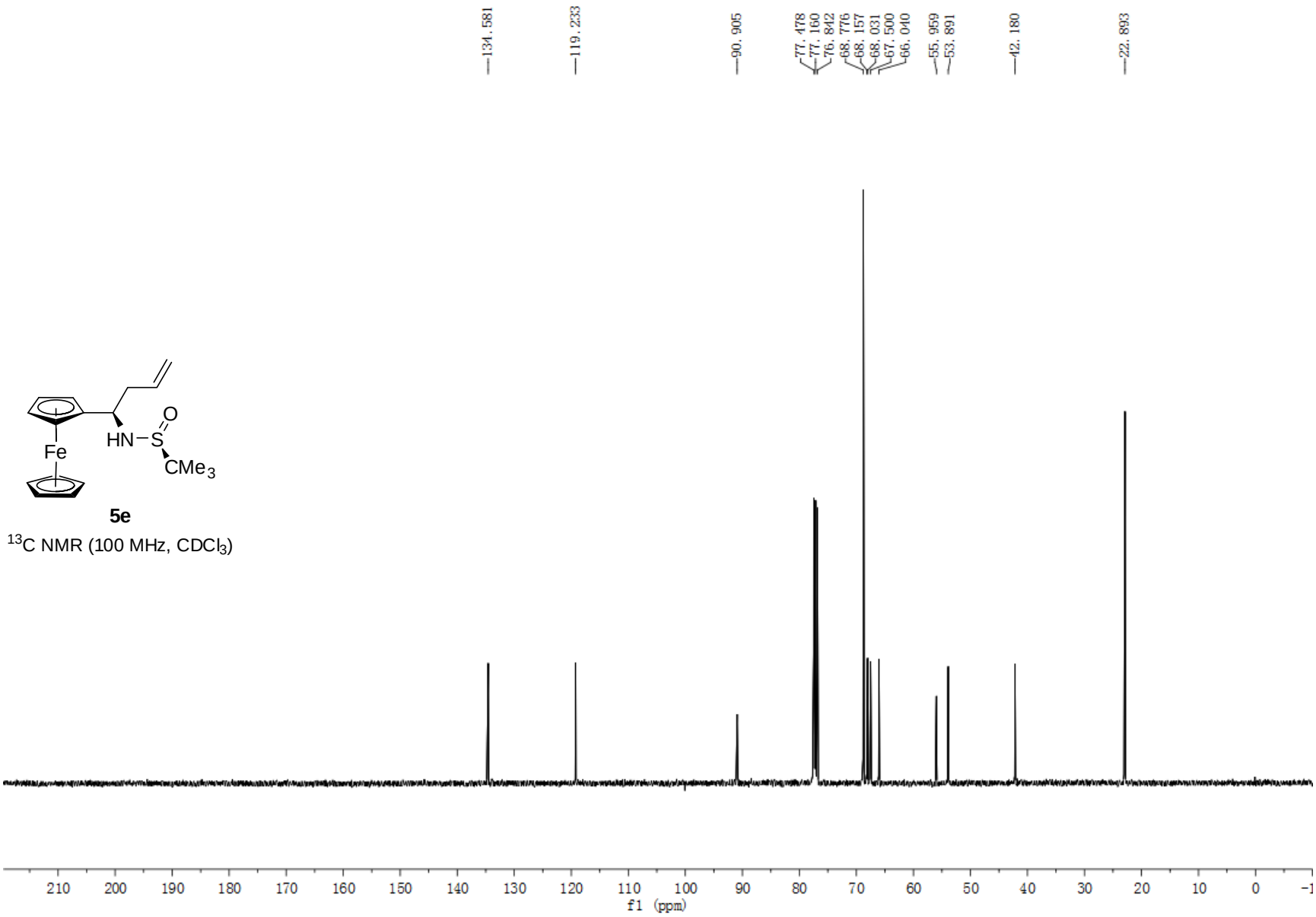
O
CMe3
5e
1H NMR (400 MHz, CDCl3)
f1 (ppm)



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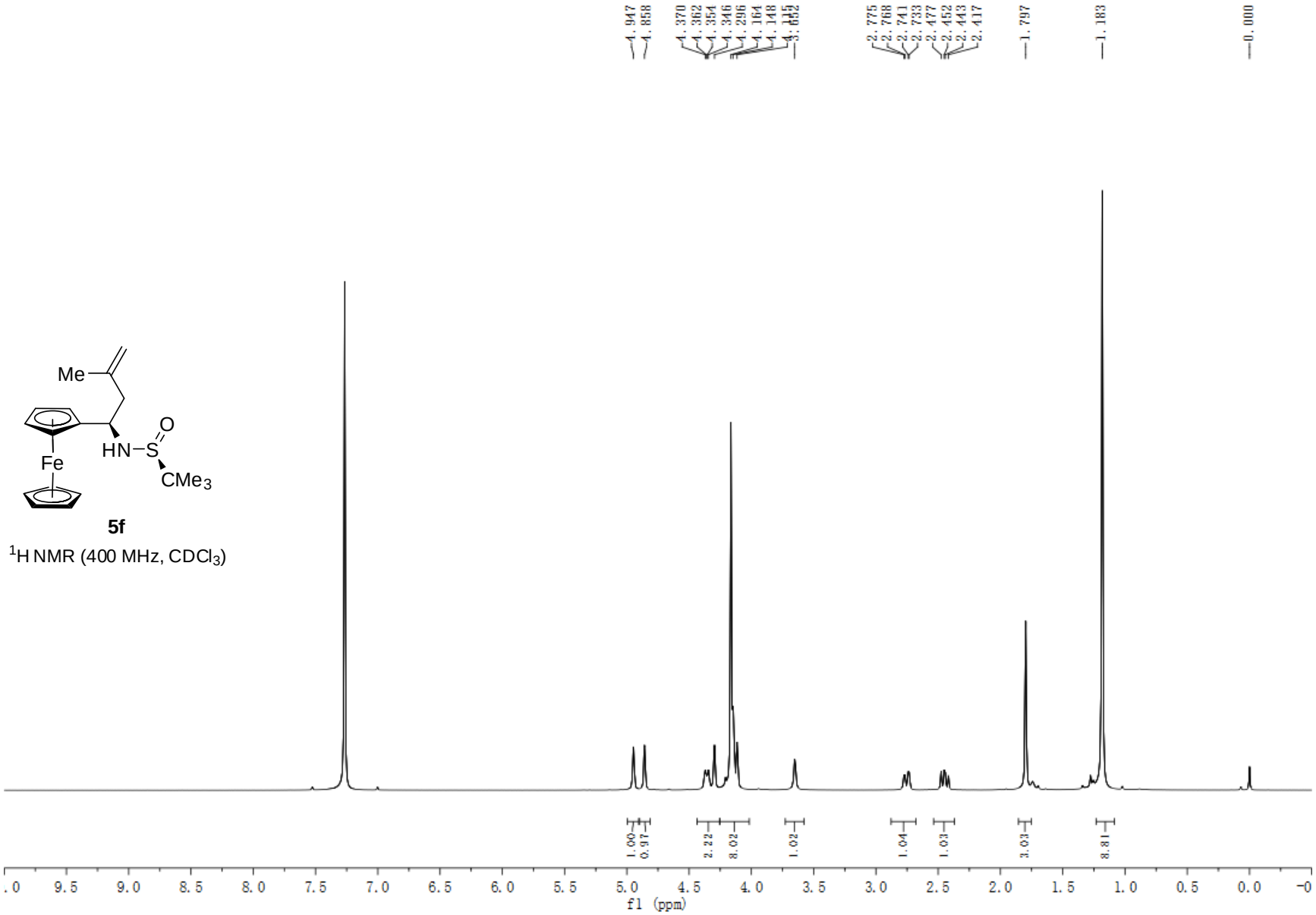

5f

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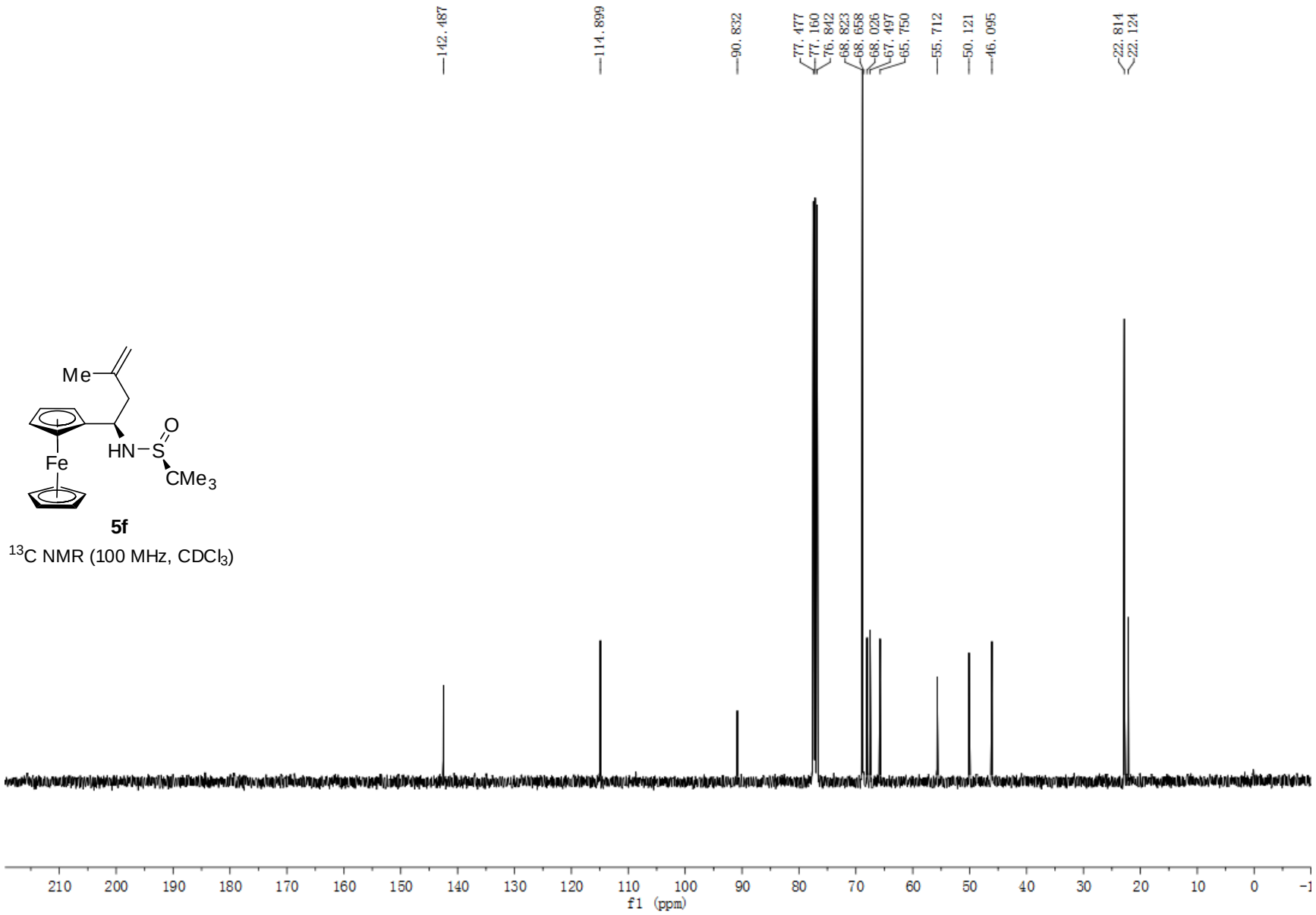

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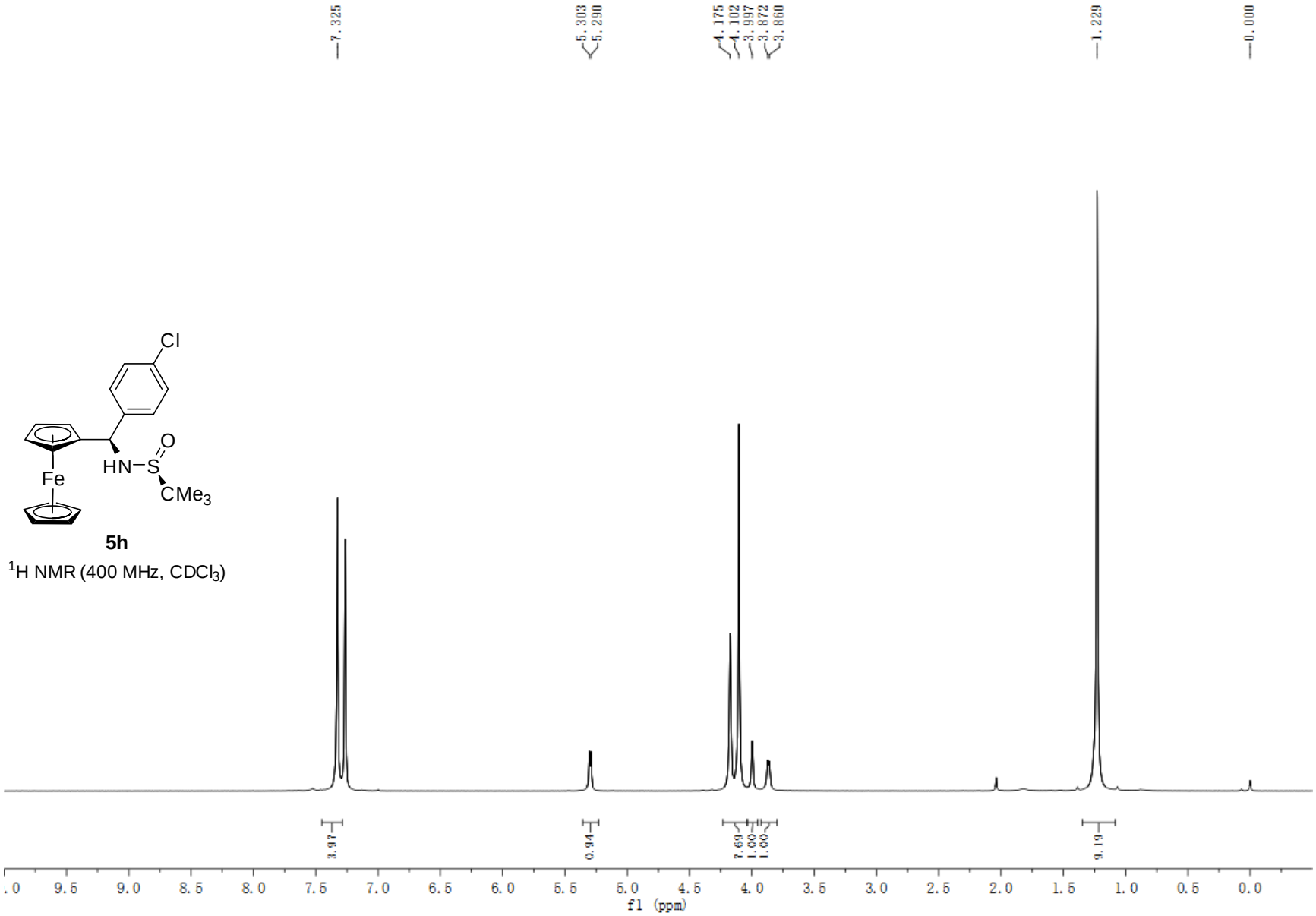
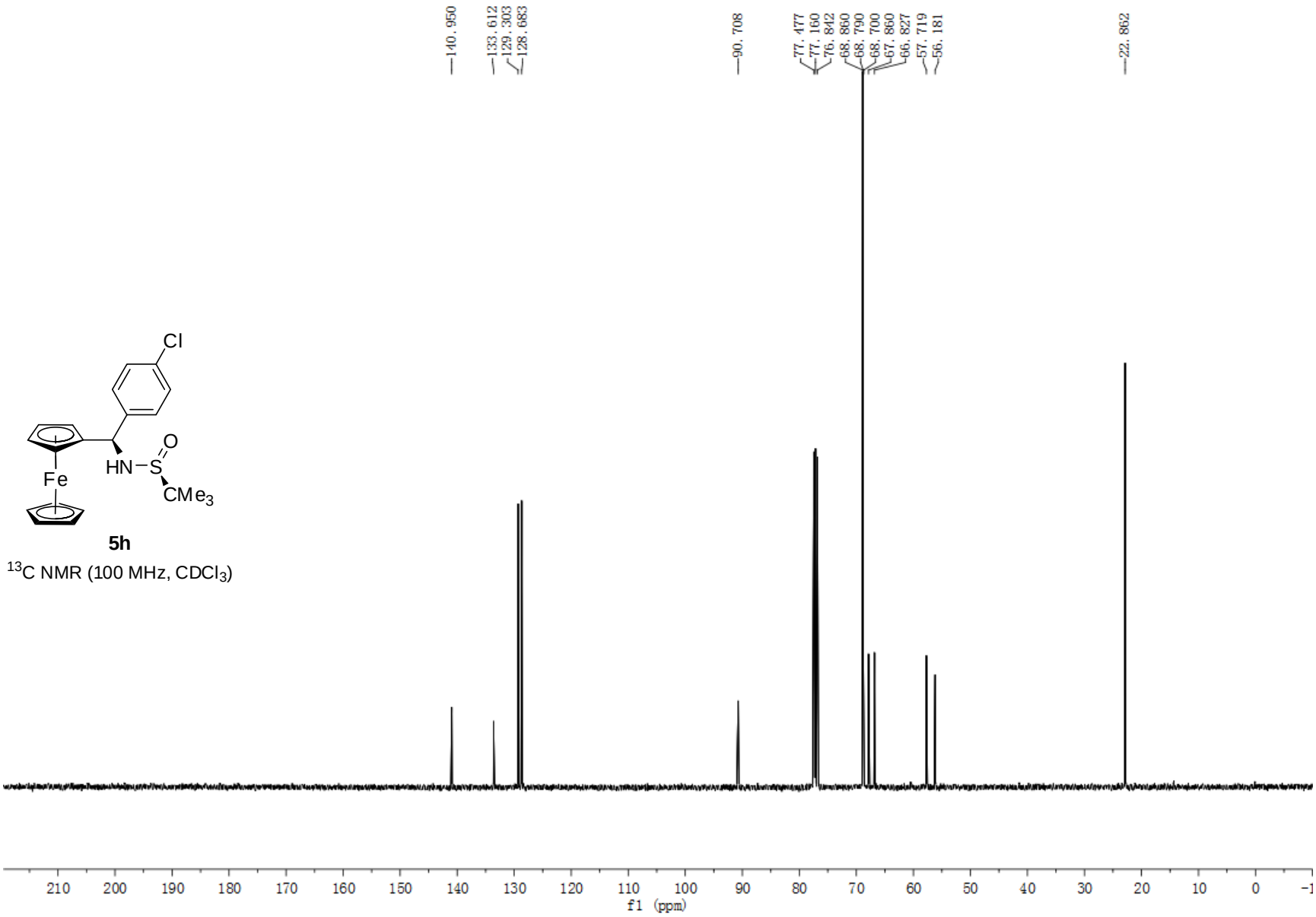


5h

^{1}H NMR (400 MHz, $CDCl_3$)



5h

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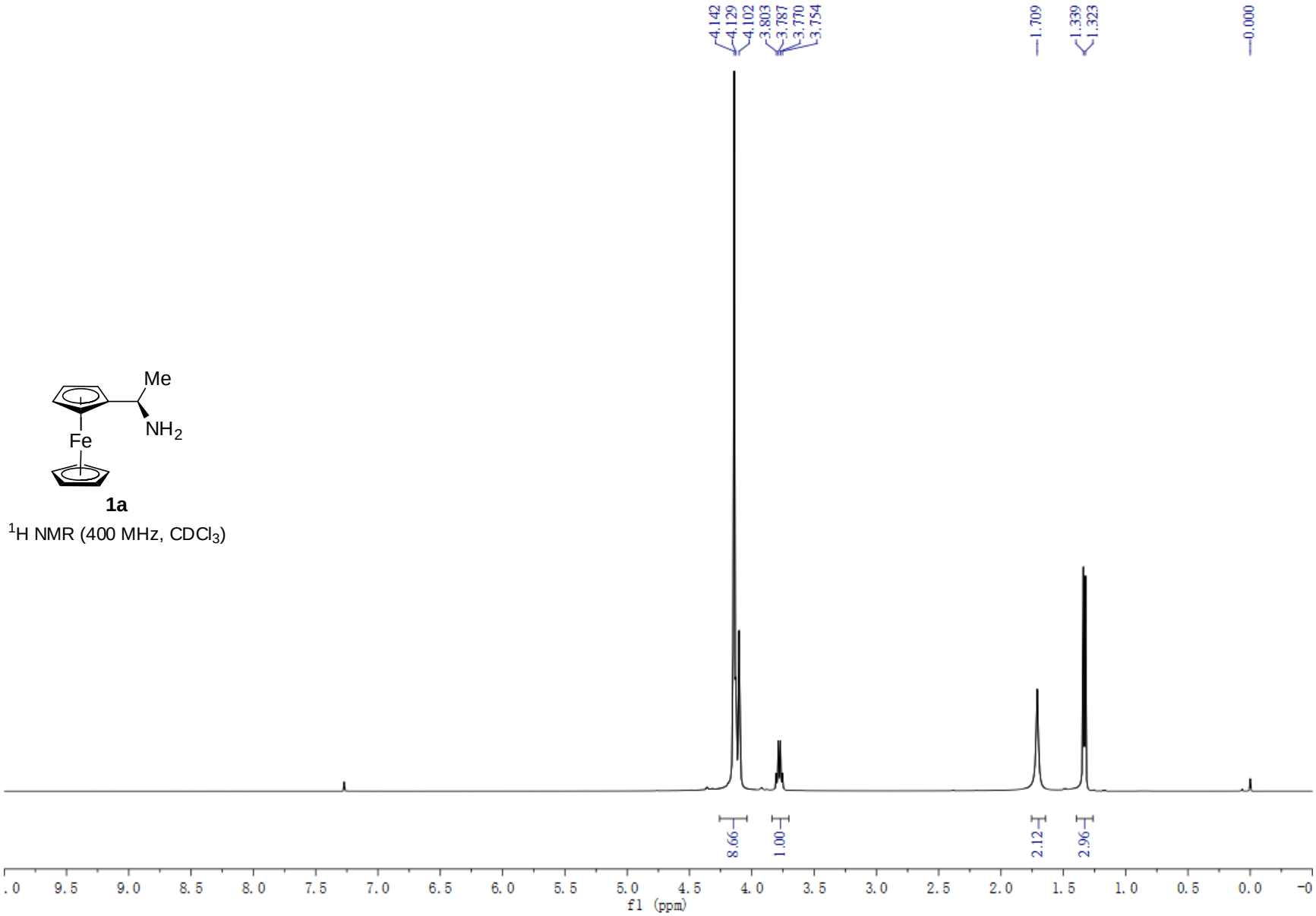
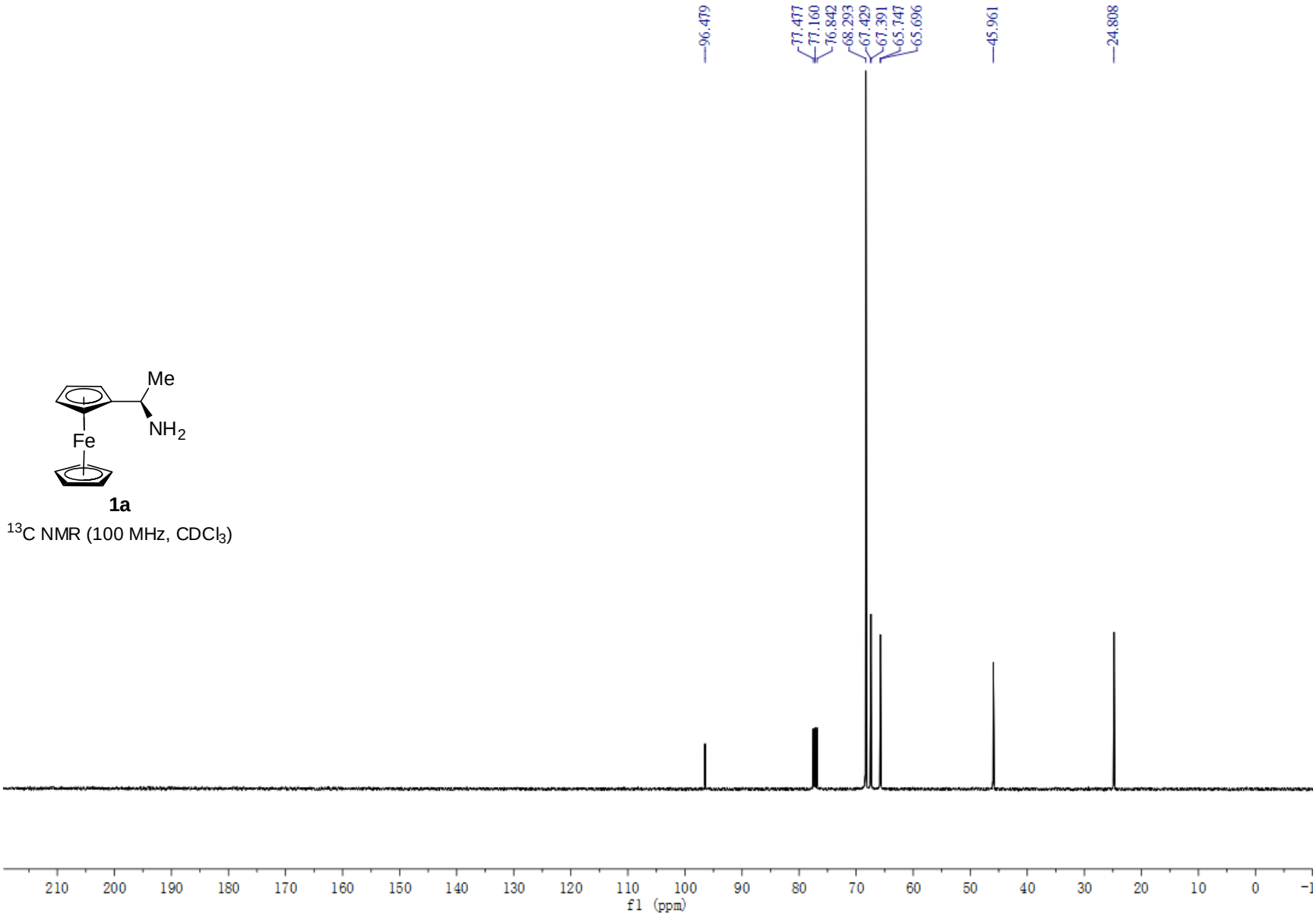


1a

^{1}H NMR (400 MHz, $CDCl_3$)



1a

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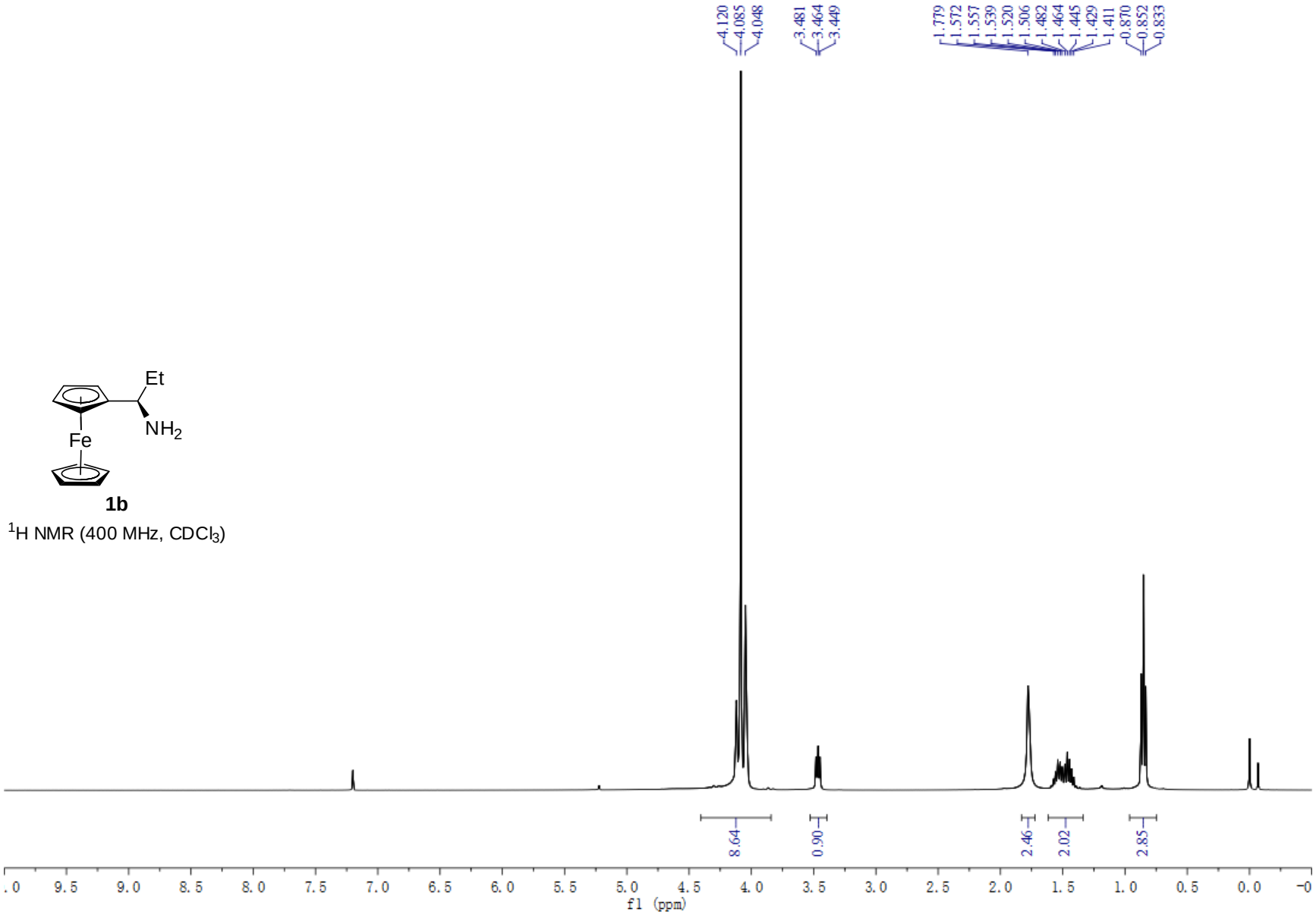
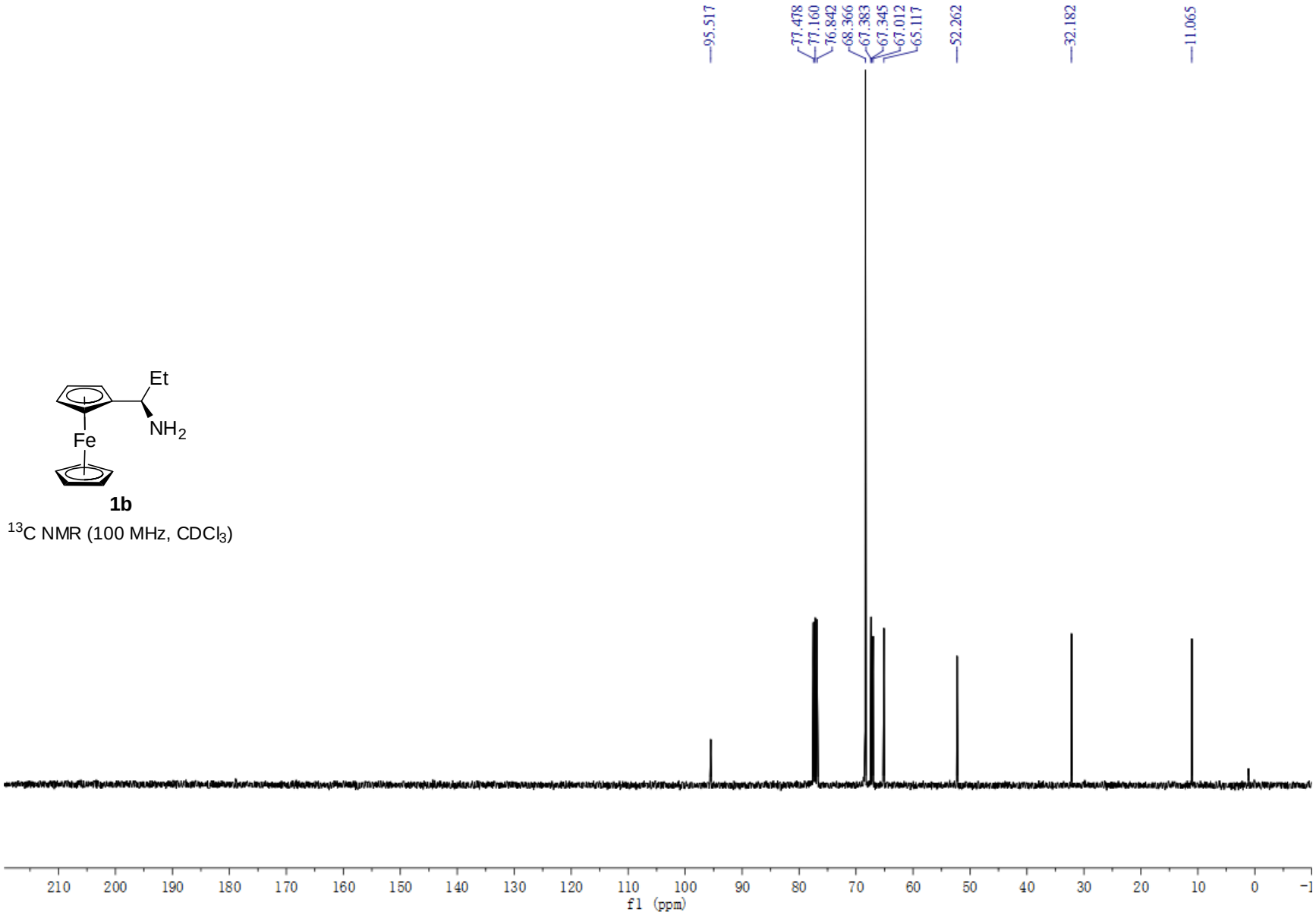


Et
NH$_2$
Fe

1b

^{1}H NMR (400 MHz, $CDCl_3$)



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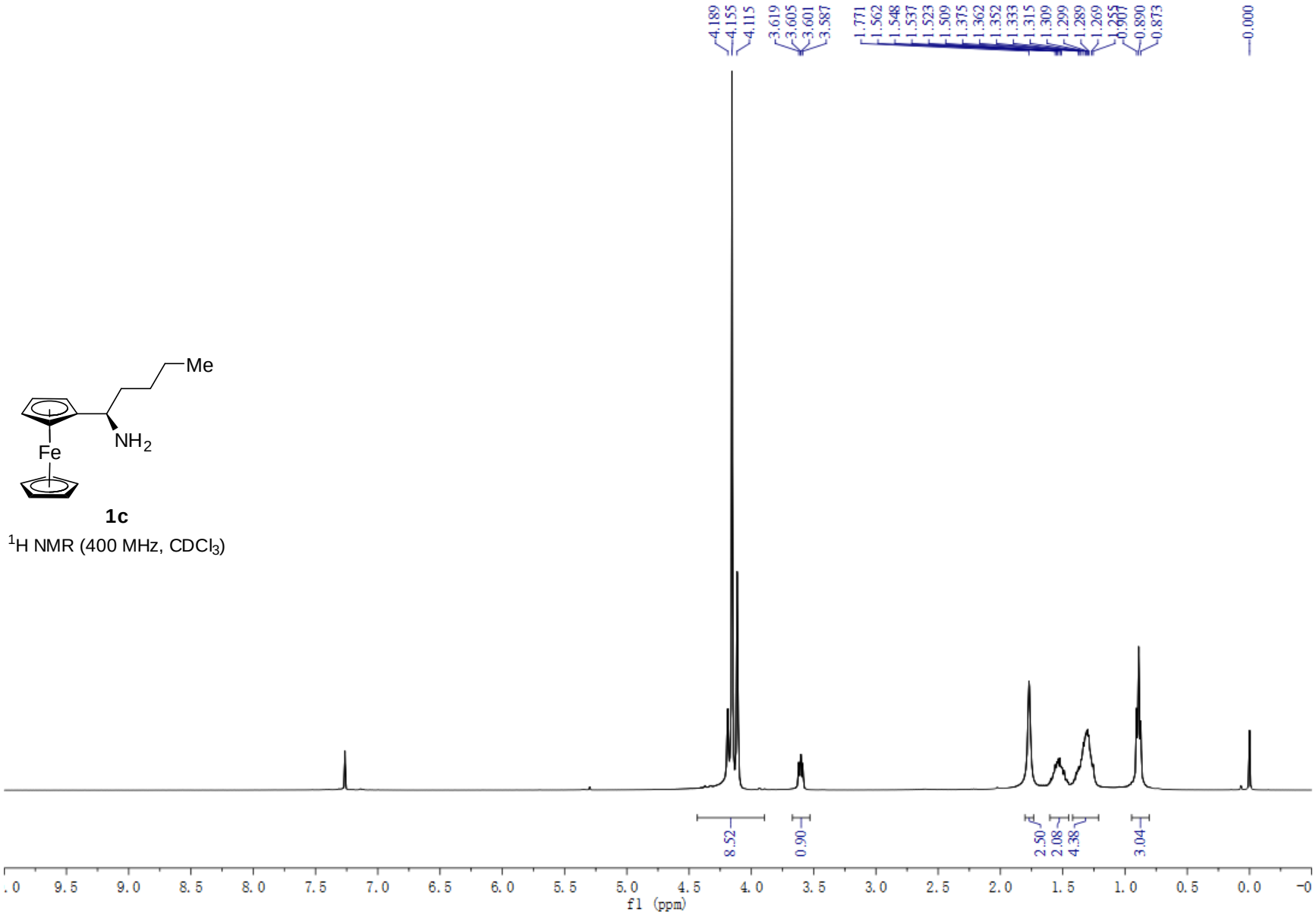

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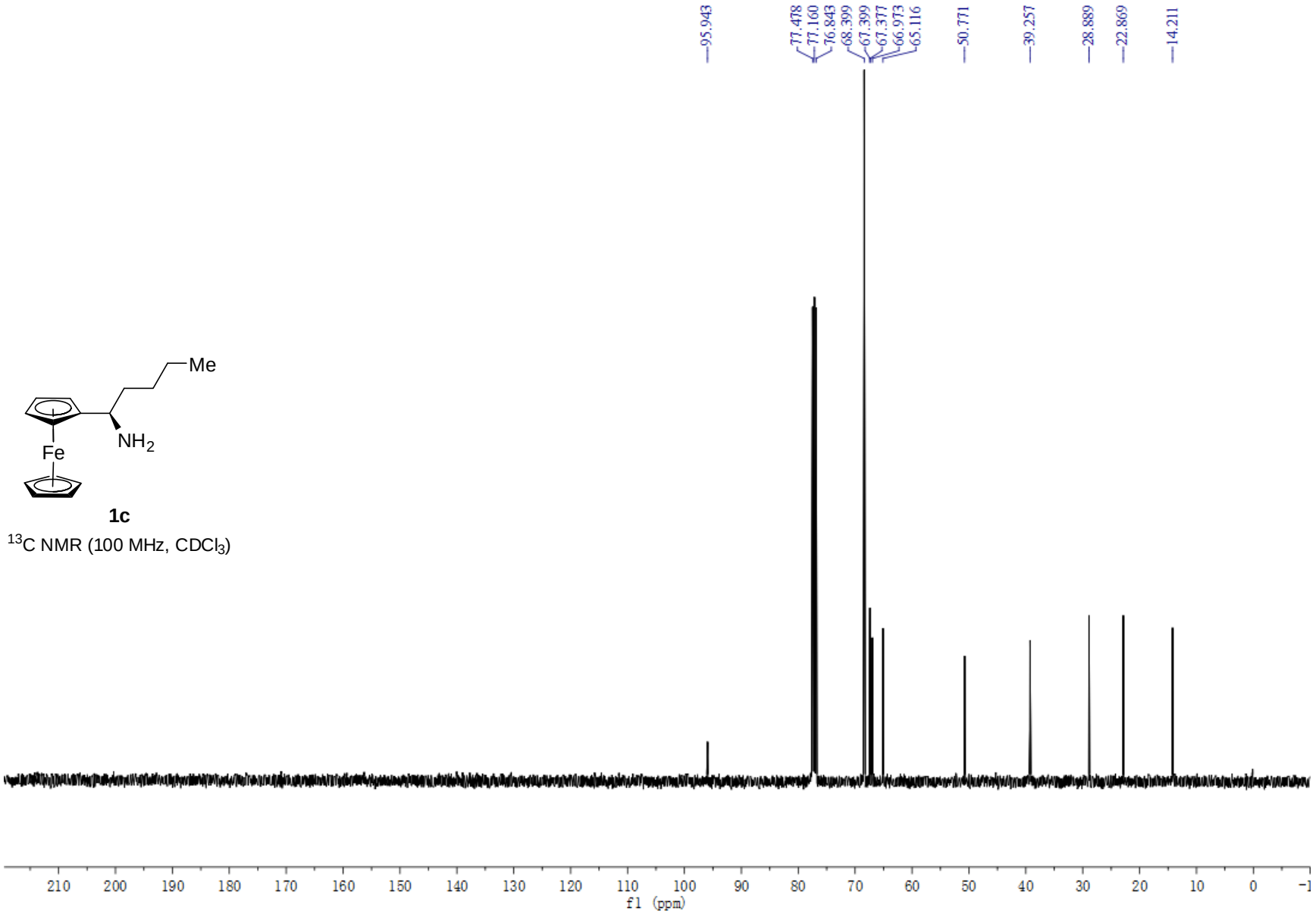

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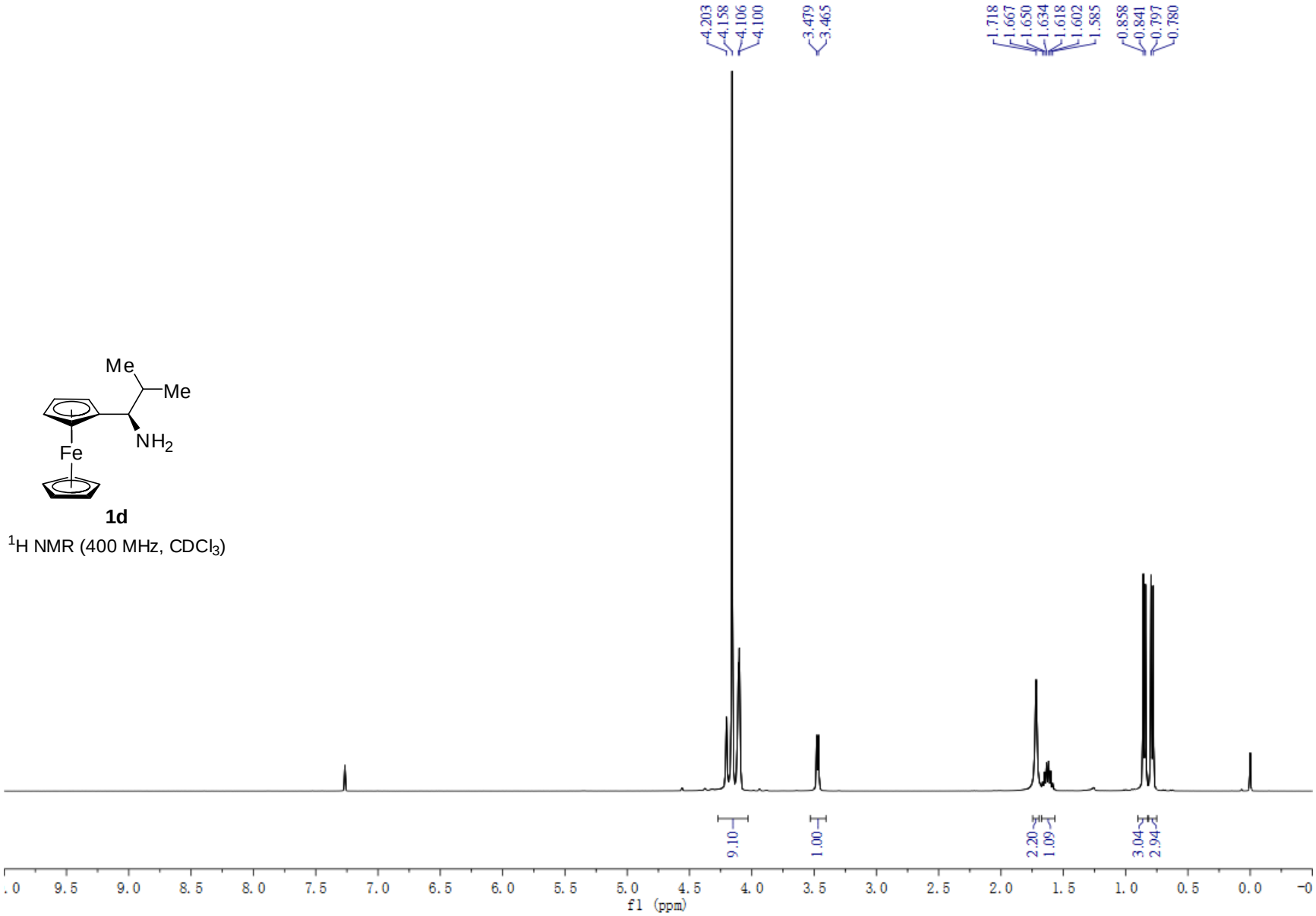

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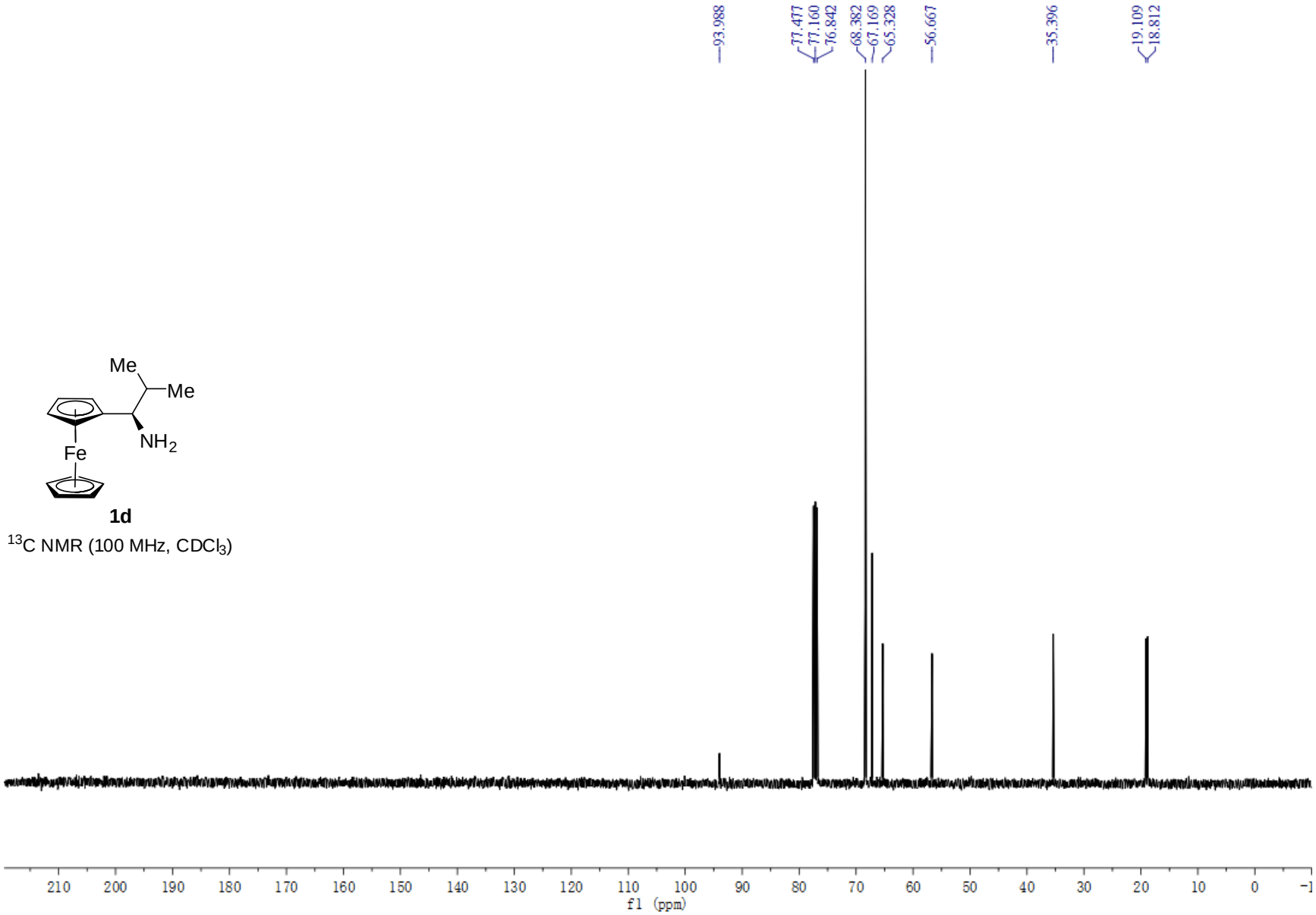

1d

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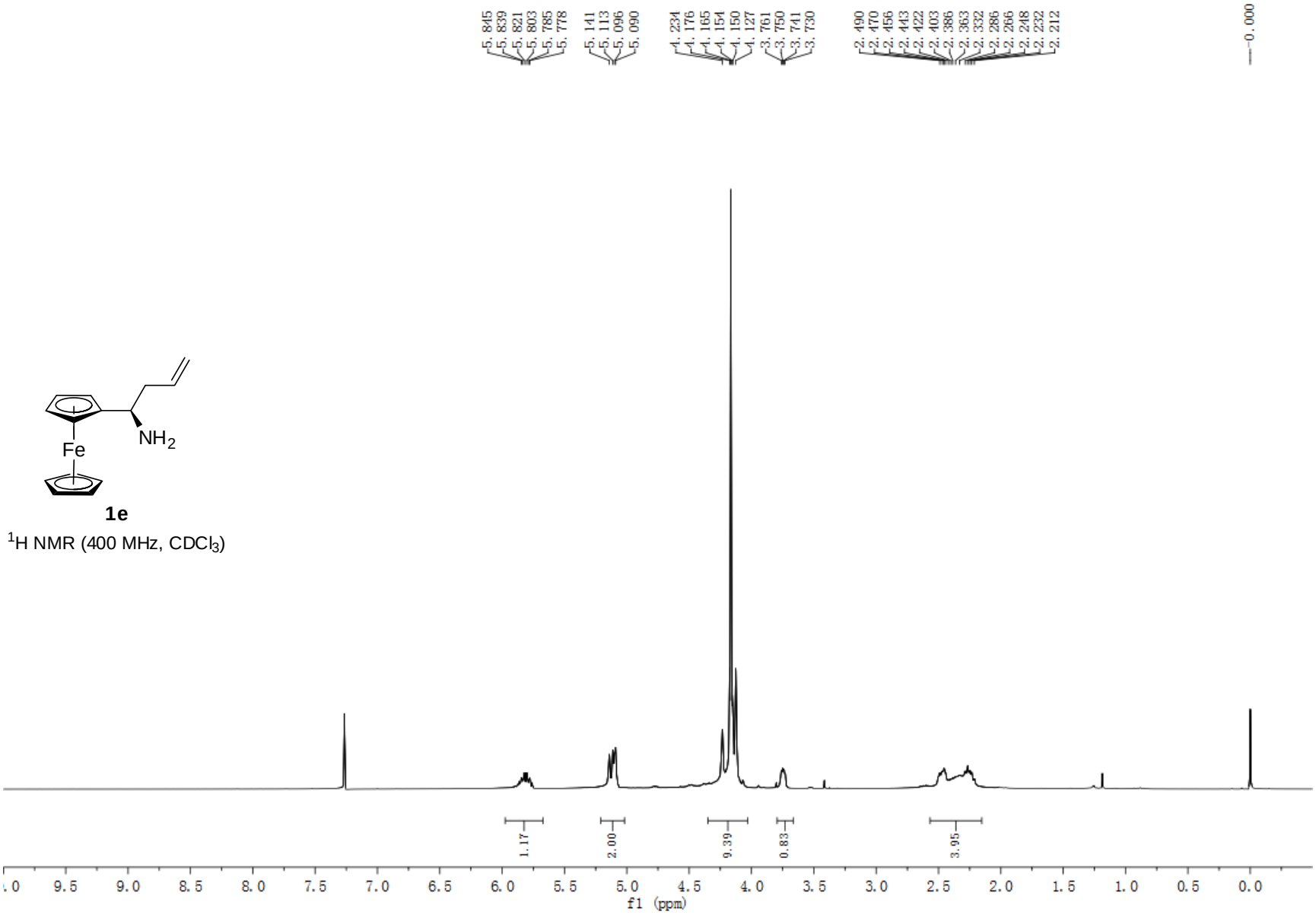

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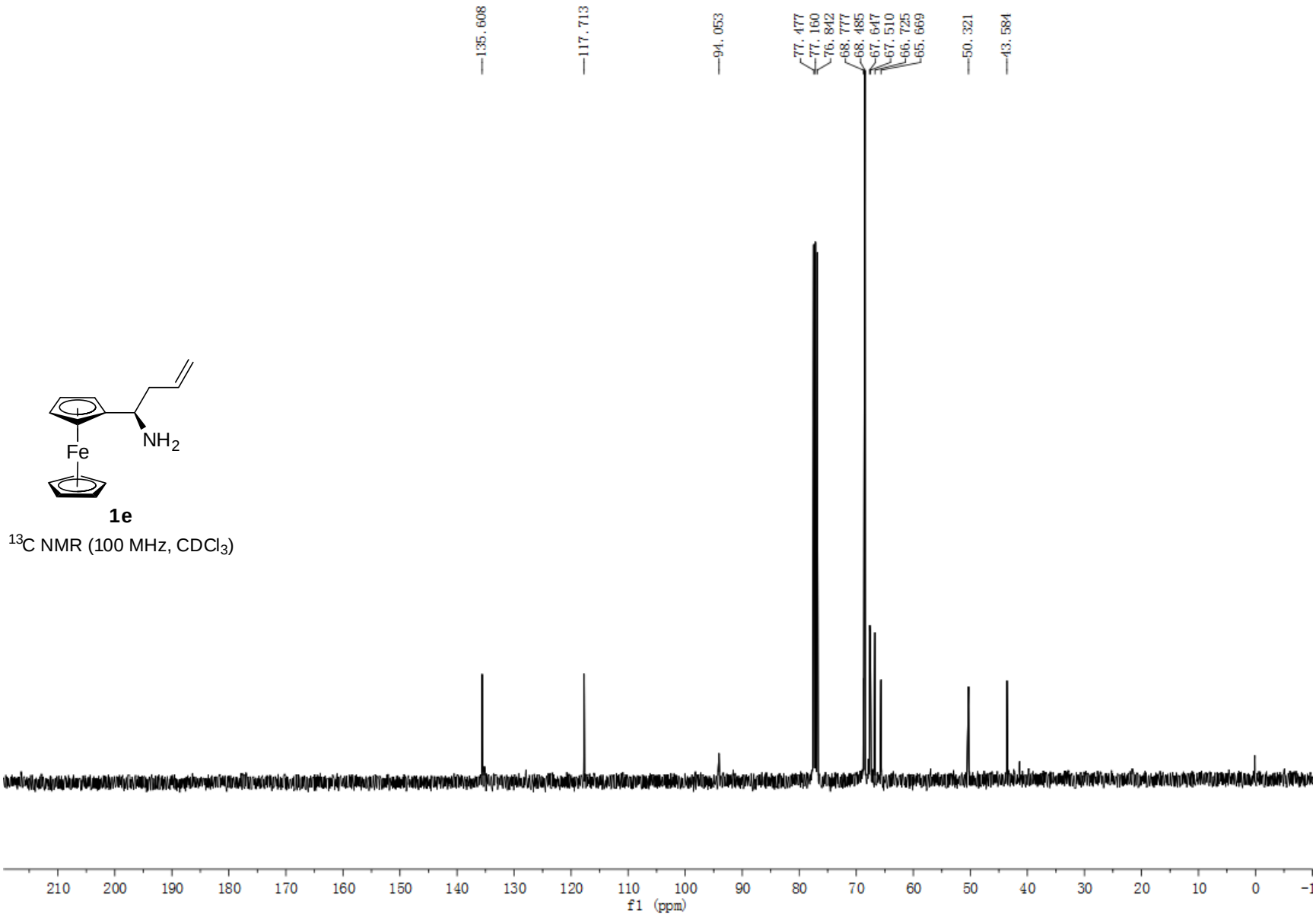

1e

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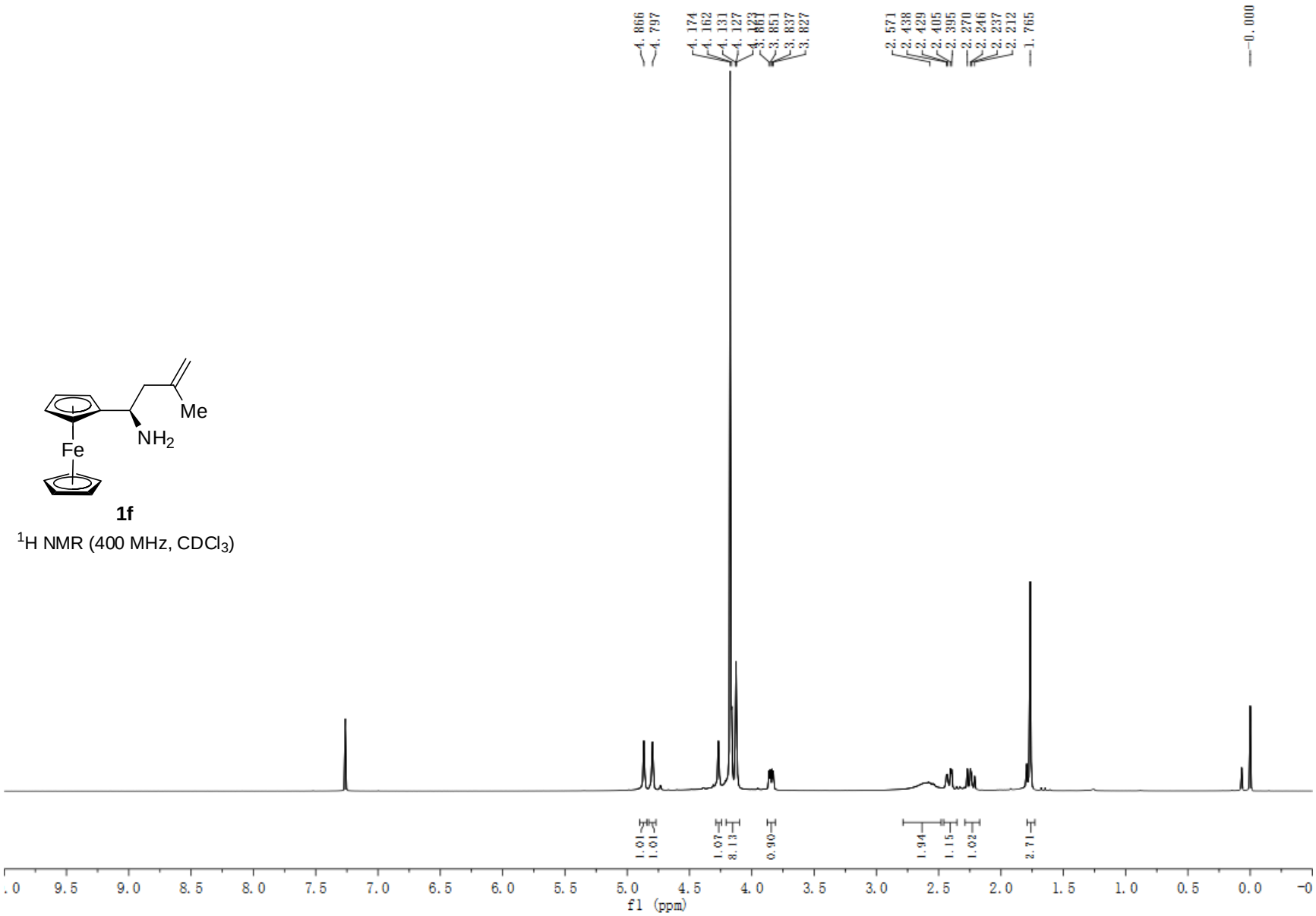

1f

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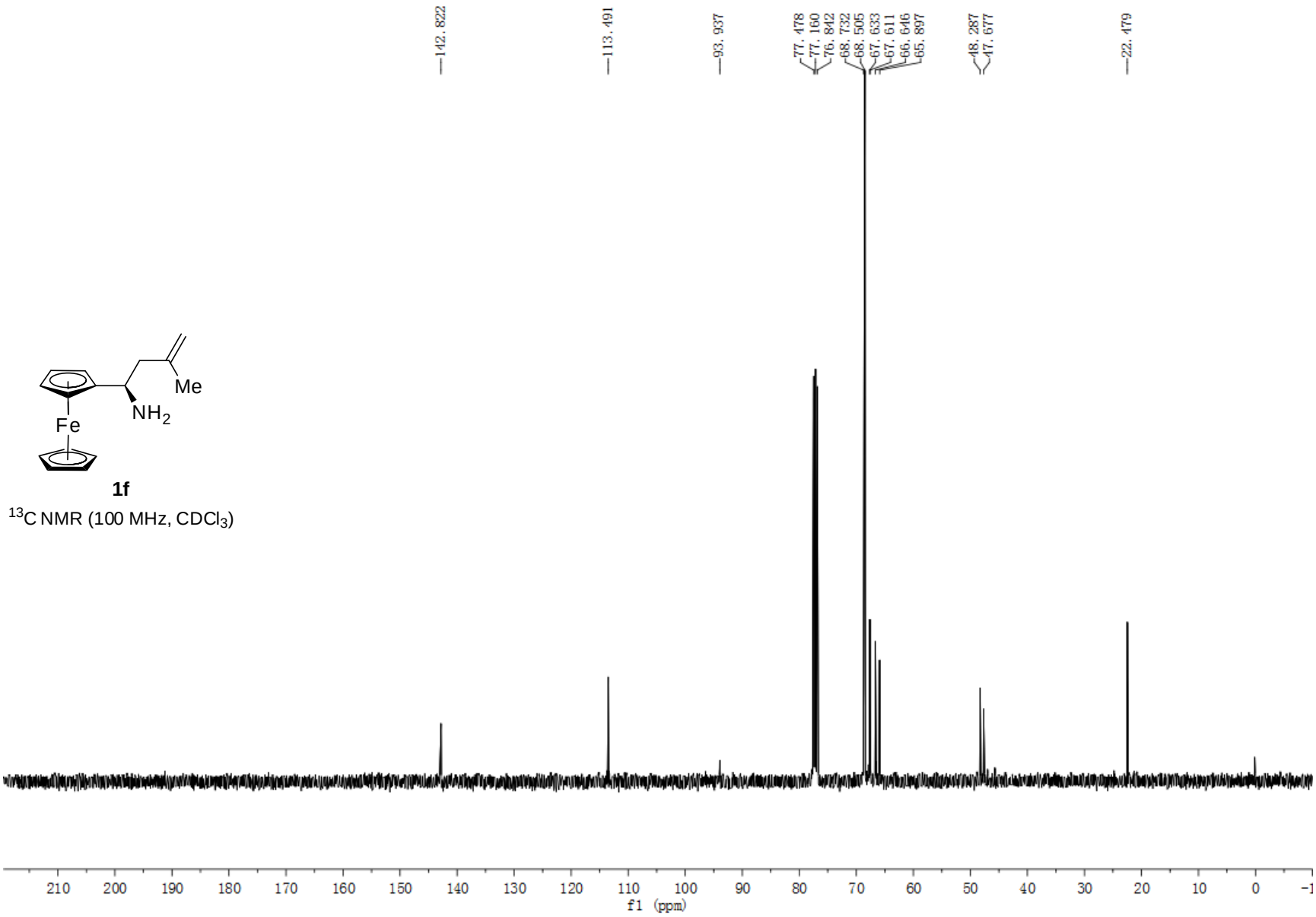

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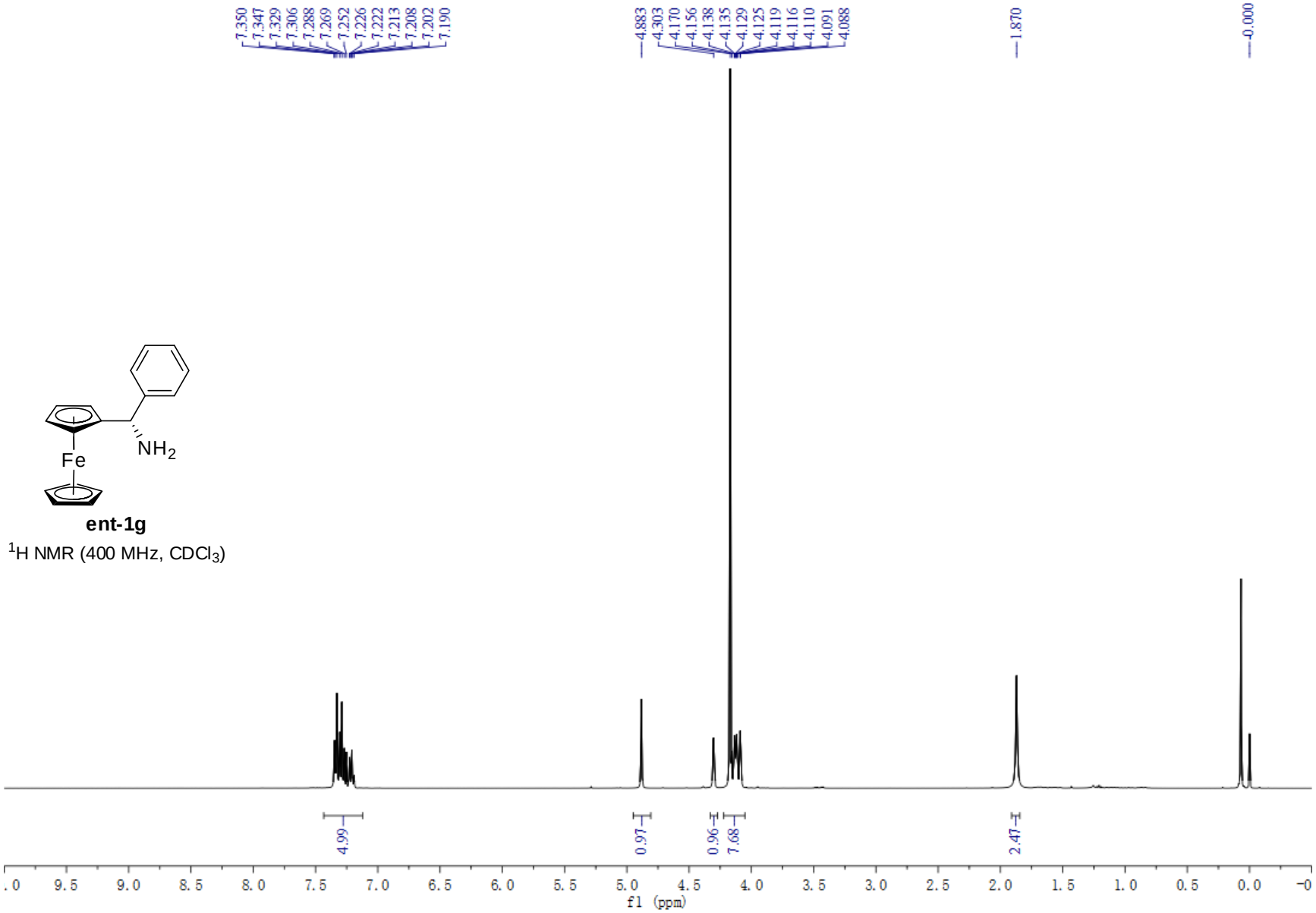

ent-1g

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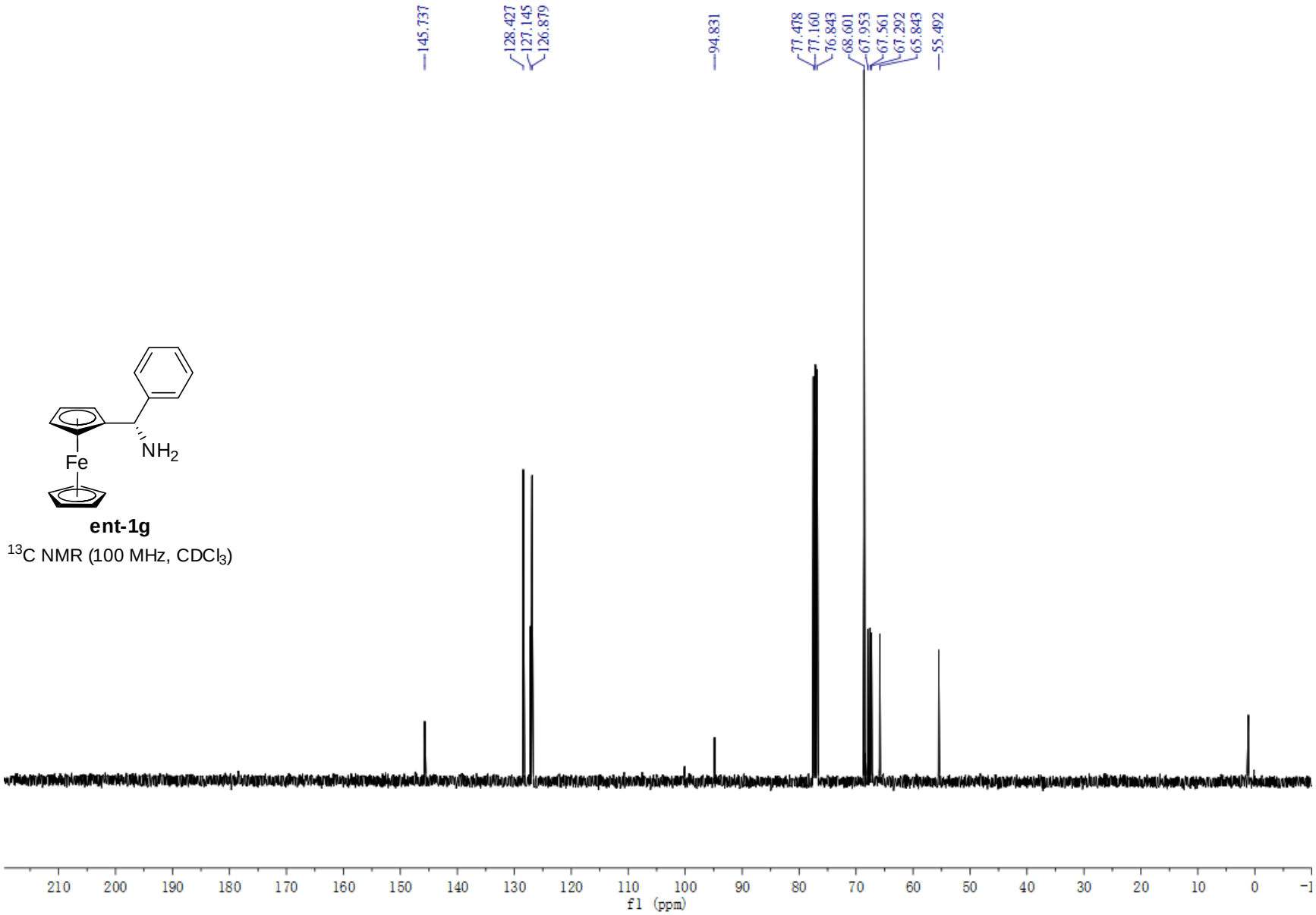

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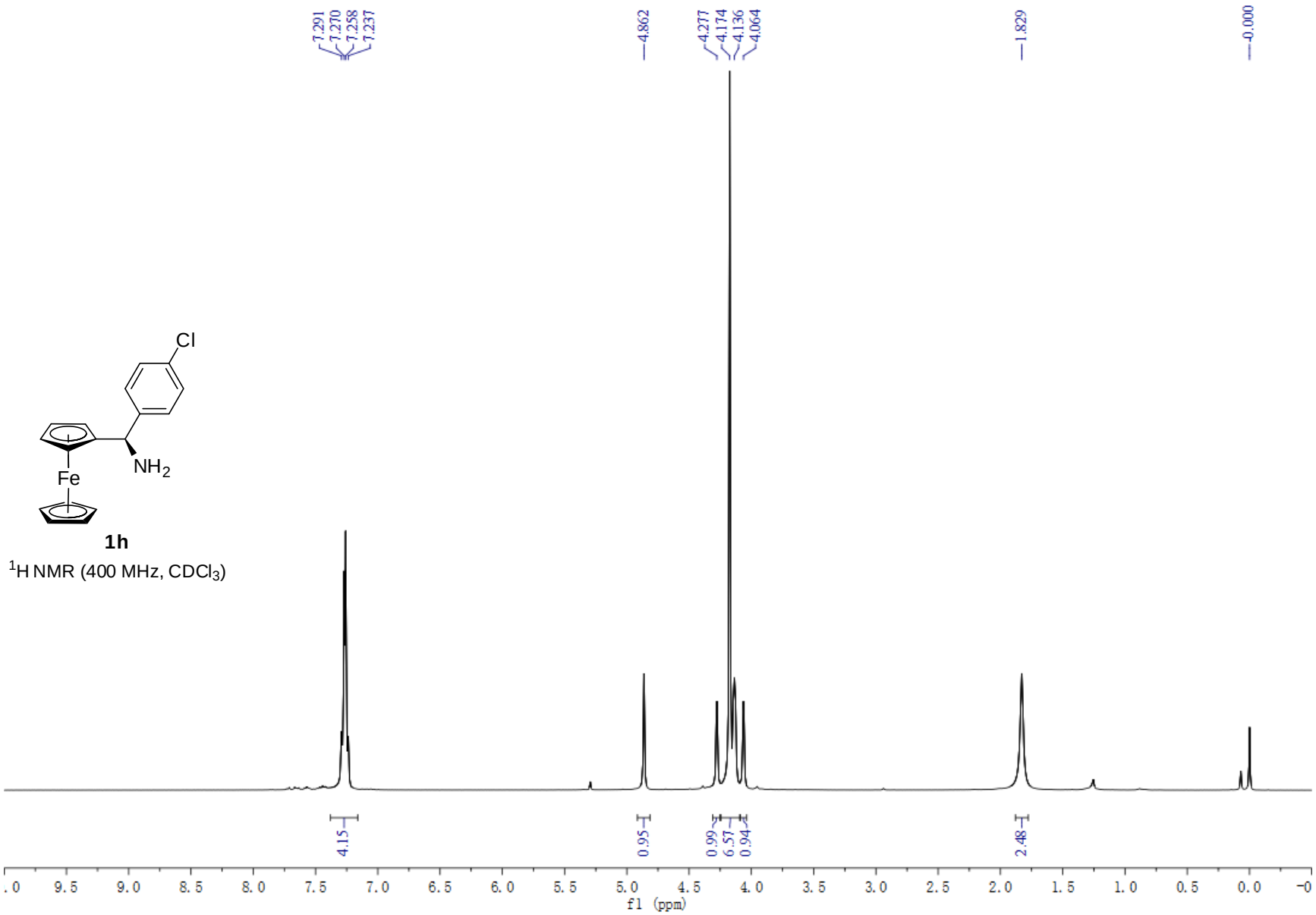

1h

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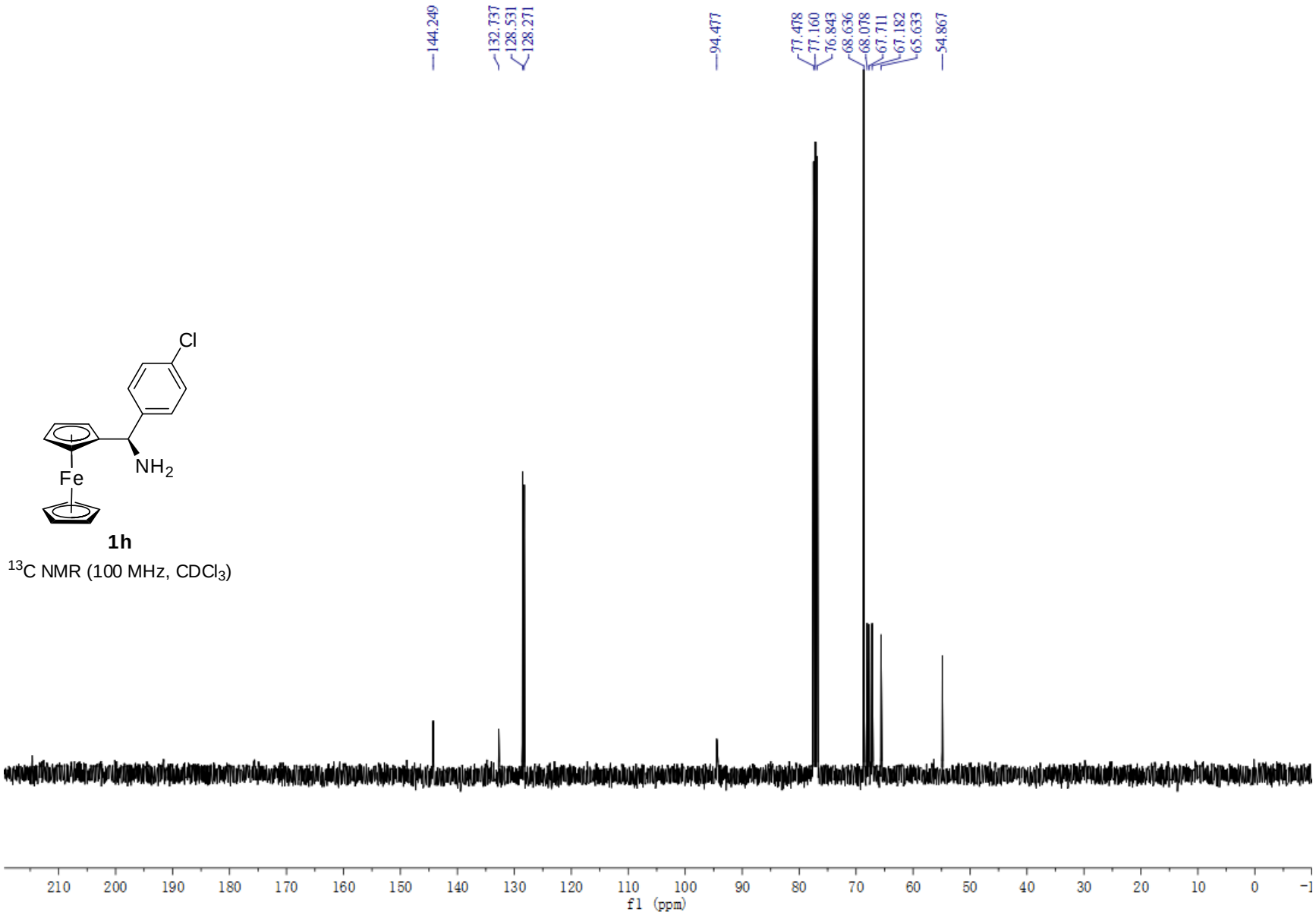

1h

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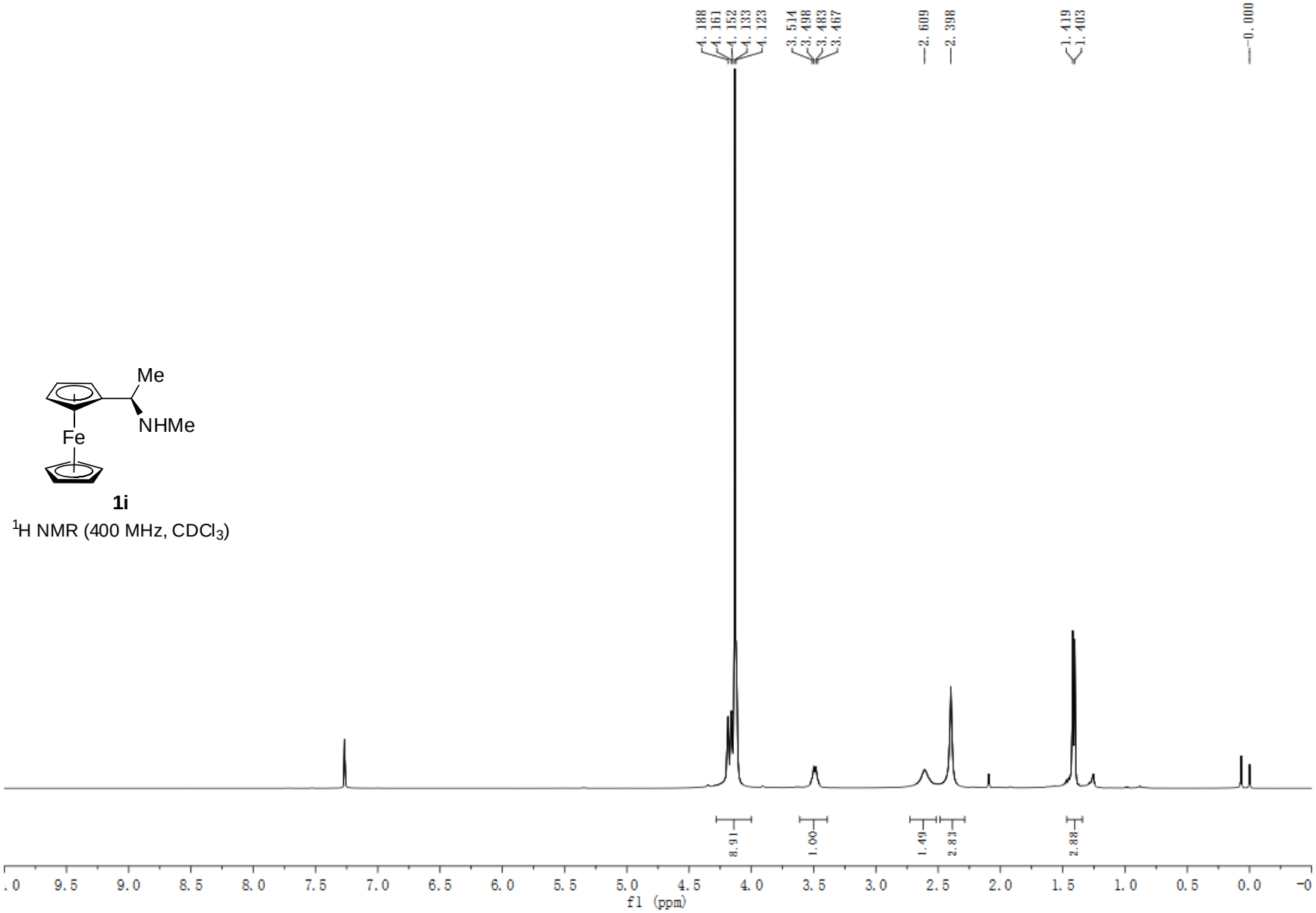

1i

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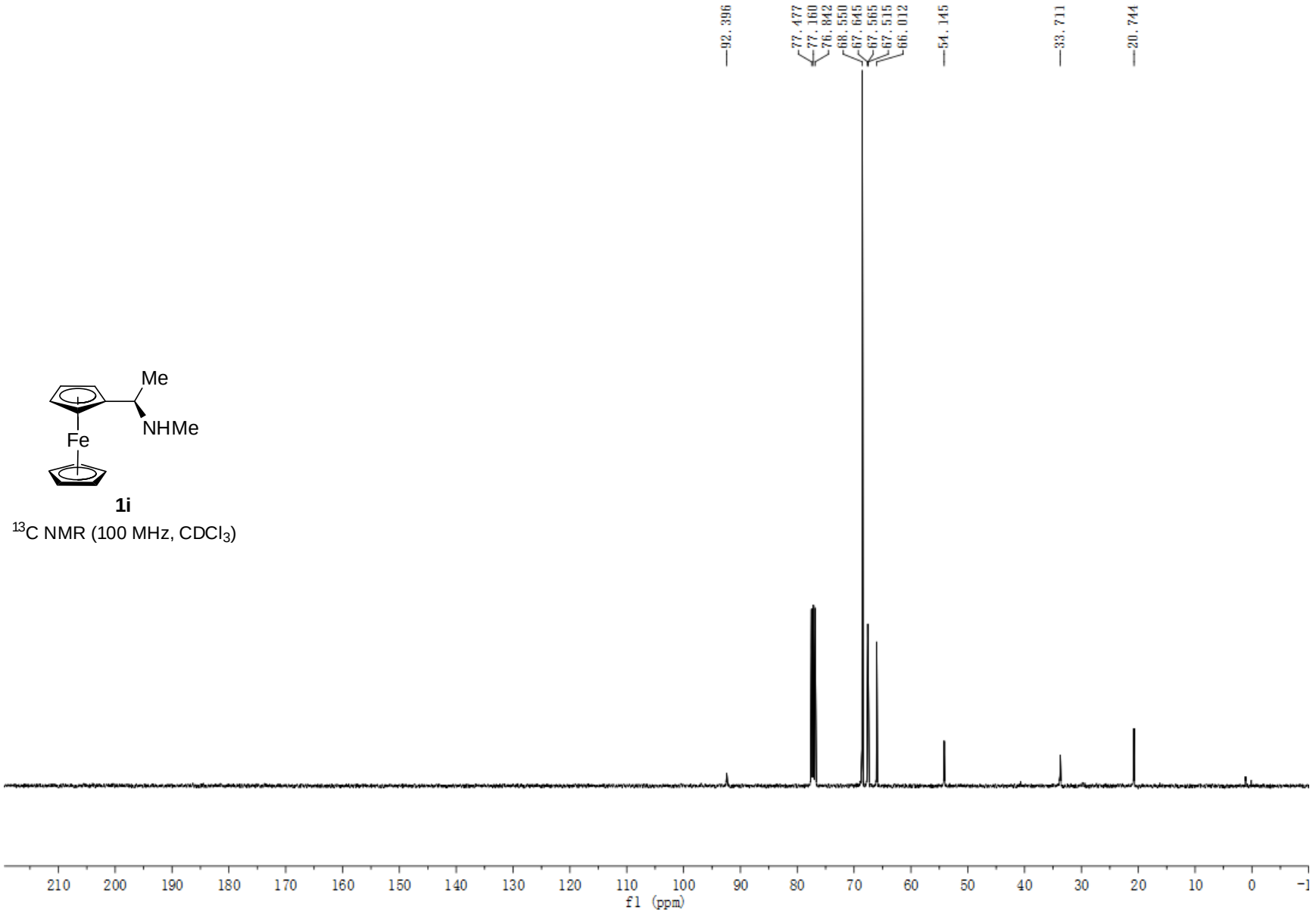

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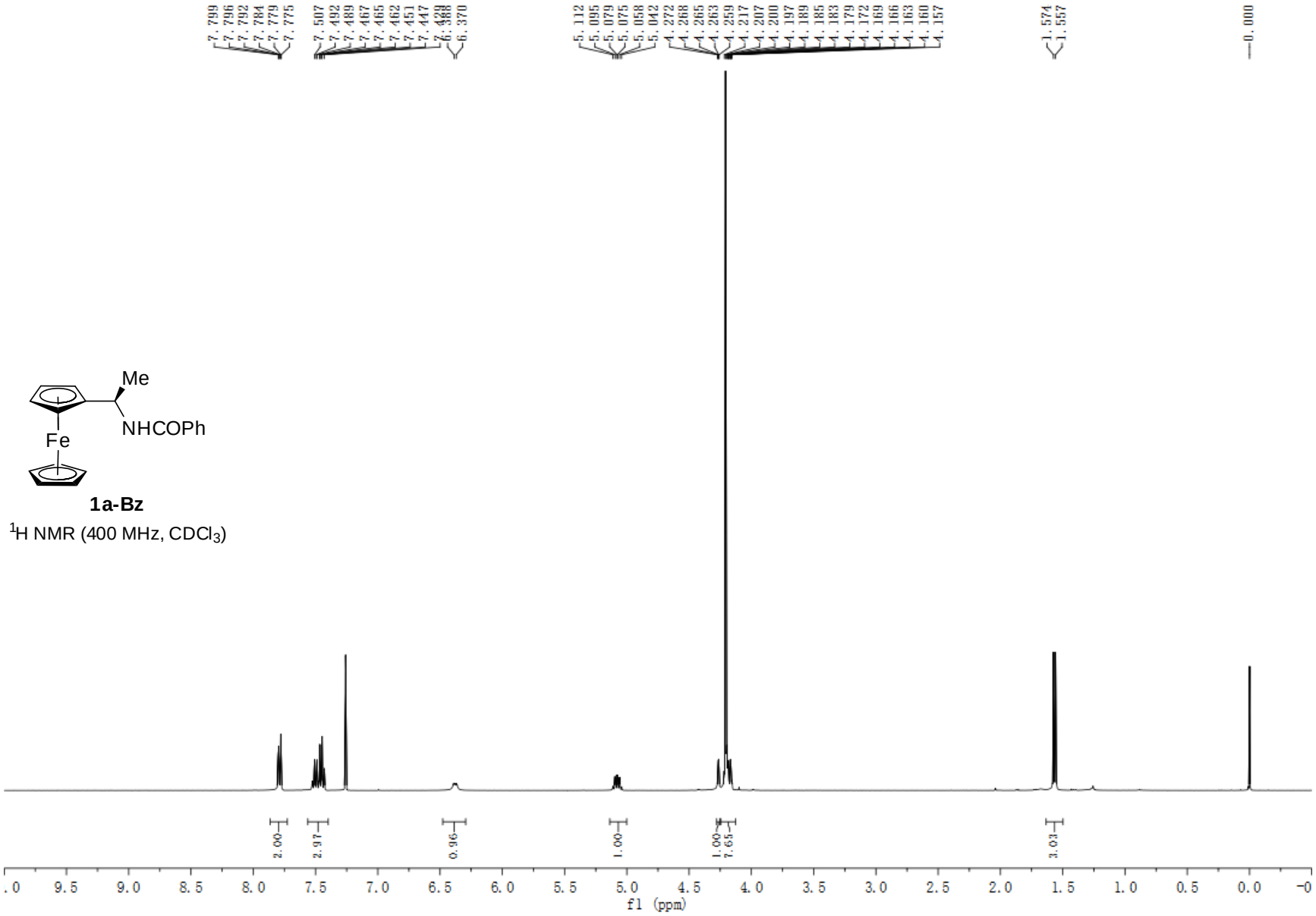
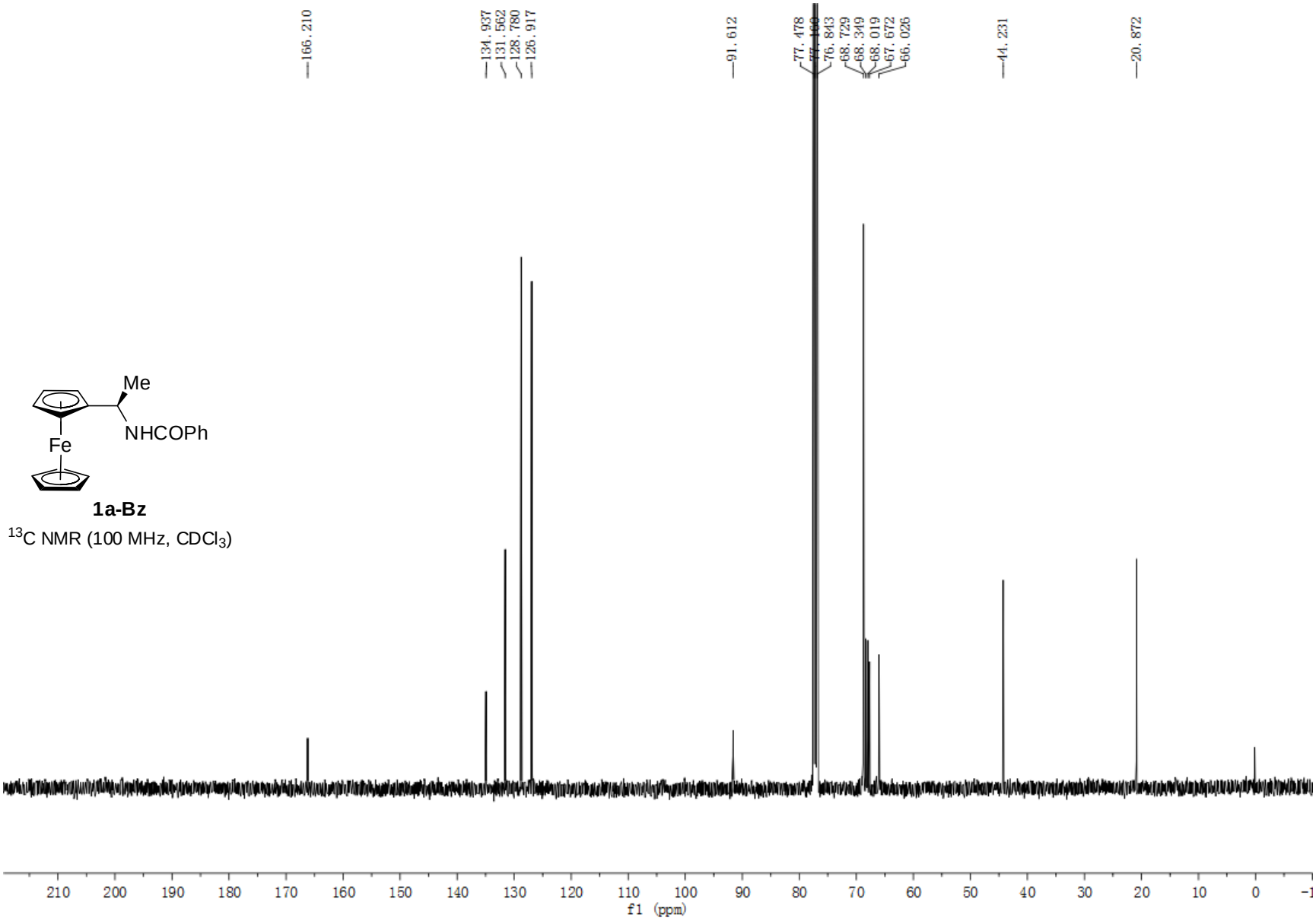
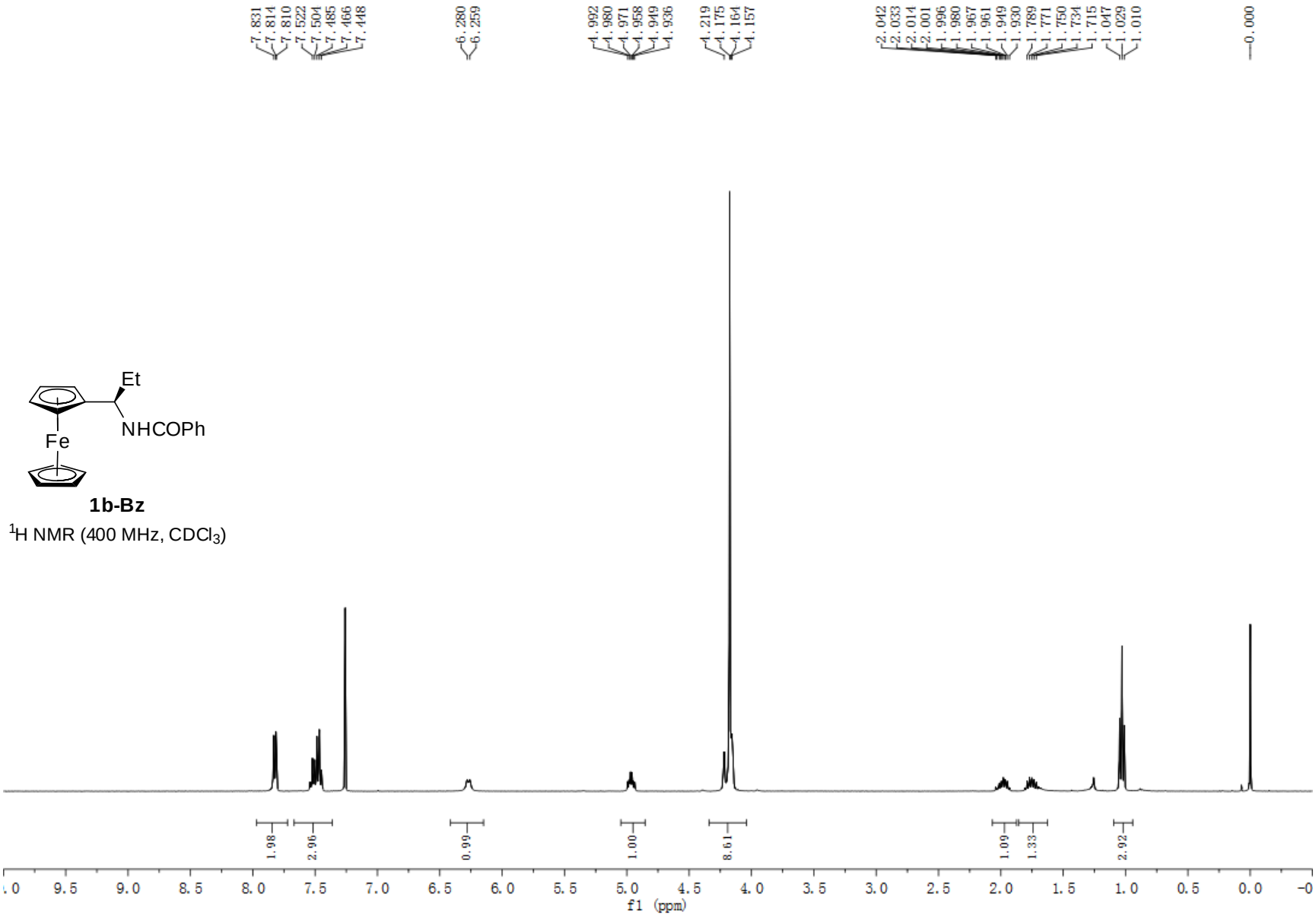
^{13}C NMR (100 MHz, $CDCl_3$)



1a-Bz

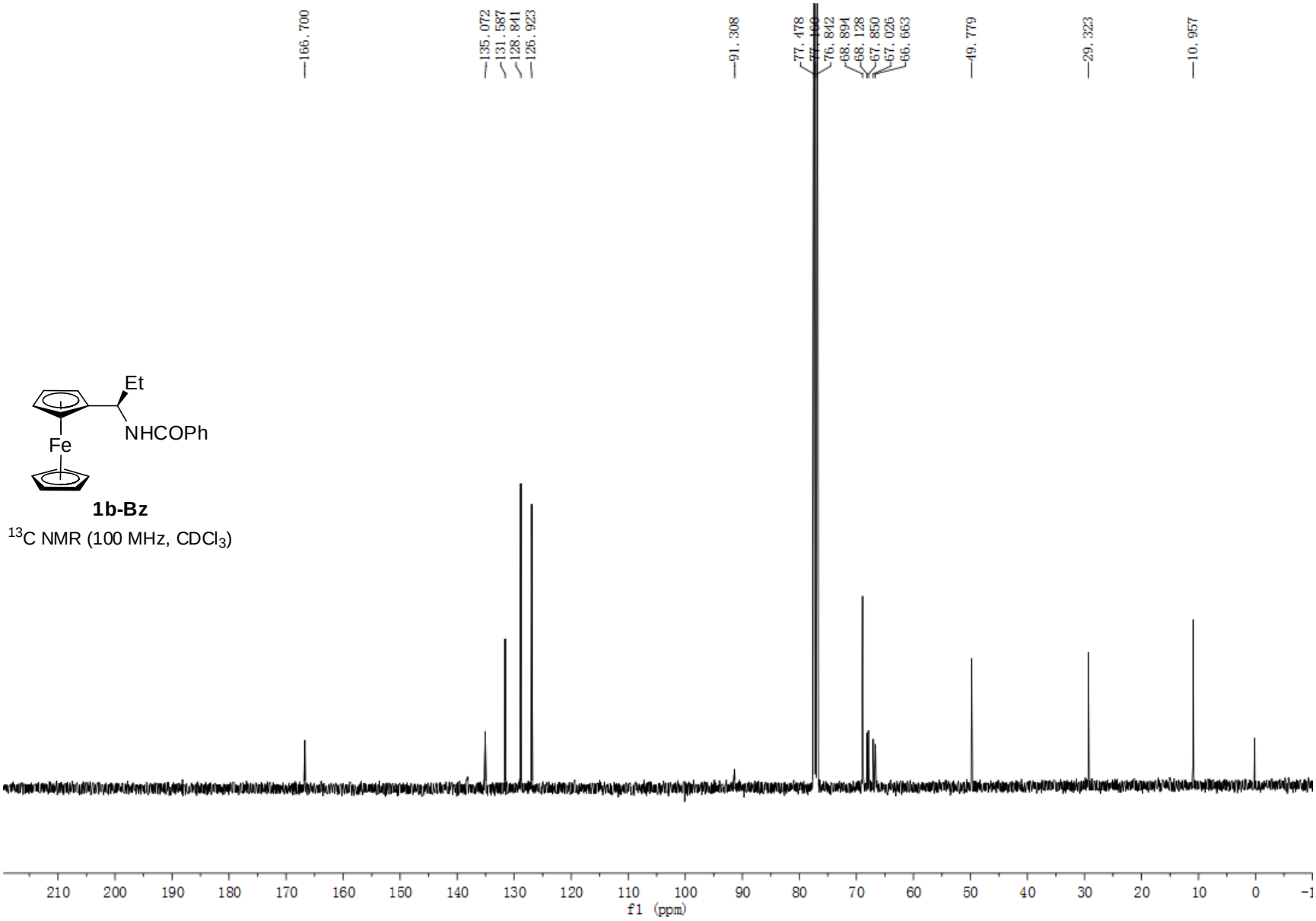
^{1}H NMR (400 MHz, $CDCl_3$)

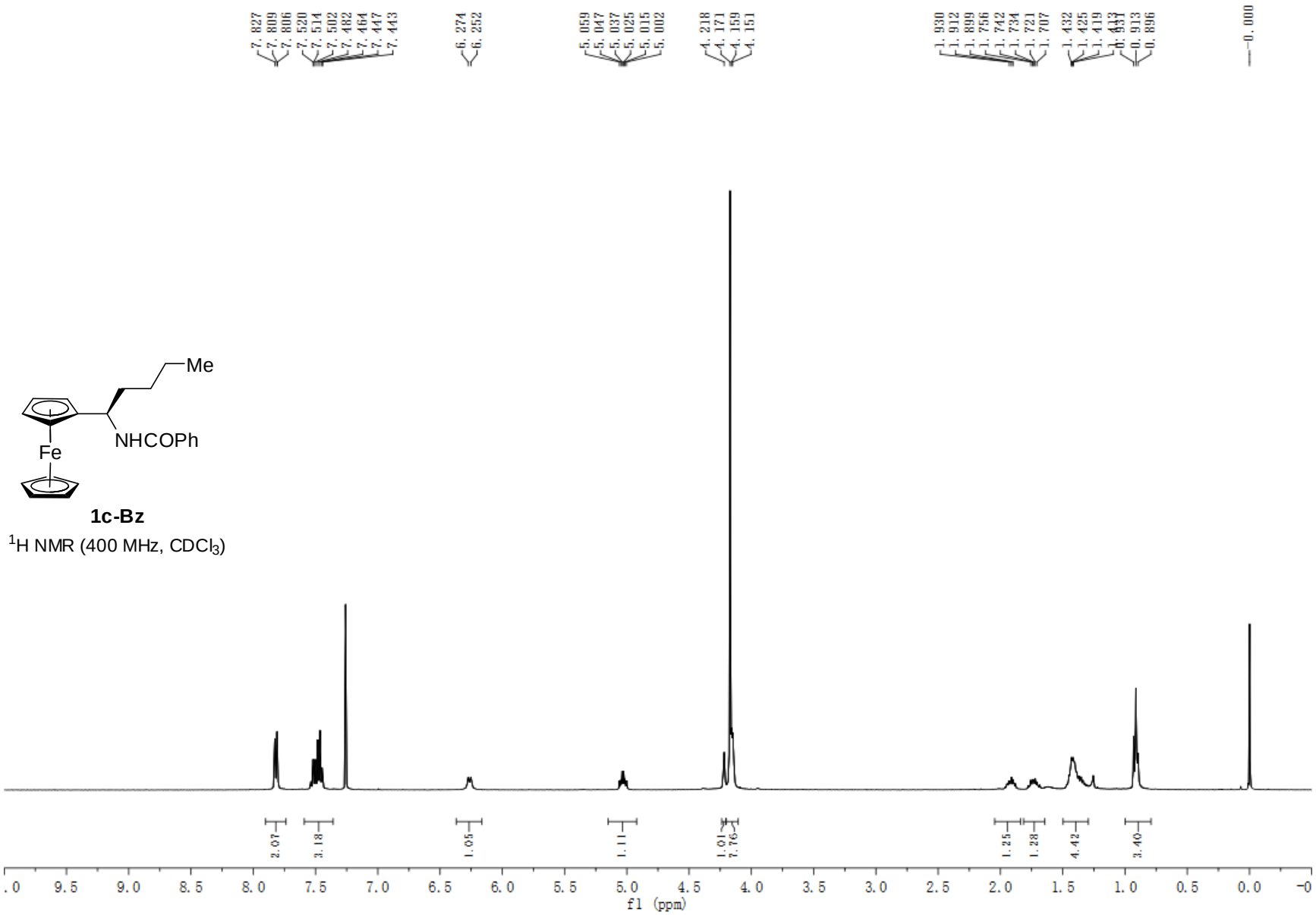

166.210
134.937
131.562
128.780
126.917
91.612
77.478
76.843
68.729
68.349
68.019
67.672
66.026
44.231
20.872
Me
NHCOPh
Fe
1a-Bz
13C NMR (100 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



1b-Bz

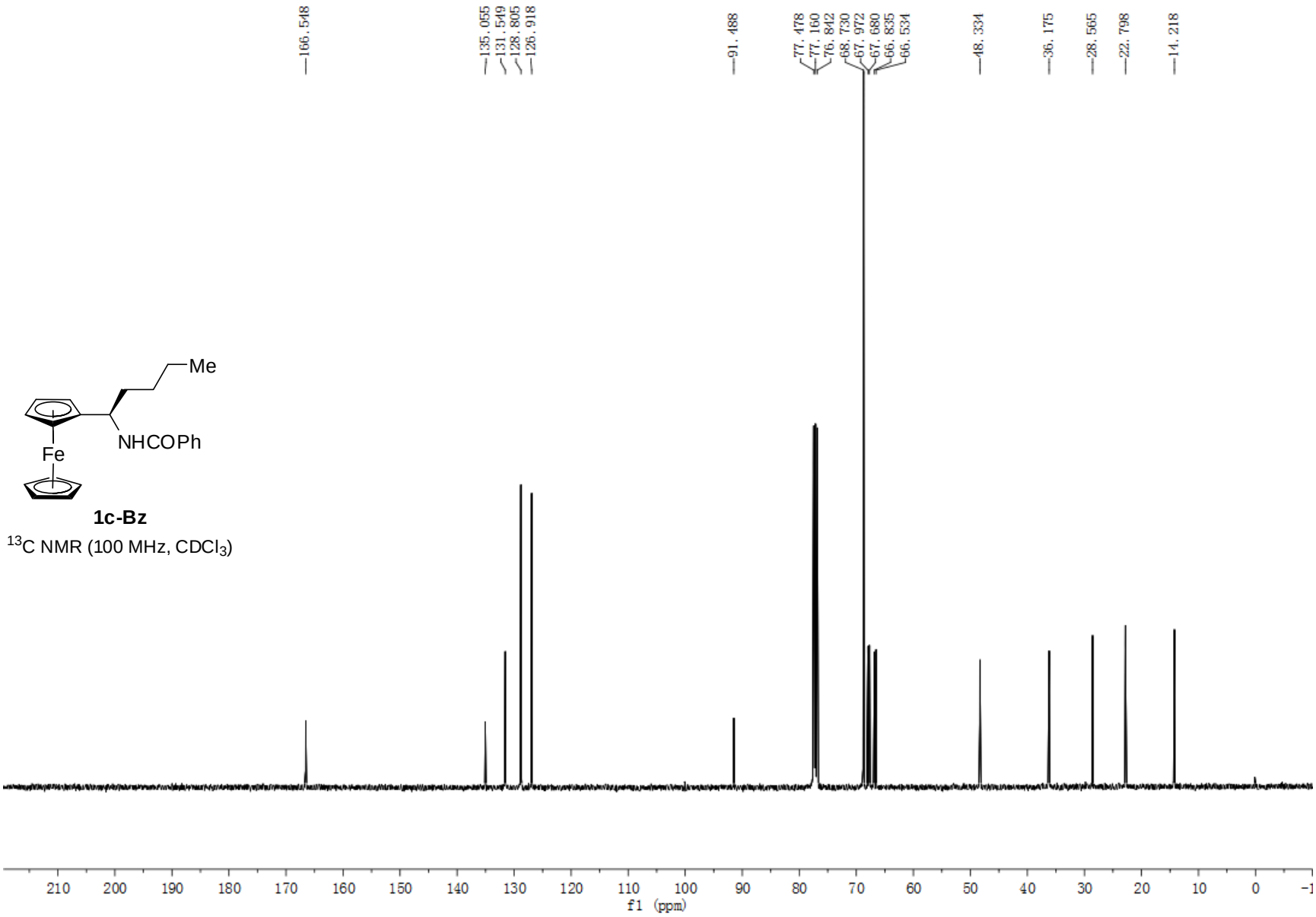
^{1}H NMR (400 MHz, $CDCl_3$)

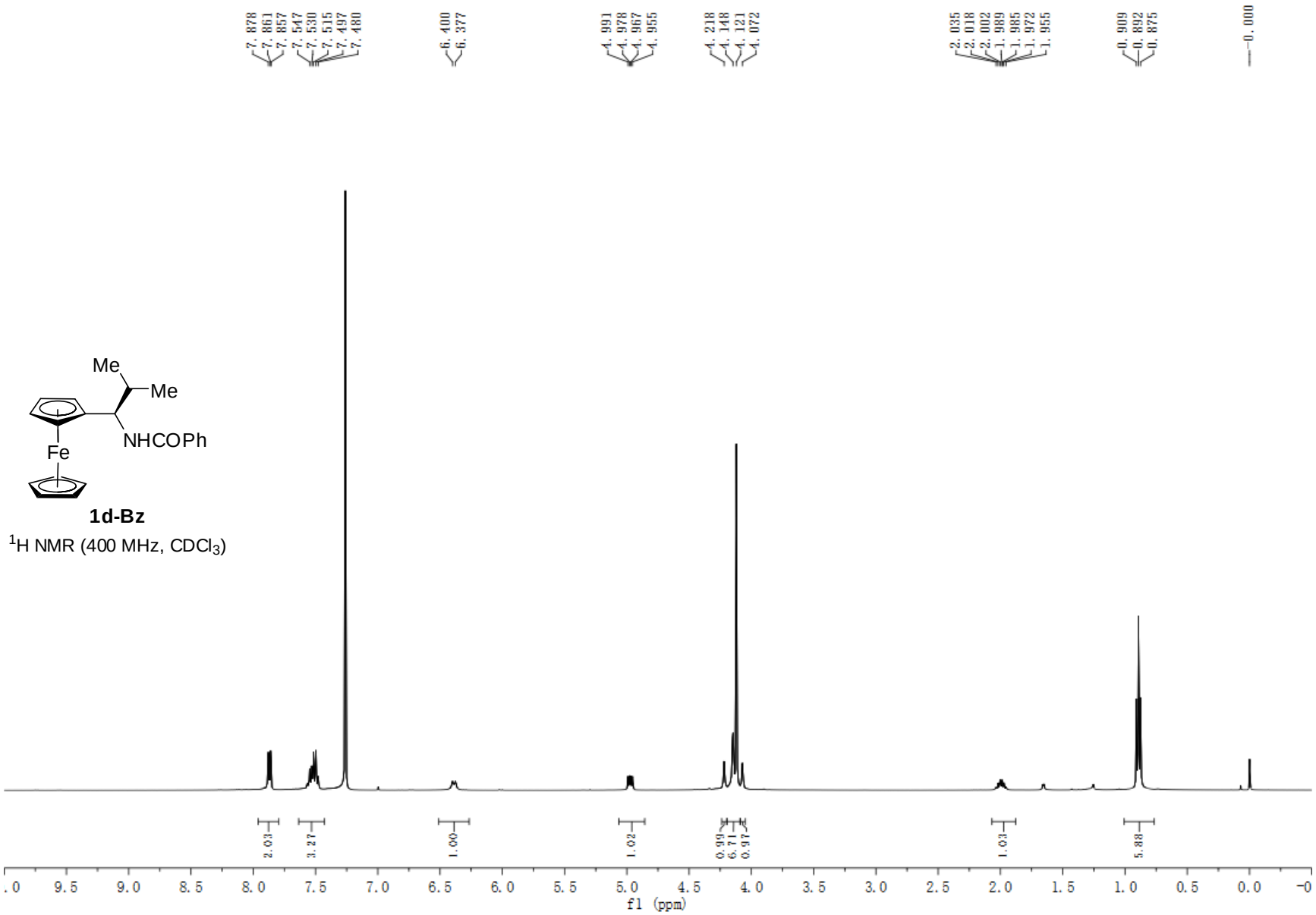

166.700
135.072
131.587
128.841
126.923
91.308
77.478
77.160
76.842
68.894
68.128
67.850
67.026
66.663
49.779
29.323
10.957
Et
NHCOPh
Fe
1b-Bz
13C NMR (100 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)



1c-Bz

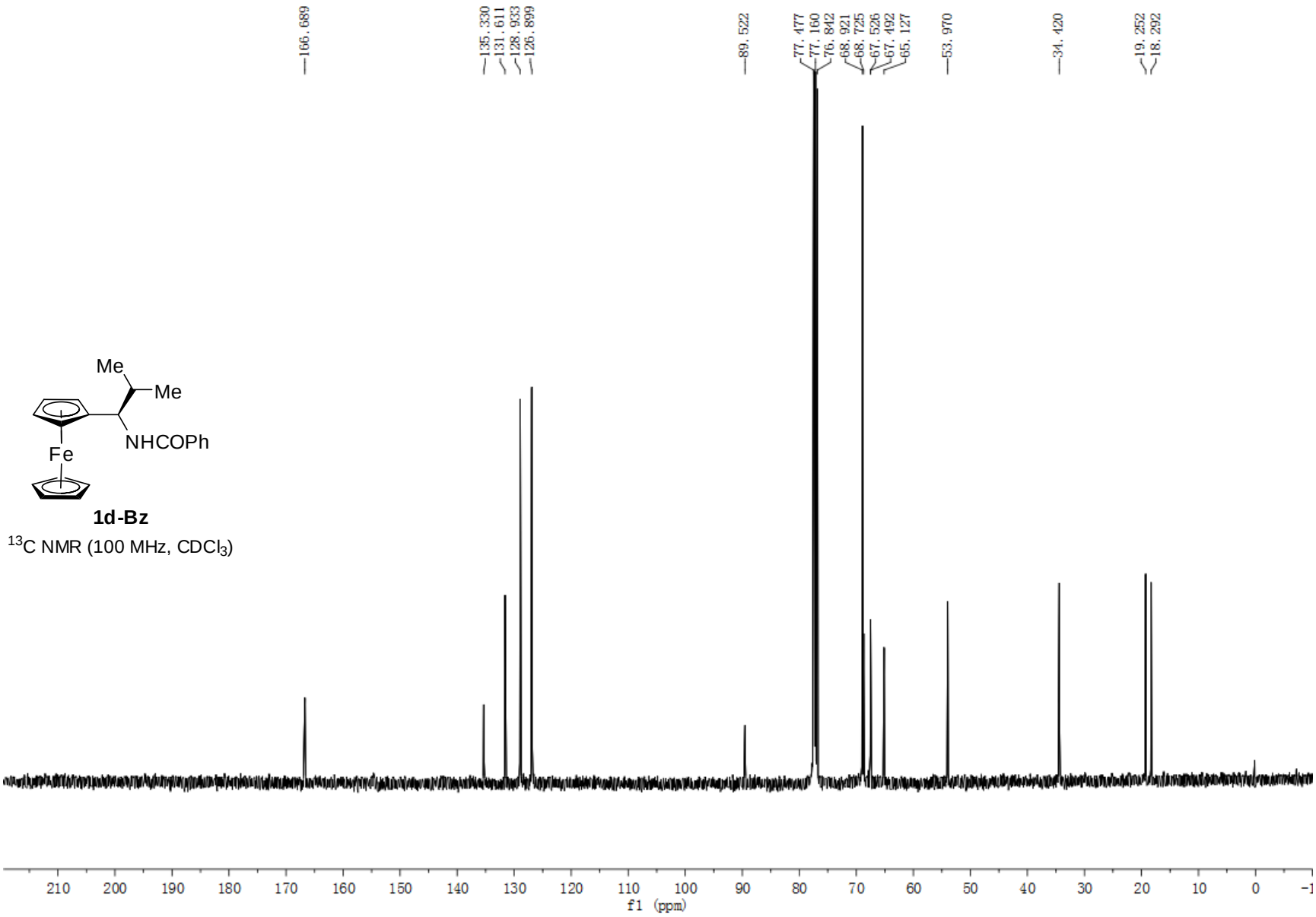
^{1}H NMR (400 MHz, $CDCl_3$)


166.548
135.055
131.549
128.805
126.918
91.488
77.478
77.160
76.842
68.730
67.972
67.680
66.835
66.534
48.334
36.175
28.565
22.798
14.218
Me
NHCOPh
Fe
1c-Bz
13C NMR (100 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)



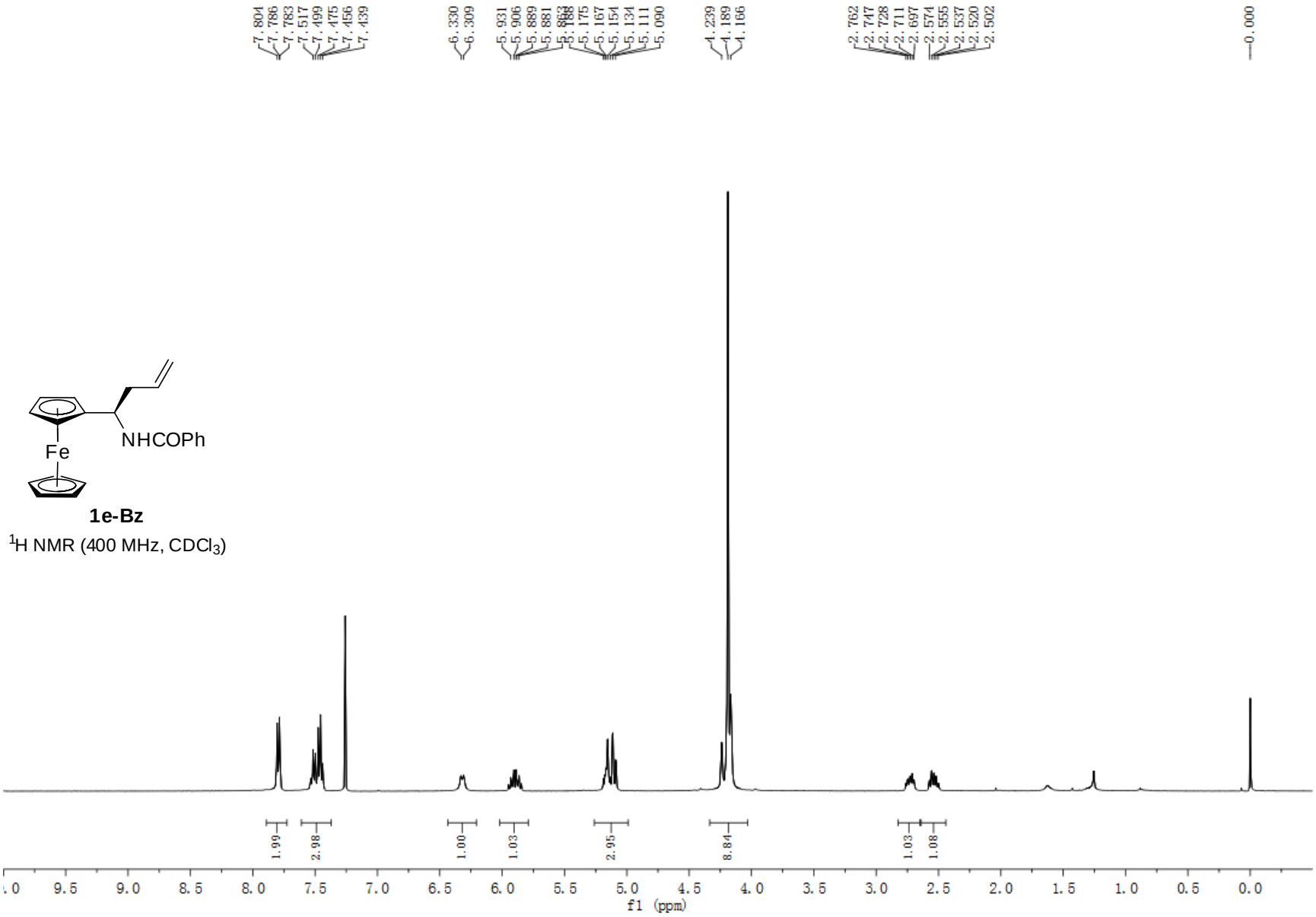
1d-Bz

^{1}H NMR (400 MHz, $CDCl_3$)



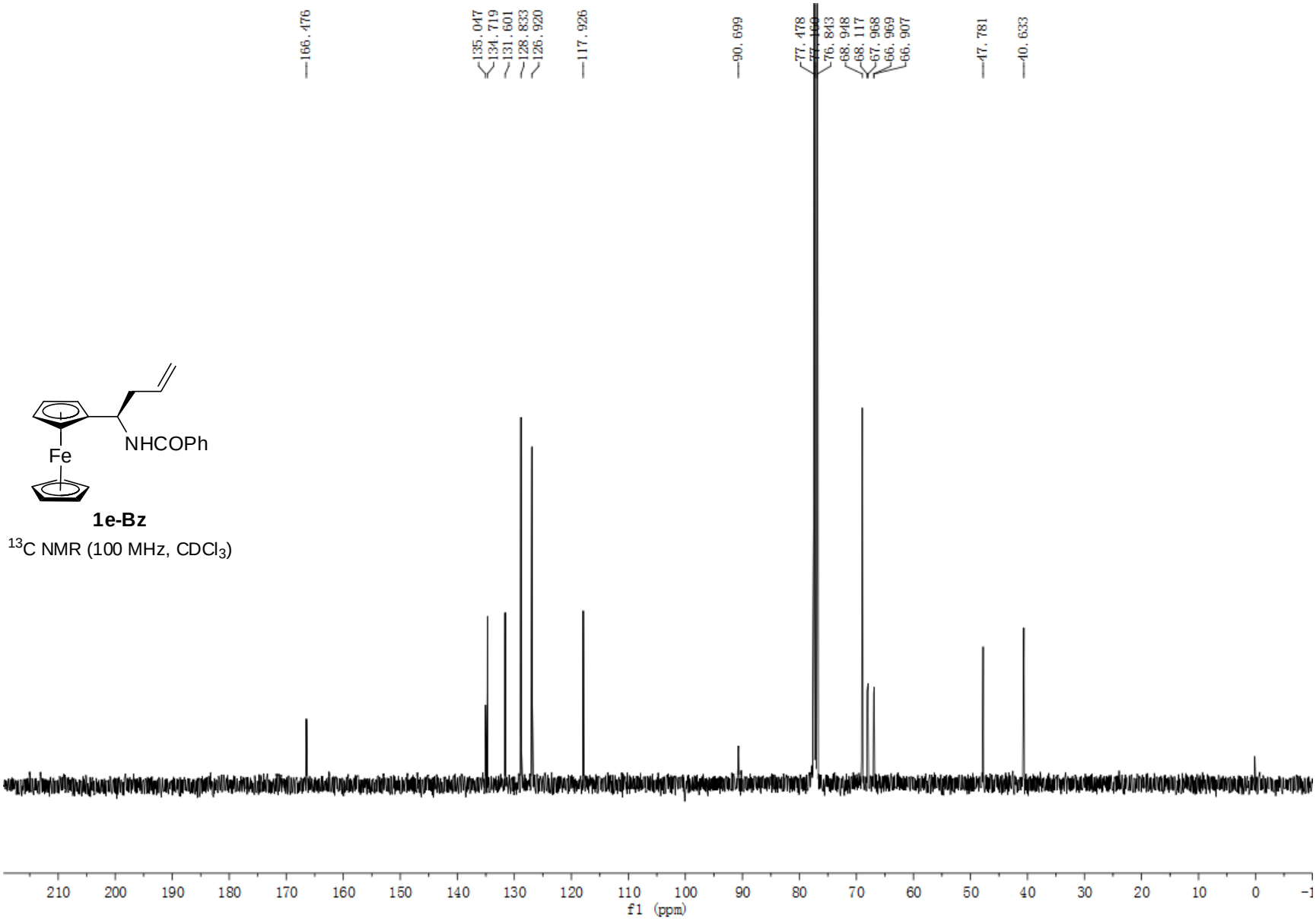
1d-Bz

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



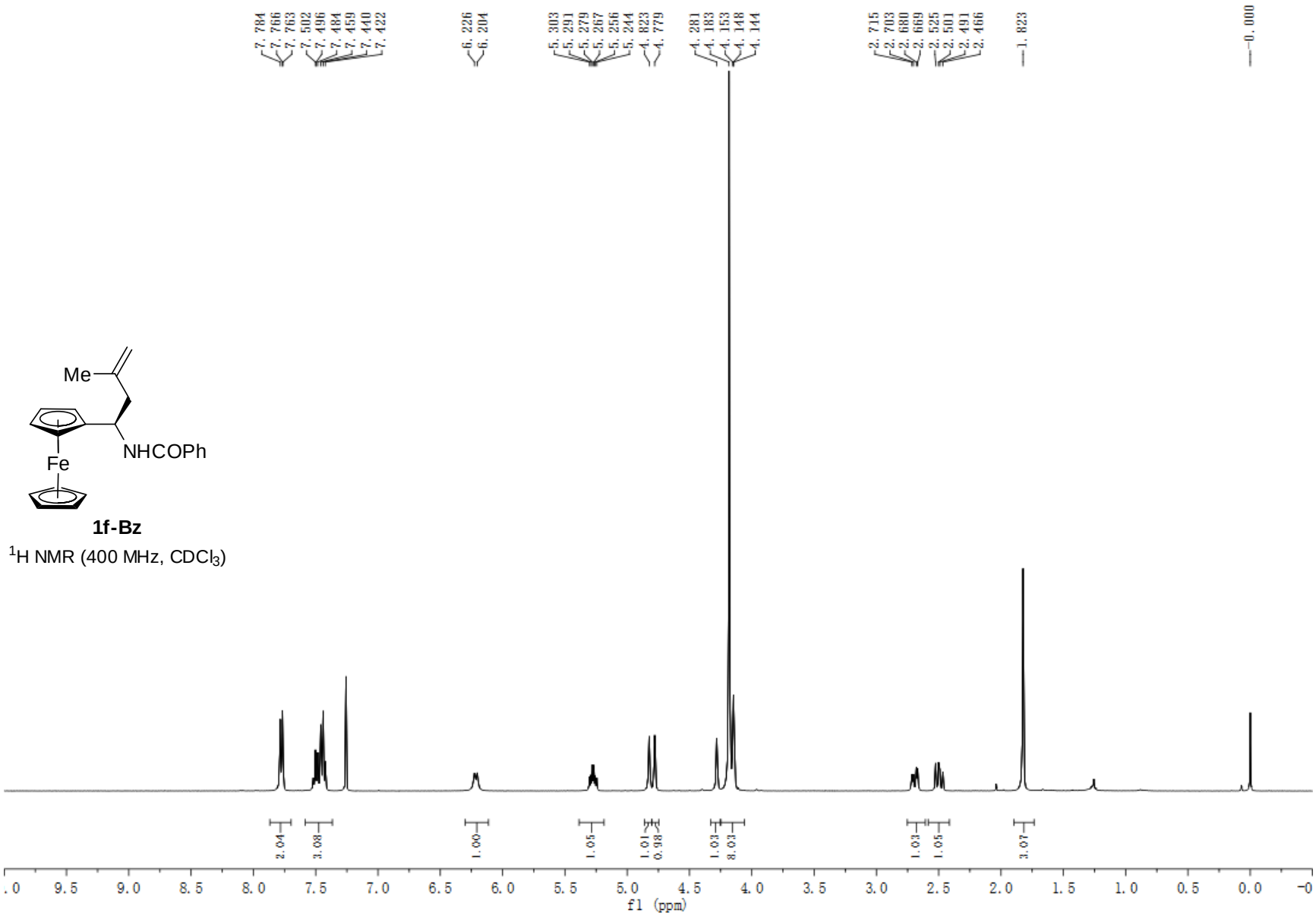
1e-Bz

^{1}H NMR (400 MHz, $CDCl_3$)



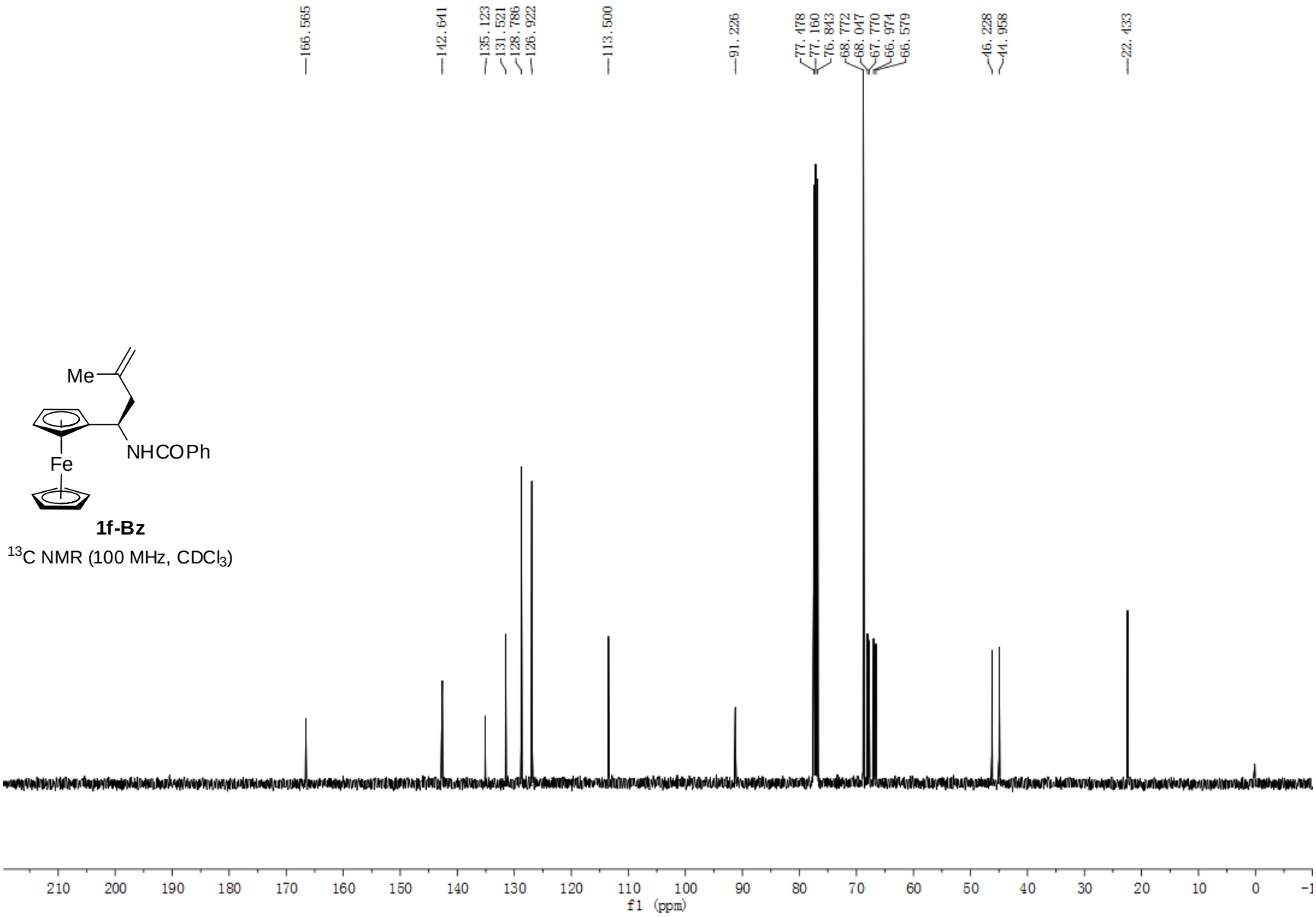
1e-Bz

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



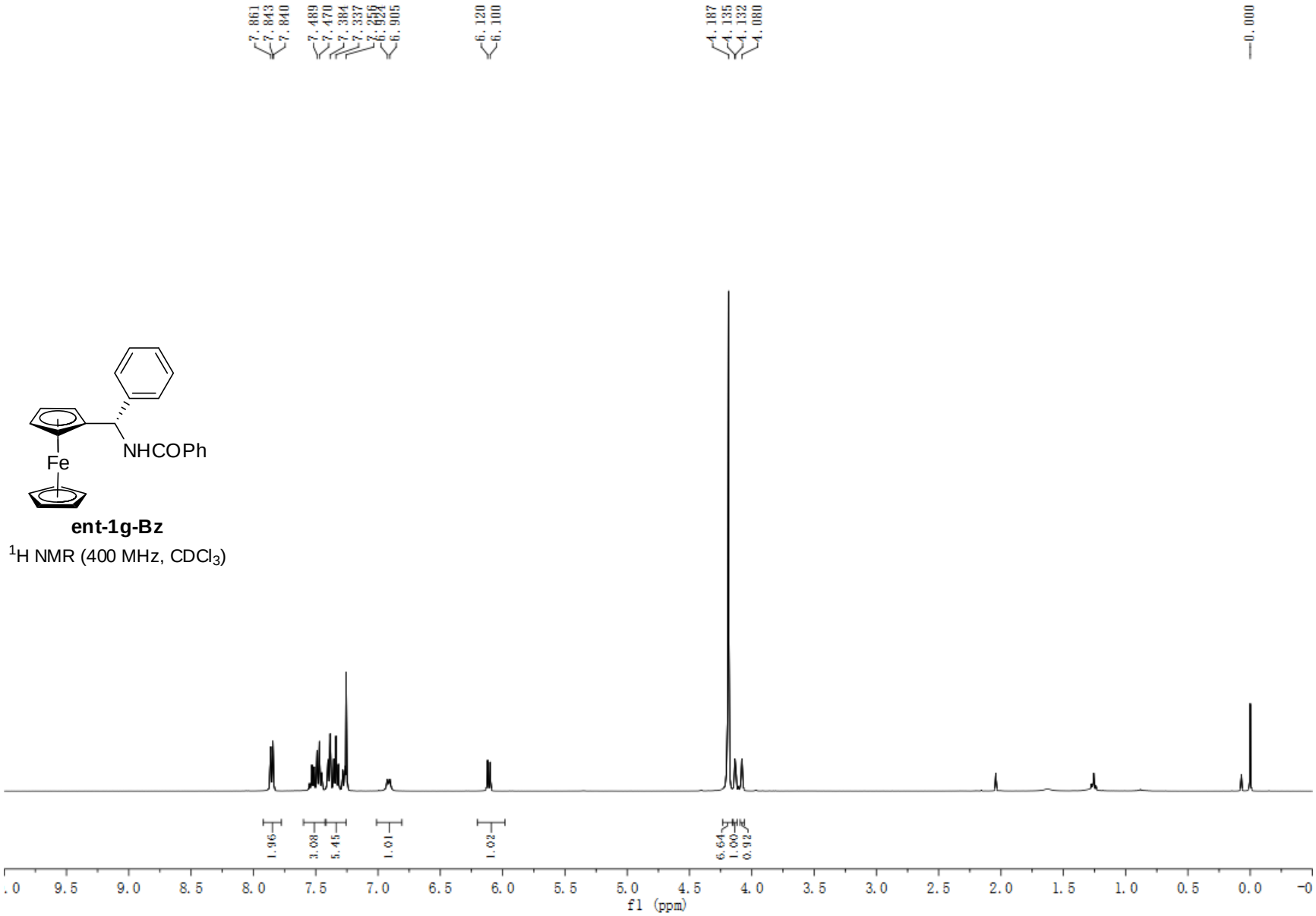
1f-Bz

^{1}H NMR (400 MHz, $CDCl_3$)



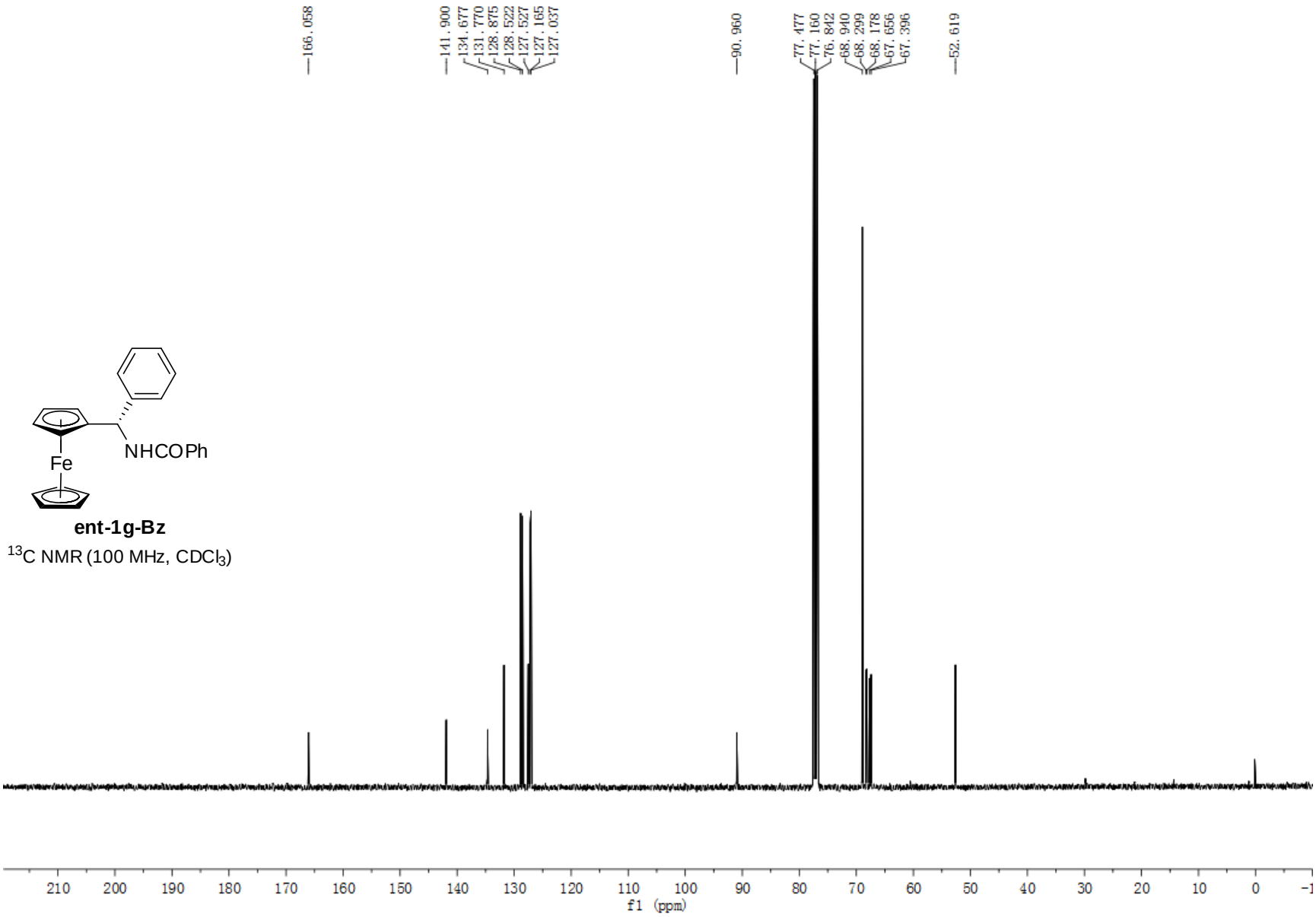
1f-Bz

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



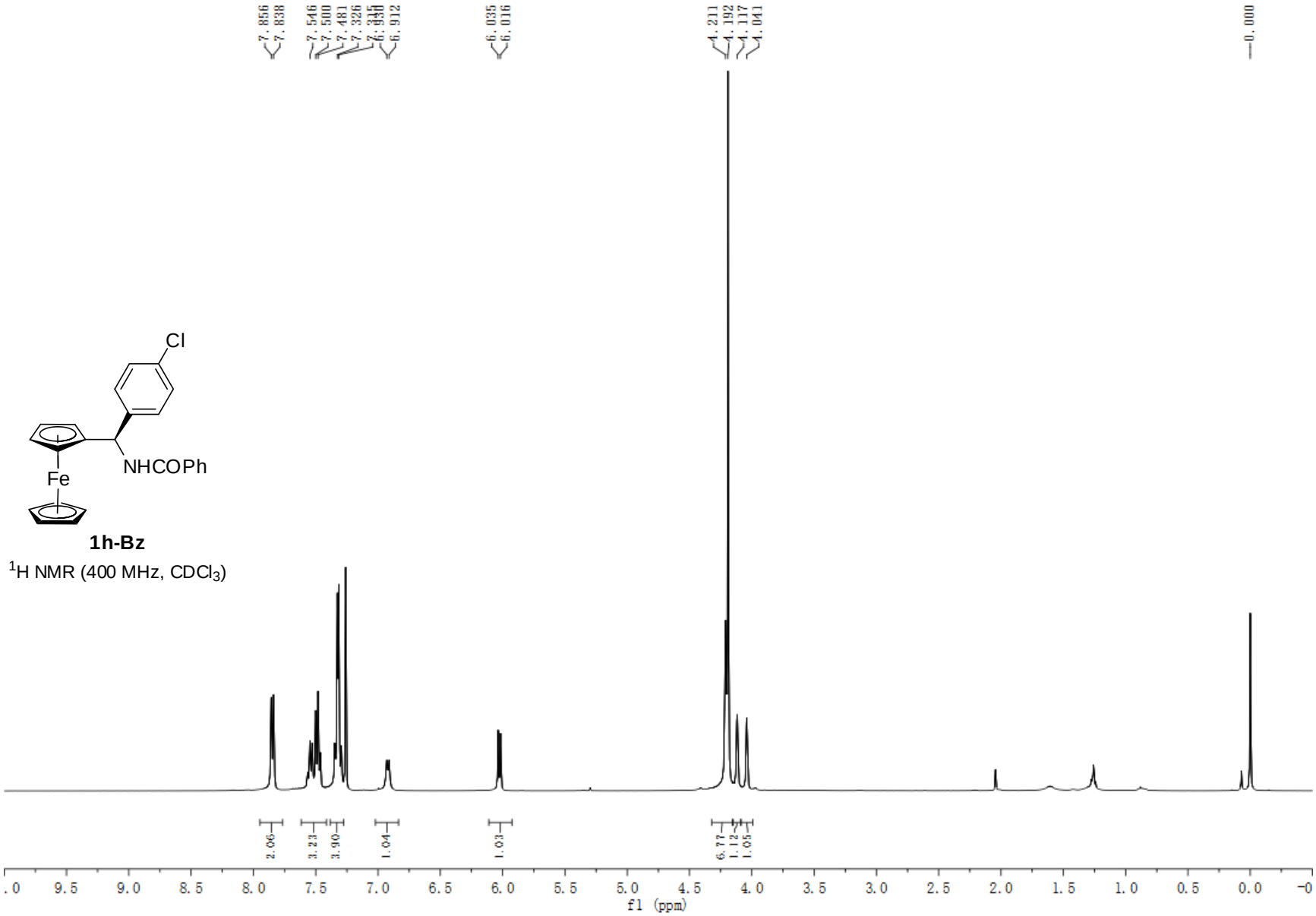
ent-1g-Bz

^{1}H NMR (400 MHz, $CDCl_3$)



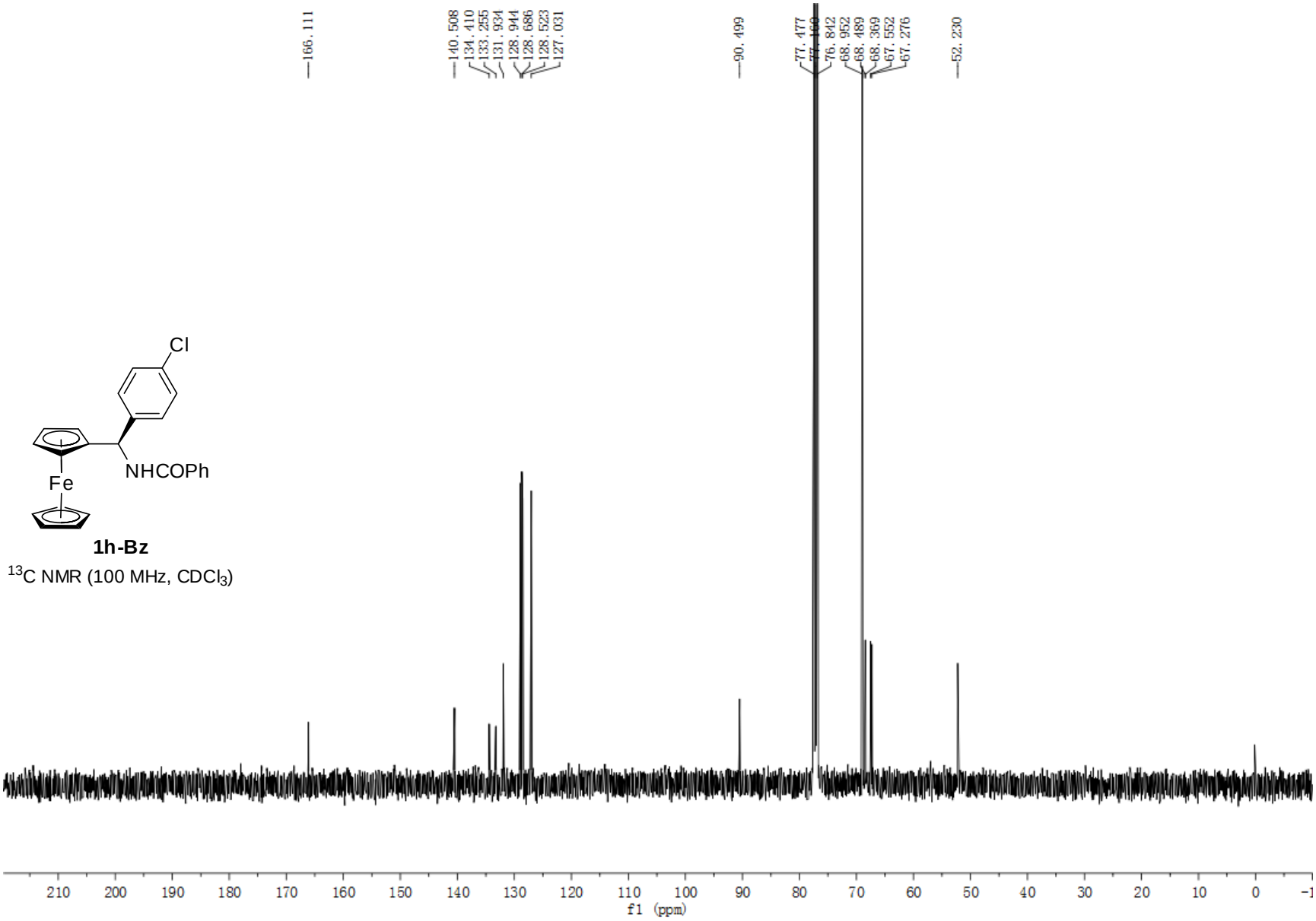
ent-1g-Bz

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



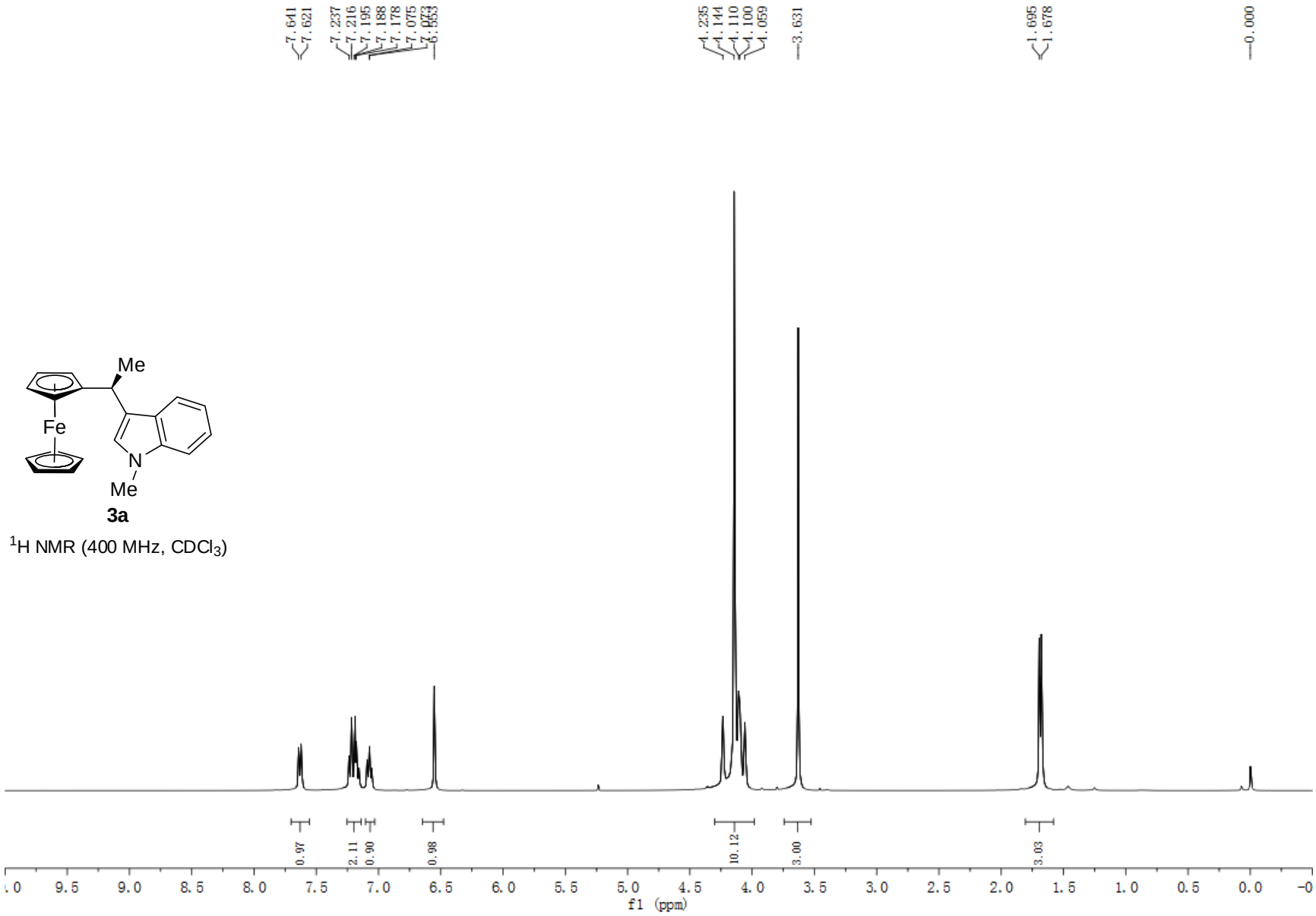
1h-Bz

^{1}H NMR (400 MHz, $CDCl_3$)



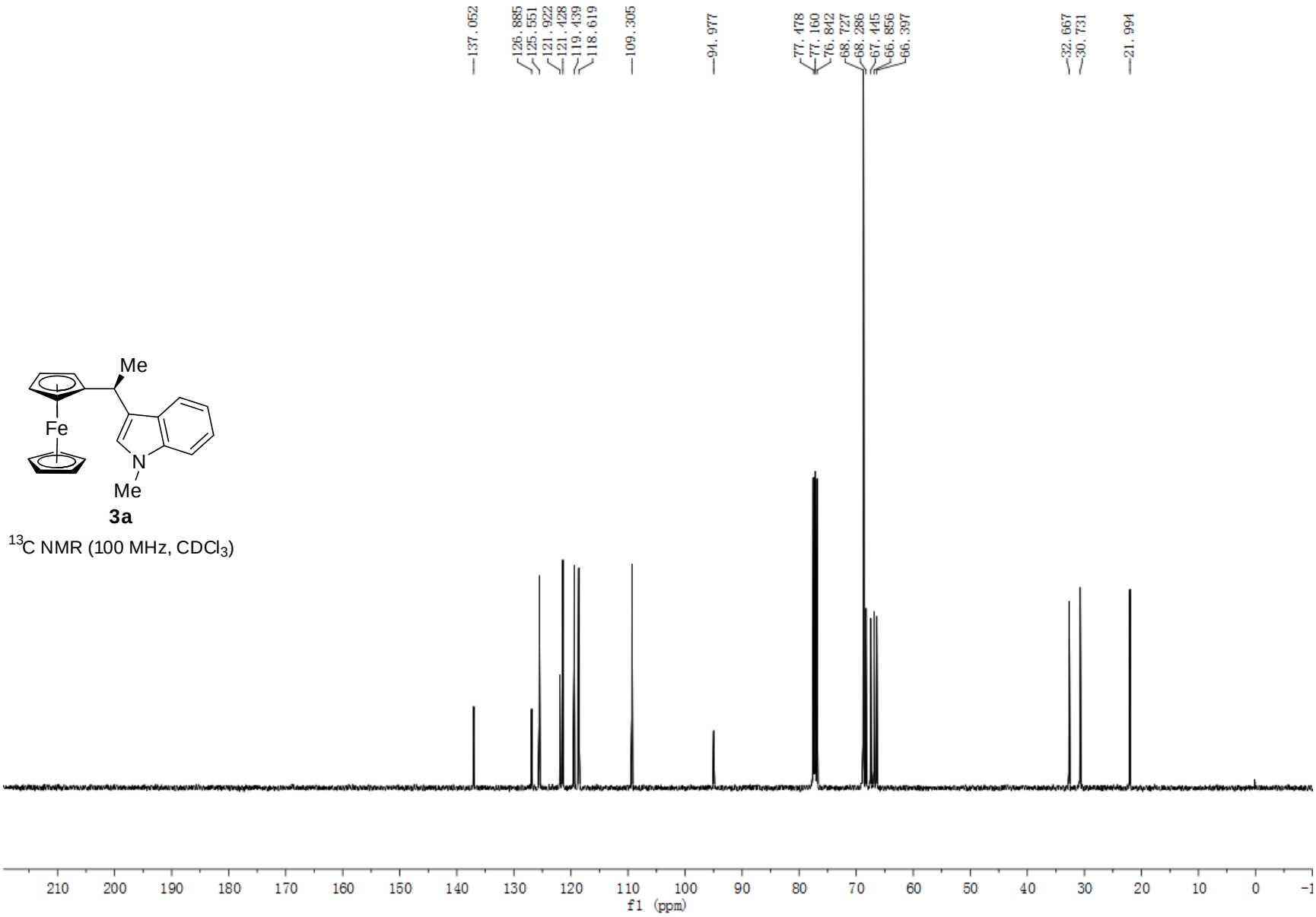
1h-Bz

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



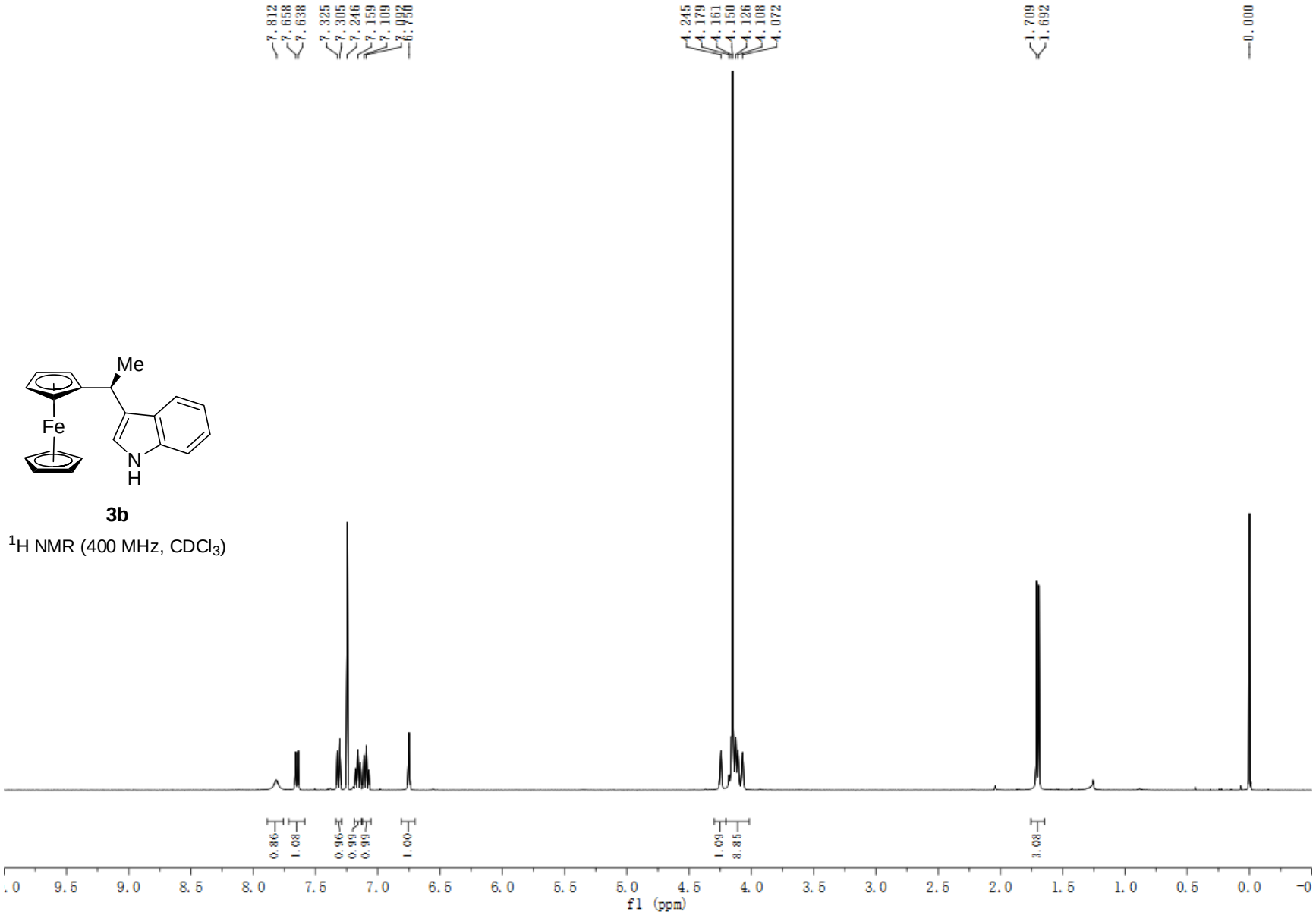
3a

^{1}H NMR (400 MHz, $CDCl_3$)



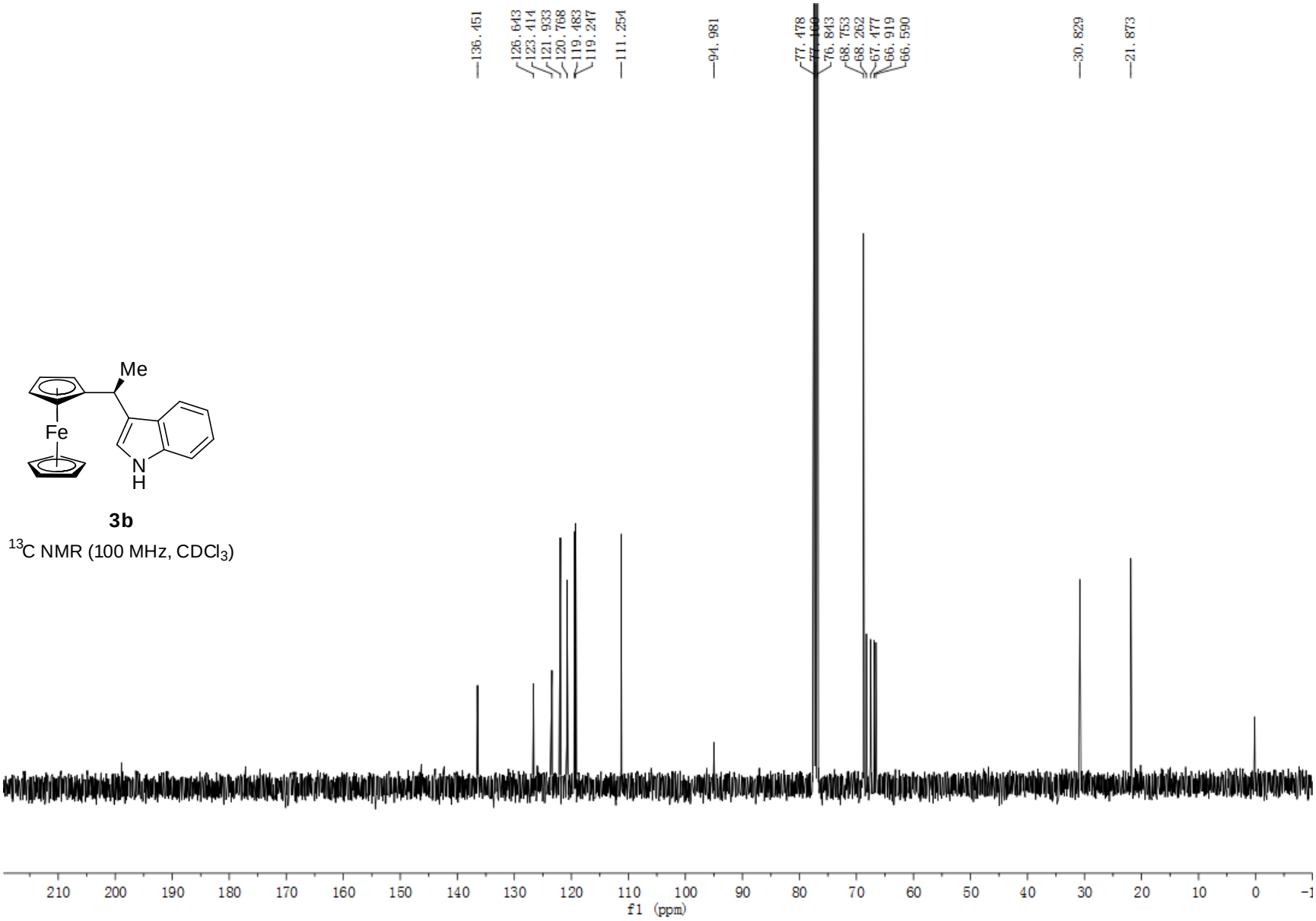
3a

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



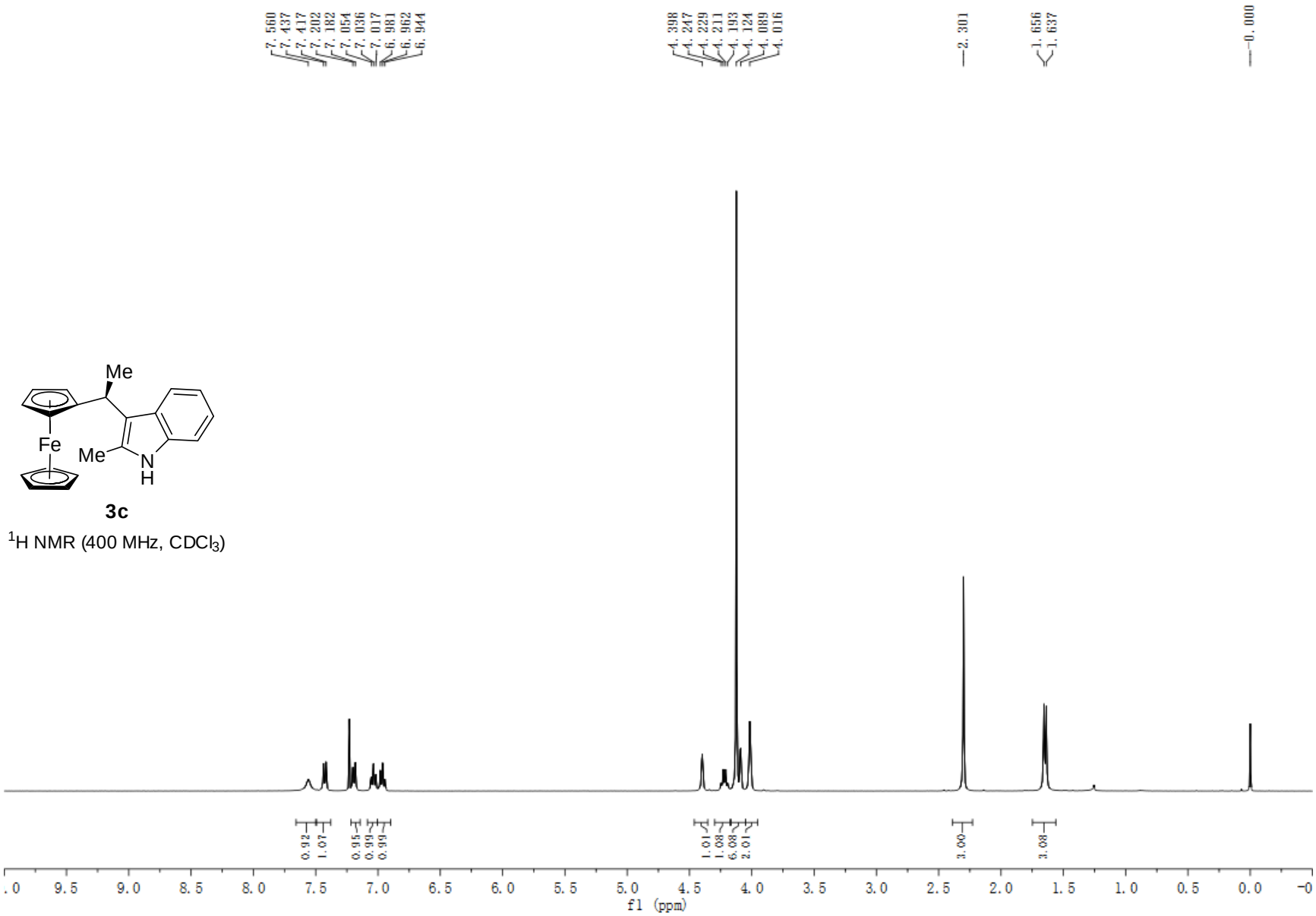
3b

^{1}H NMR (400 MHz, $CDCl_3$)



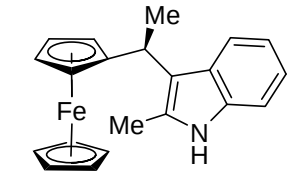
3b

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



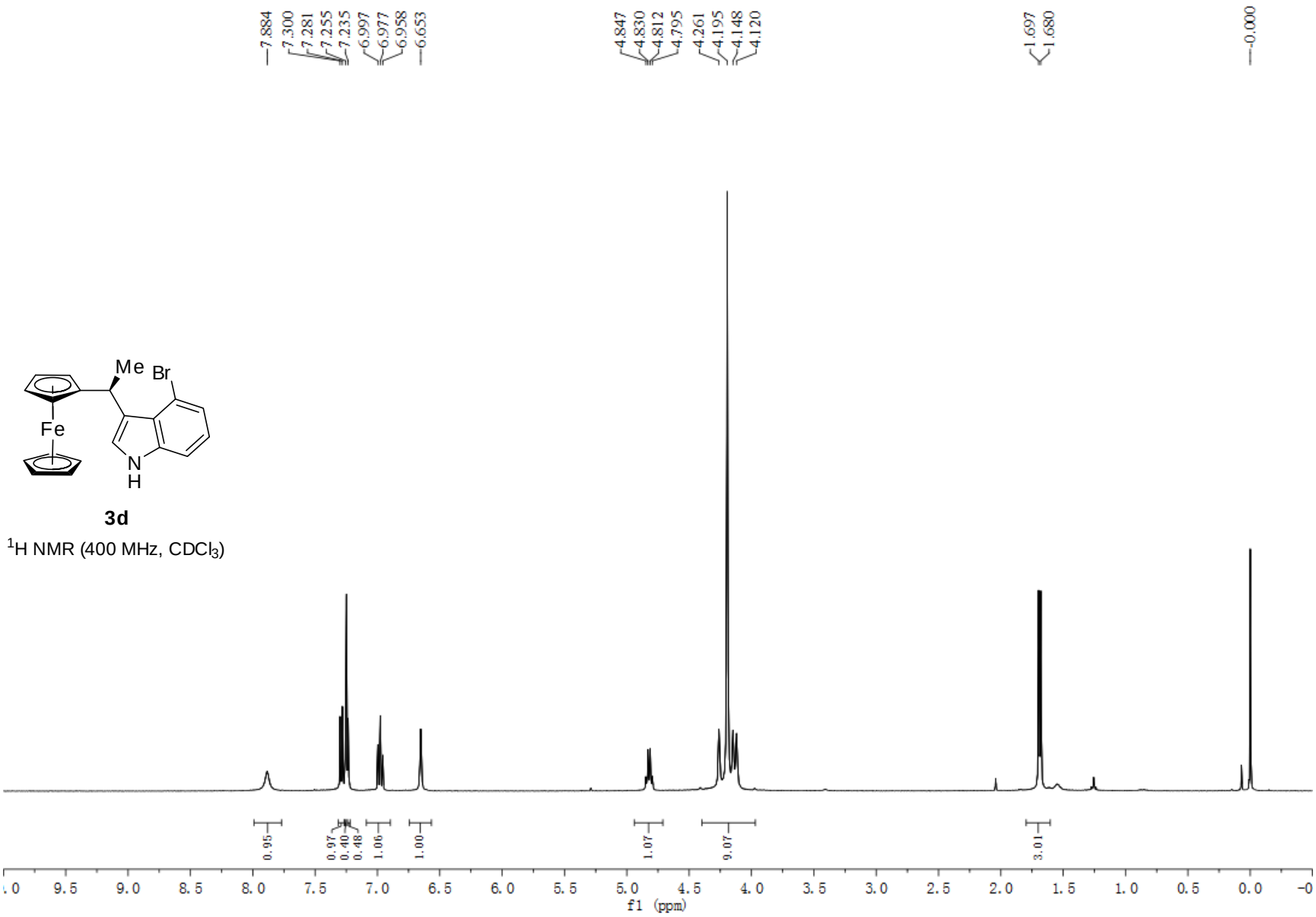
3c

^{1}H NMR (400 MHz, $CDCl_3$)



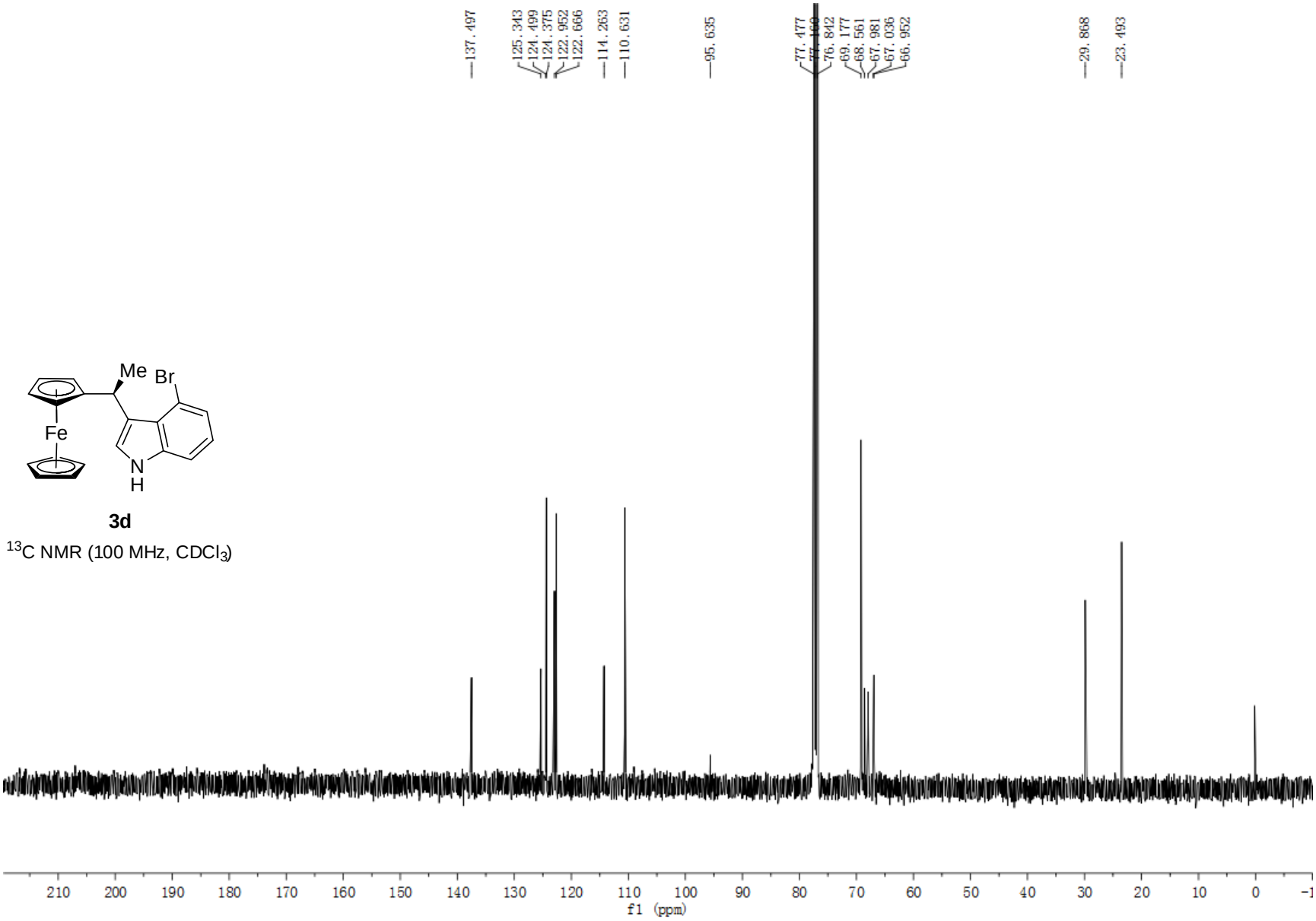
3c

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



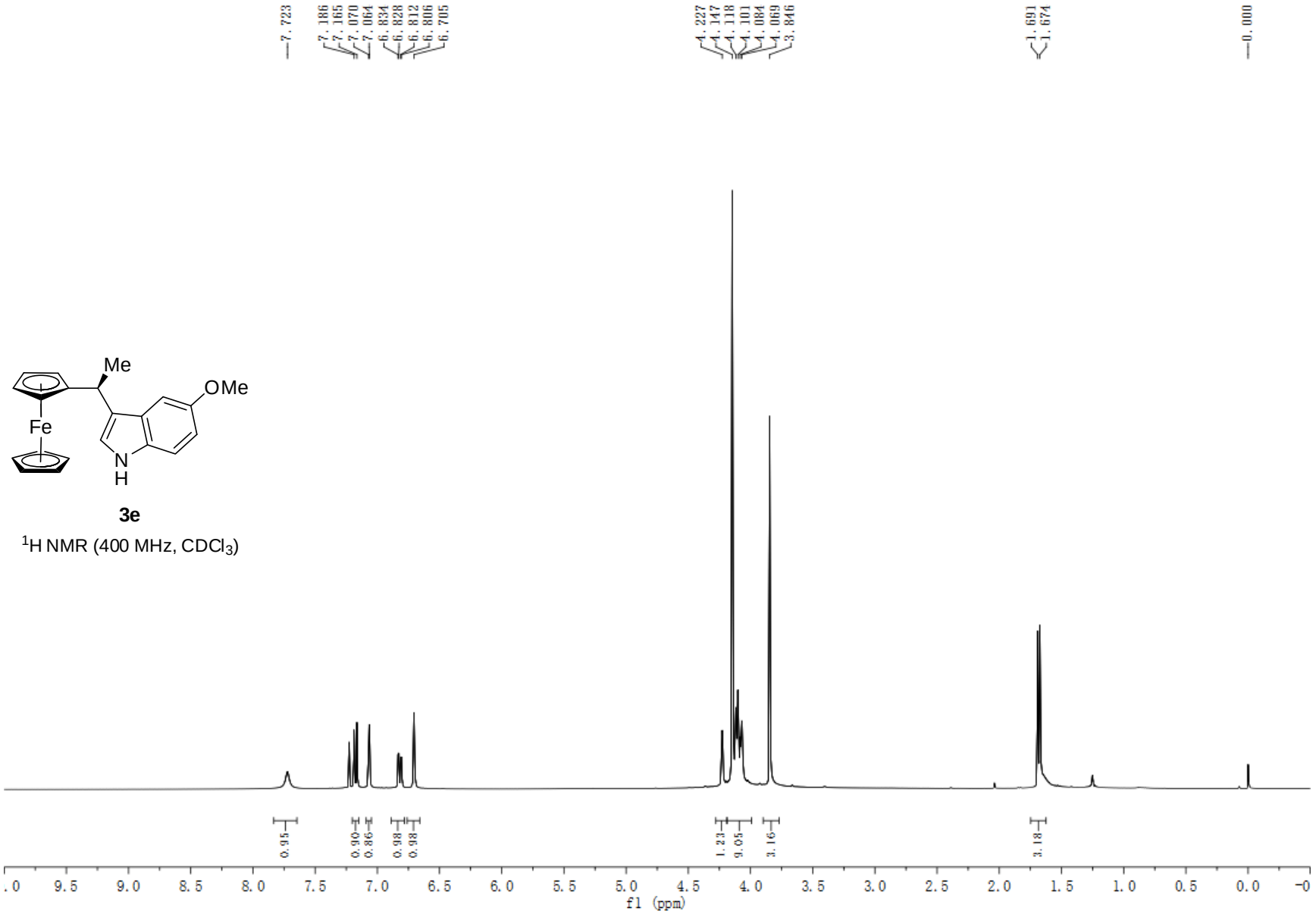
3d

^{1}H NMR (400 MHz, $CDCl_3$)



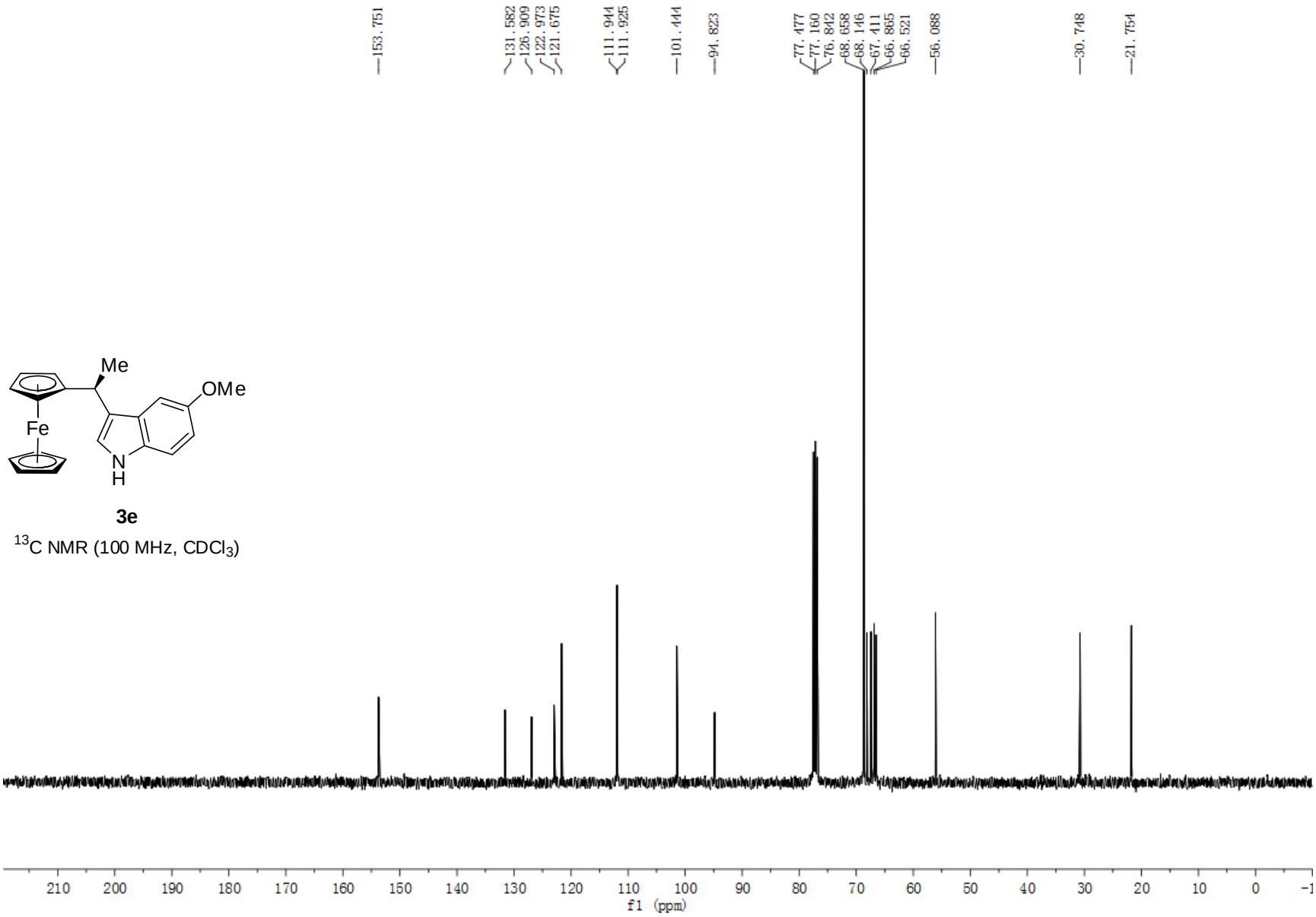
3d

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



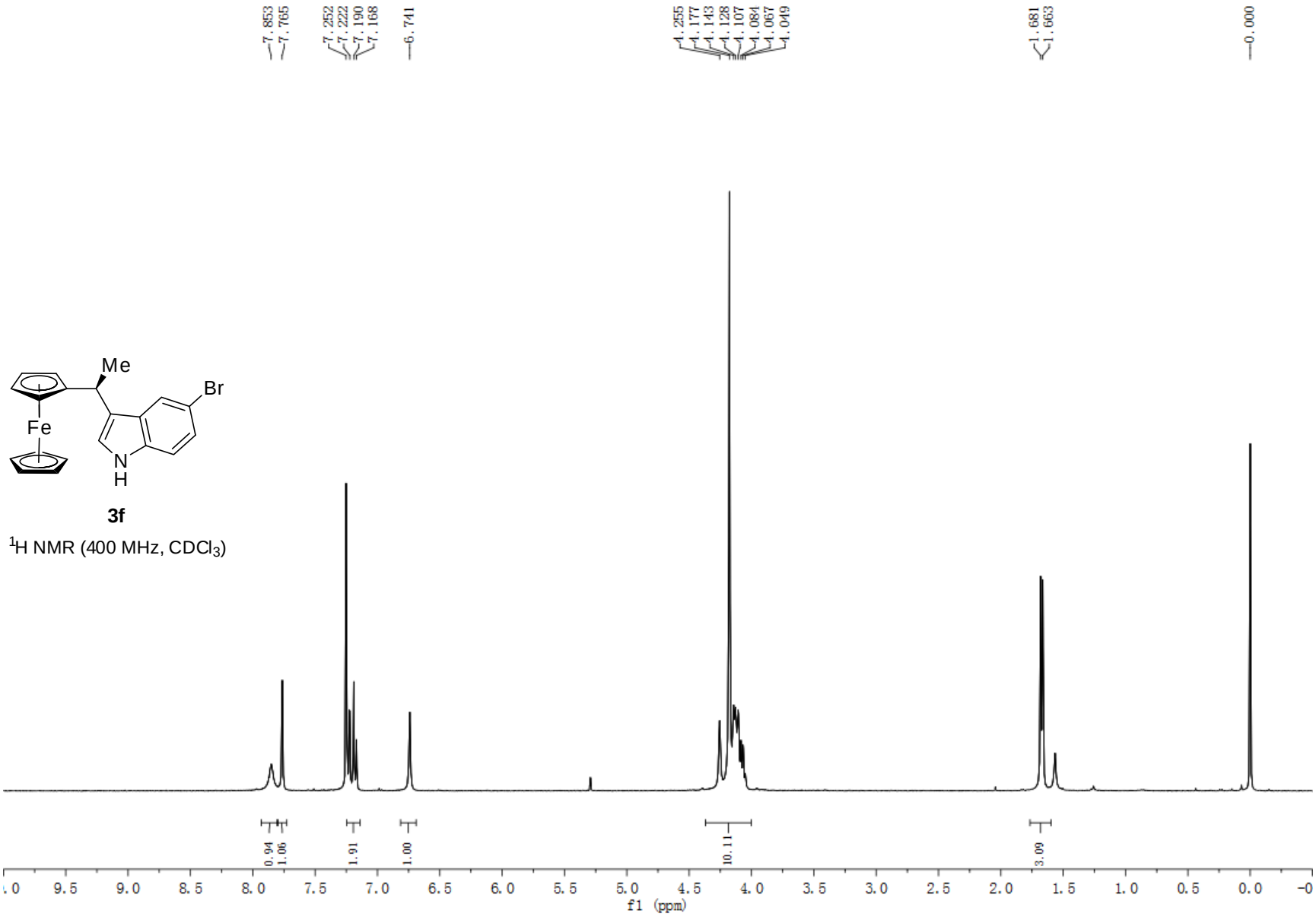
3e

^{1}H NMR (400 MHz, $CDCl_3$)



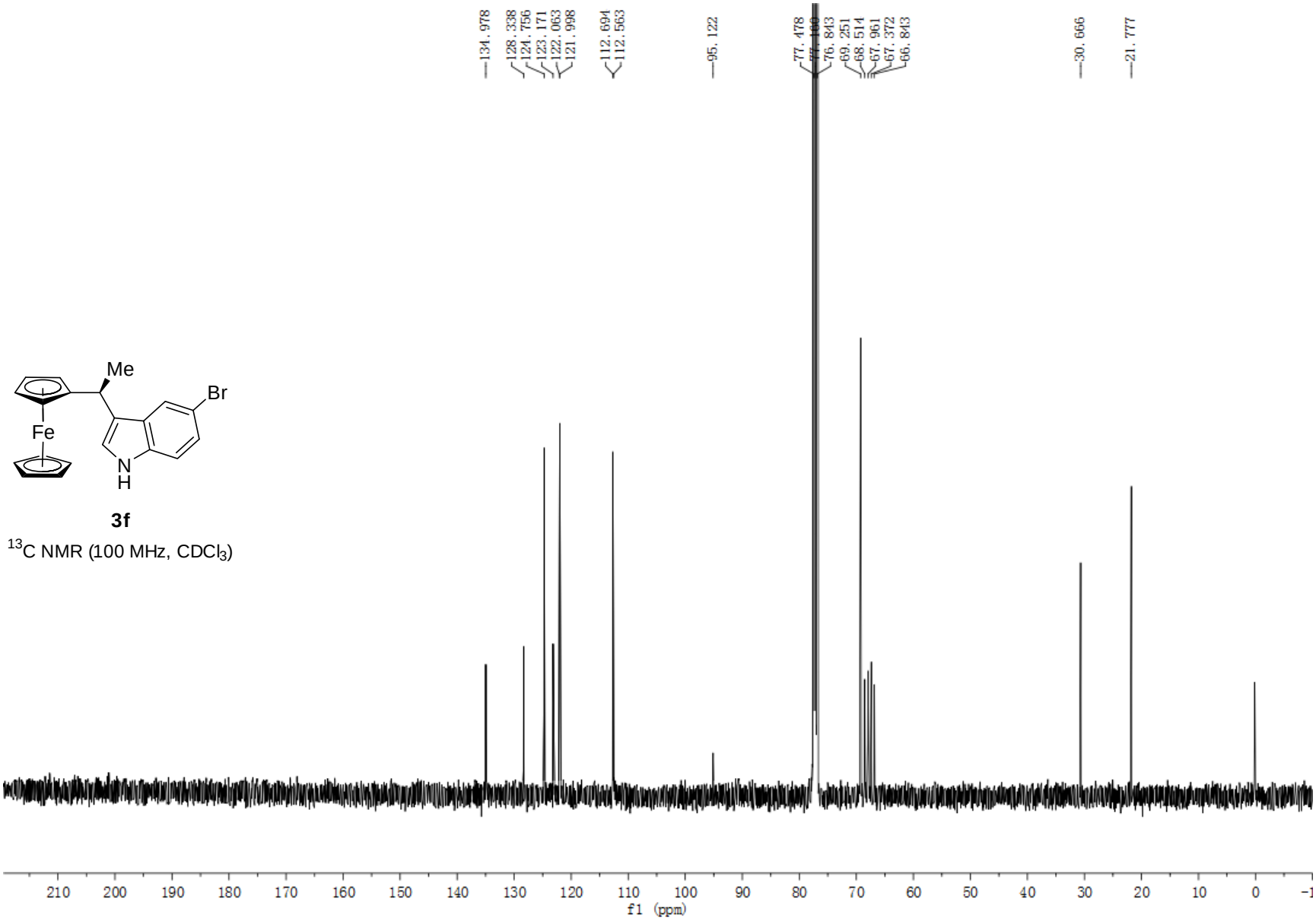
3e

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



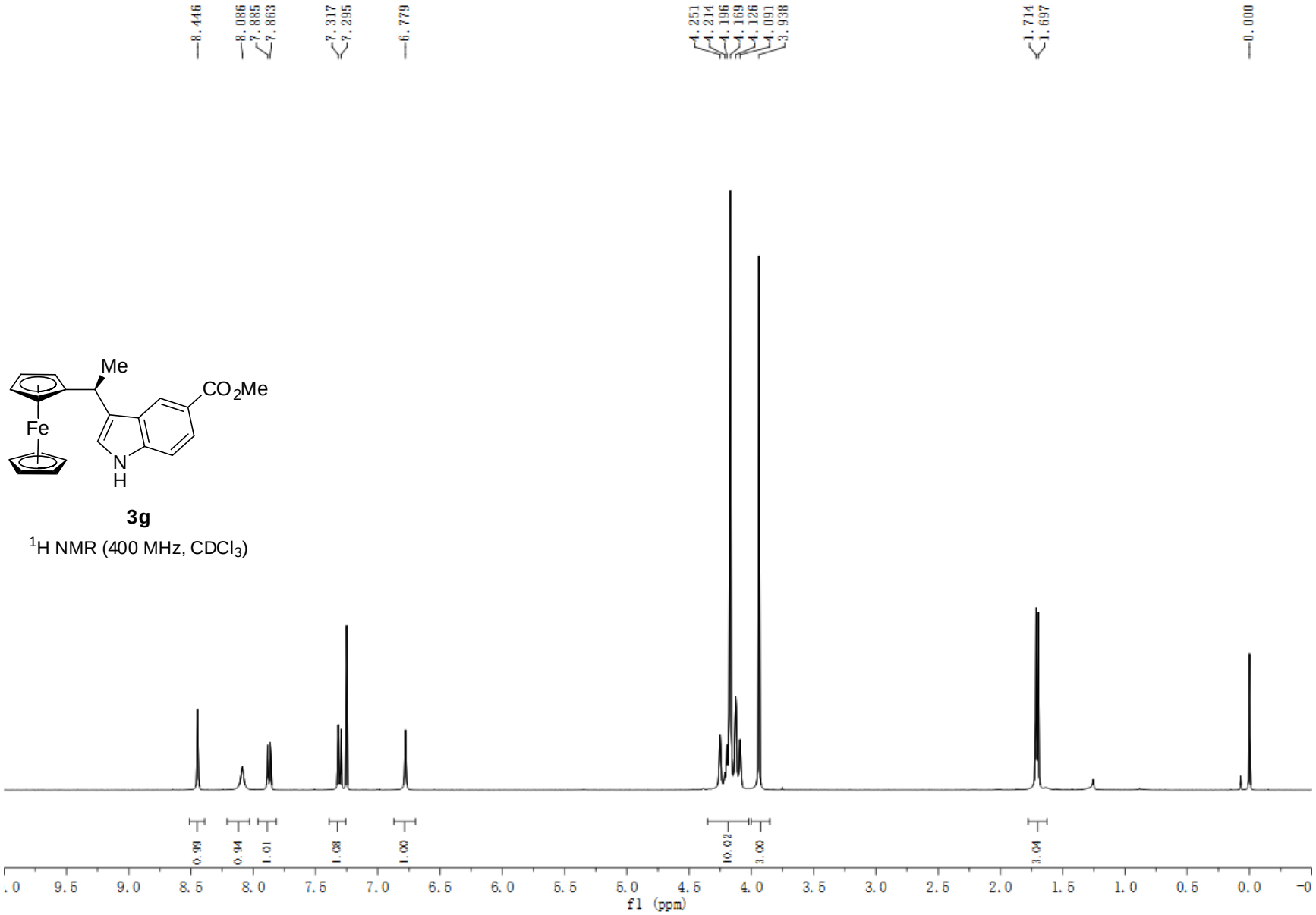
3f

^{1}H NMR (400 MHz, $CDCl_3$)



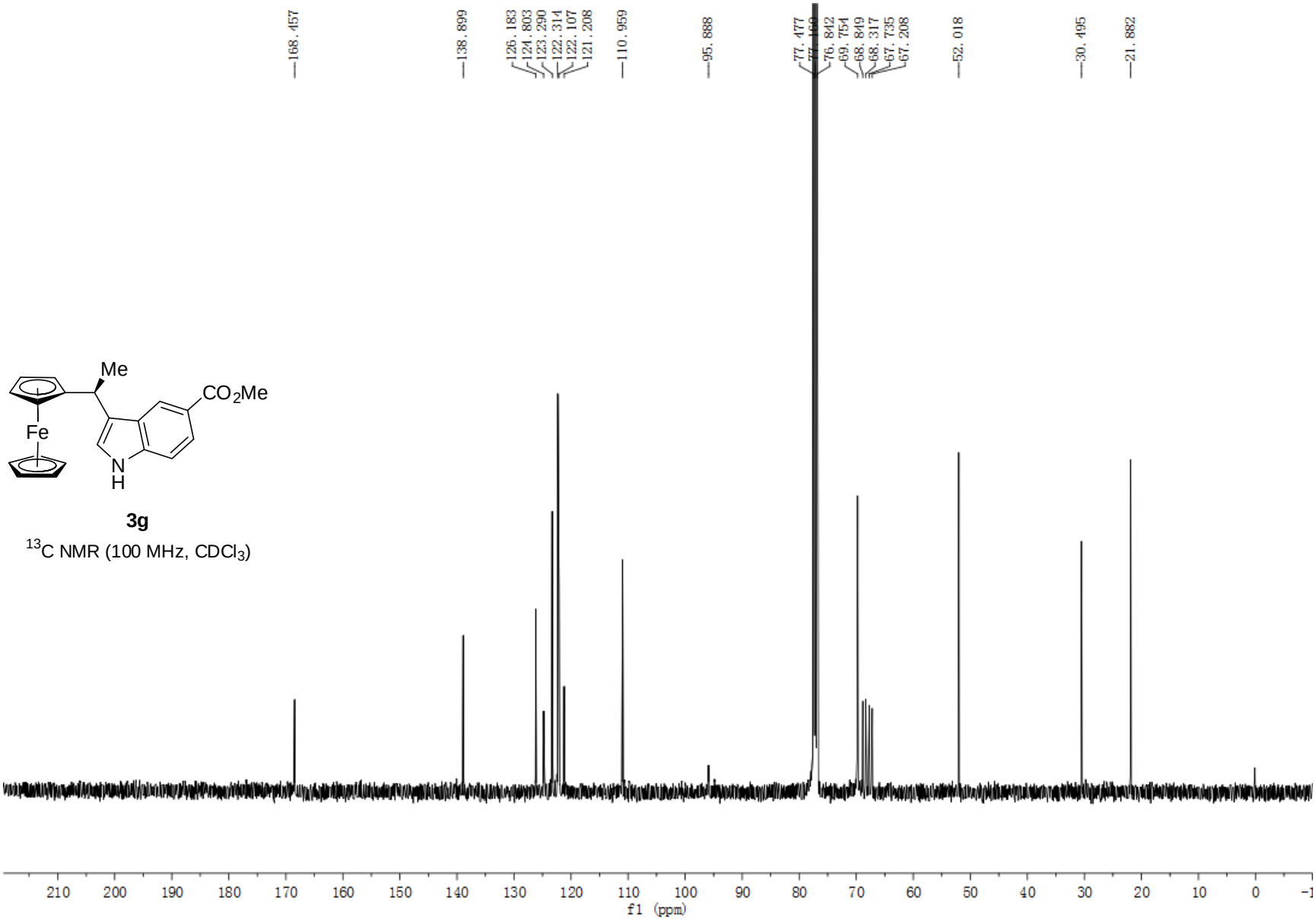
3f

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



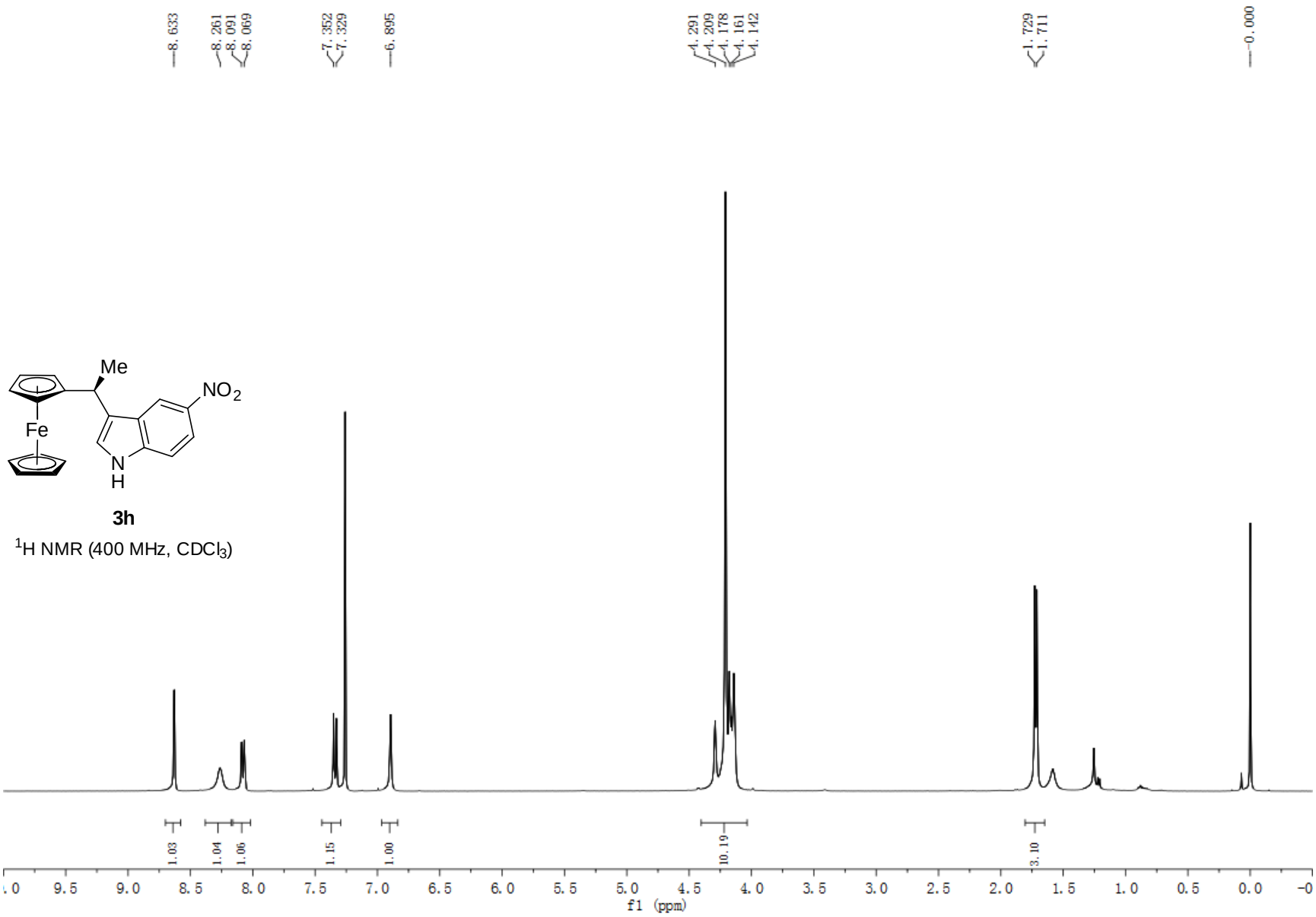
3g

^{1}H NMR (400 MHz, $CDCl_3$)



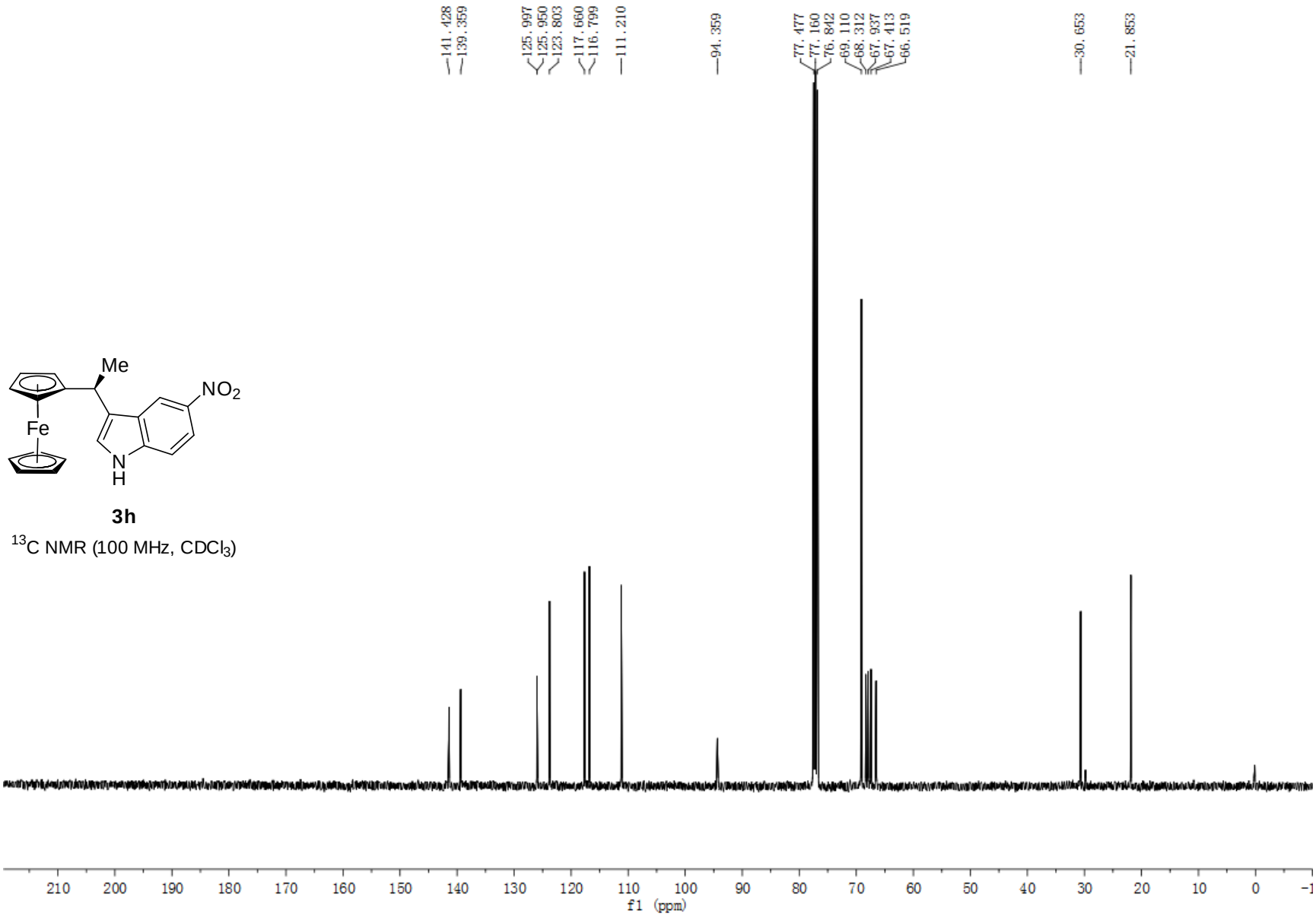
3g

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



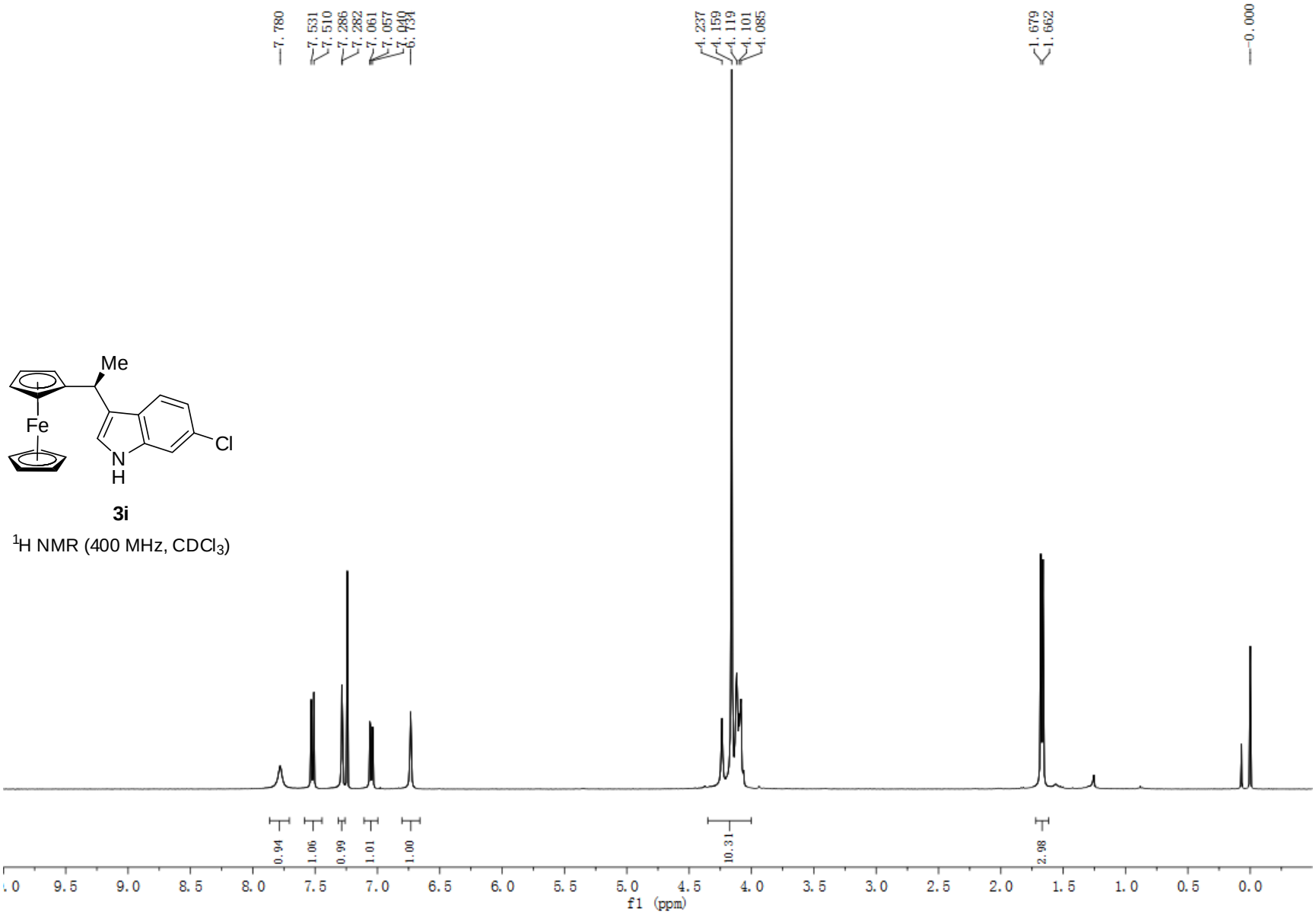
3h

^{1}H NMR (400 MHz, $CDCl_3$)



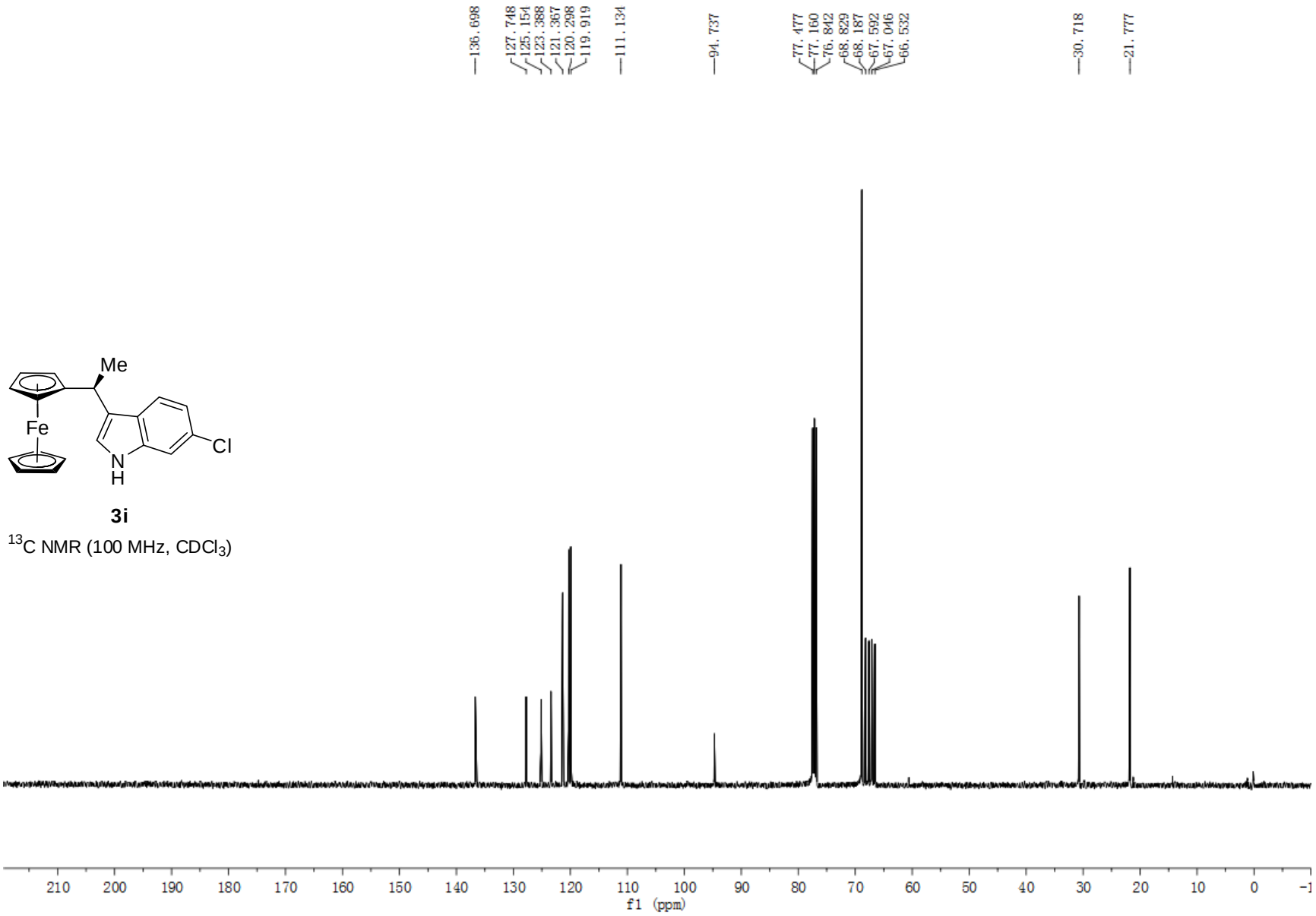
3h

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



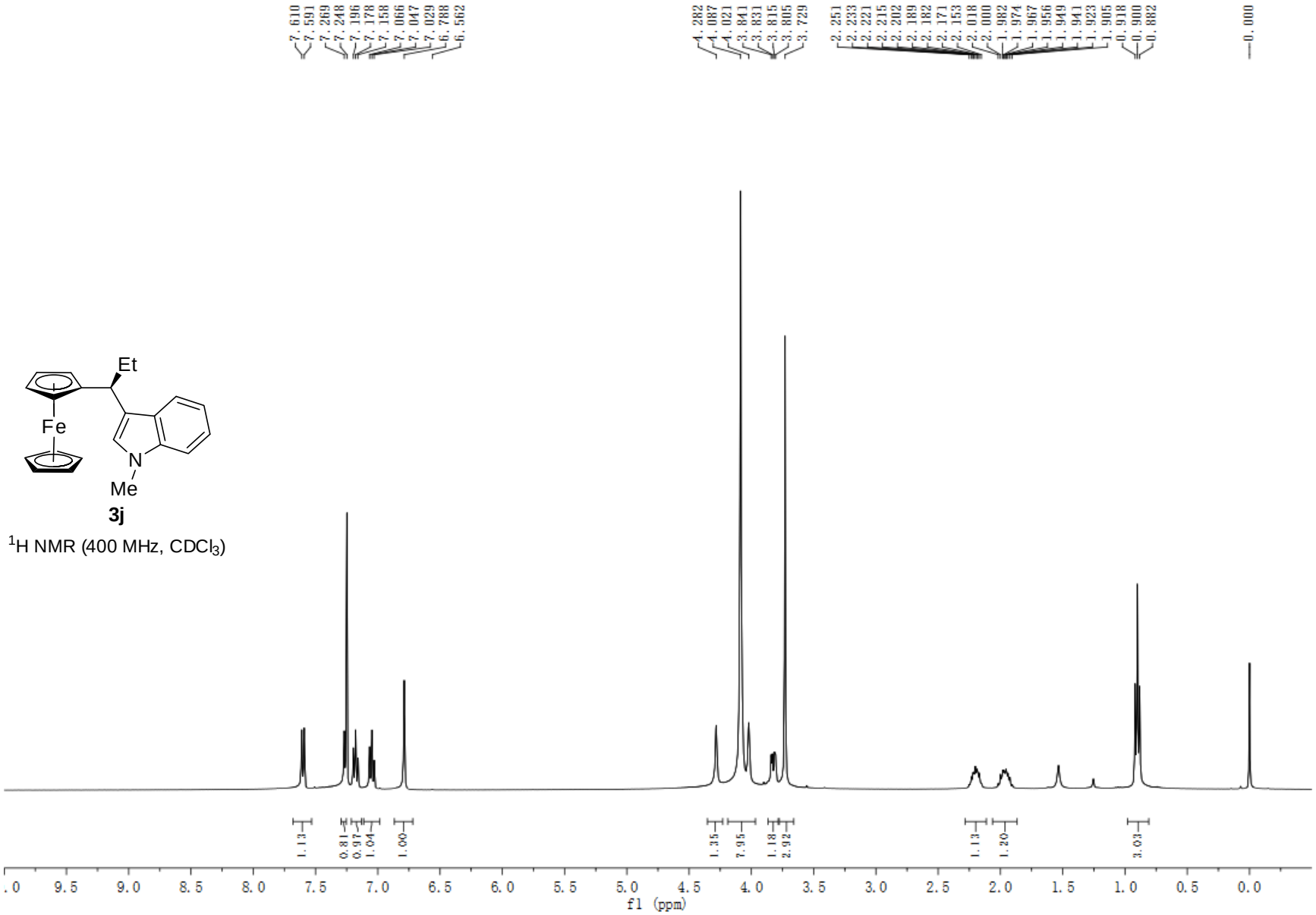
3i

^{1}H NMR (400 MHz, $CDCl_3$)



3i

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



Et

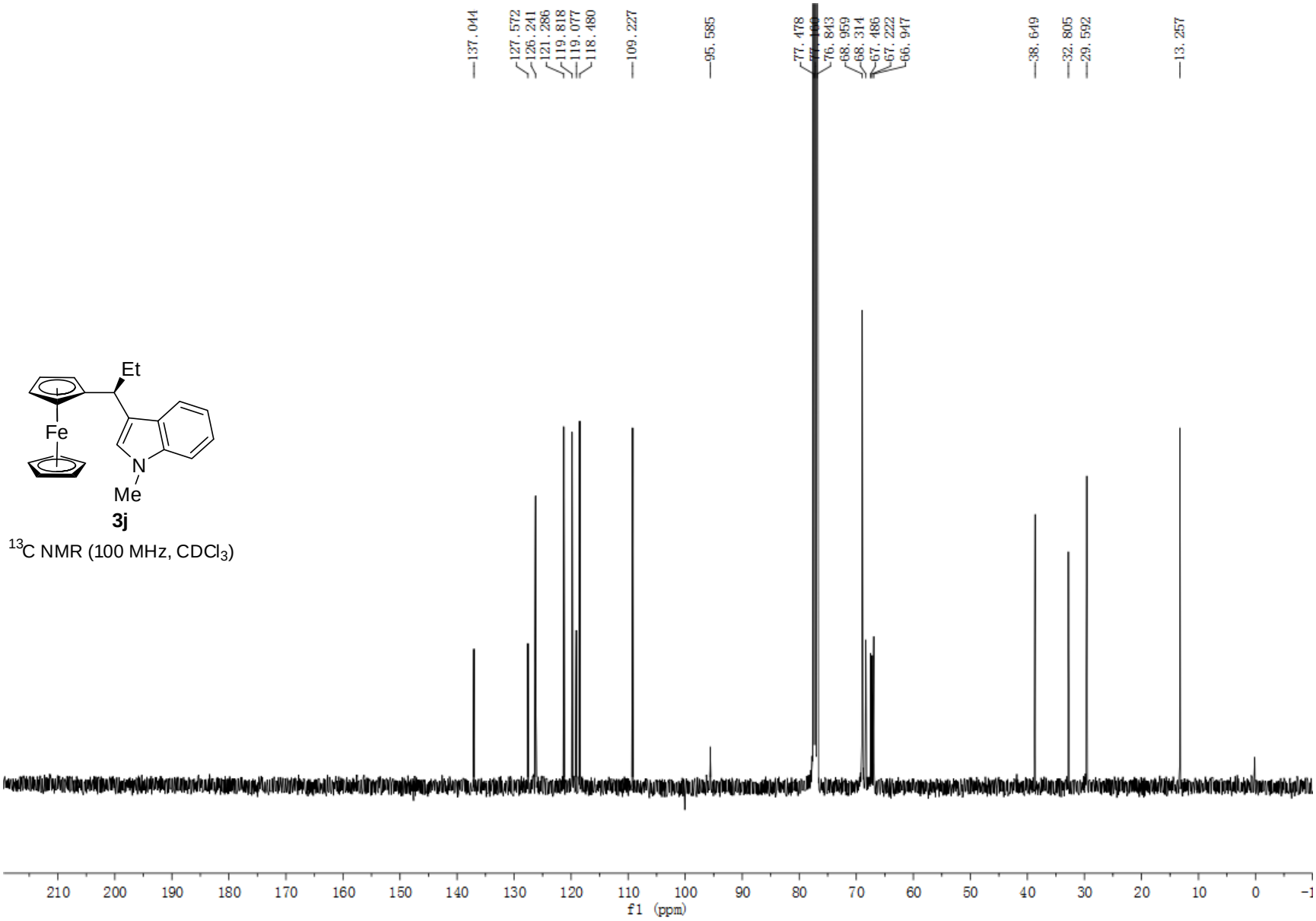
Fe

N

Me

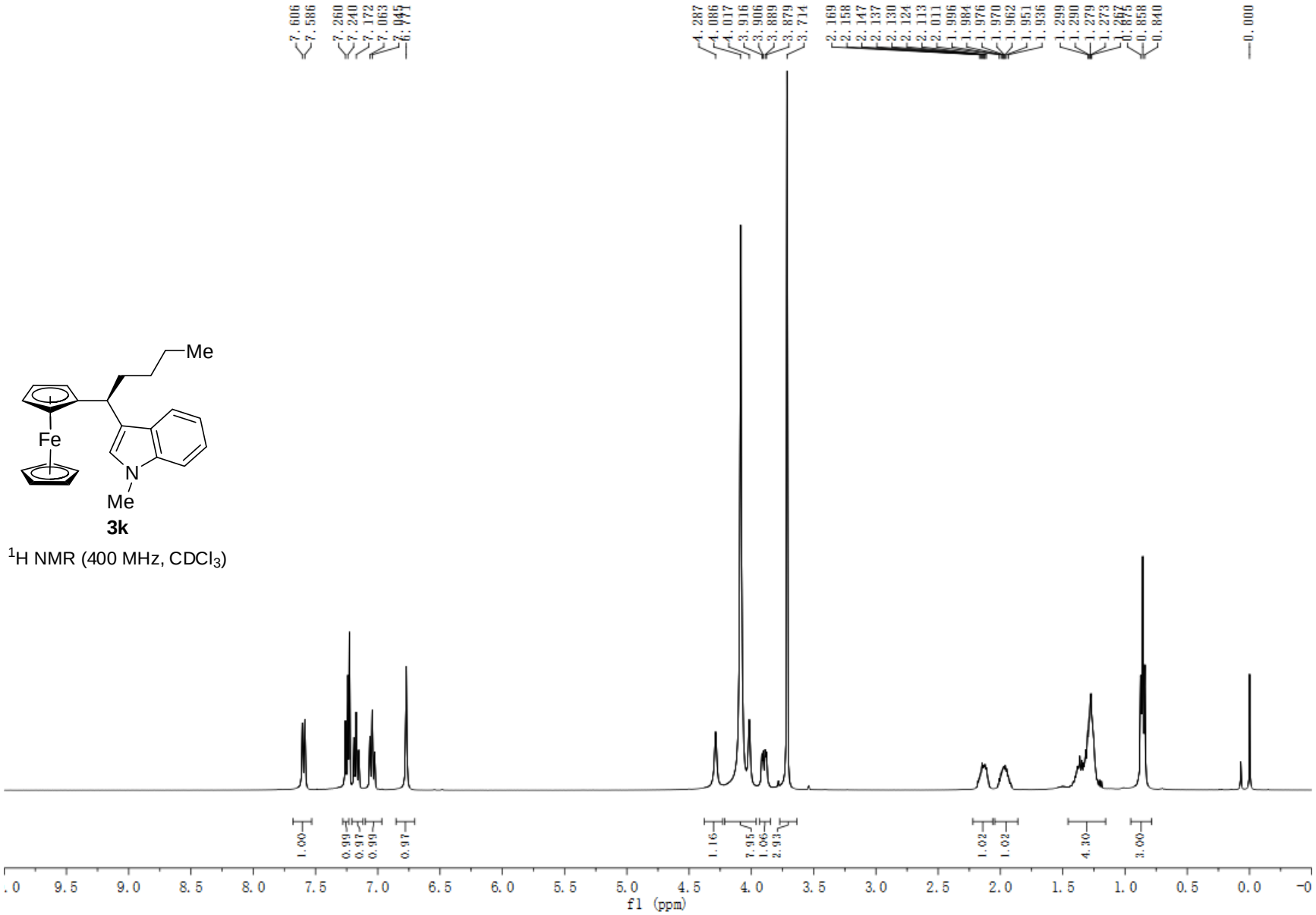
3j

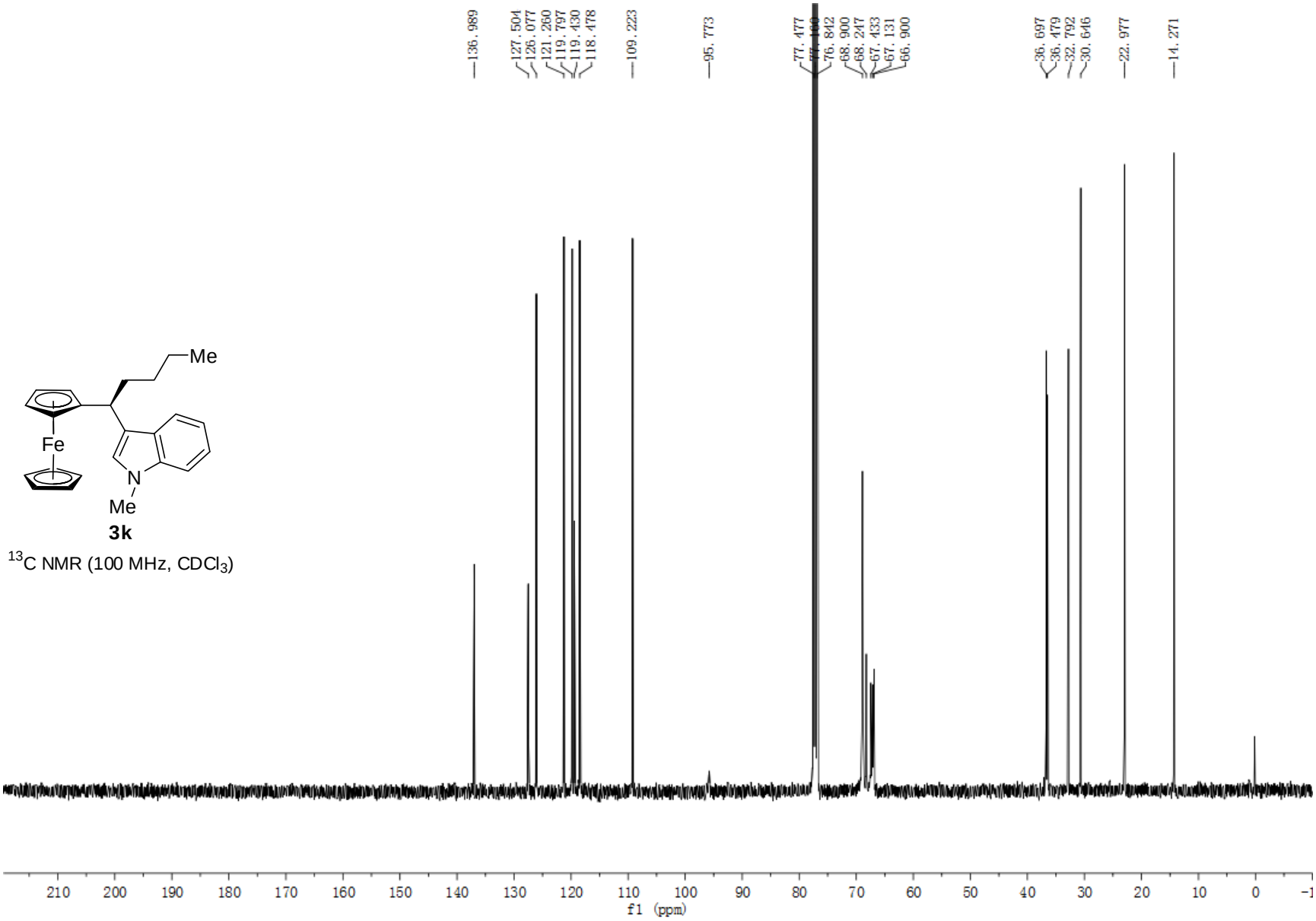
^{1}H NMR (400 MHz, $CDCl_3$)



3j

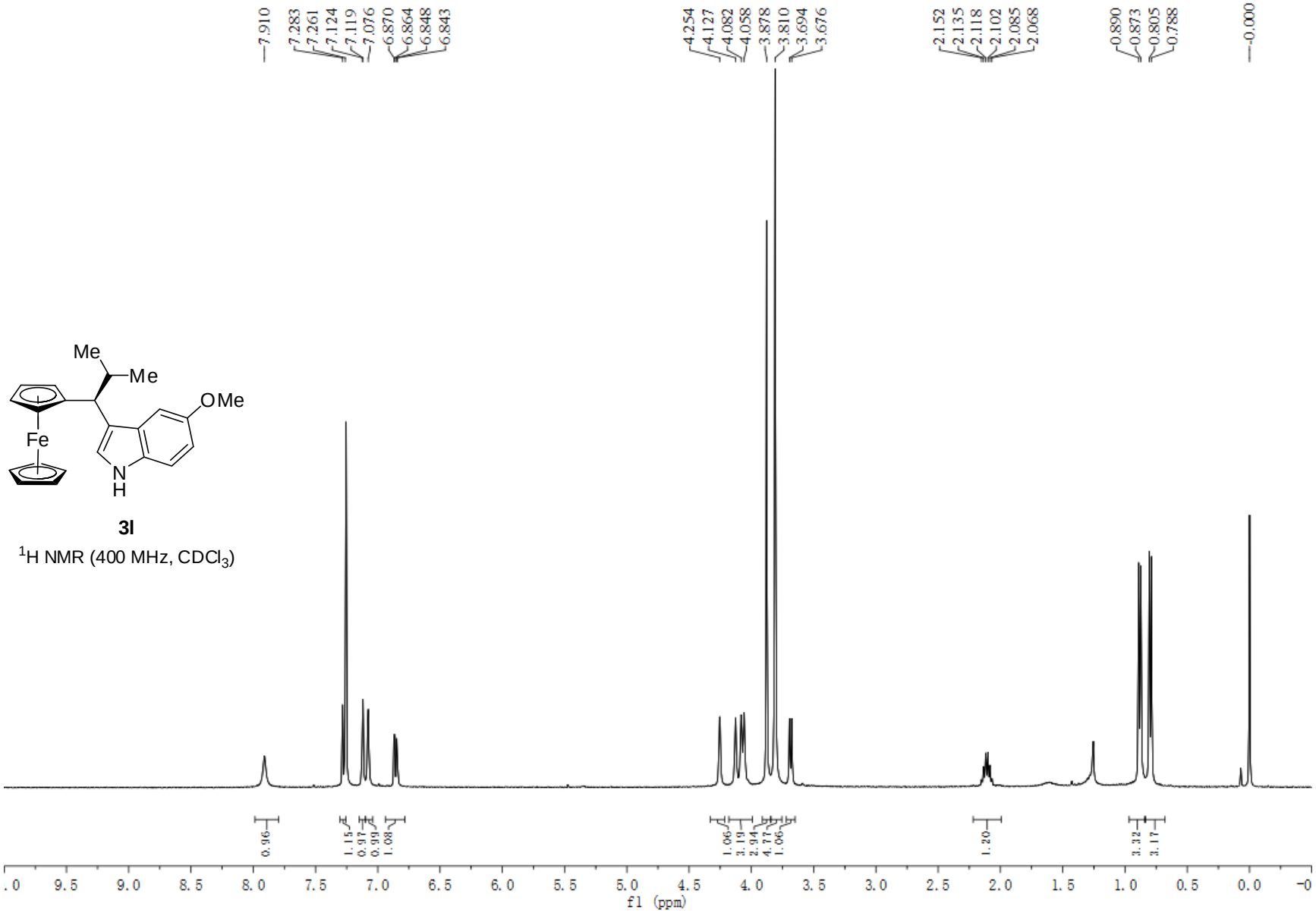
^{13}C NMR (100 MHz, $CDCl_3$)


Me
Fe
N
Me
3k
1H NMR (400 MHz, CDCl3)
f1 (ppm)



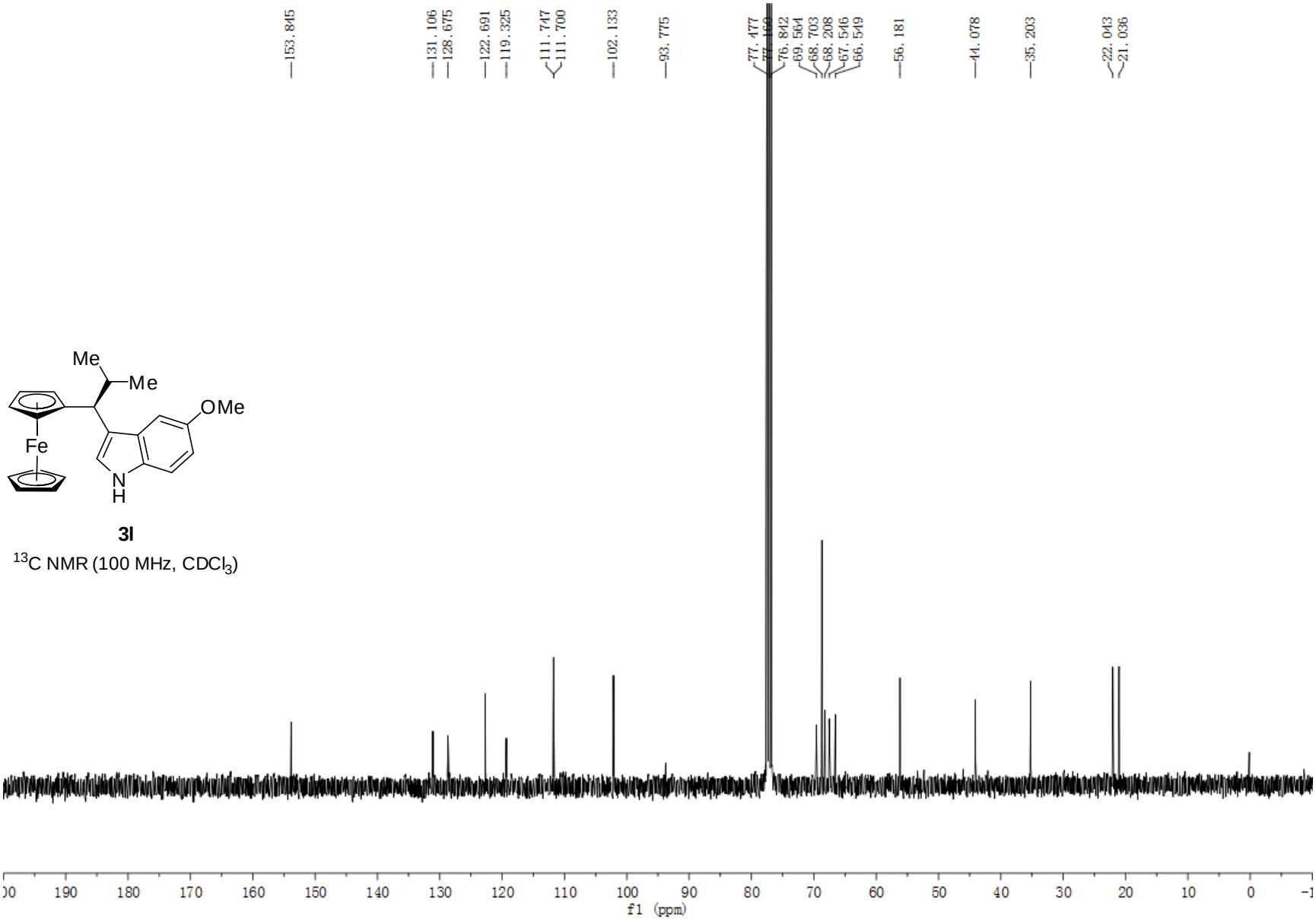
3k

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



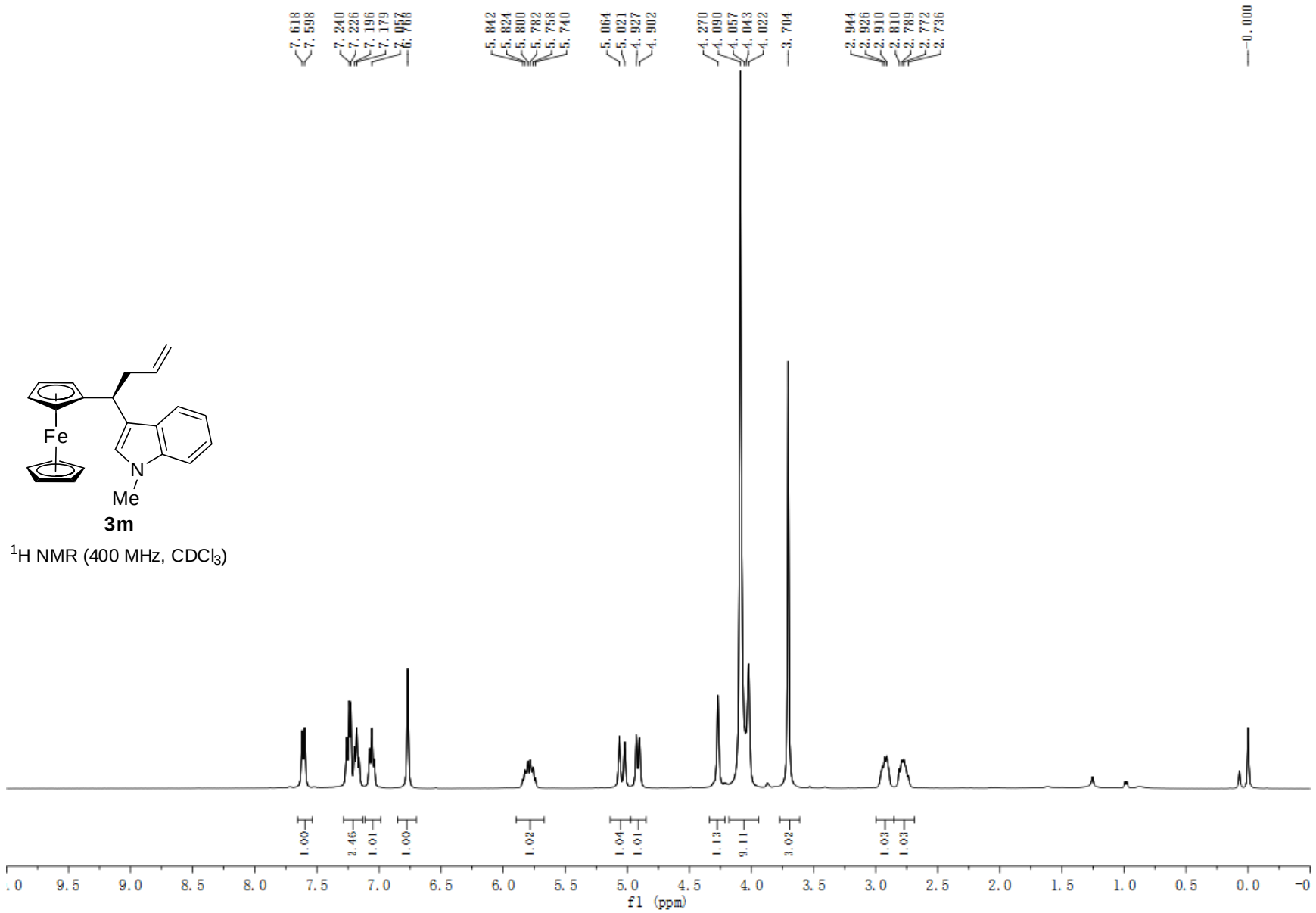
3l

^{1}H NMR (400 MHz, $CDCl_3$)



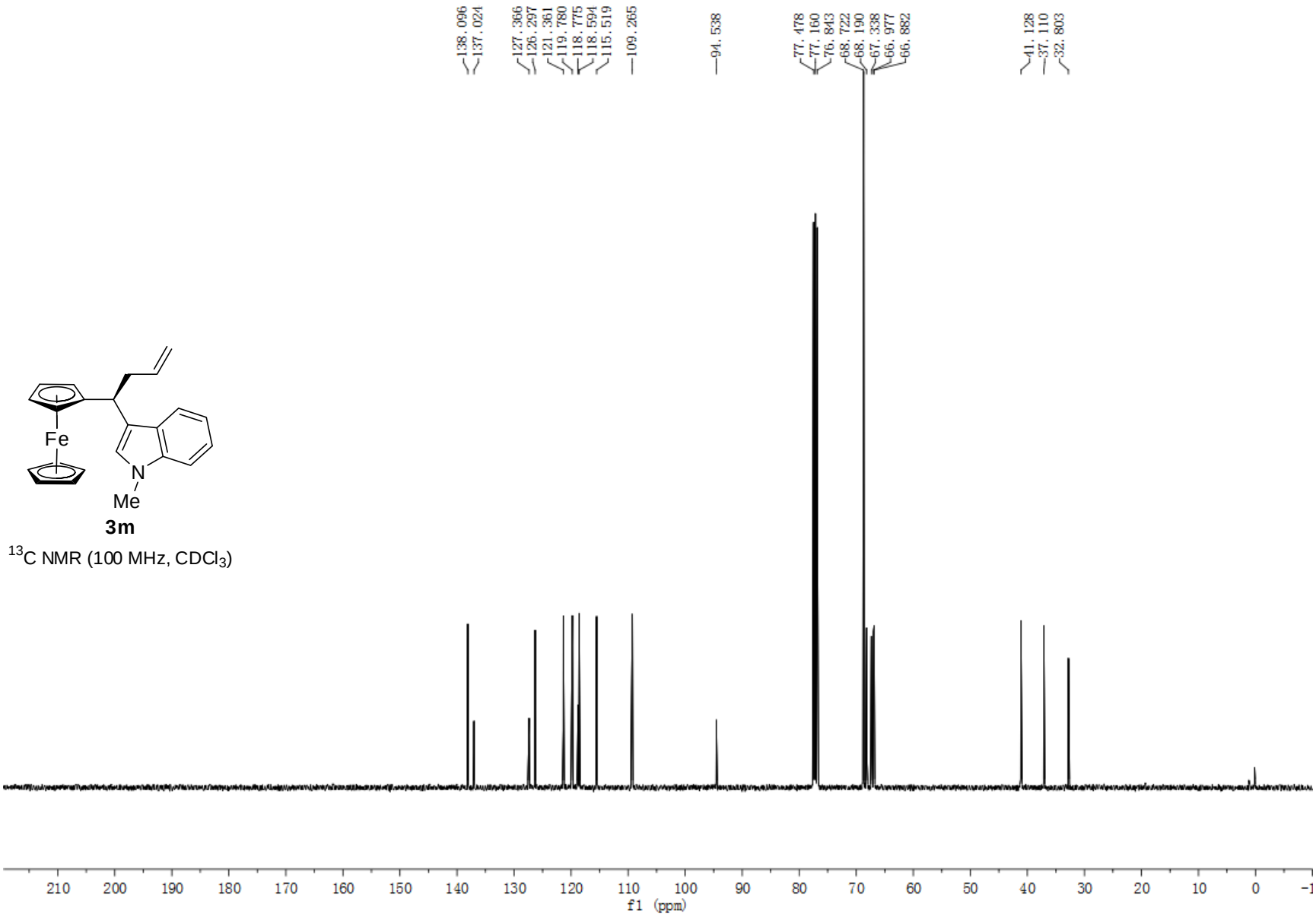
3l

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



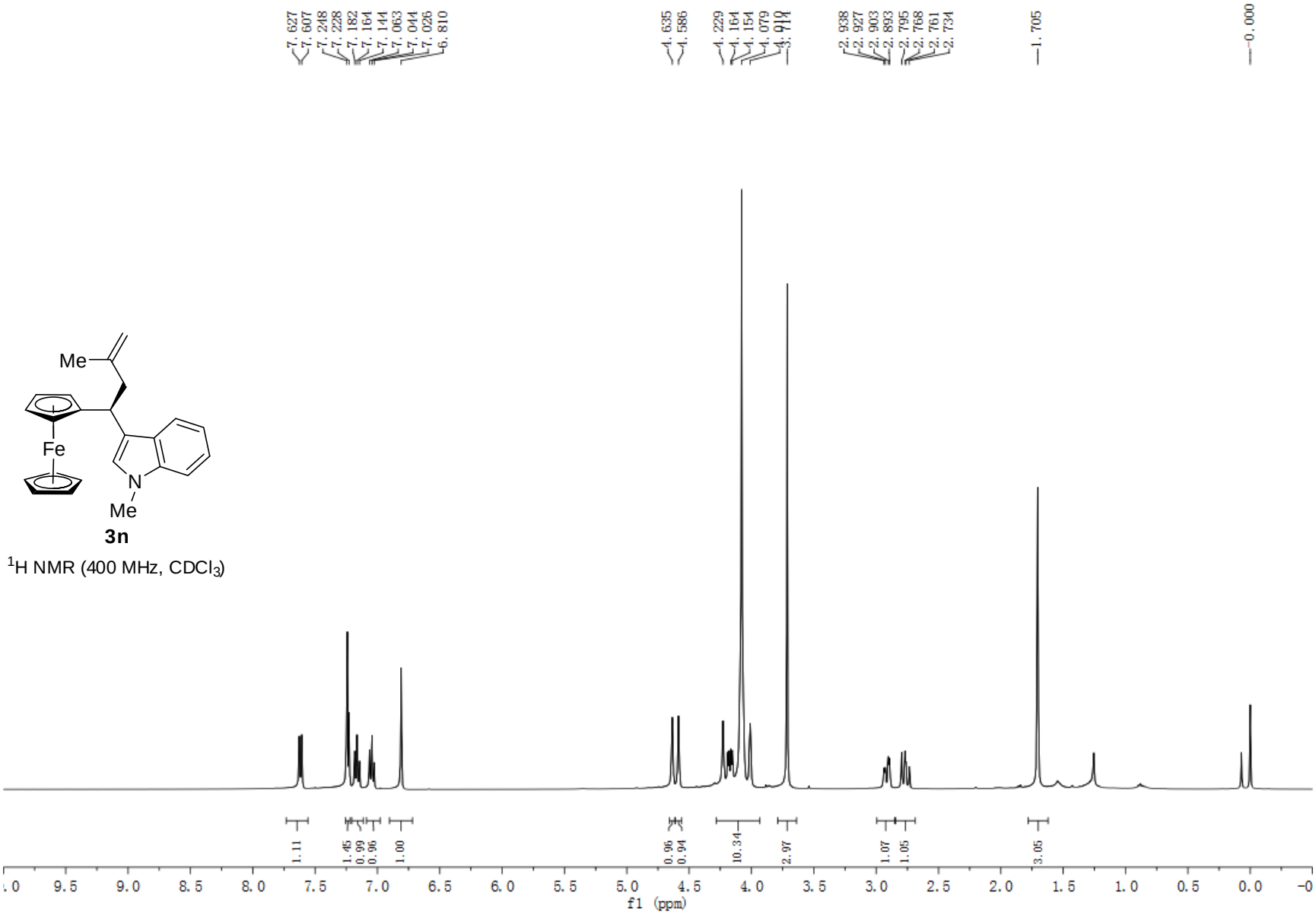
3m

^{1}H NMR (400 MHz, $CDCl_3$)



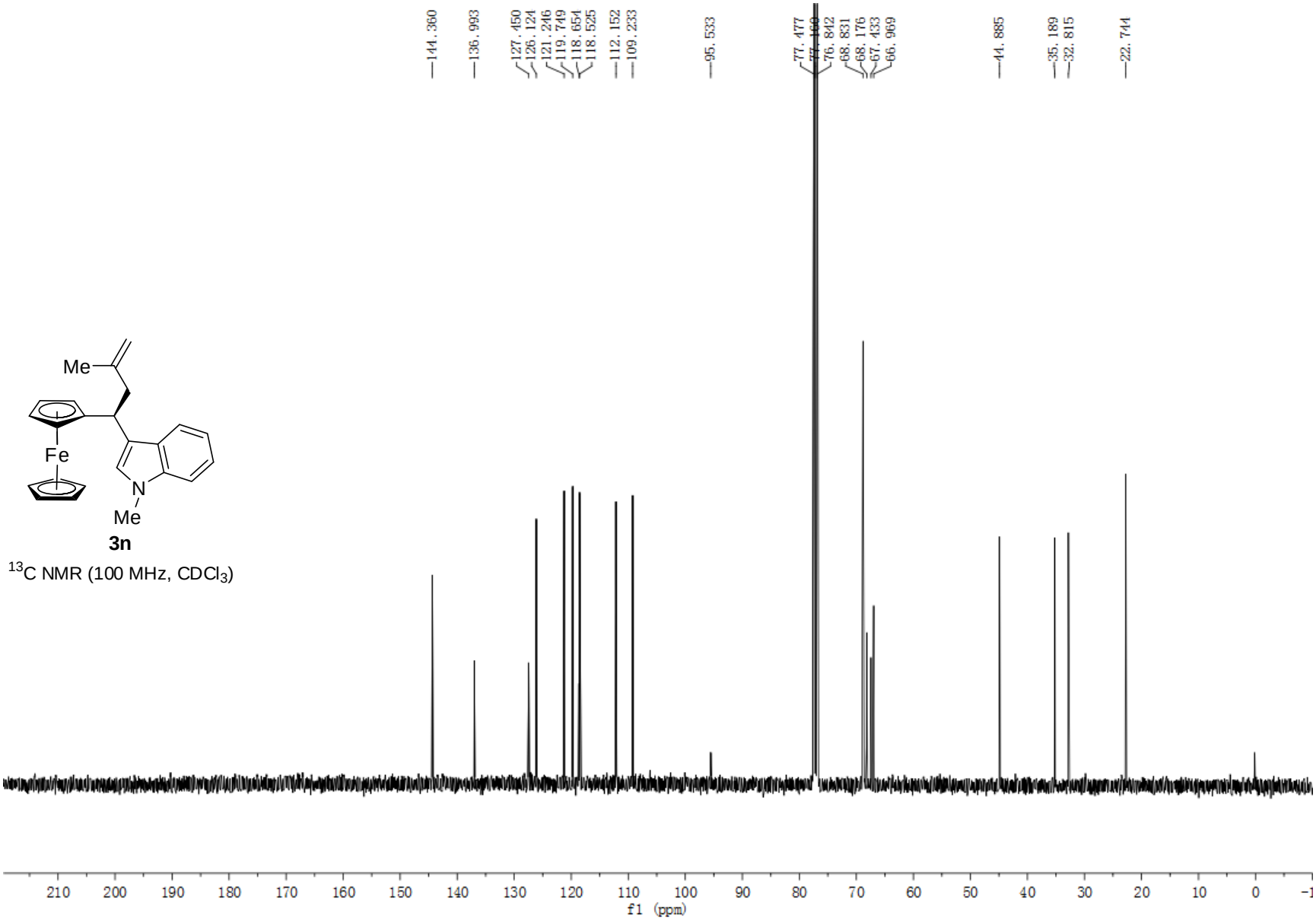
3m

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



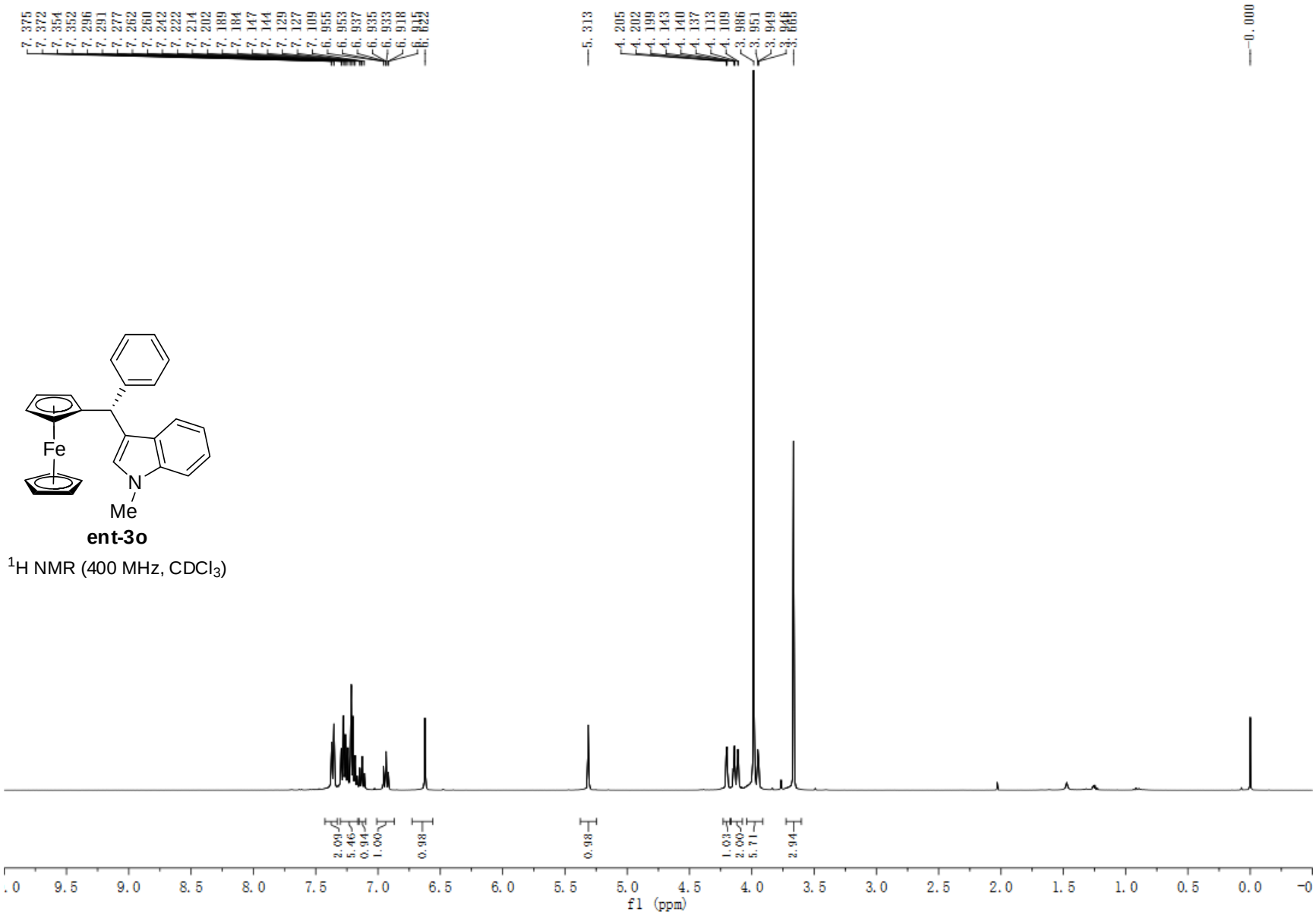
3n

^{1}H NMR (400 MHz, $CDCl_3$)



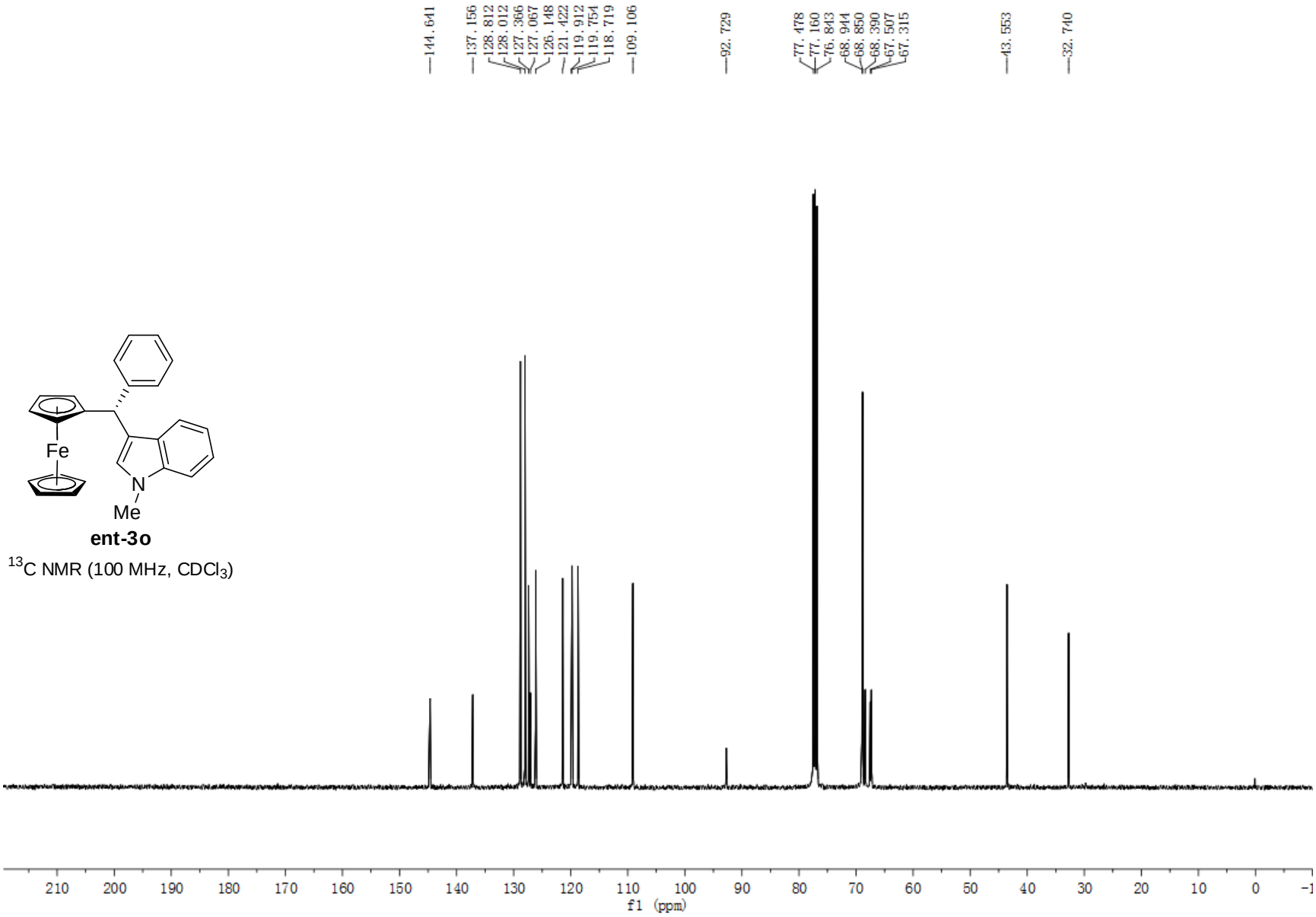
3n

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



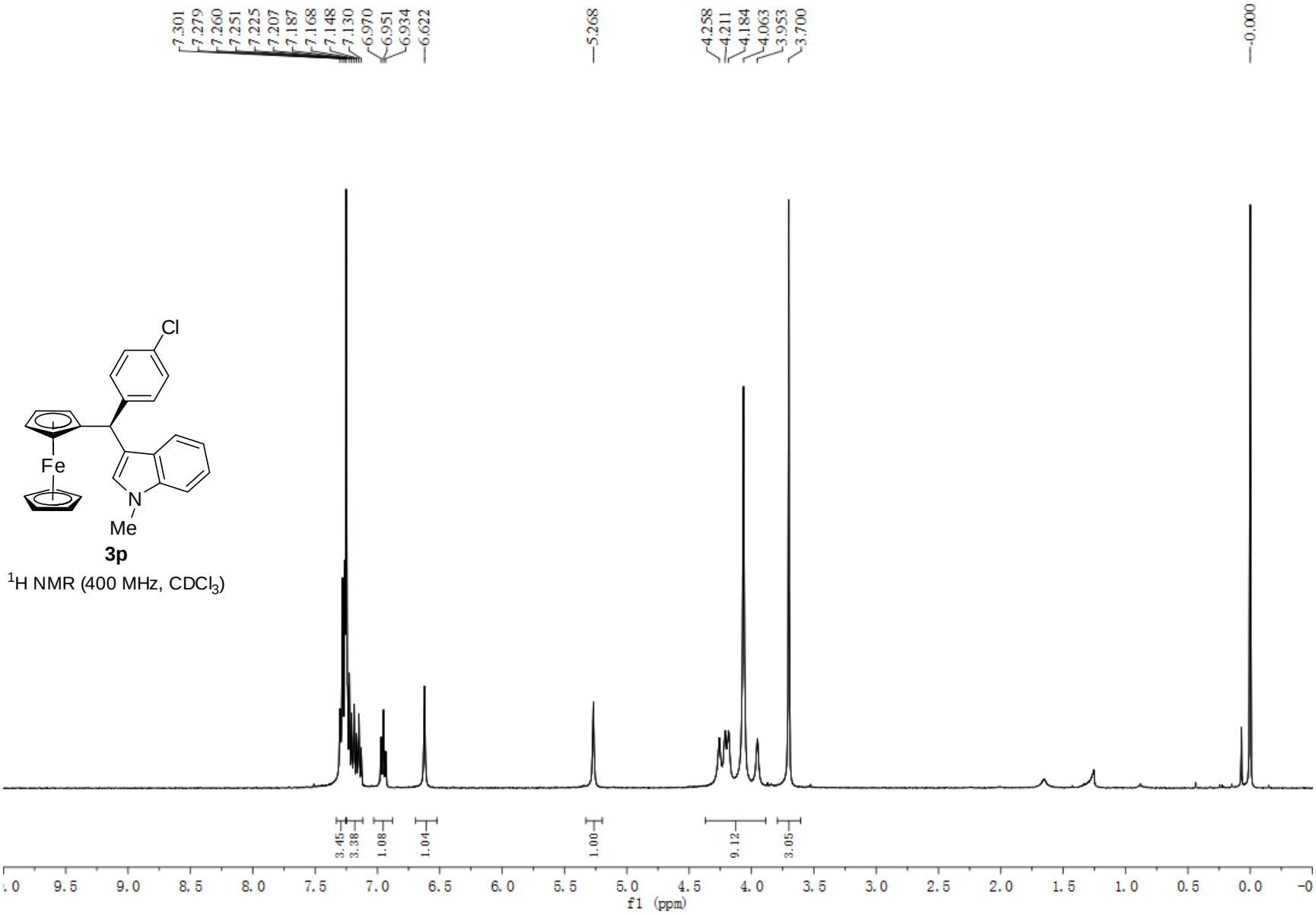
ent-3o

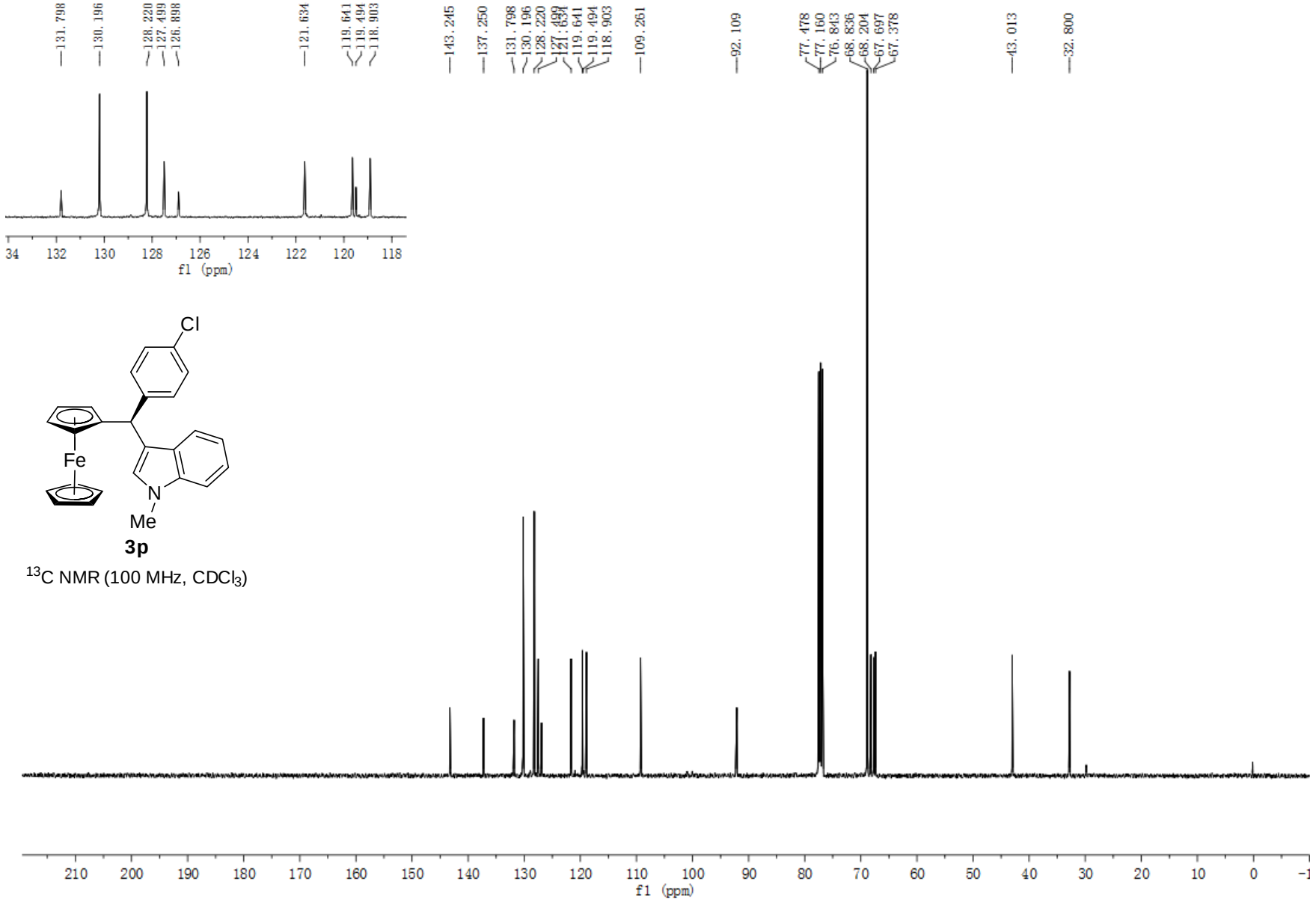
^{1}H NMR (400 MHz, $CDCl_3$)



ent-3o

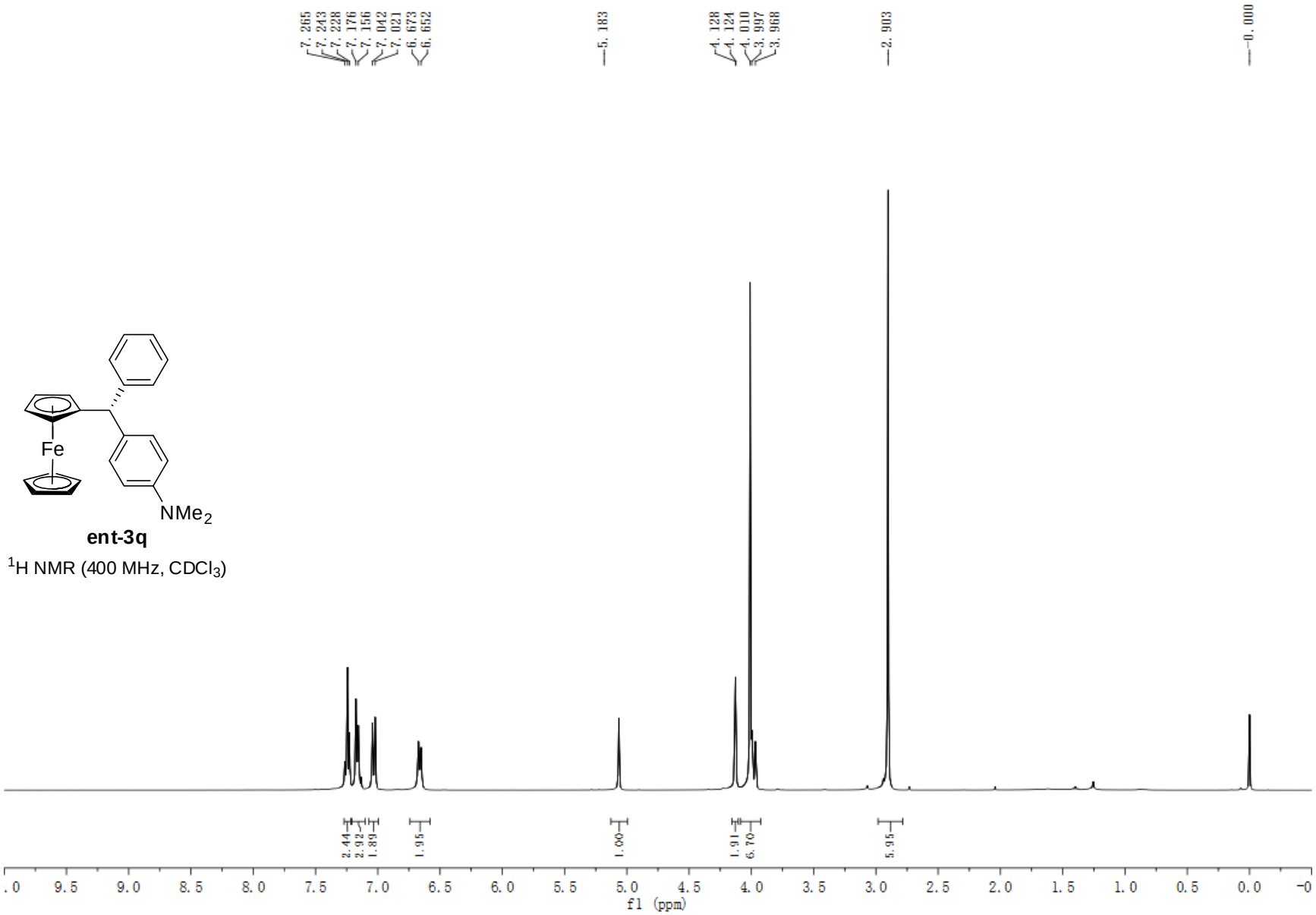
^{13}C NMR (100 MHz, $CDCl_3$)


7.301
7.279
7.260
7.251
7.225
7.207
7.187
7.168
7.148
7.130
6.970
6.951
6.934
6.622
5.268
4.258
4.211
4.184
4.063
3.953
3.700
0.000
Cl
Fe
N
Me
3p
1H NMR (400 MHz, CDCl3)
3.45
3.38
1.08
1.04
1.00
9.12
3.05
f1 (ppm)



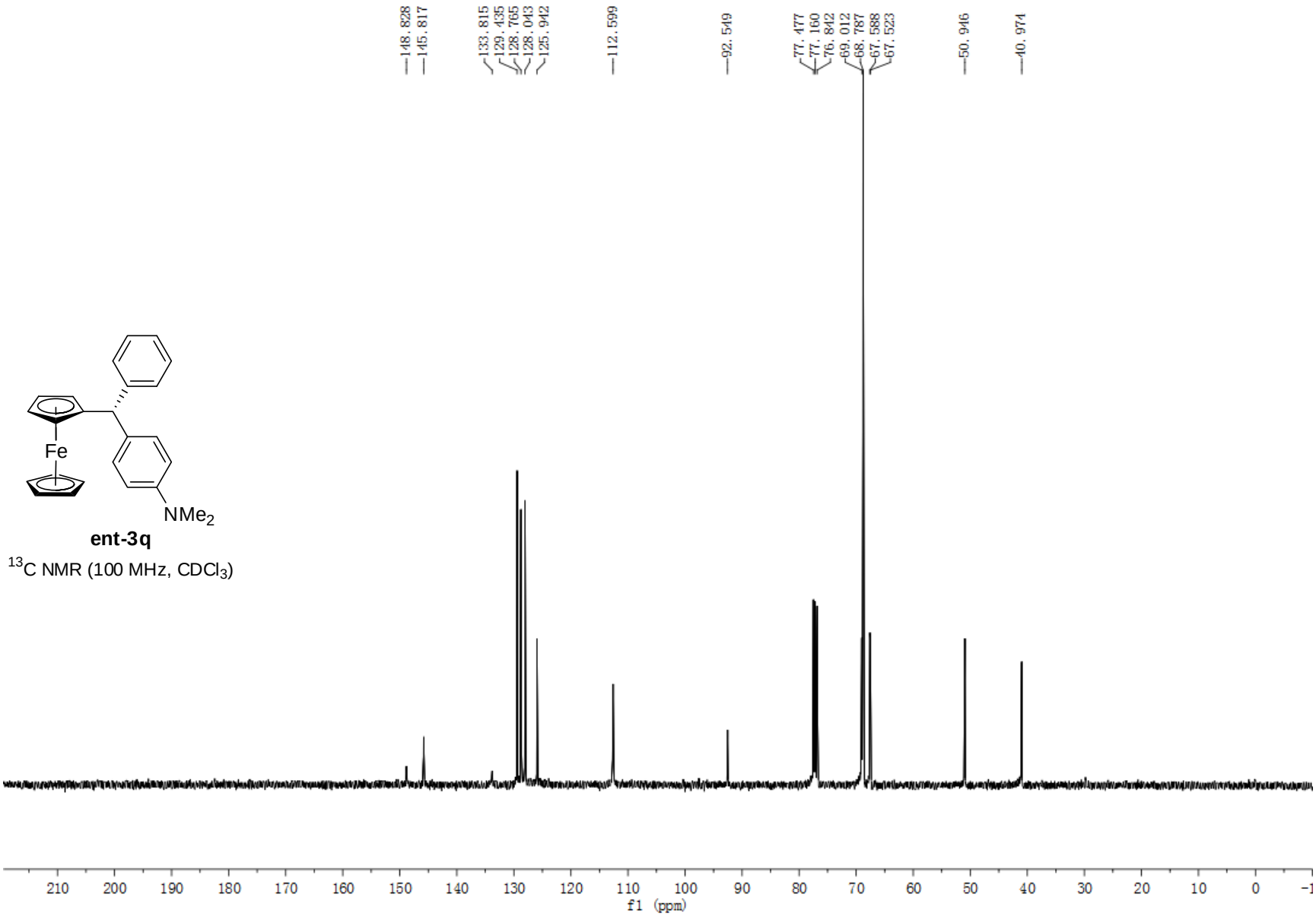
3p

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



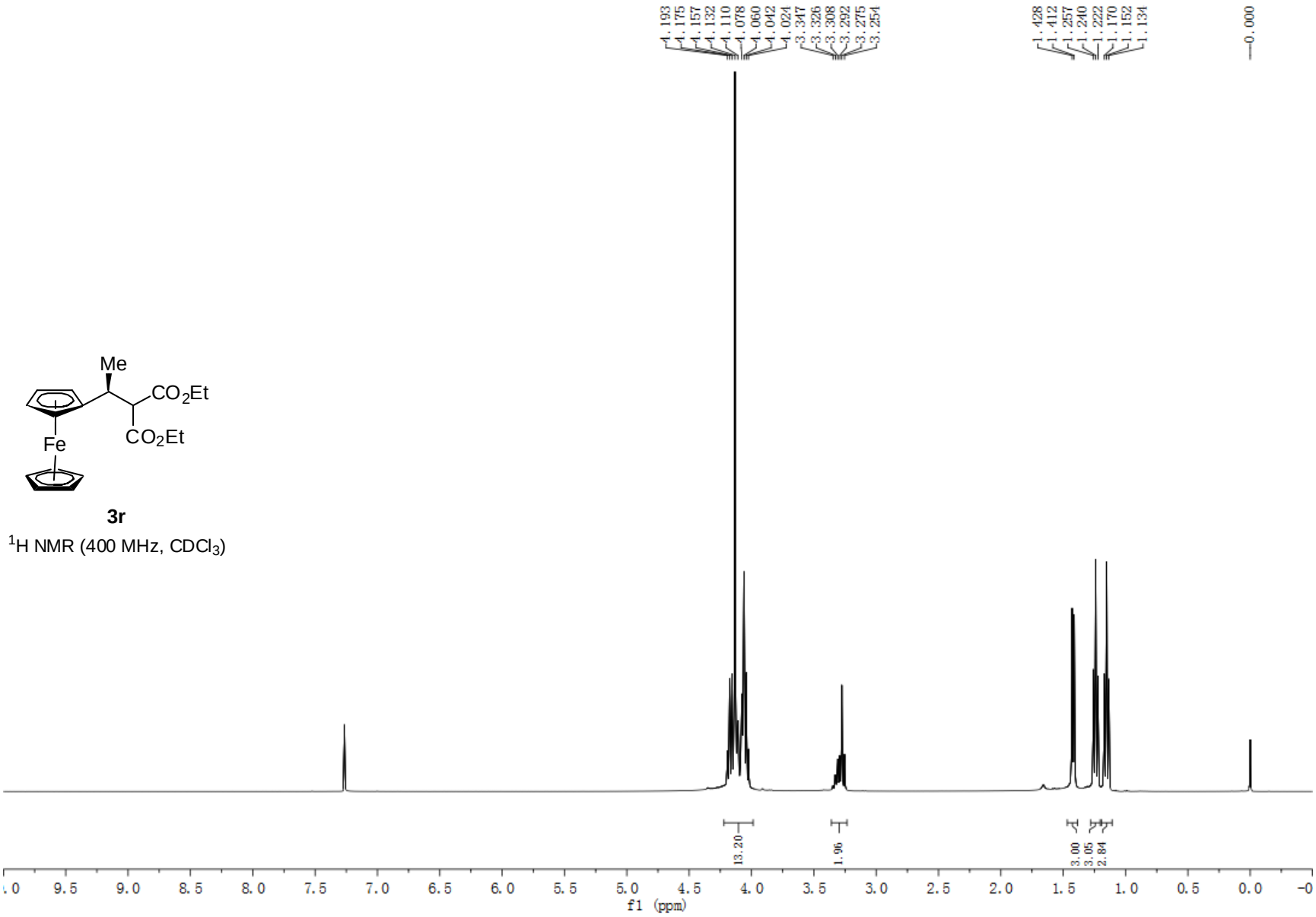
ent-3q

^{1}H NMR (400 MHz, $CDCl_3$)



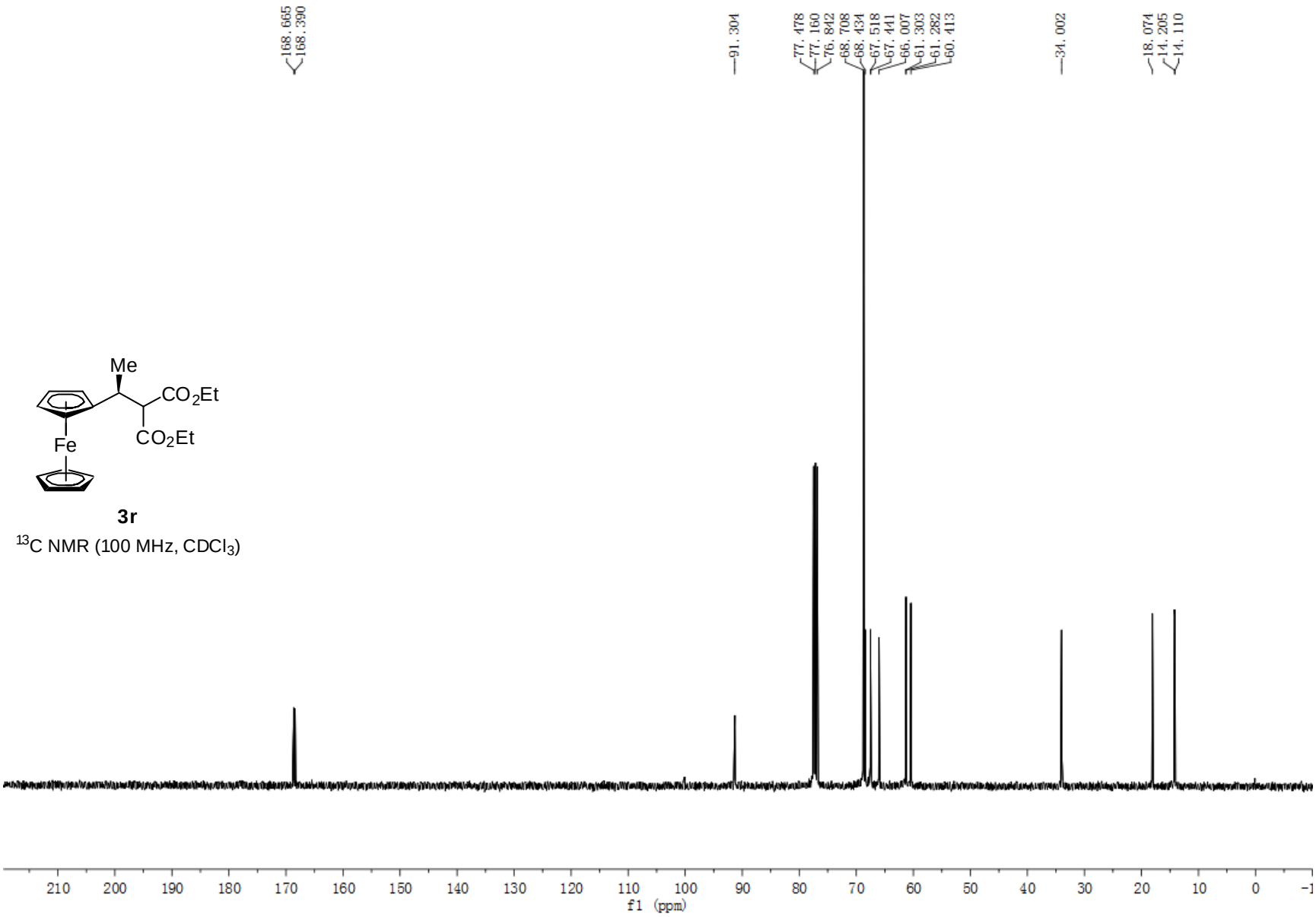
ent-3q

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



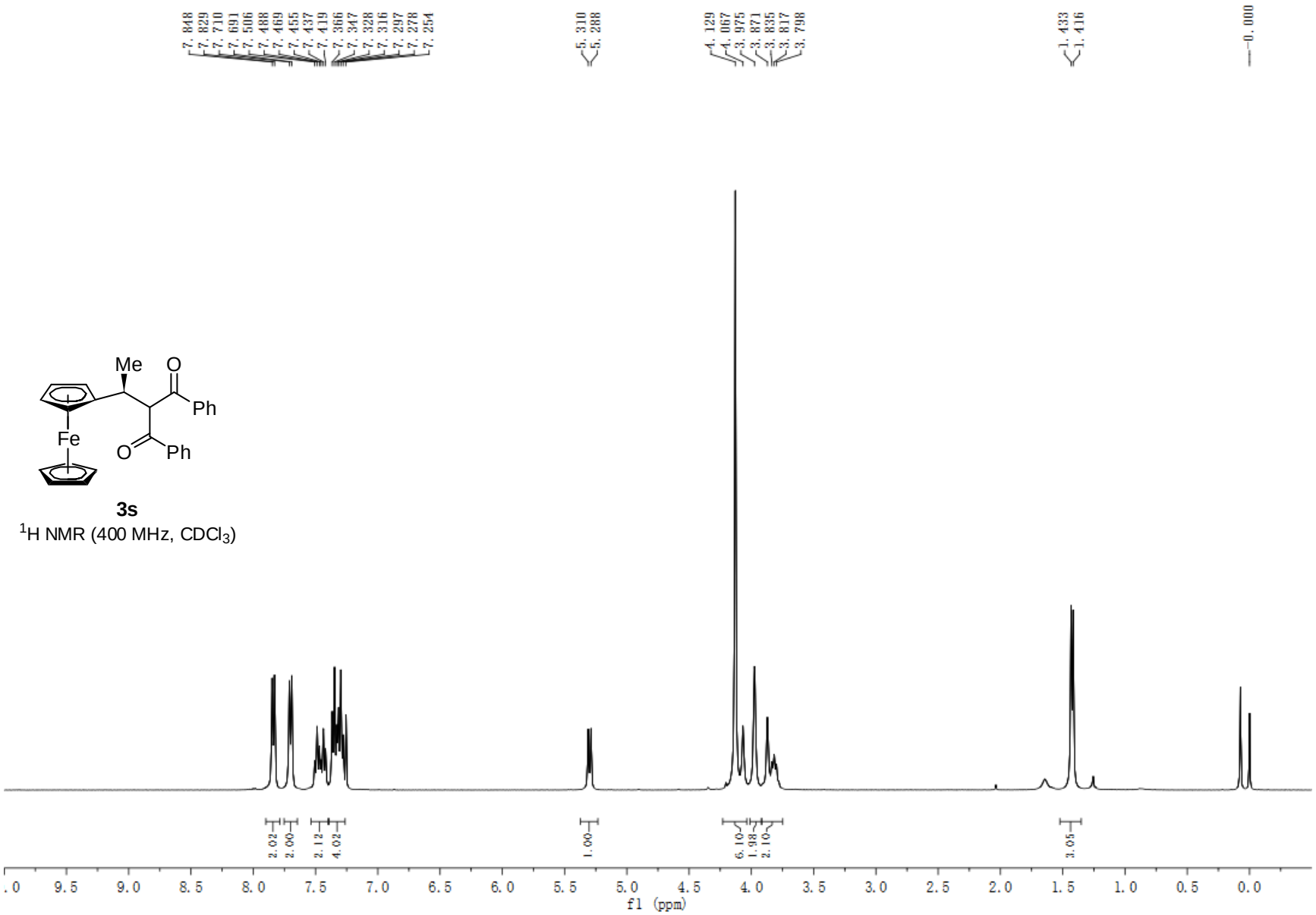
3r

^{1}H NMR (400 MHz, $CDCl_3$)



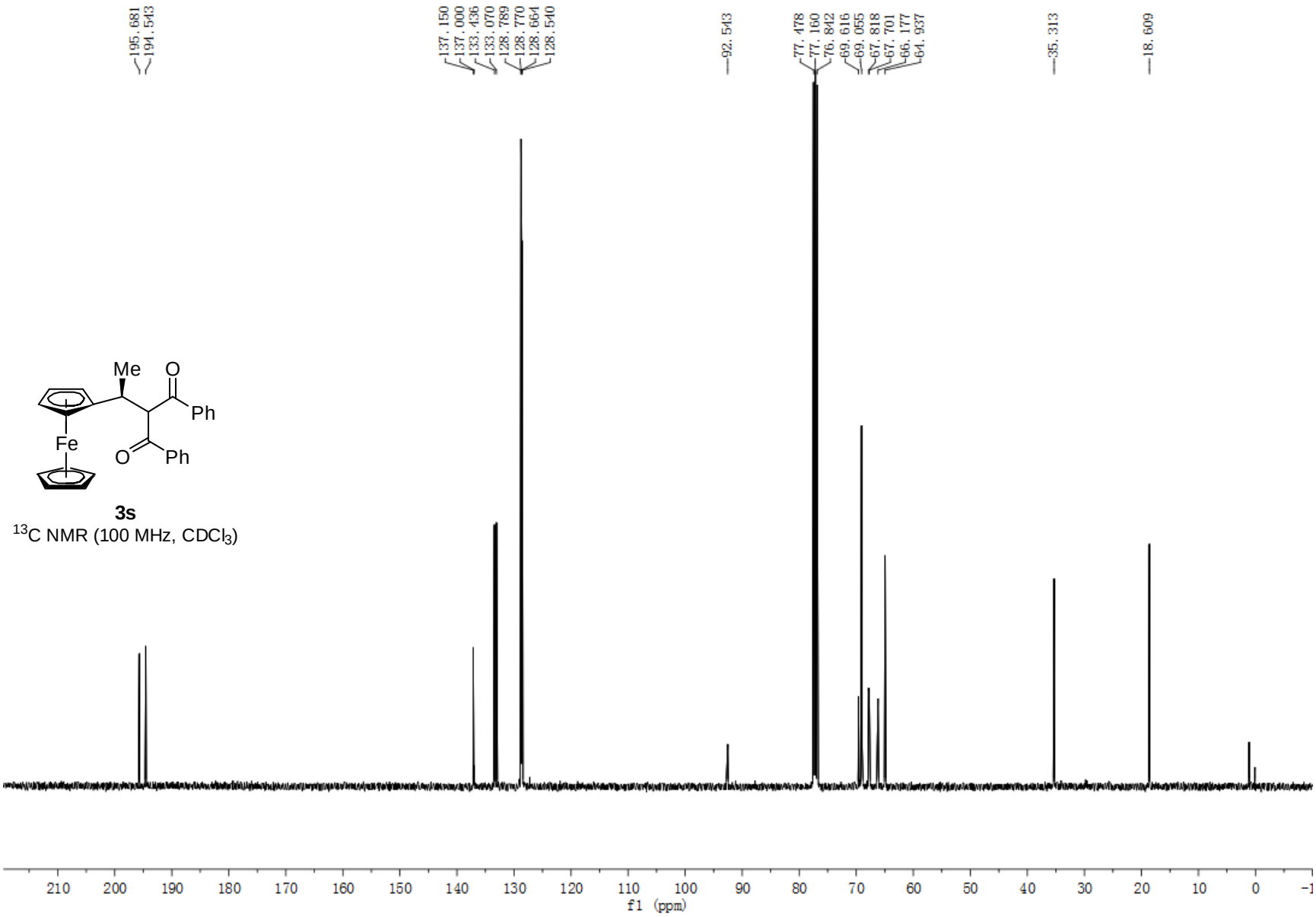
3r

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



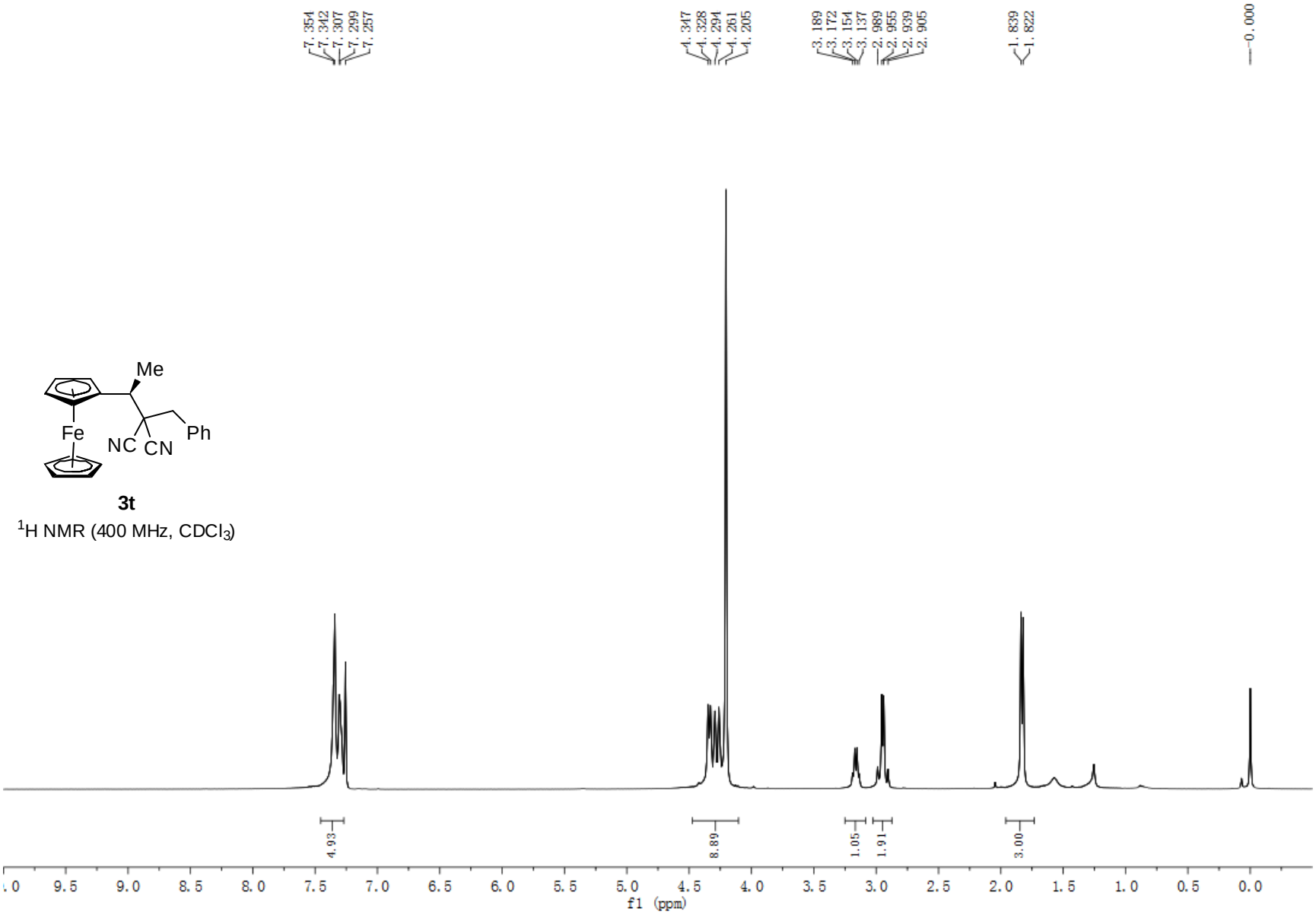
3s

^{1}H NMR (400 MHz, $CDCl_3$)



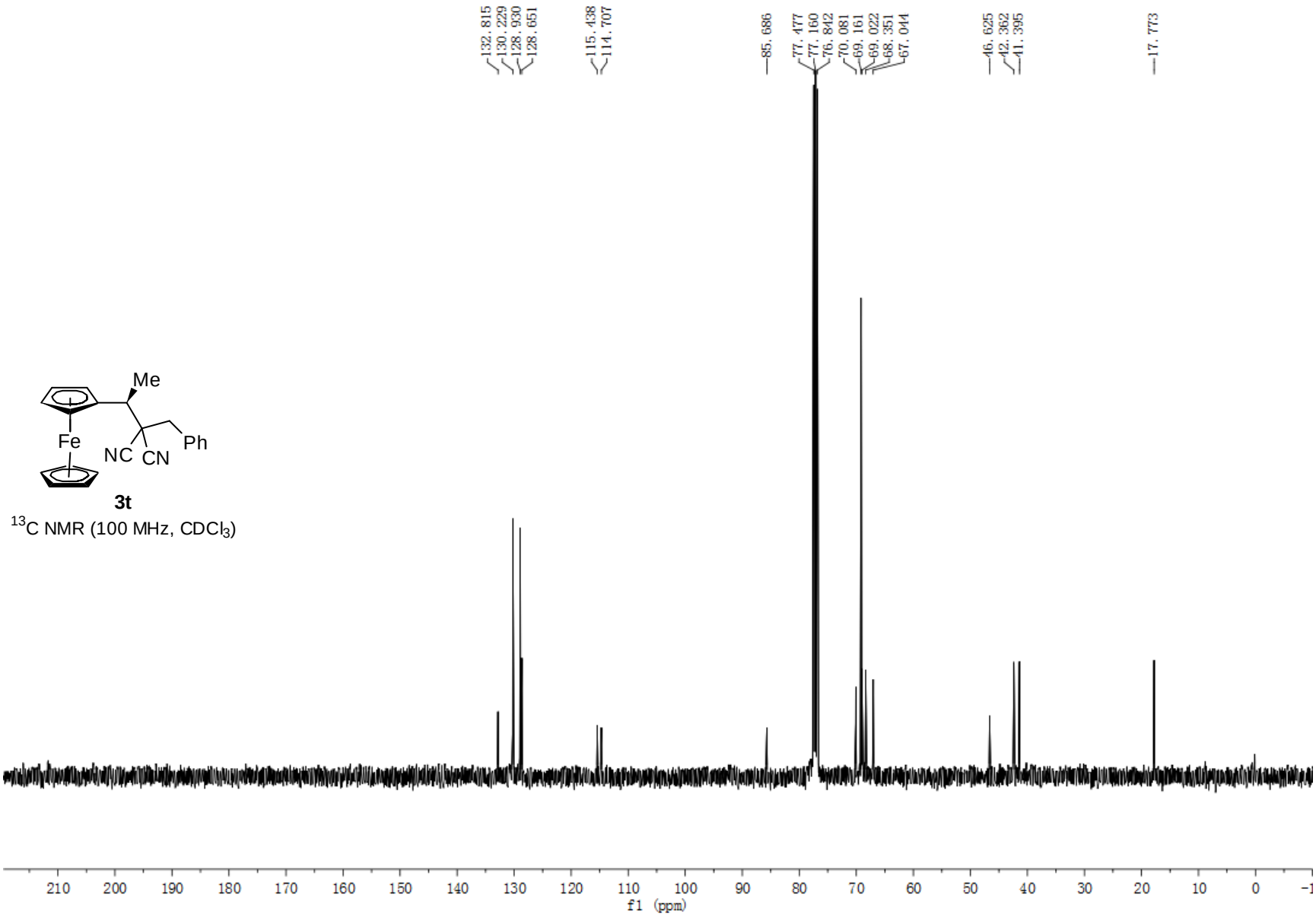
3s

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



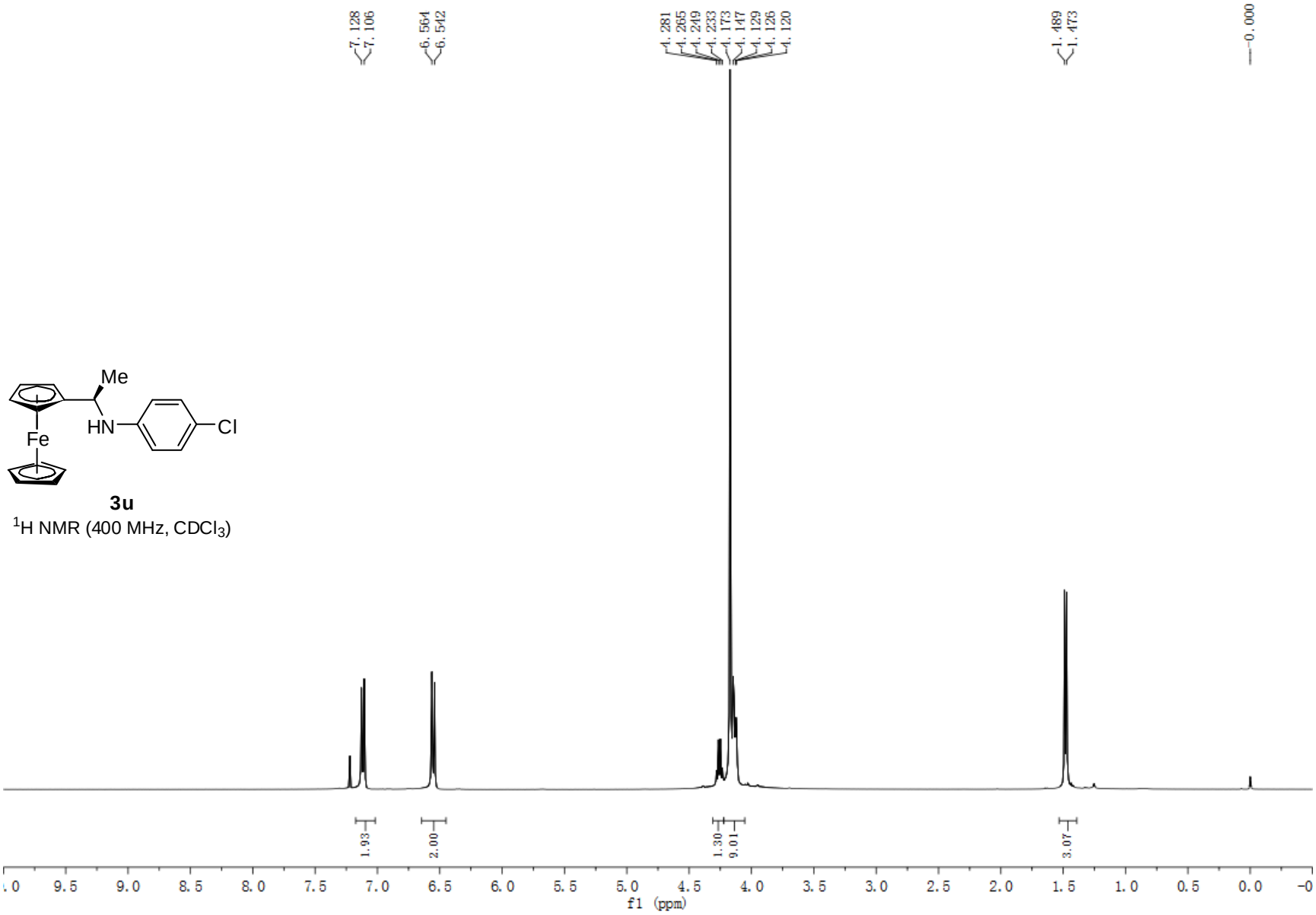
3t

^{1}H NMR (400 MHz, $CDCl_3$)



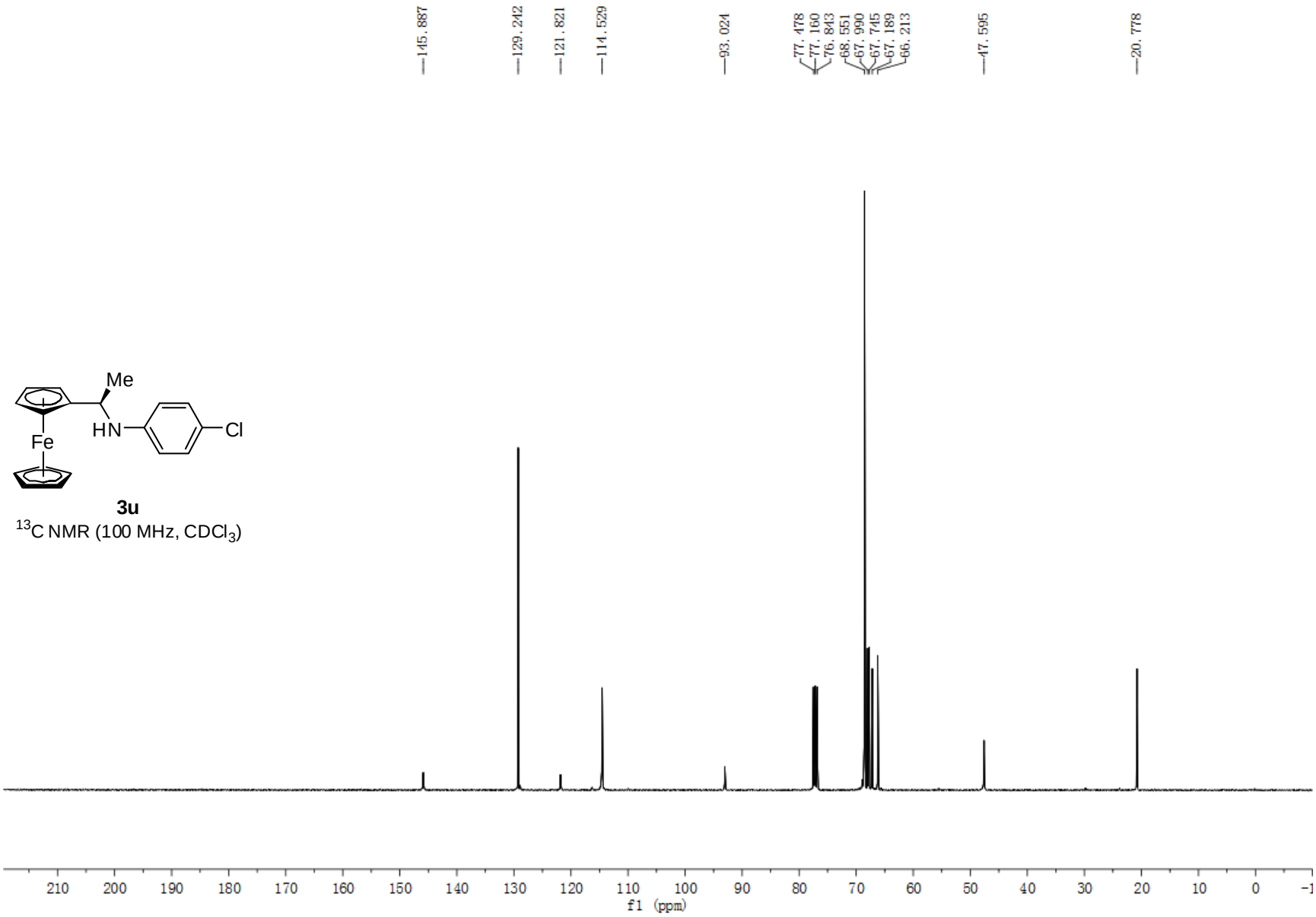
3t

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



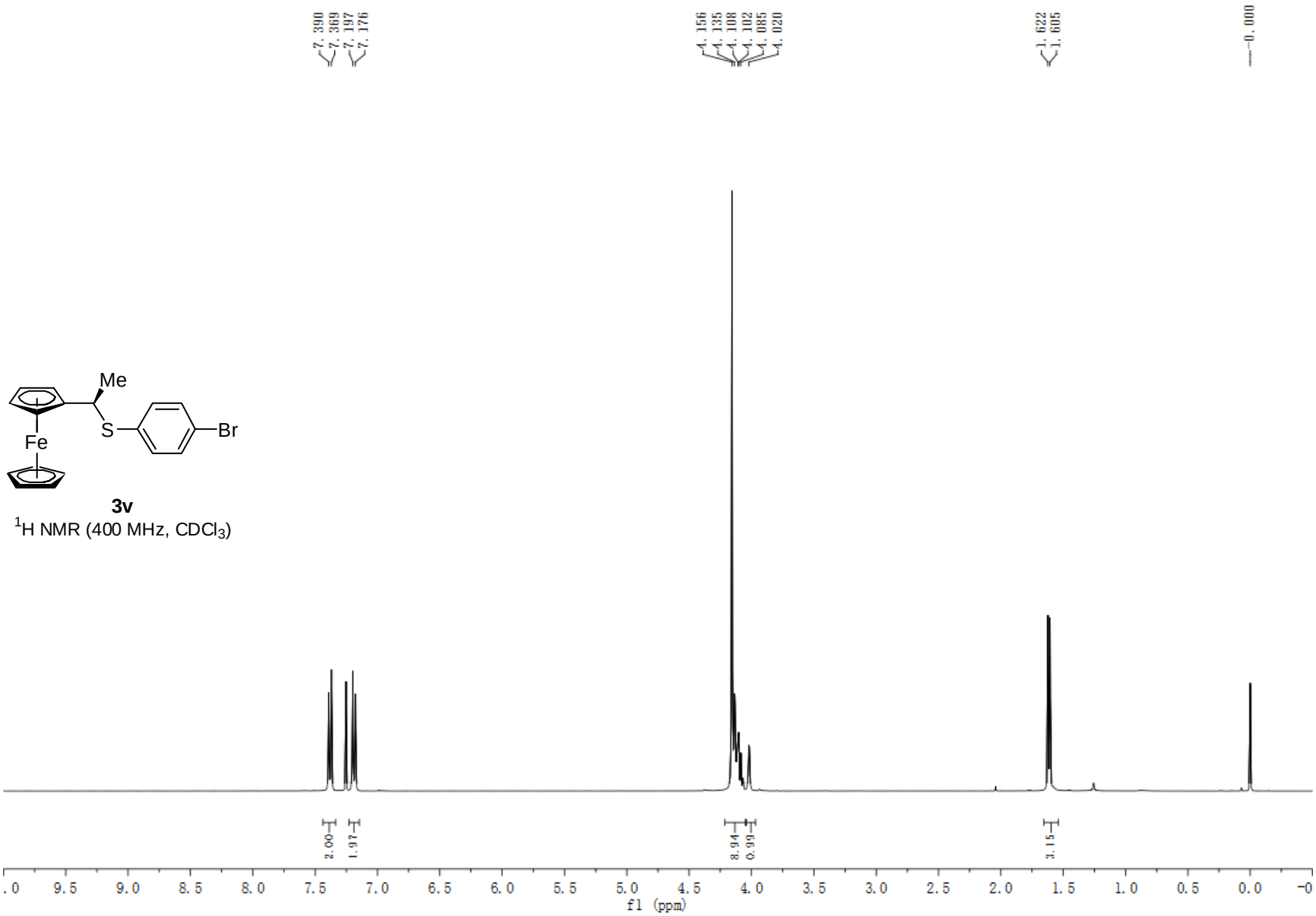
3u

^{1}H NMR (400 MHz, $CDCl_3$)



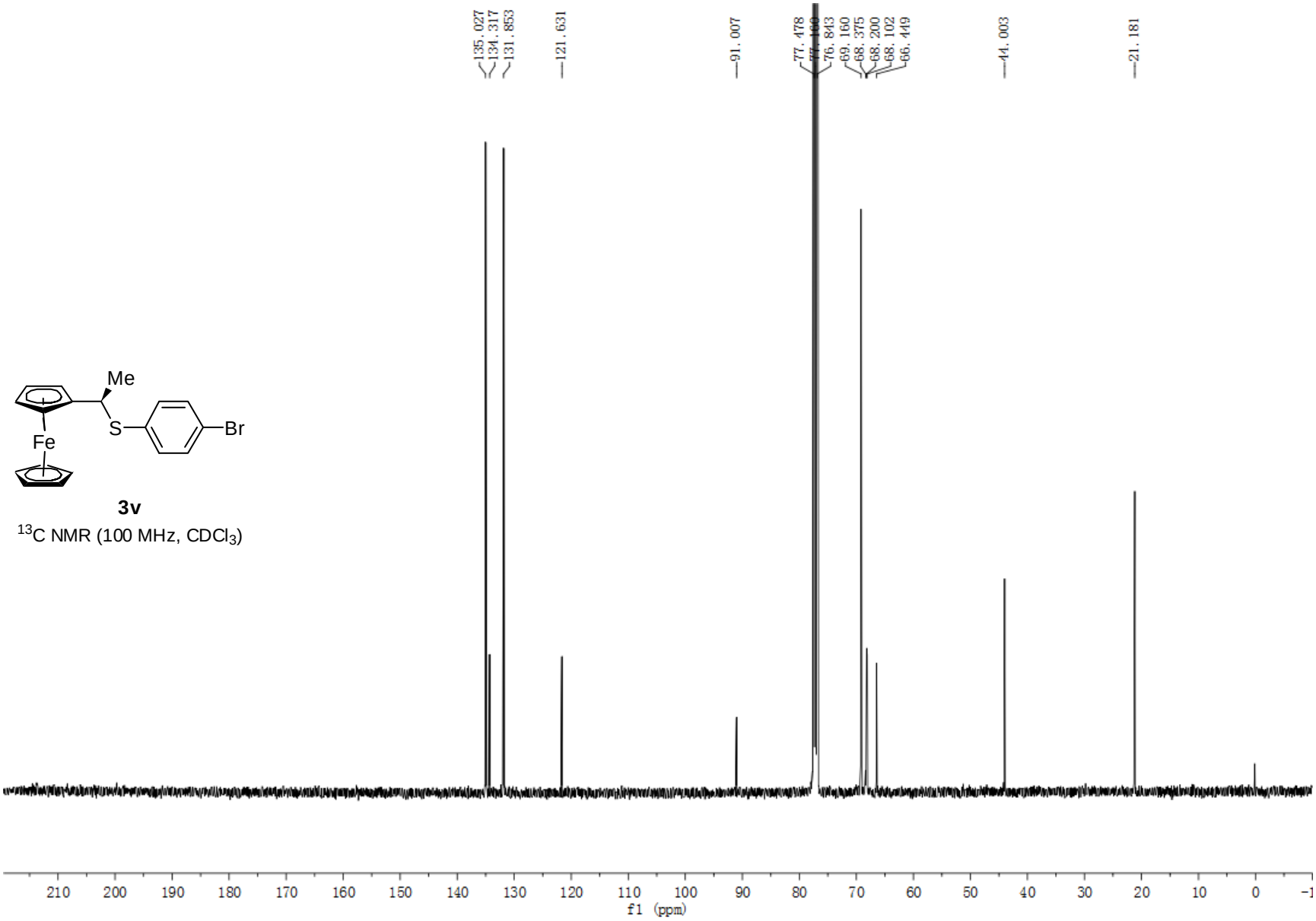
3u

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



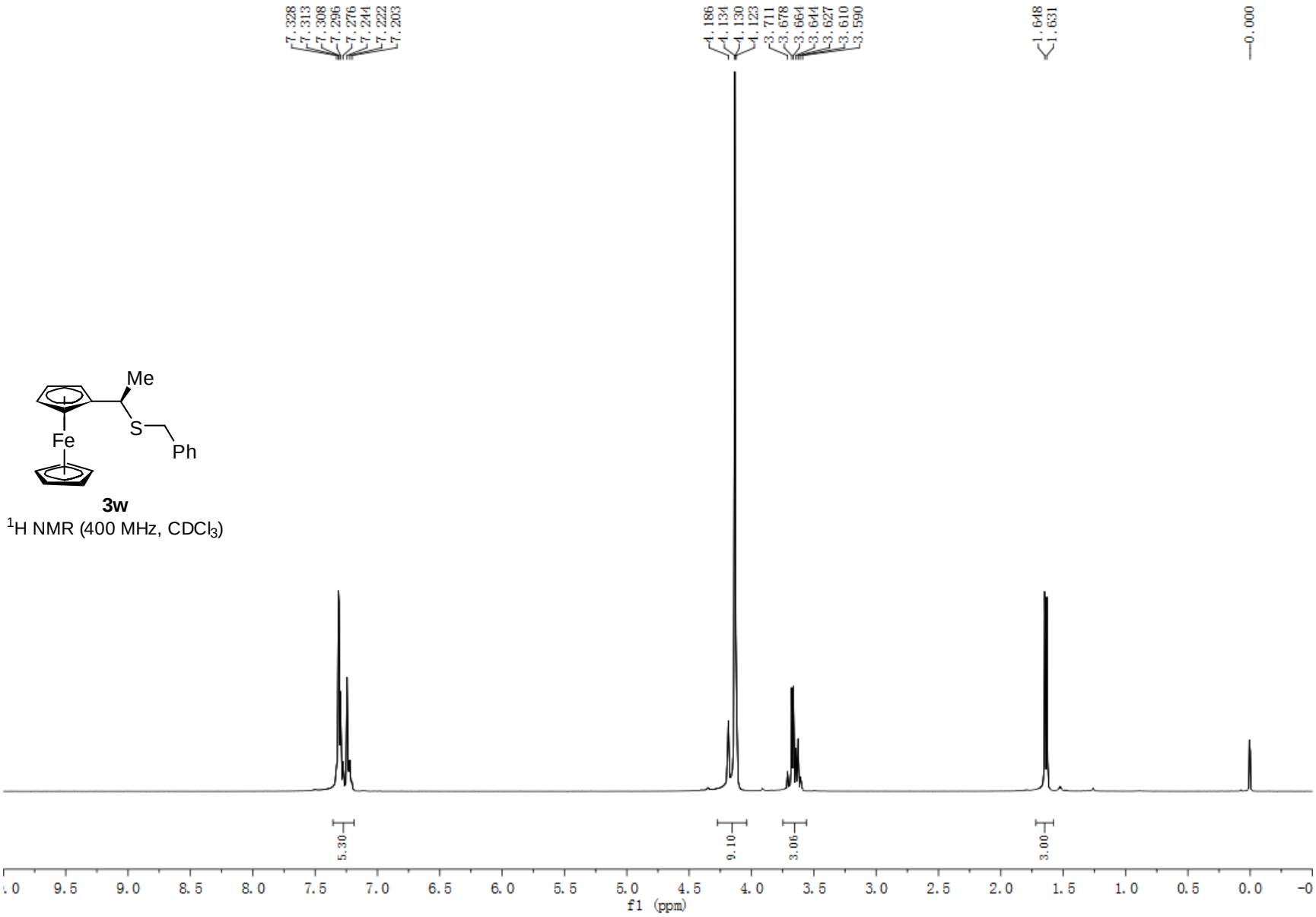
3v

^{1}H NMR (400 MHz, $CDCl_3$)



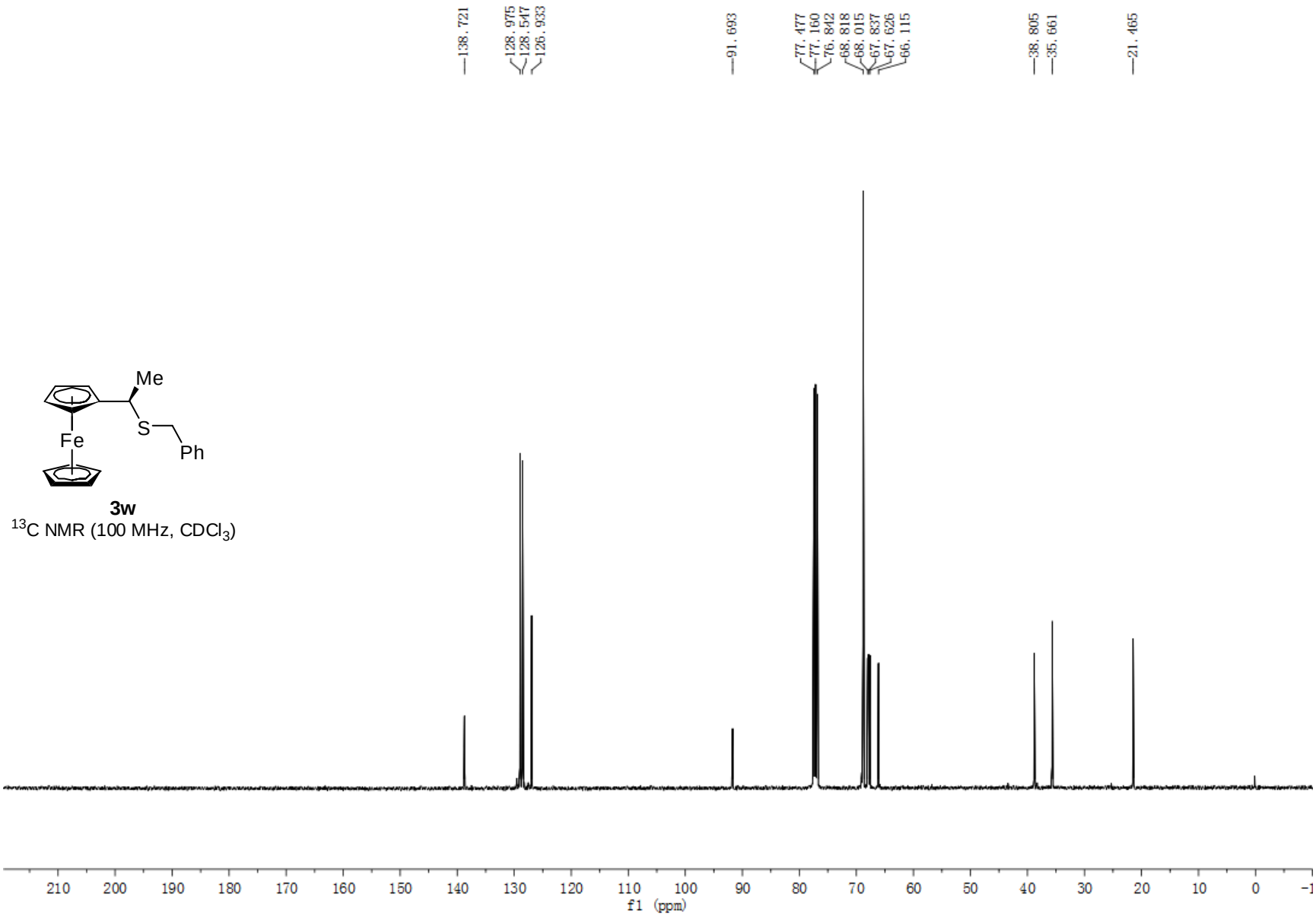
3v

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



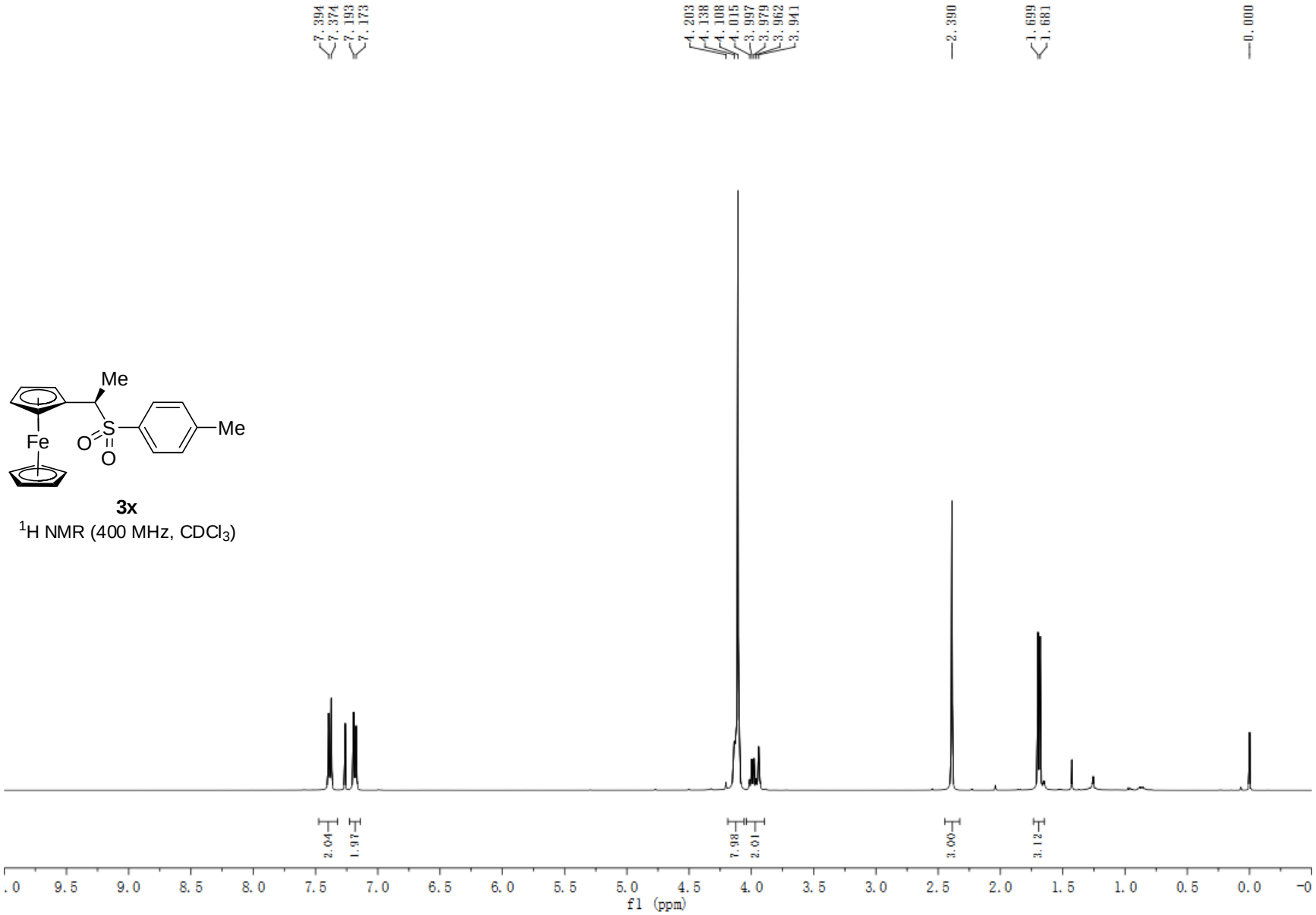
3w

^{1}H NMR (400 MHz, $CDCl_3$)



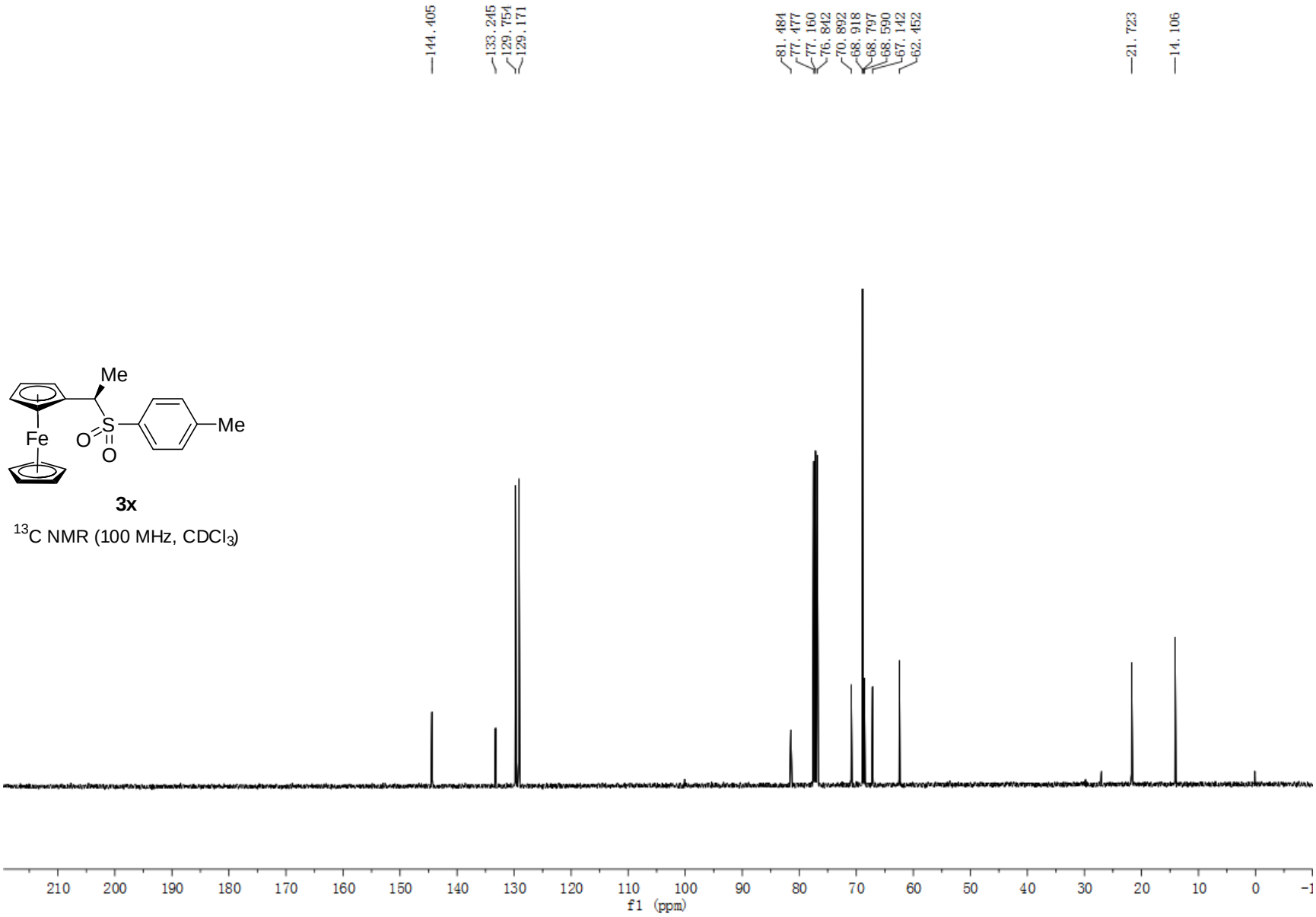
3w

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



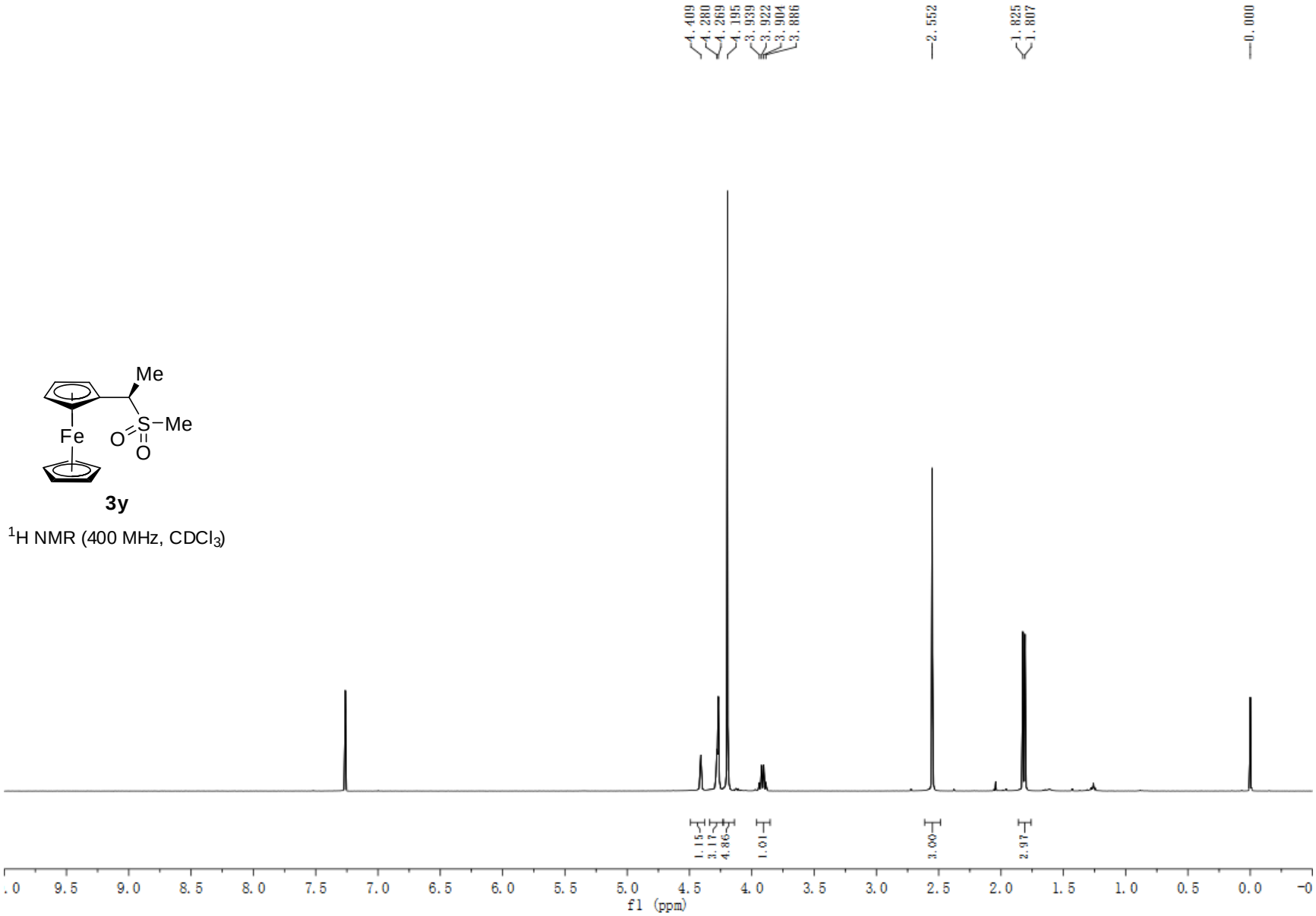
3x

^{1}H NMR (400 MHz, $CDCl_3$)



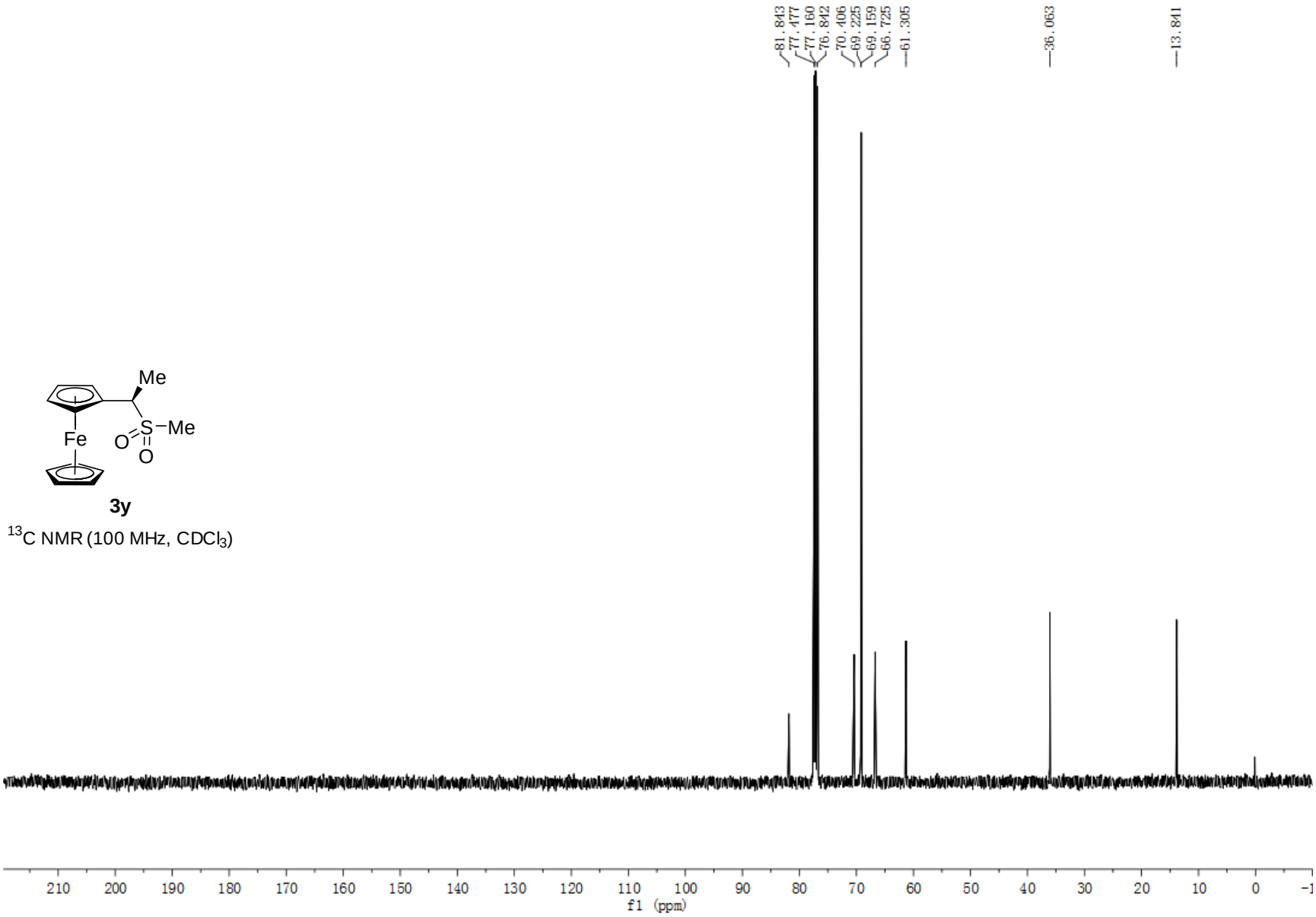
3x

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



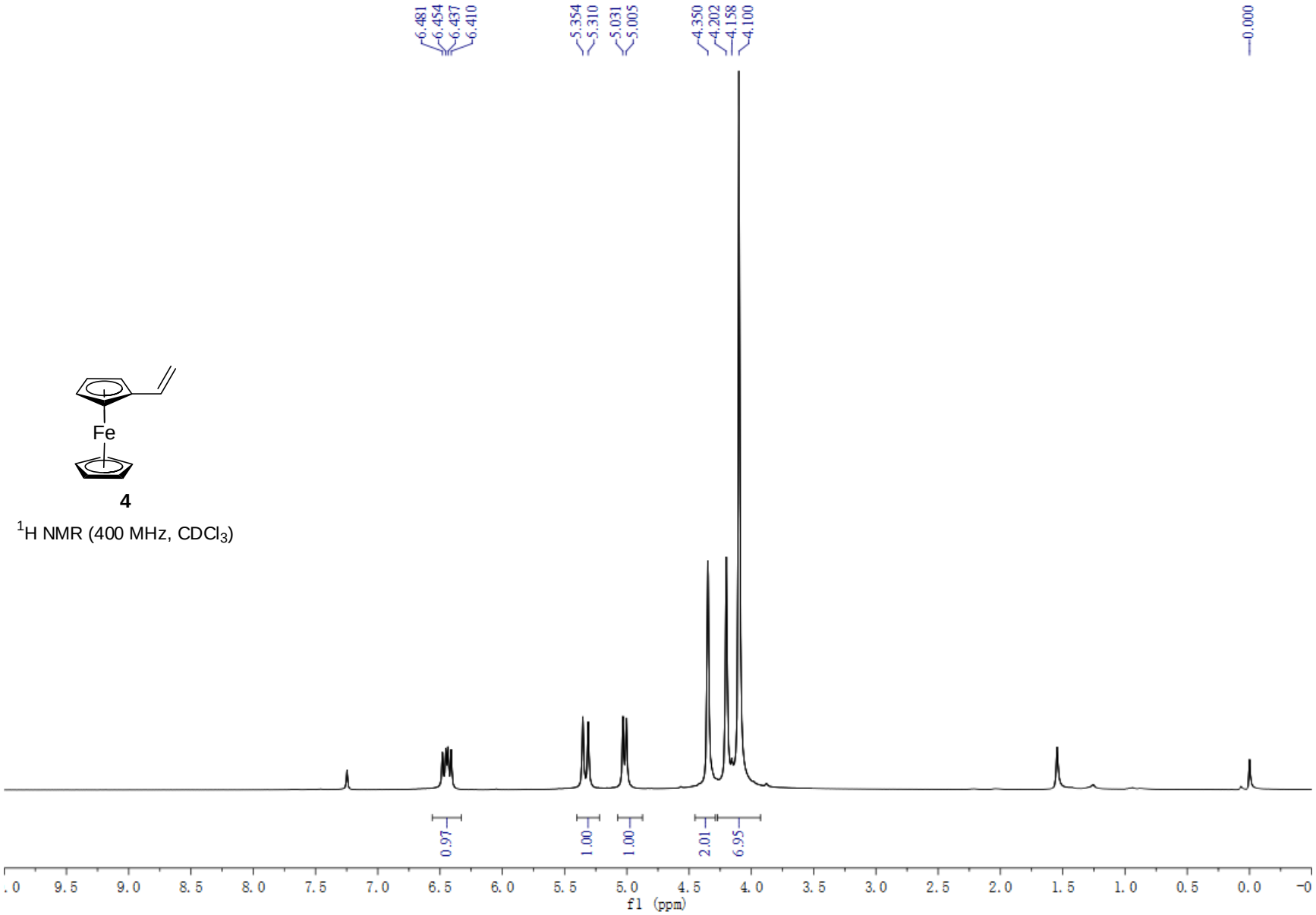
3y

^{1}H NMR (400 MHz, $CDCl_3$)



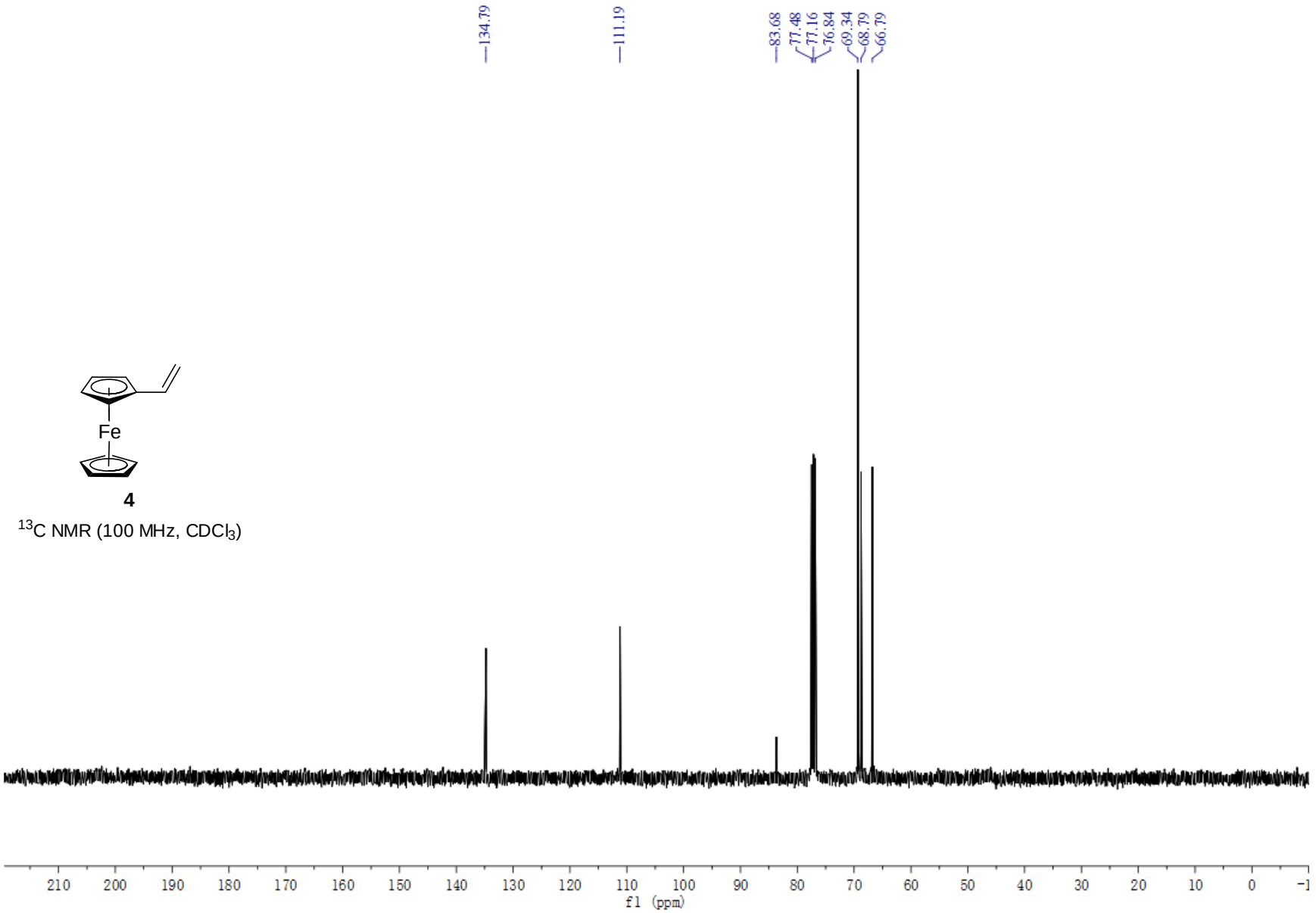
3y

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



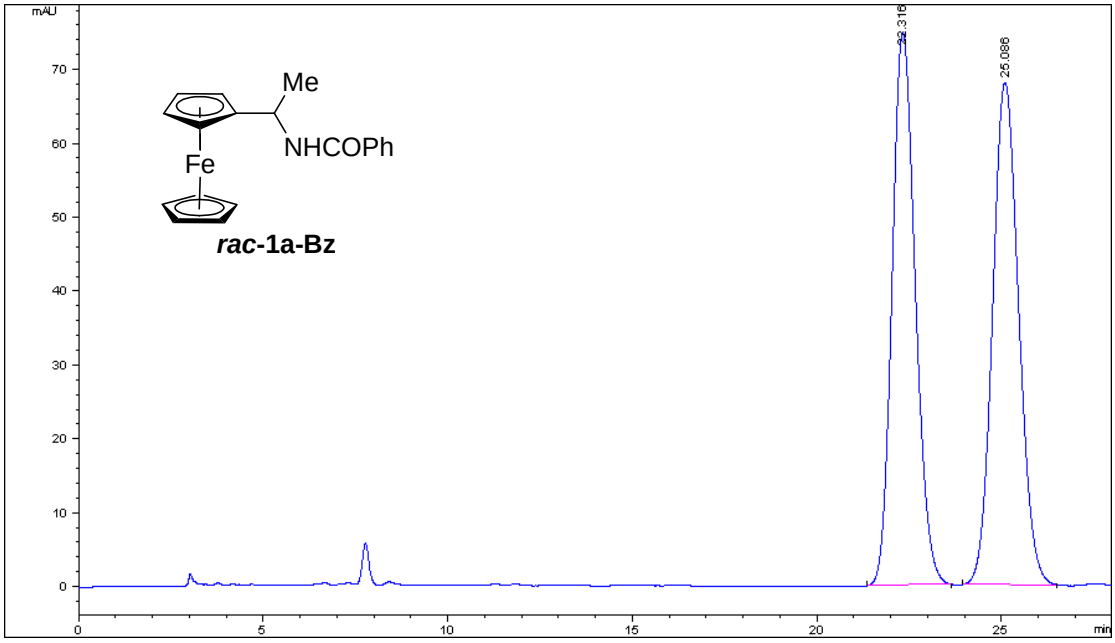
4

^{1}H NMR (400 MHz, $CDCl_3$)

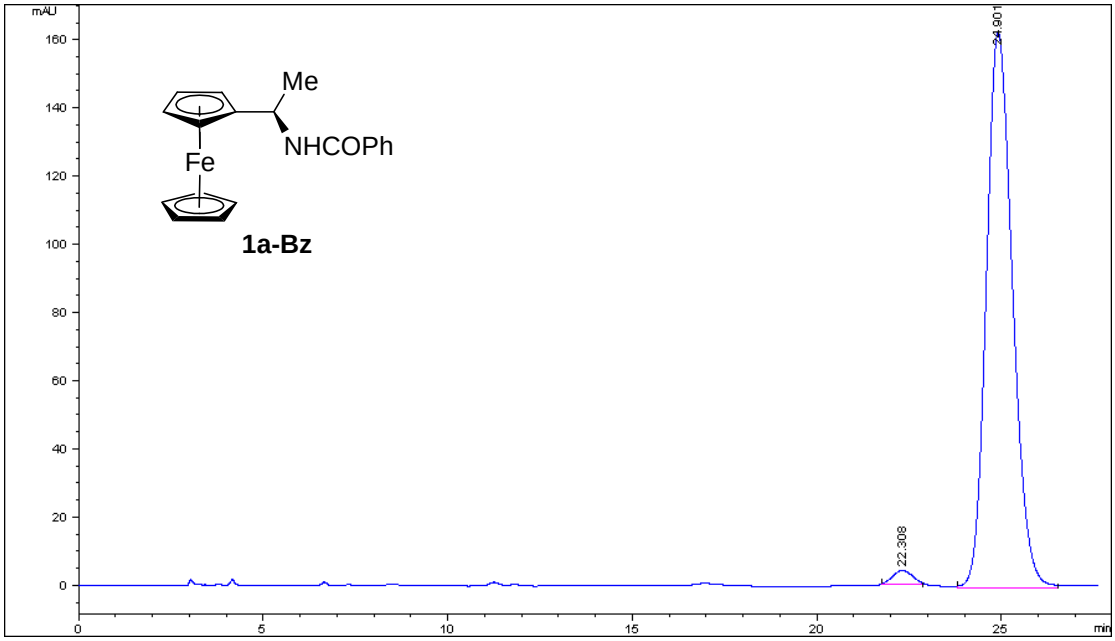


4

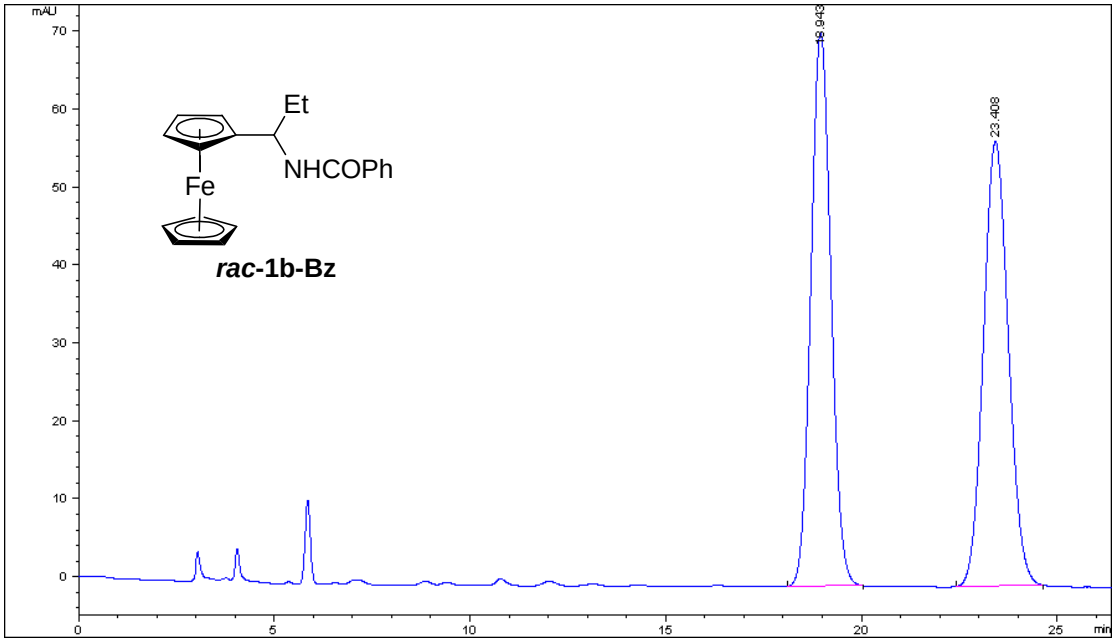
^{13}C NMR (100 MHz, $CDCl_3$)



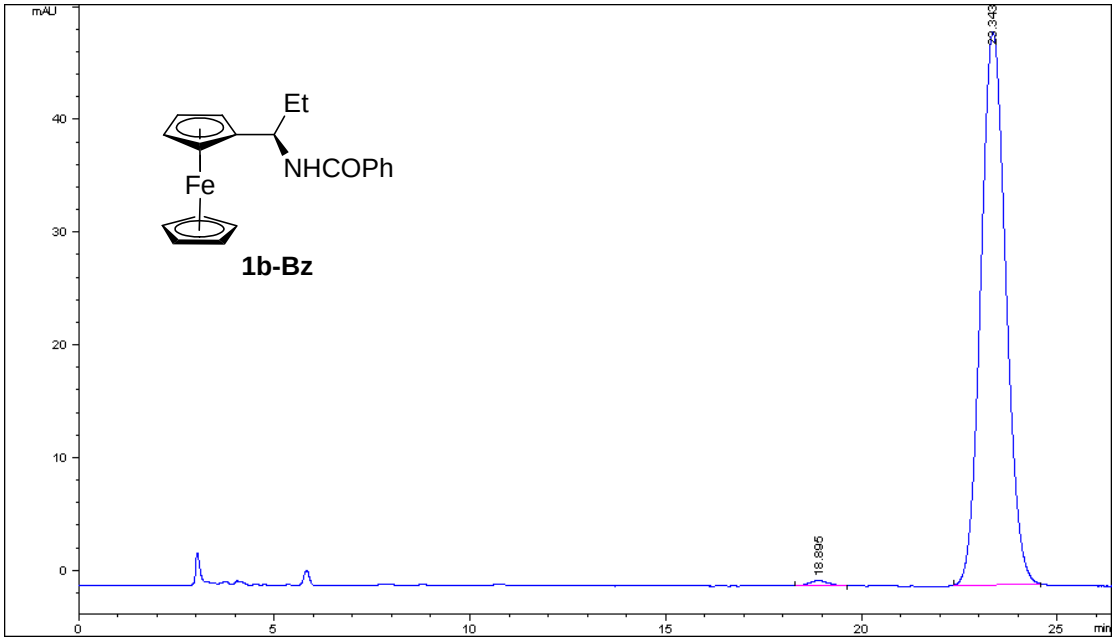
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	22.316	3270	74.9	0.6785	0.814	49.451
2	25.086	3342.6	68	0.764	0.873	50.549



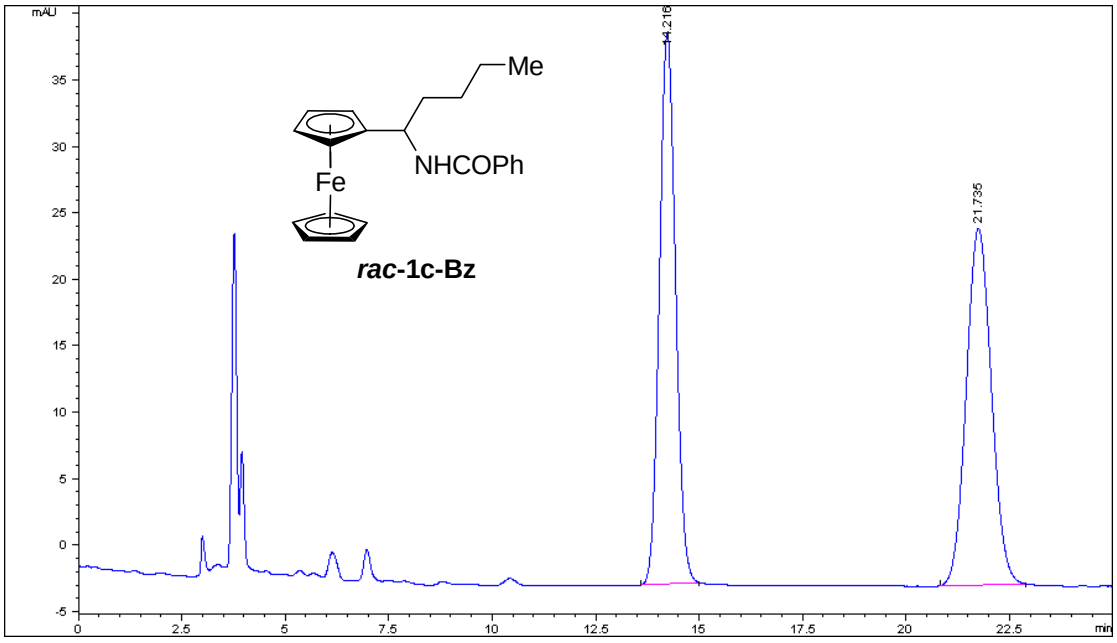
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	22.308	171.8	4.3	0.664	0.947	2.091
2	24.901	8044.1	163	0.8225	0.797	97.909



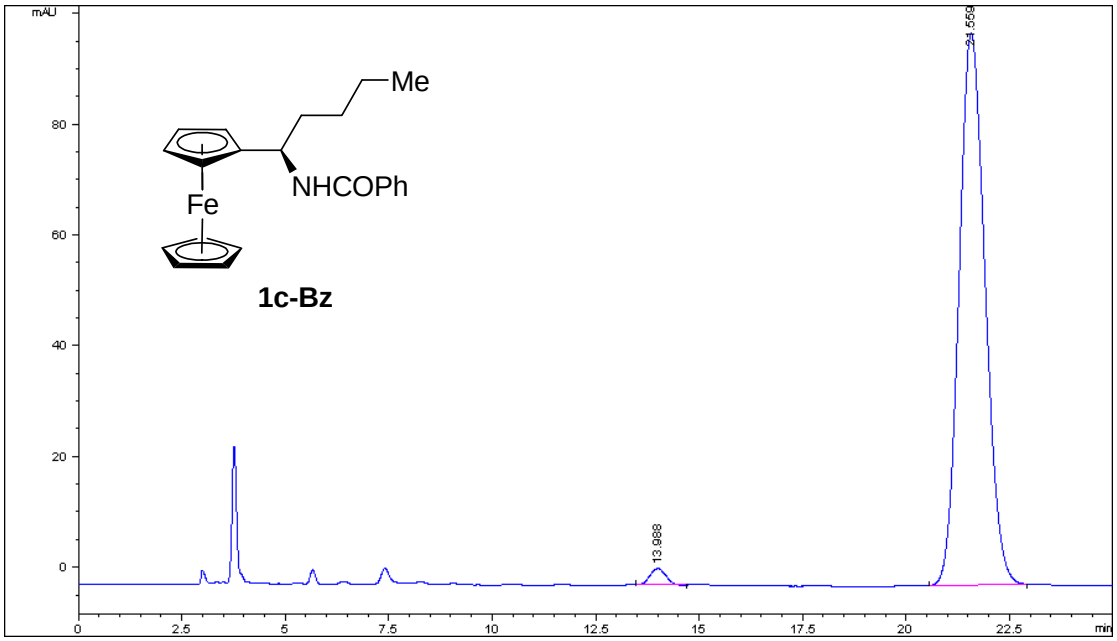
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	18.943	2537.5	71.1	0.5559	0.911	50.039
2	23.408	2533.5	57.1	0.6878	0.887	49.961



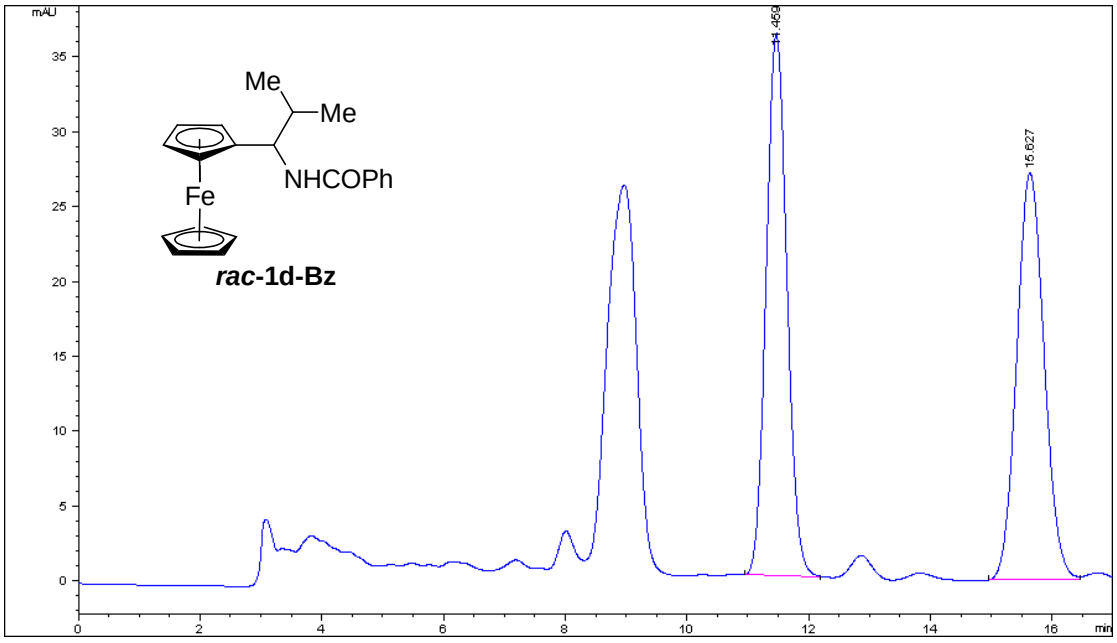
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	18.895	15.3	4.5E-1	0.5705	0.968	0.696
2	23.343	2188.8	49.1	0.6936	0.89	99.304



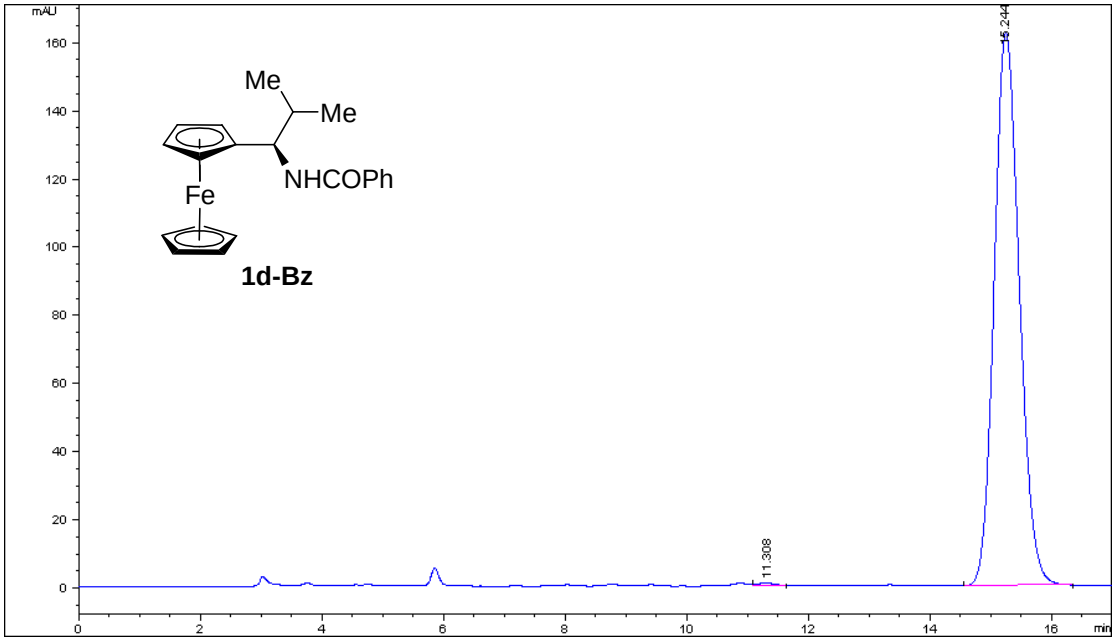
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	14.216	1128.5	41.5	0.4238	0.9	49.862
2	21.735	1134.8	26.9	0.6647	0.905	50.138



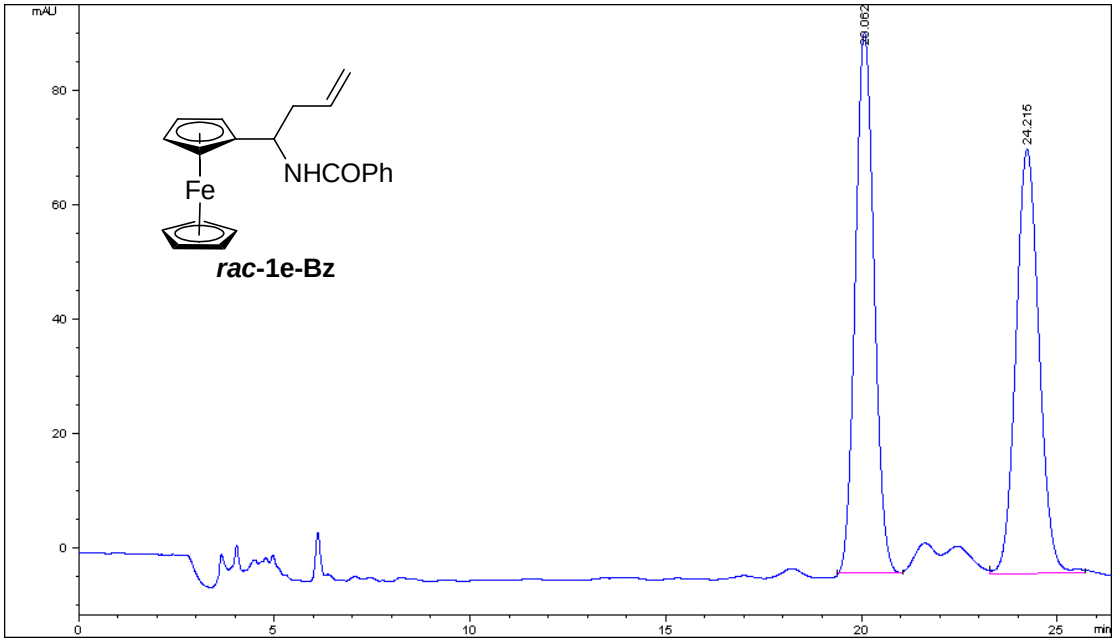
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	13.988	77.8	3	0.4086	0.969	1.751
2	21.559	4362.8	99.7	0.6882	0.83	98.249



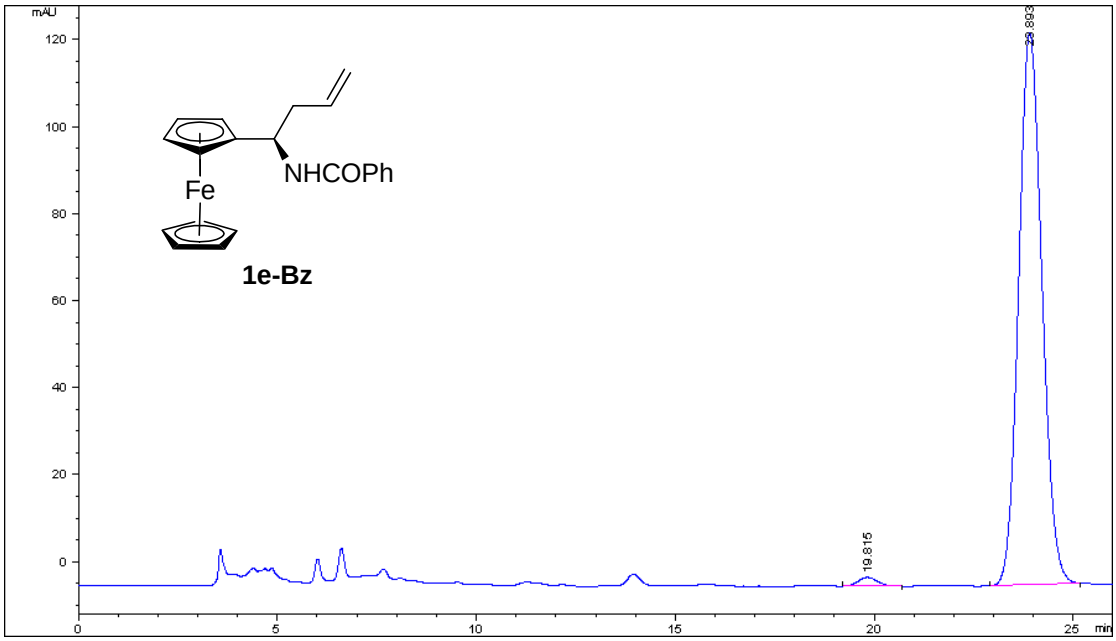
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	11.459	856.8	36.2	0.3707	0.905	50.065
2	15.627	854.6	27.2	0.4904	0.899	49.935



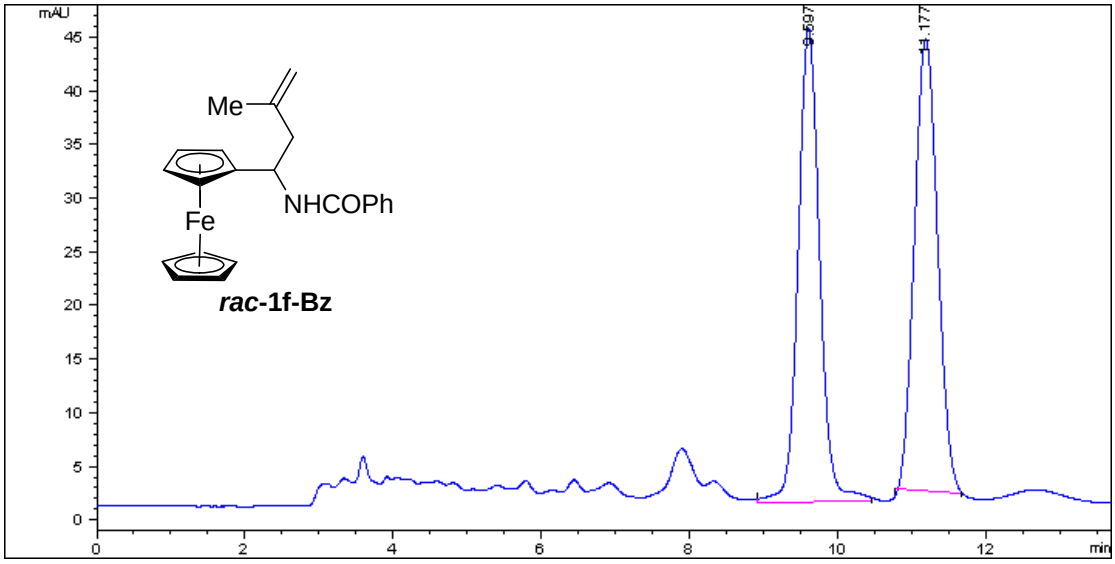
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	11.308	20.5	9.1E-1	0.3763	0.744	0.437
2	15.244	4661.9	162.3	0.4457	0.821	99.563



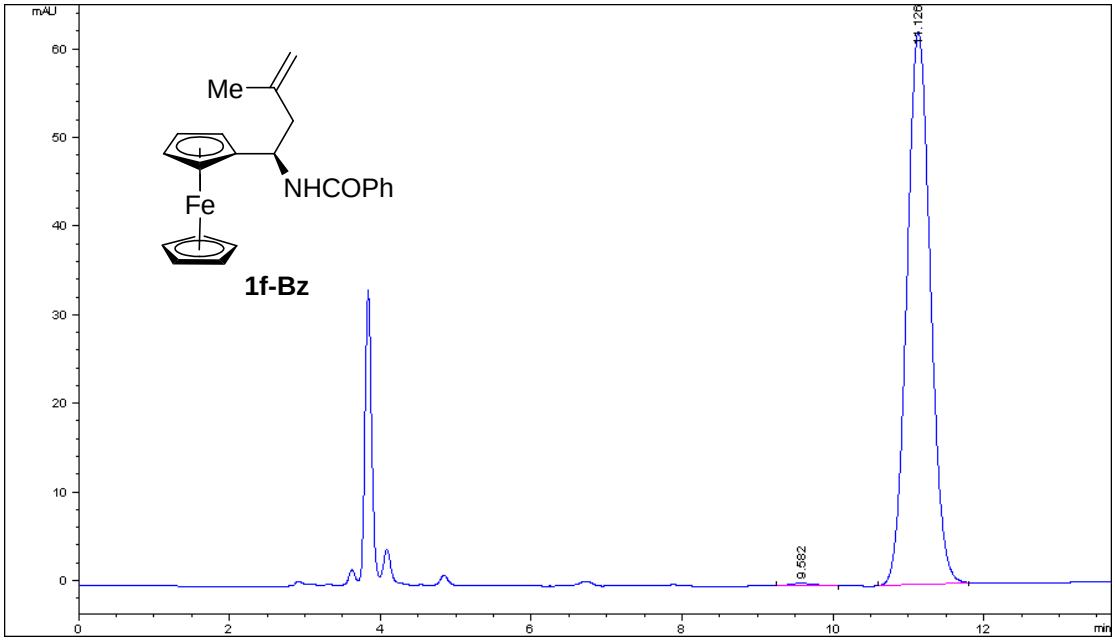
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	20.062	3157.5	94.7	0.5556	0.906	50.774
2	24.215	3061.3	74.4	0.686	0.892	49.226



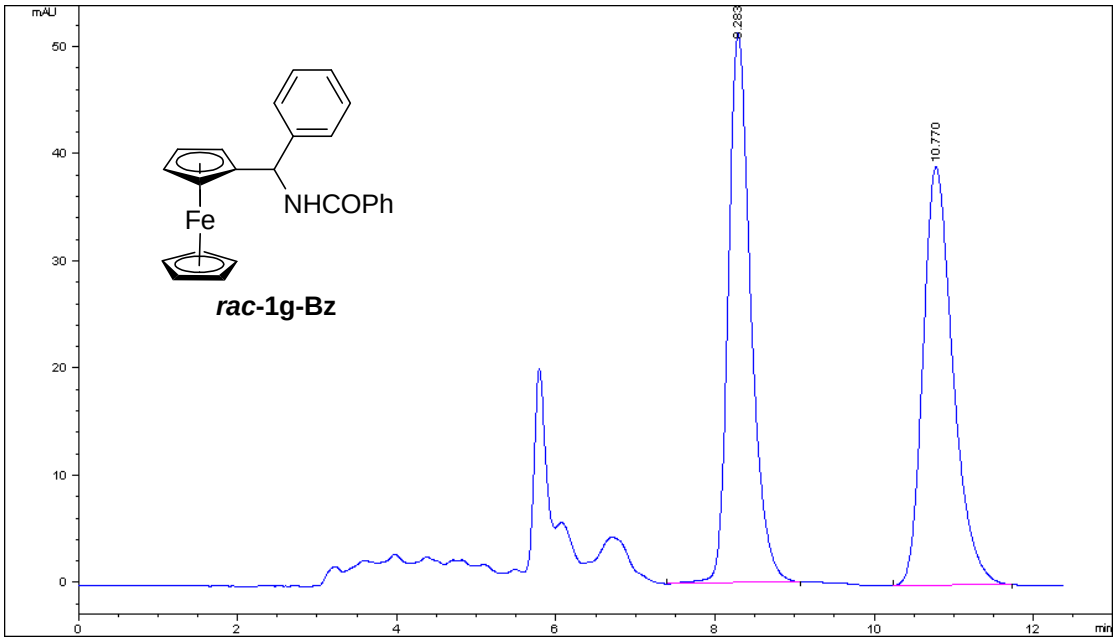
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	19.815	69	2	0.5079	0.878	1.318
2	23.893	5164.5	126.8	0.634	0.862	98.682



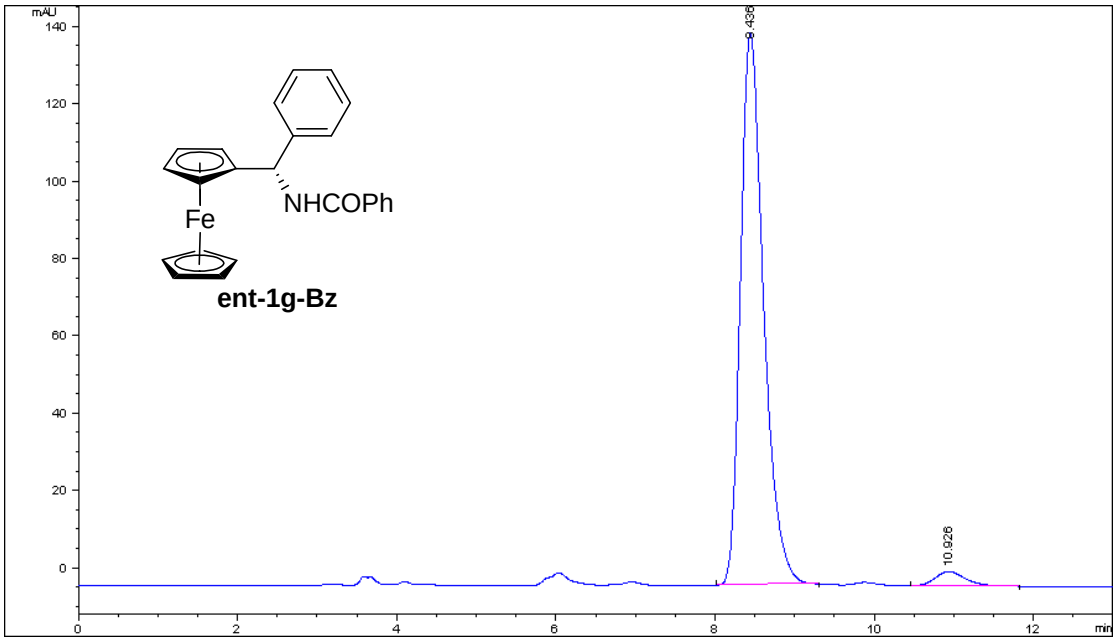
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	9.597	897.8	44.2	0.3388	0.914	49.469
2	11.177	917.1	42.2	0.3623	0.914	50.531



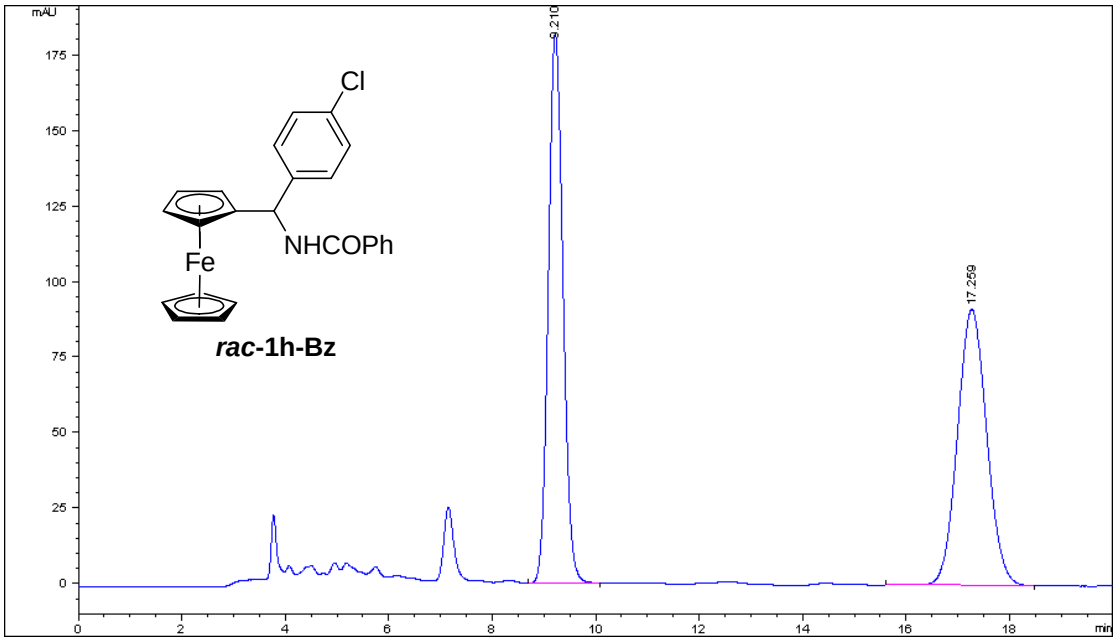
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	9.582	7	3E-1	0.3846	0.82	0.517
2	11.126	1352.3	62.4	0.3375	0.915	99.483



Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	8.283	1009.4	51.3	0.298	0.727	49.657
2	10.77	1023.4	39	0.399	0.718	50.343

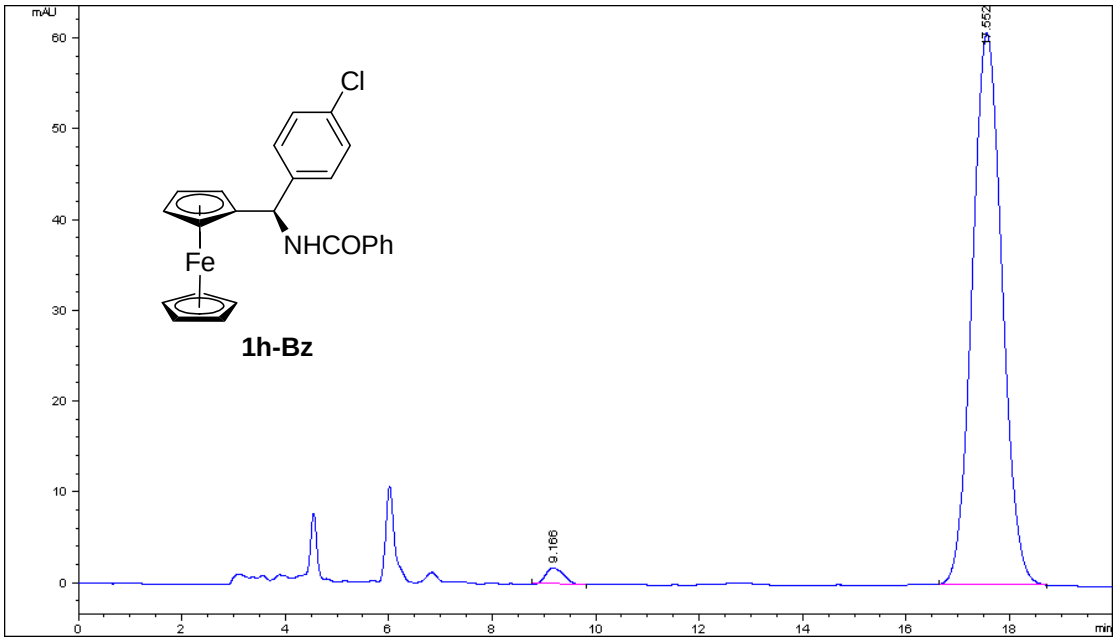


Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	8.436	2890.9	142.8	0.3076	0.684	96.753
2	10.926	97	3.7	0.403	0.756	3.247



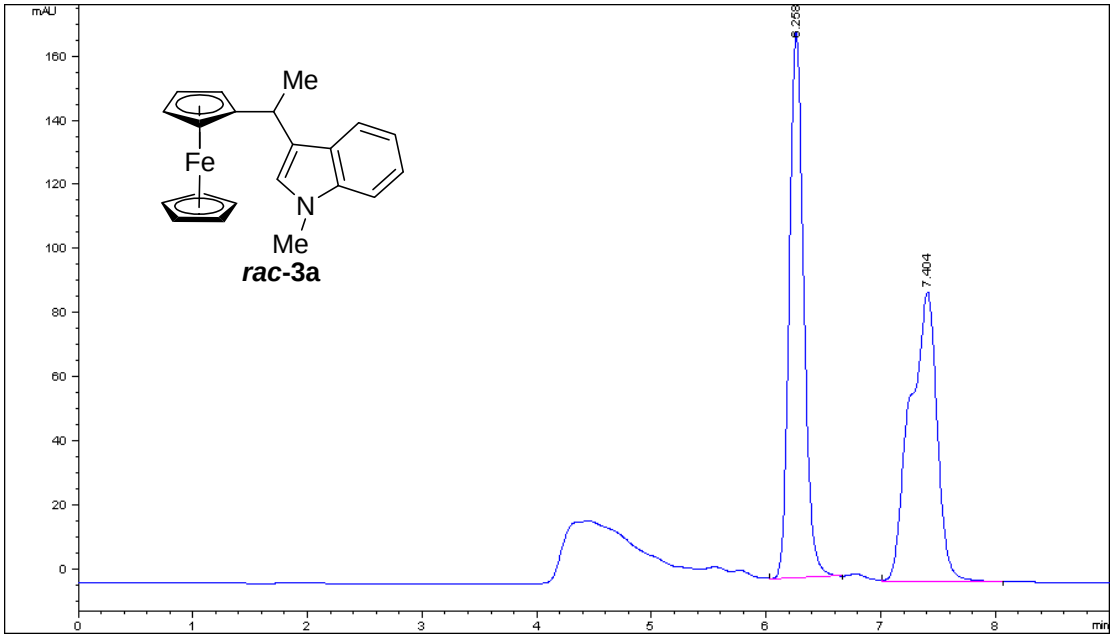
***rac*-1h-Bz**

Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	9.21	3587.9	182	0.3072	0.876	49.890
2	17.259	3603.8	91.4	0.6145	0.932	50.110

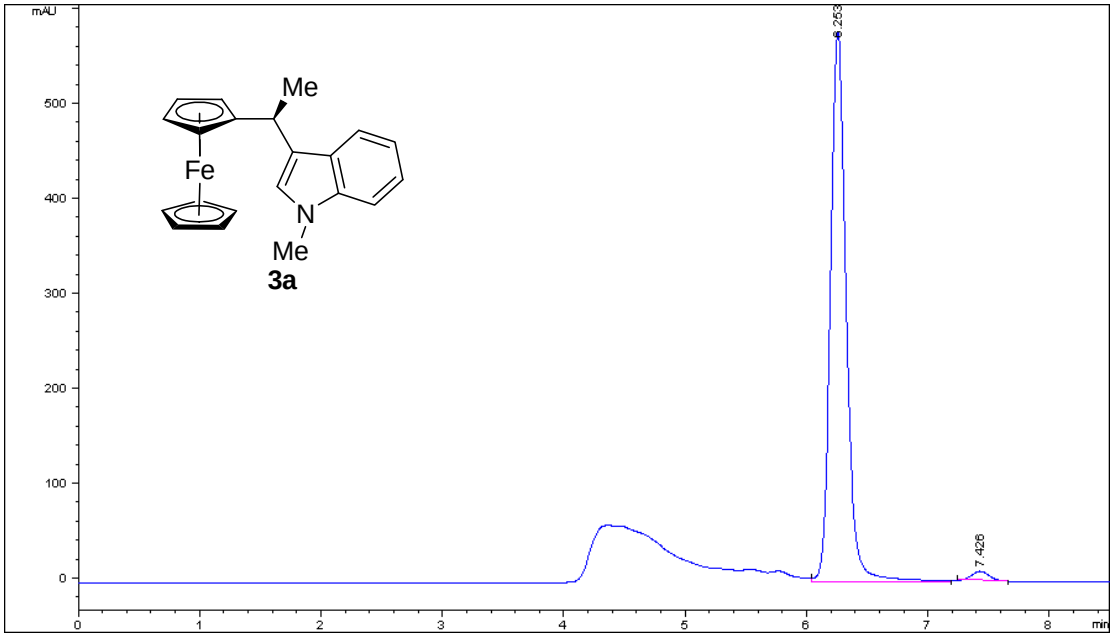


1h-Bz

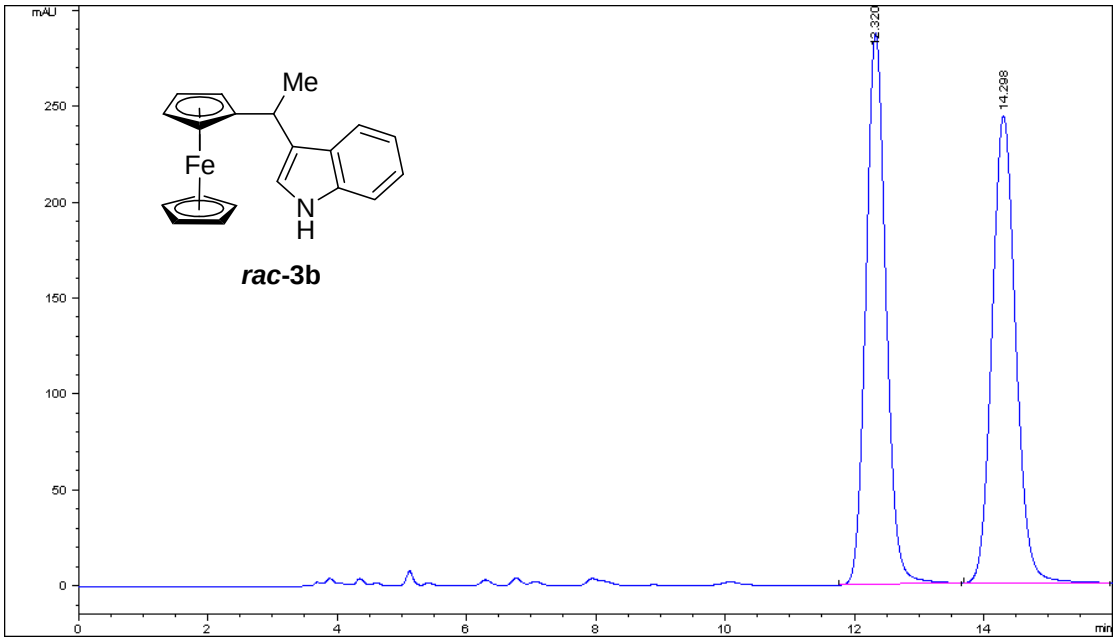
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	9.166	44.1	1.8	0.3789	0.701	1.772
2	17.552	2443.5	60.8	0.6278	0.929	98.228



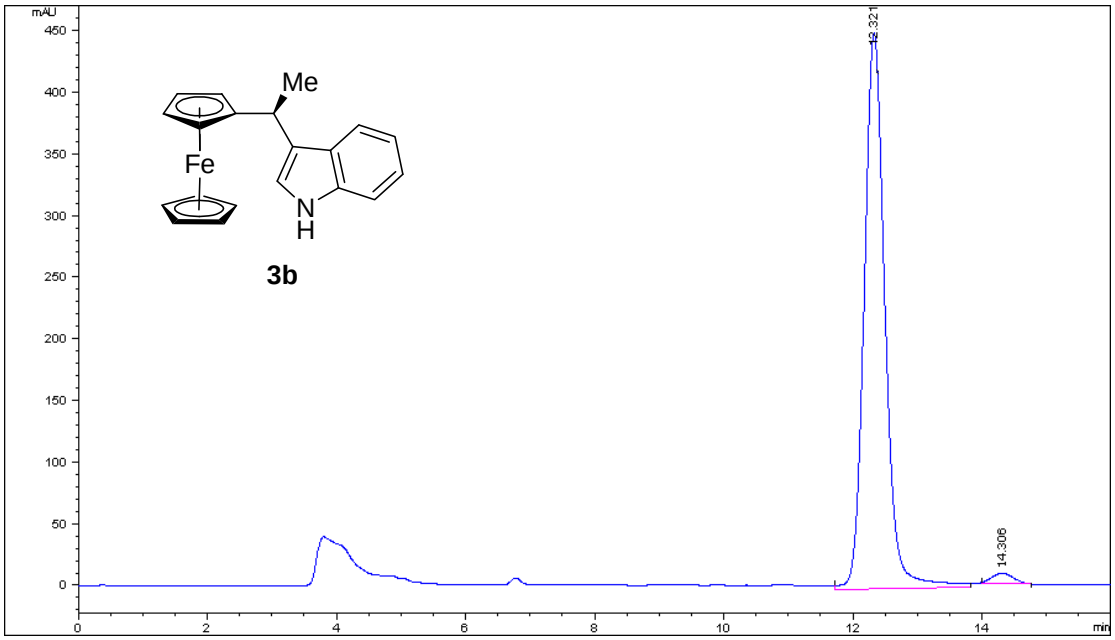
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	6.258	1492.5	170.3	0.1461	0.854	50.166
2	7.404	1482.7	90.4	0.2276	1.724	49.834



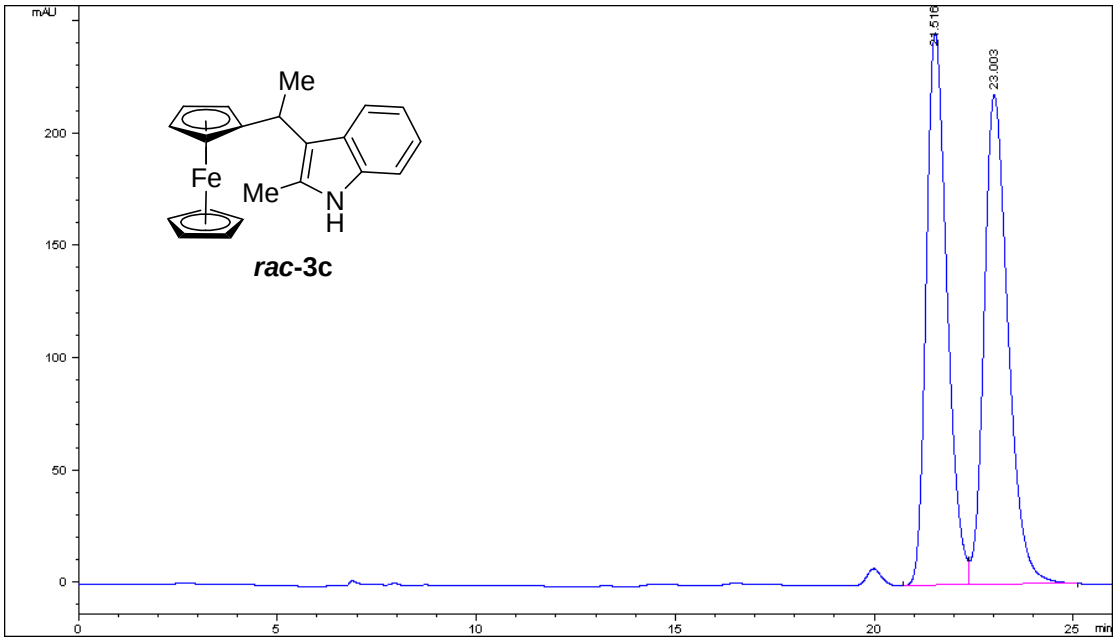
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	6.253	5259.6	579.5	0.1379	0.8	98.103
2	7.426	101.7	10	0.1693	0.92	1.897



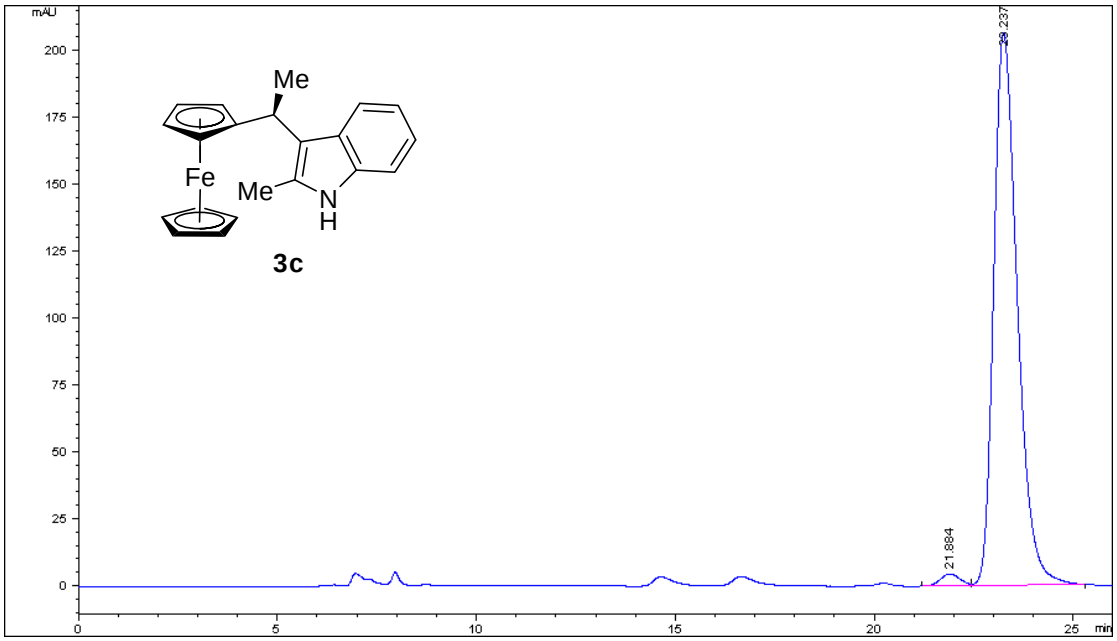
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	12.32	6218.3	287.6	0.3338	0.866	49.948
2	14.298	6231.3	244.1	0.3954	0.871	50.052



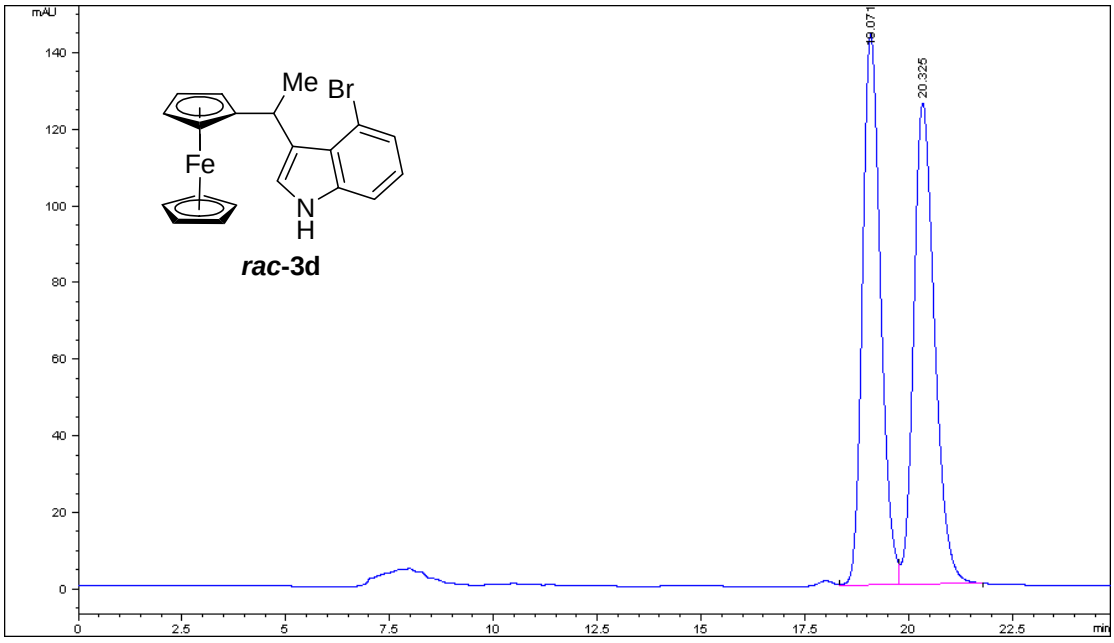
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	12.321	10172.2	451.3	0.3757	0.847	97.808
2	14.306	227.9	9.2	0.4118	0.9	2.192



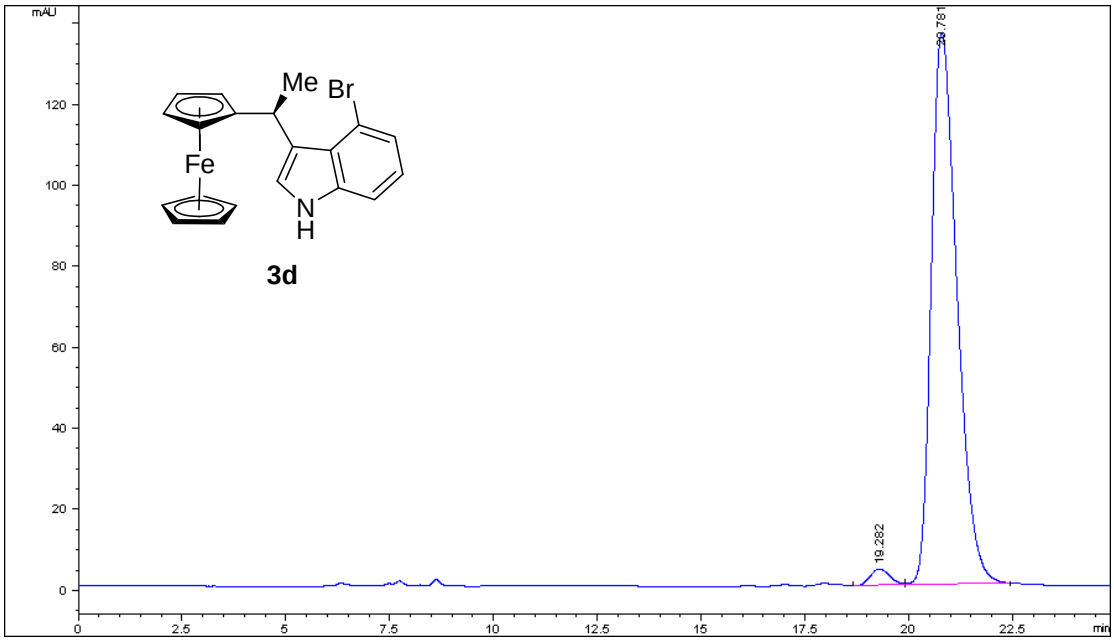
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	21.516	8923.2	245.7	0.5591	0.703	49.372
2	23.003	9150.1	218	0.6425	0.687	50.628



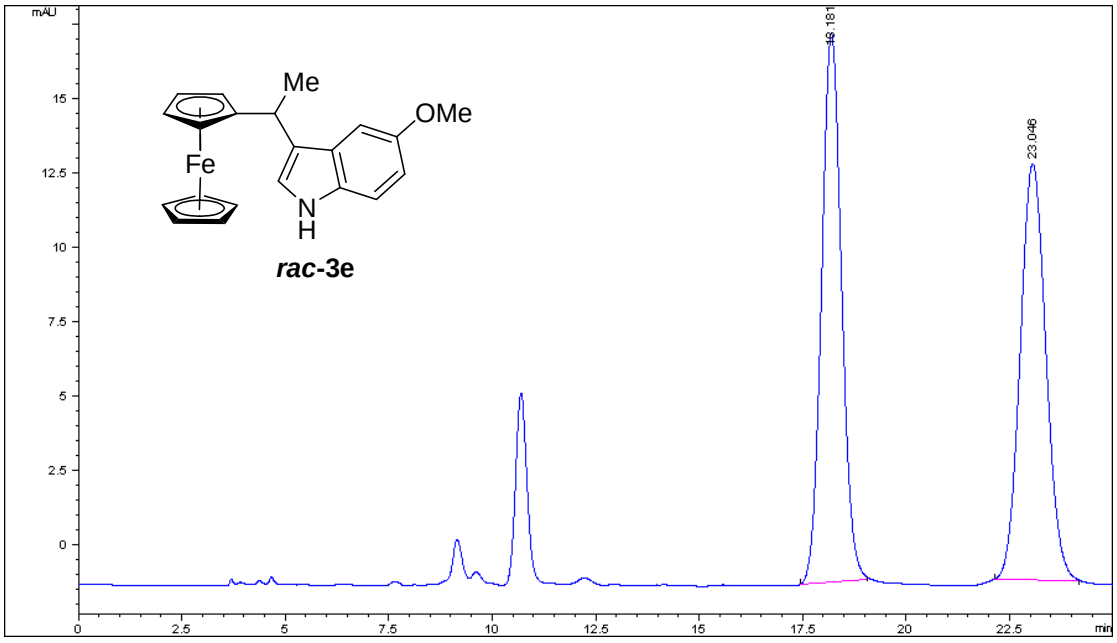
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	21.884	153.6	4.5	0.5293	0.888	1.773
2	23.237	8508.4	206.4	0.6323	0.669	98.227



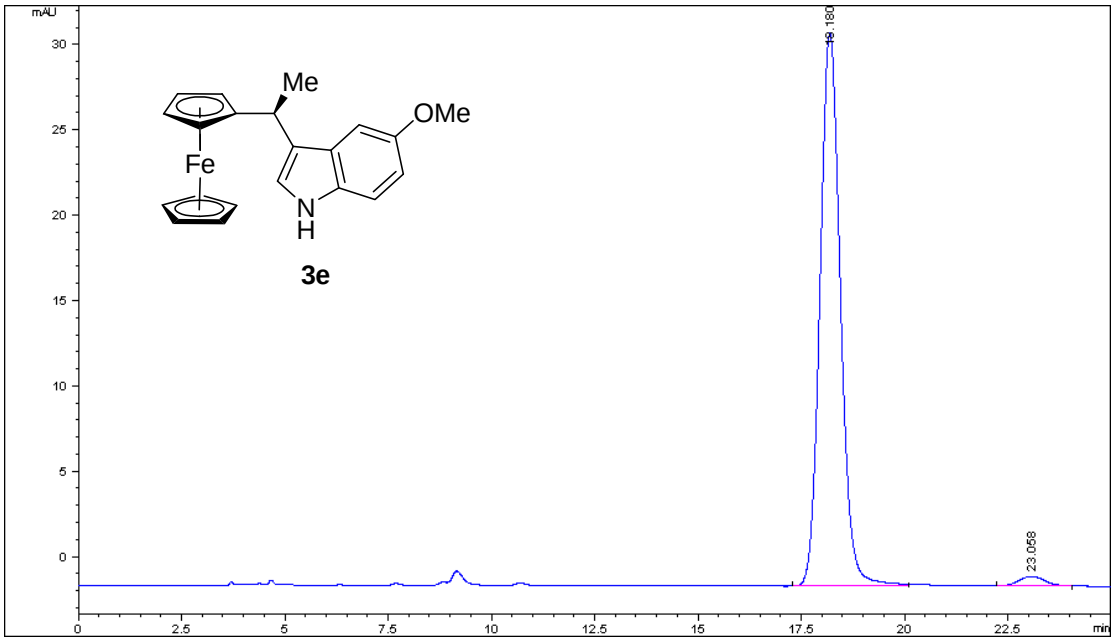
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	19.071	4382.3	144	0.4685	0.777	49.942
2	20.325	4392.4	125.6	0.5363	0.715	50.058



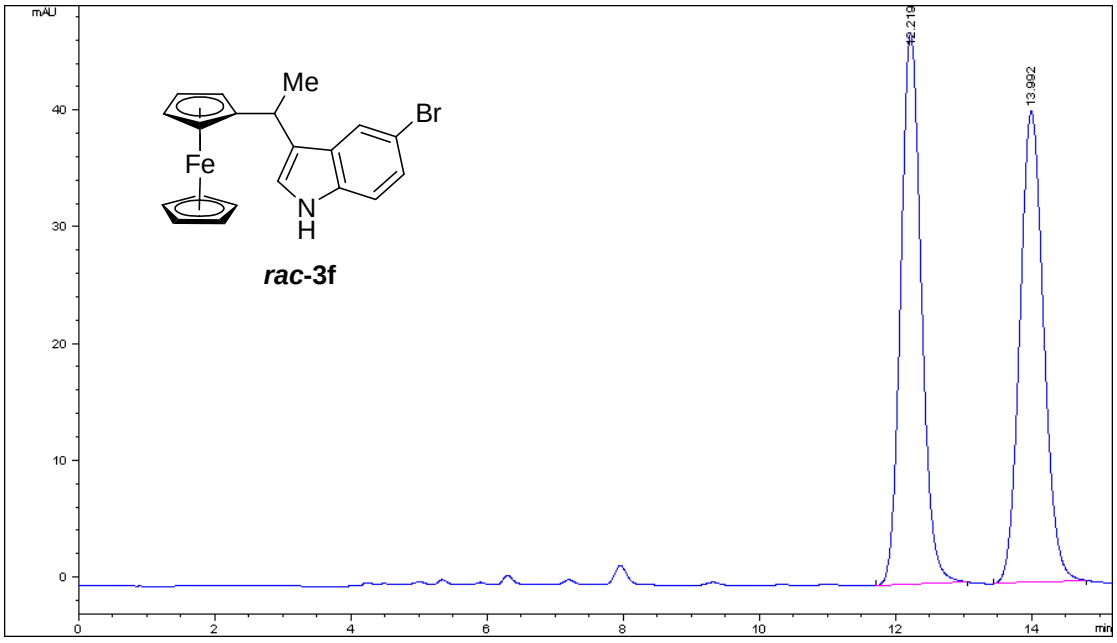
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	19.282	126.5	4	0.5275	0.977	2.112
2	20.781	5861.3	136.1	0.6656	0.638	97.888



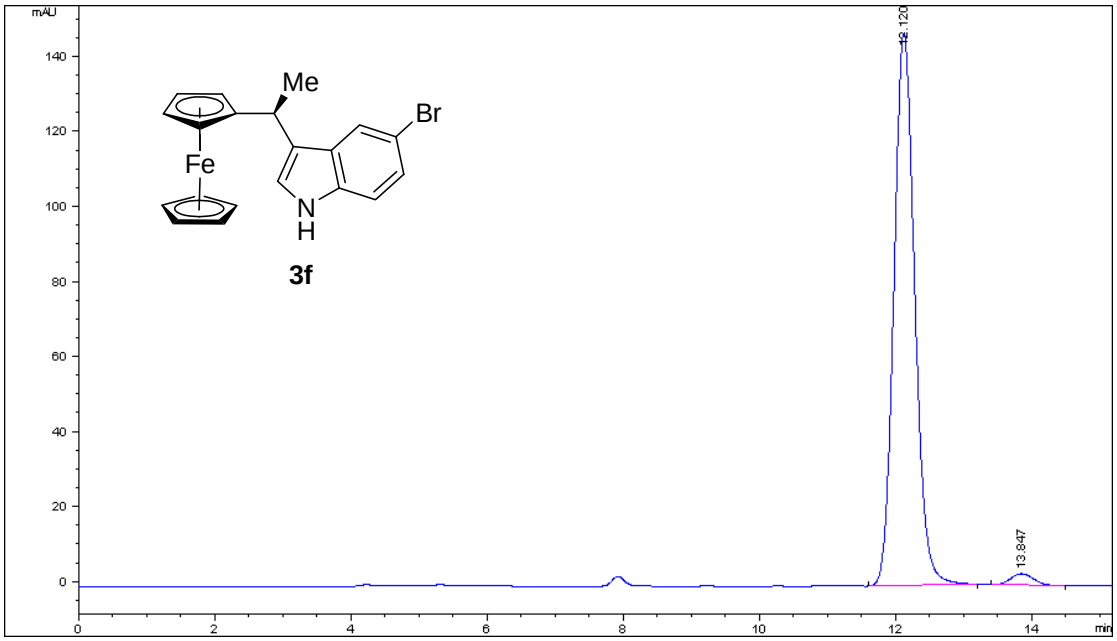
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	18.181	620	18.5	0.5169	0.917	50.487
2	23.046	608.1	14	0.6745	0.916	49.513



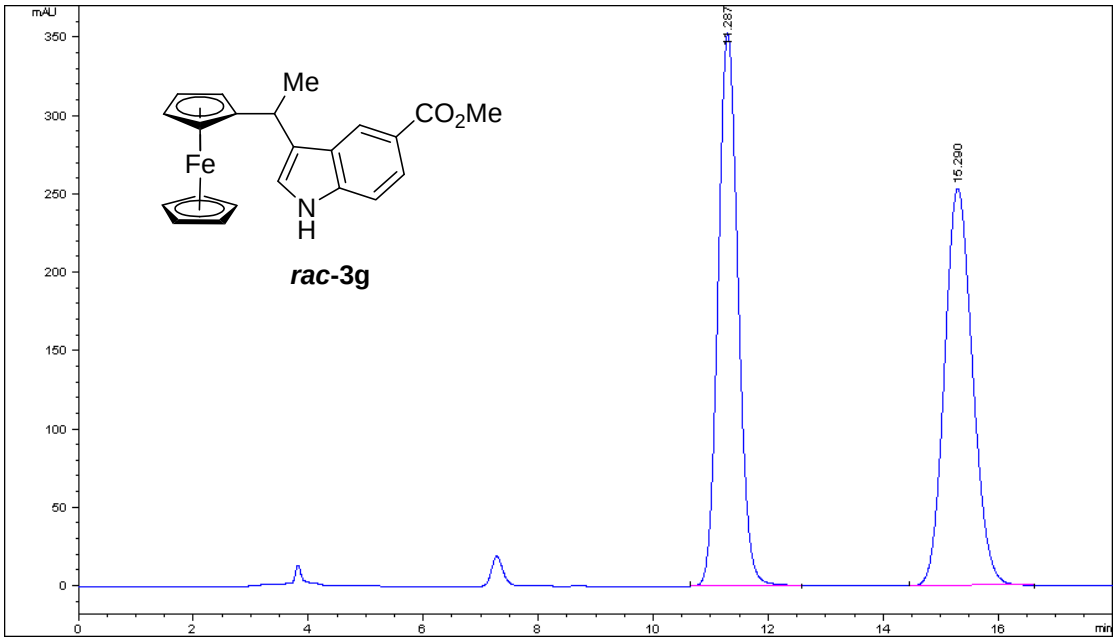
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	18.18	1114.2	32.4	0.5731	0.882	97.823
2	23.058	24.8	5.7E-1	0.7251	0.895	2.177



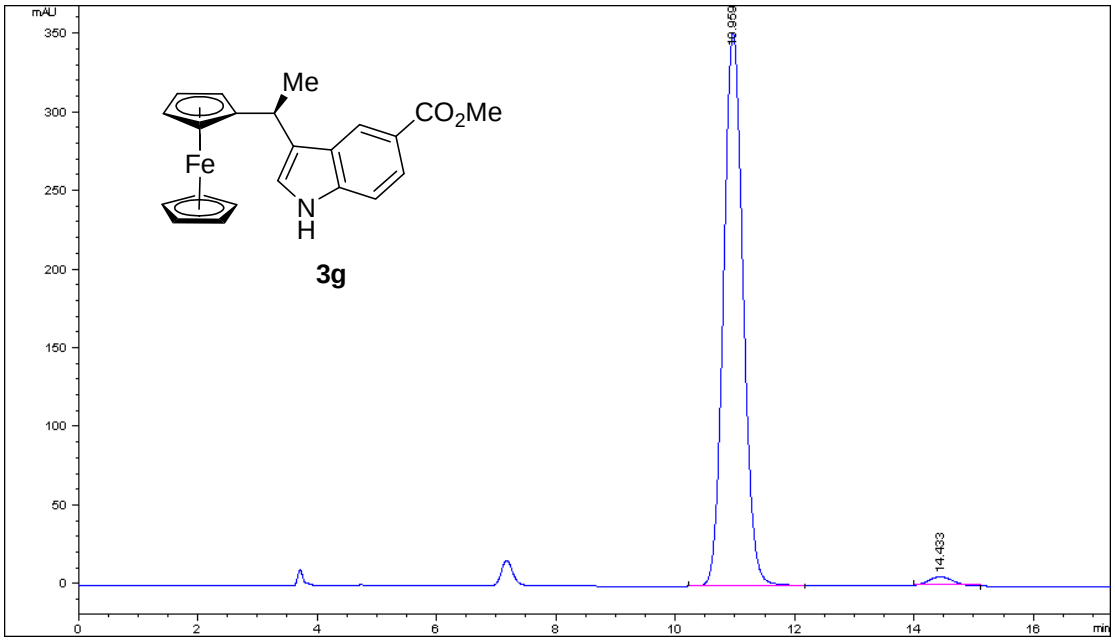
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	12.219	995.2	47.2	0.3273	0.871	50.255
2	13.992	985.1	40.4	0.3776	0.887	49.745



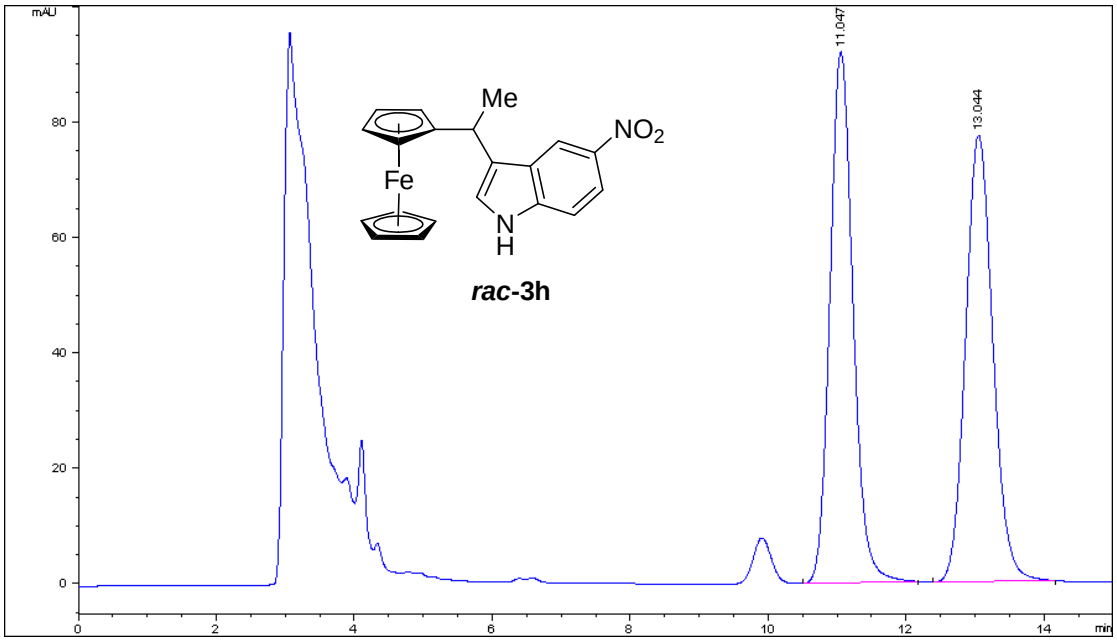
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	12.12	3129.2	147.3	0.328	0.862	97.762
2	13.847	71.6	3	0.3718	0.877	2.238



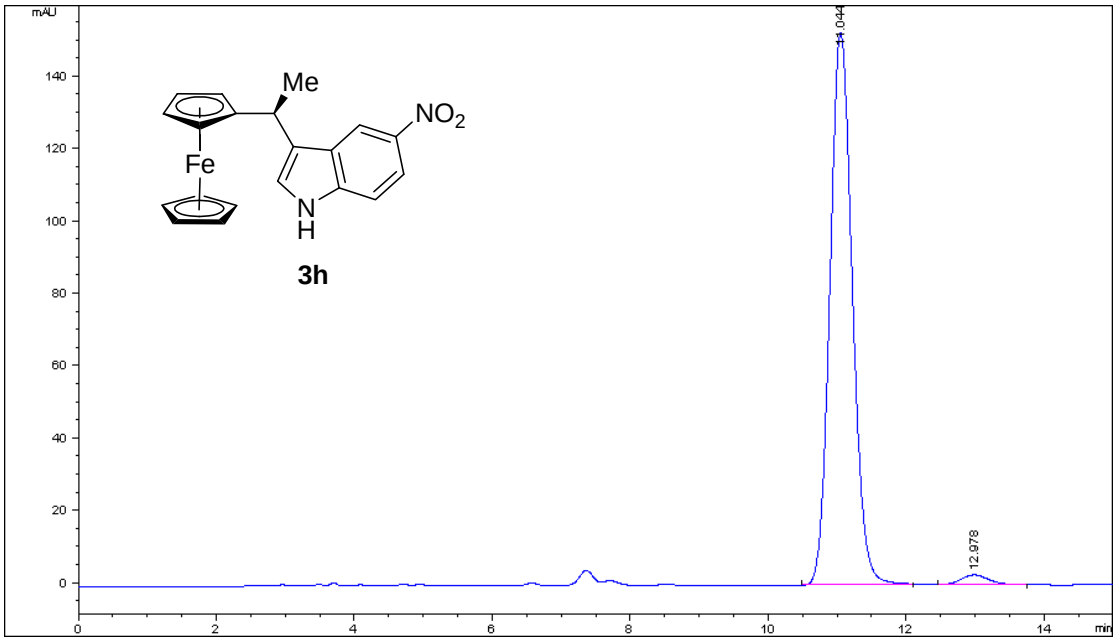
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	11.287	8529.5	352.9	0.3767	0.87	49.816
2	15.29	8592.5	253.6	0.5263	0.854	50.184



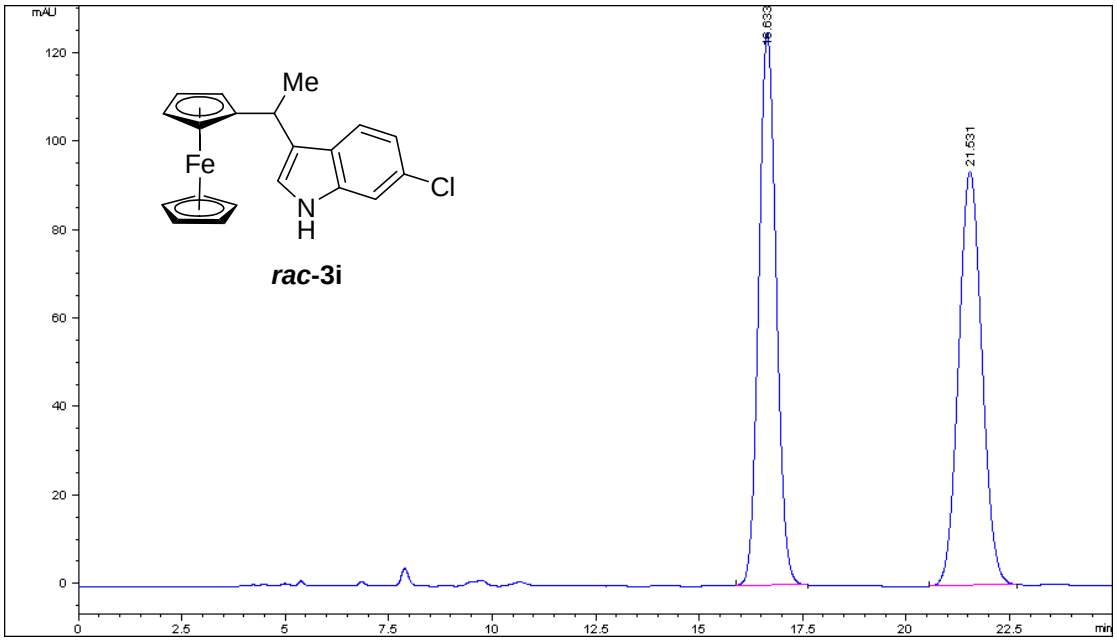
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	10.959	8012.7	351.4	0.3548	0.897	98.151
2	14.433	150.9	5.4	0.463	0.968	1.849



Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	11.047	2139.5	92	0.3601	0.844	50.136
2	13.044	2127.8	77.3	0.4258	0.866	49.864

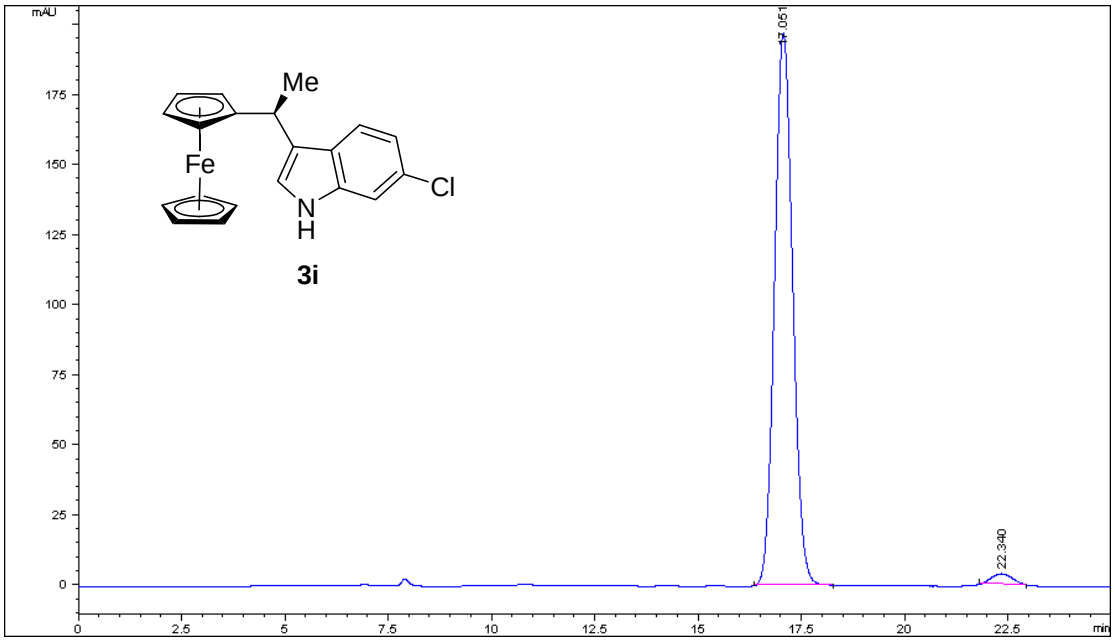


Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	11.044	3442.2	152.5	0.3506	0.864	97.889
2	12.978	74.2	2.7	0.4312	0.848	2.111



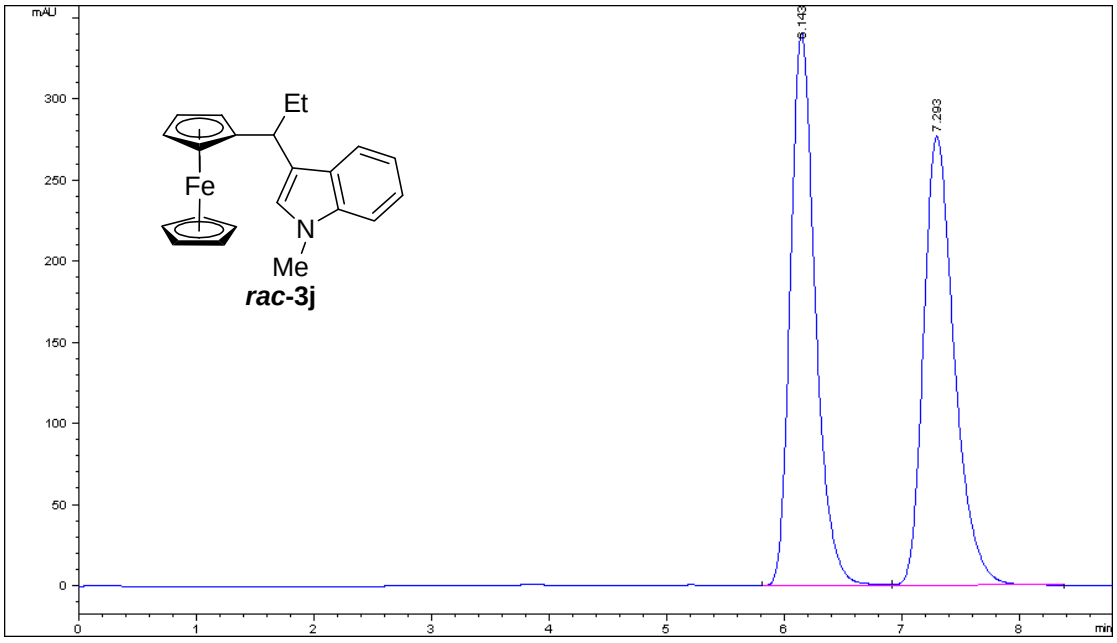
***rac*-3i**

Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	16.633	3662.6	124.8	0.4589	0.904	49.953
2	21.531	3669.5	93.6	0.609	0.917	50.047

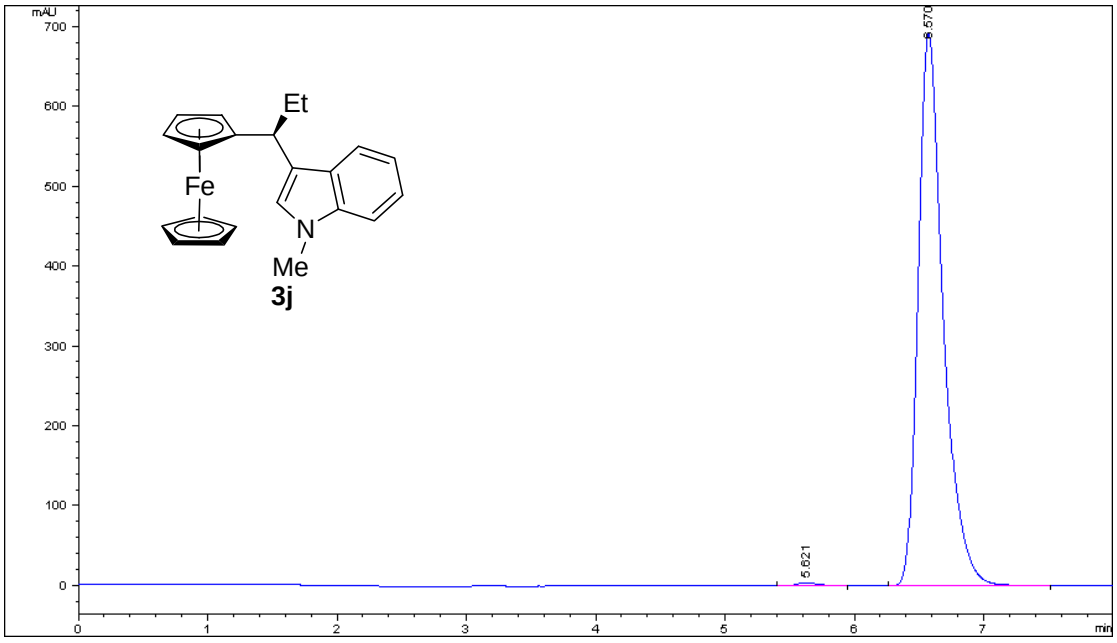


3i

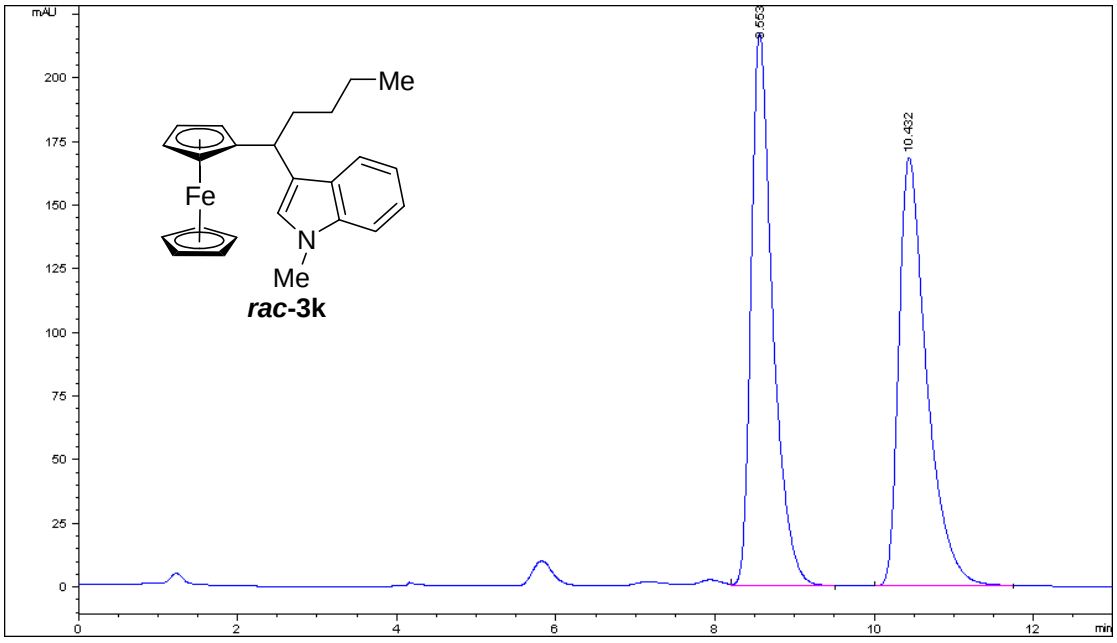
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	17.051	6019.6	197.1	0.5091	0.901	97.698
2	22.34	141.9	3.9	0.6034	0.89	2.302



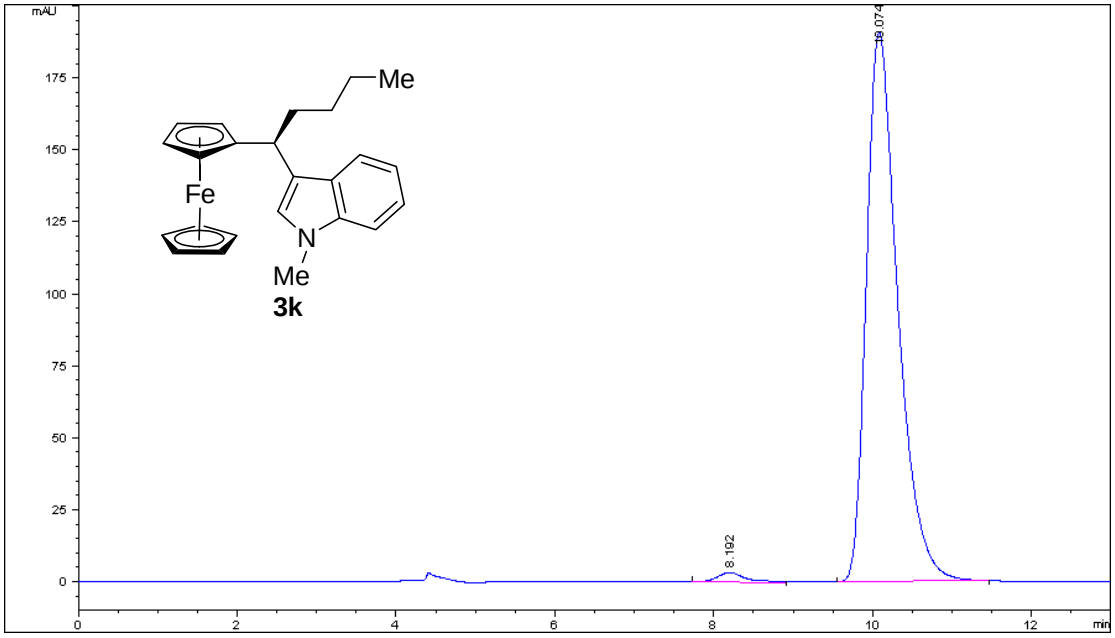
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	6.143	5014.9	340.4	0.2258	0.757	49.920
2	7.293	5030.9	276.9	0.2775	0.706	50.080



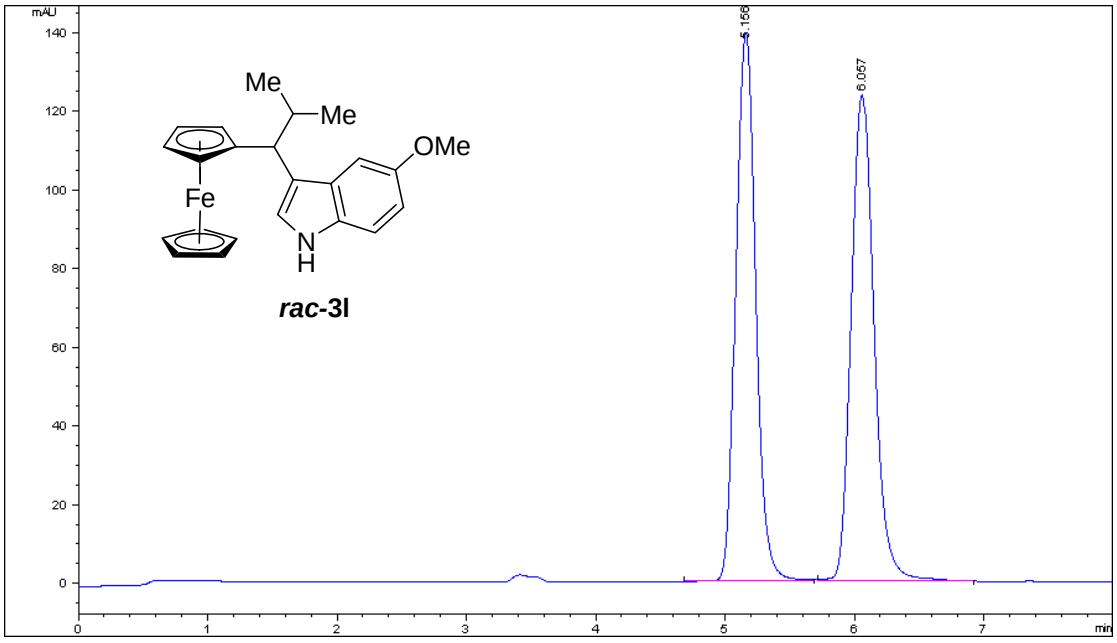
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	5.621	47.6	4.3	0.1695	0.706	0.503
2	6.57	9413.2	692.1	0.2038	0.658	99.497



Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	8.553	4091.5	217	0.2811	0.598	50.011
2	10.432	4089.7	168.2	0.3623	0.539	49.989

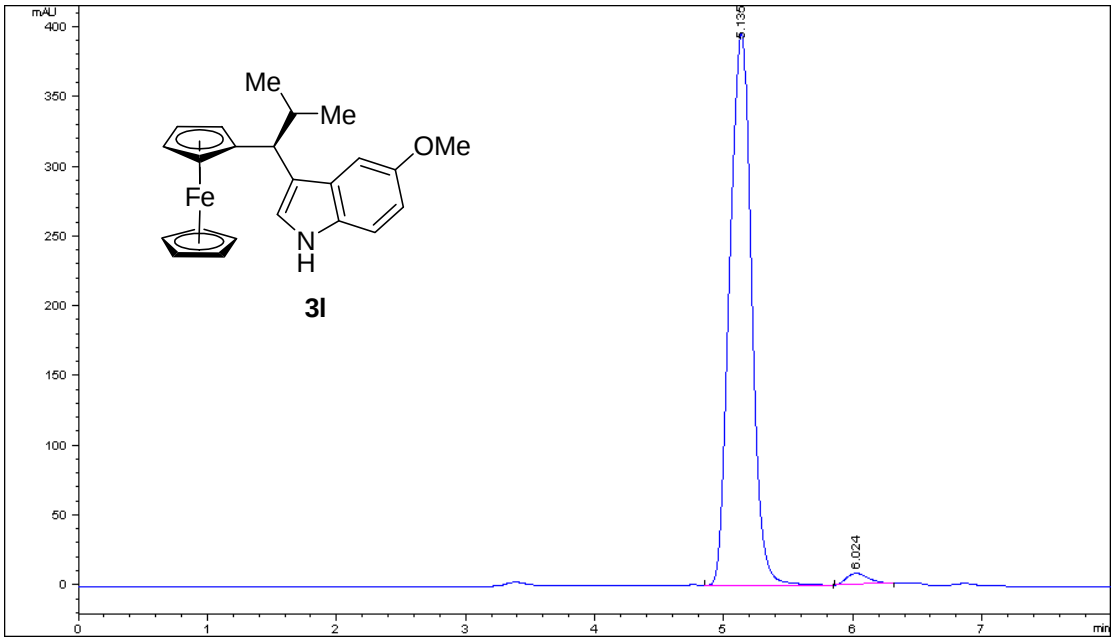


Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	8.192	96.9	3.6	0.4538	0.711	1.812
2	10.074	5252.7	190.9	0.4585	0.646	98.188



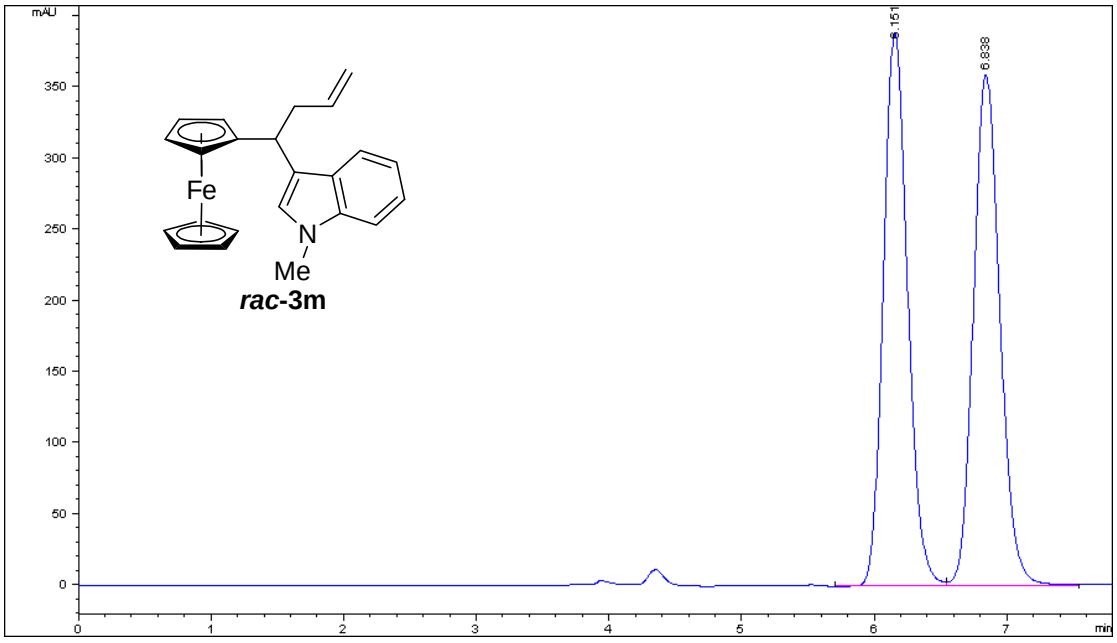
***rac*-3l**

Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	5.156	1501.8	139.4	0.1693	0.922	49.699
2	6.057	1520	123.7	0.1914	0.857	50.301

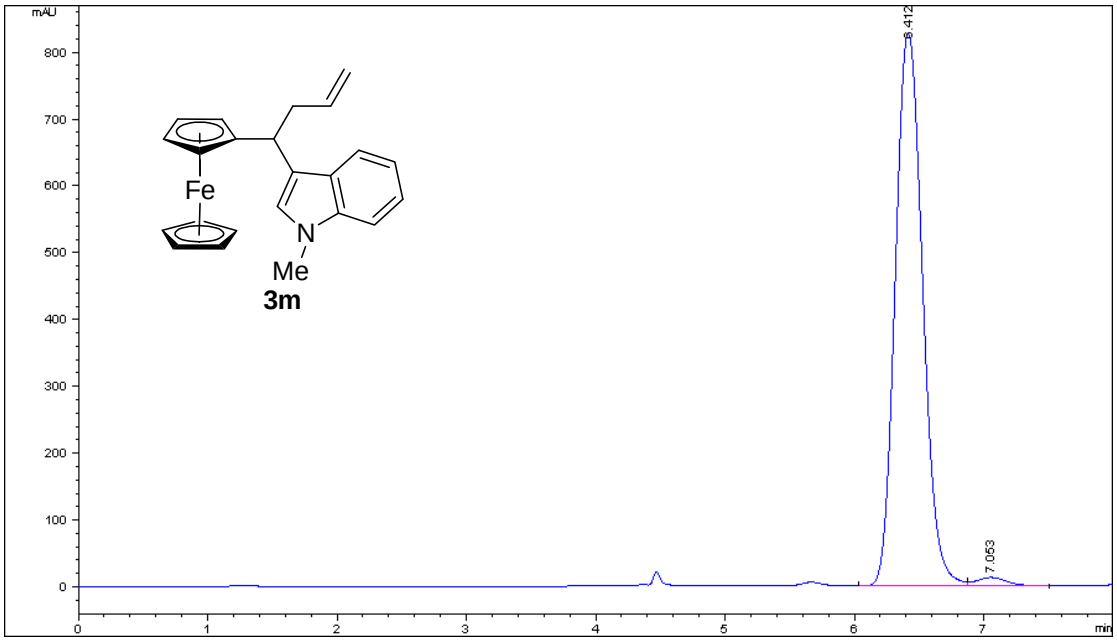


3l

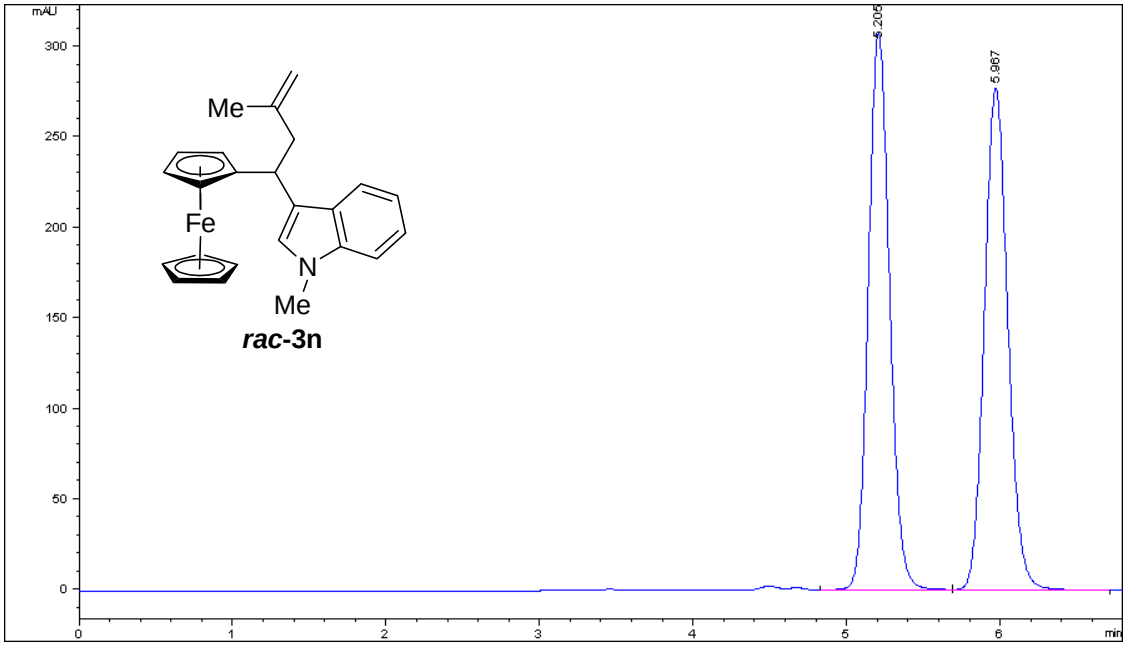
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	5.135	4654.9	396.3	0.1909	1.111	97.883
2	6.024	100.7	8.1	0.2068	0.745	2.117



Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	6.151	4958.2	389	0.1982	0.845	49.740
2	6.838	5010	359.9	0.2163	0.84	50.260

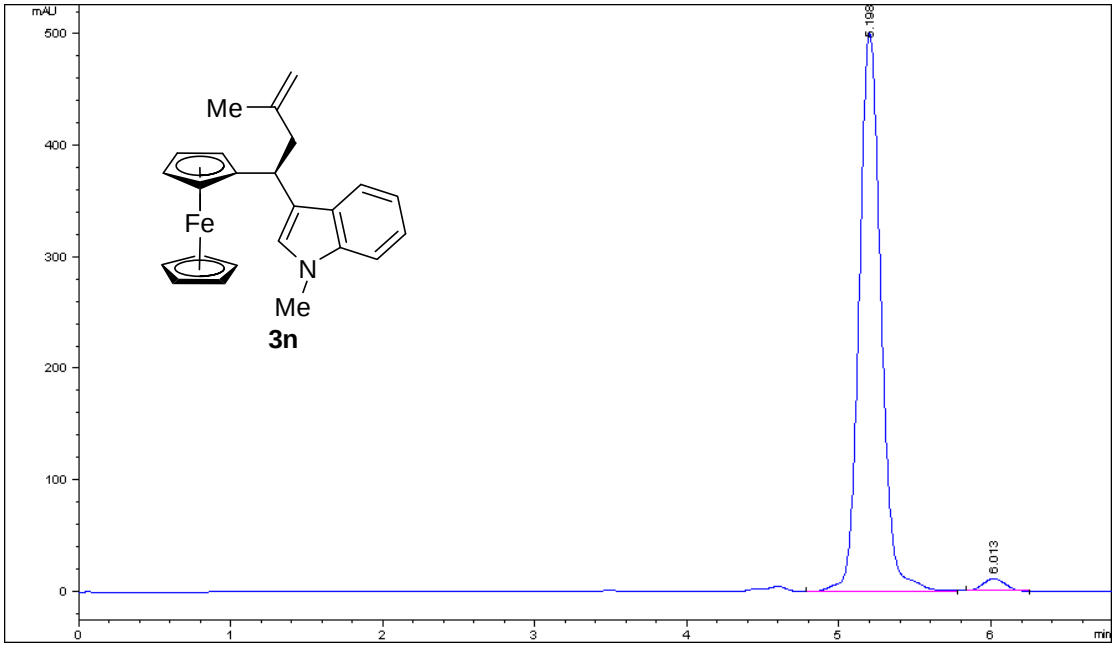


Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	6.412	12072.1	827	0.23	0.845	98.348
2	7.053	202.7	12.5	0.2457	0.849	1.652



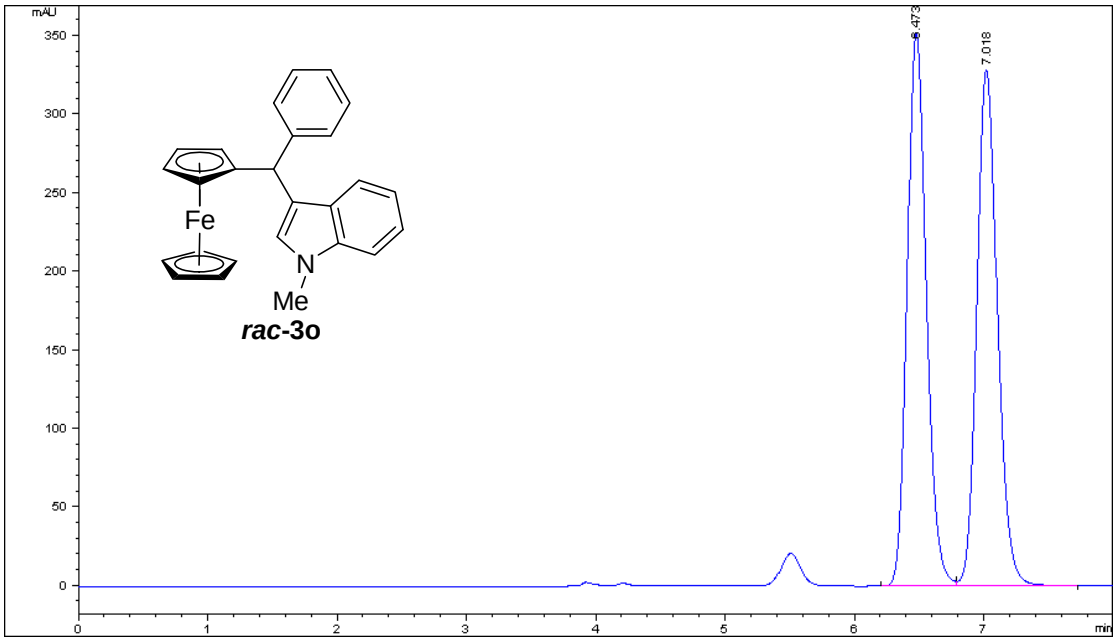
***rac*-3n**

Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	5.205	2978.7	308.4	0.1505	0.883	50.097
2	5.967	2967.1	277.6	0.1655	0.86	49.903



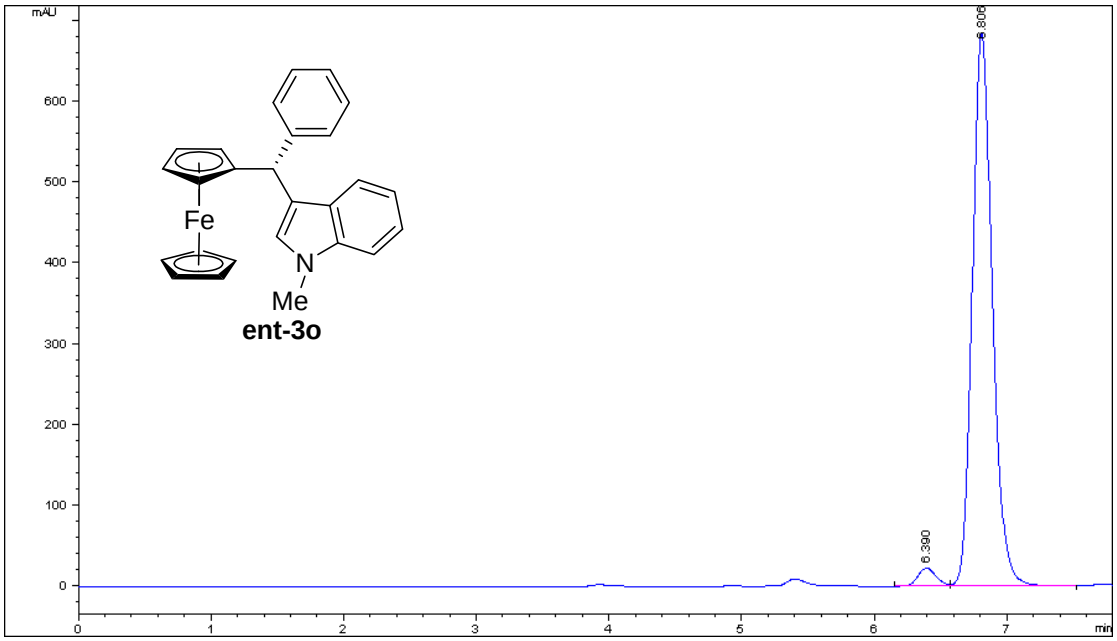
3n

Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	5.198	5005	501.5	0.1528	0.876	97.811
2	6.013	112	11	0.162	0	2.189



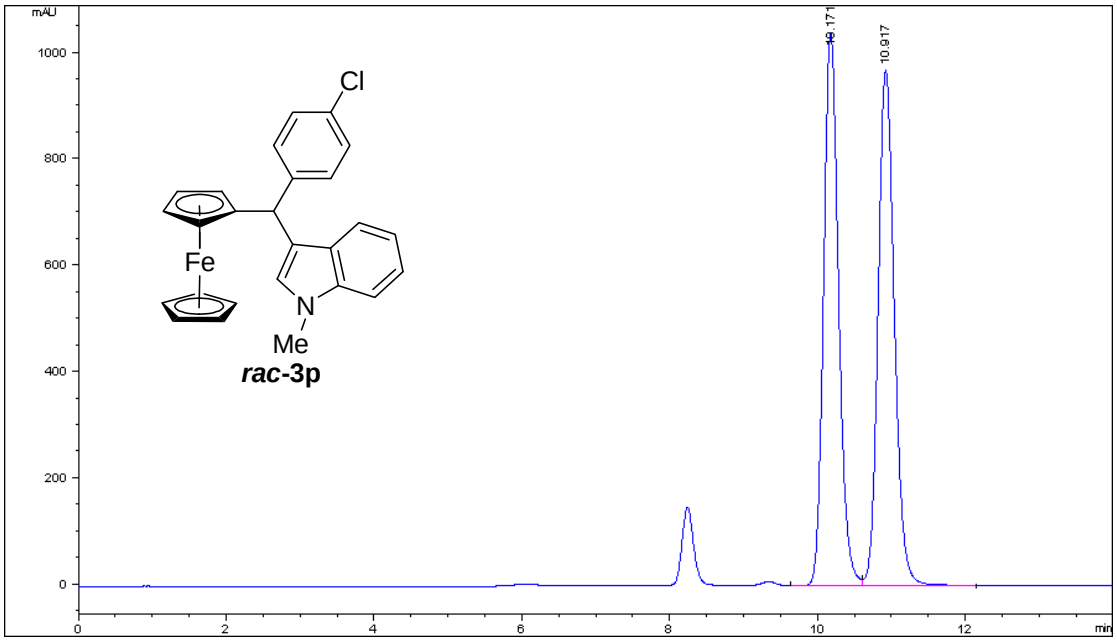
***rac*-3o**

Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	6.473	3617.1	352	0.1577	0.821	49.870
2	7.018	3635.9	328.6	0.1713	0.828	50.130

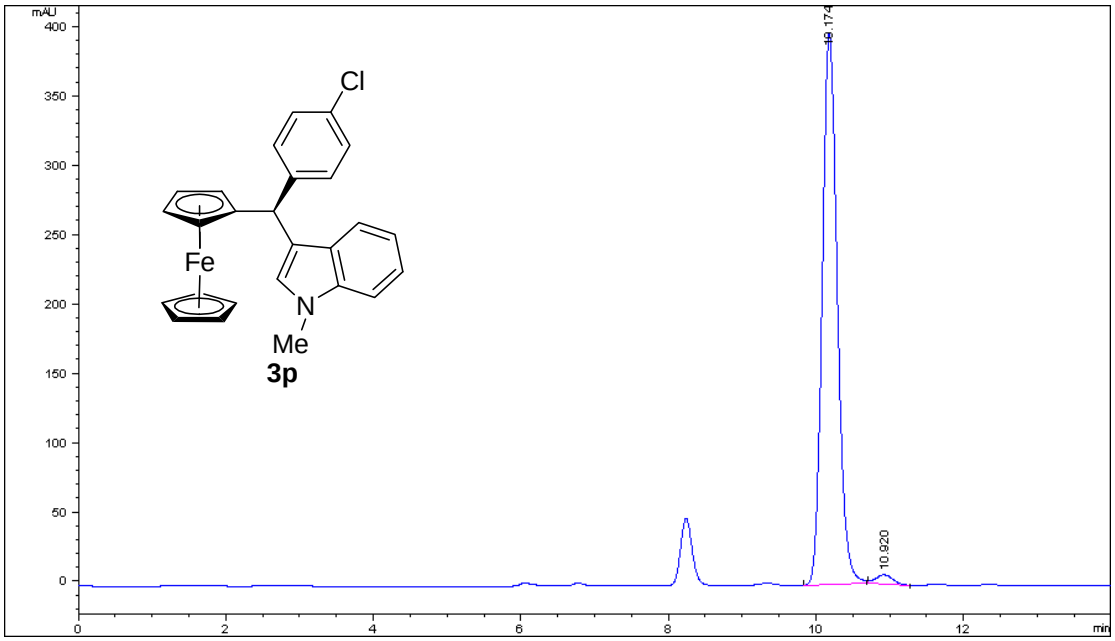


ent-3o

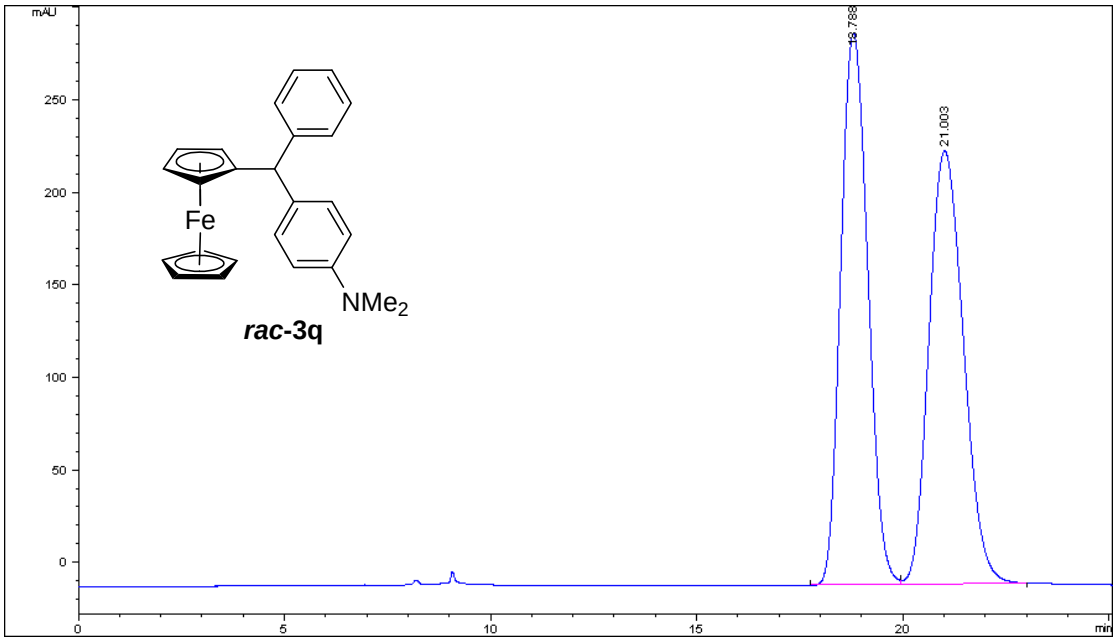
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	6.39	217.3	22.5	0.149	0.862	2.932
2	6.806	7193	686	0.1616	0.814	97.068



Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	10.171	14736.1	1040	0.2177	0.825	49.628
2	10.917	14957.1	971.1	0.2365	0.818	50.372

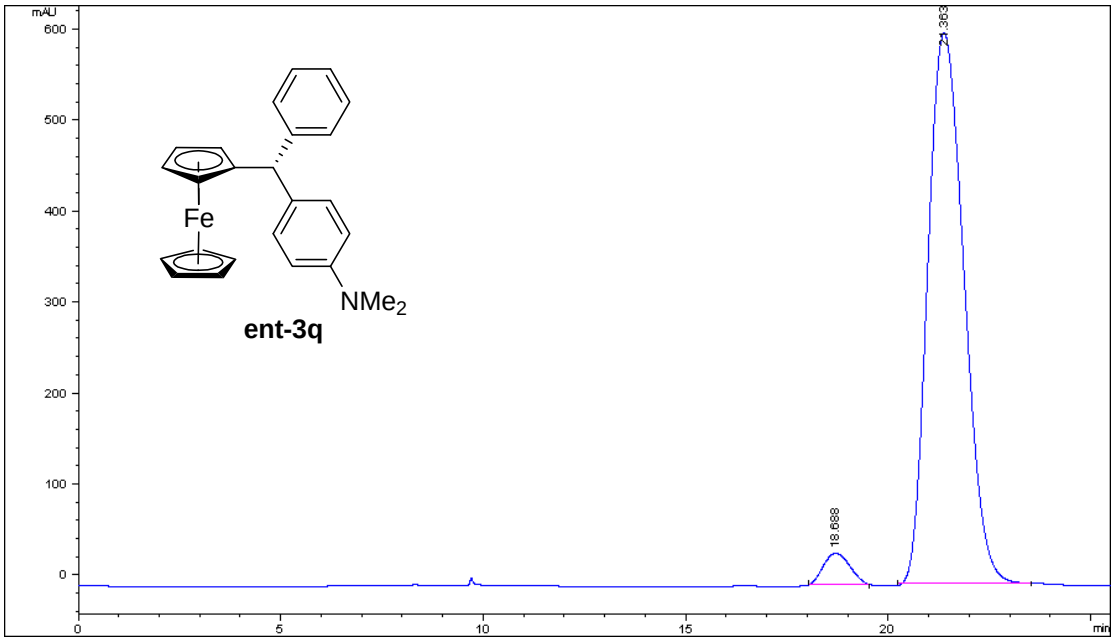


Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	10.174	5671.2	397.8	0.1989	0	98.027
2	10.92	114.2	6.9	0.2772	0.832	1.973



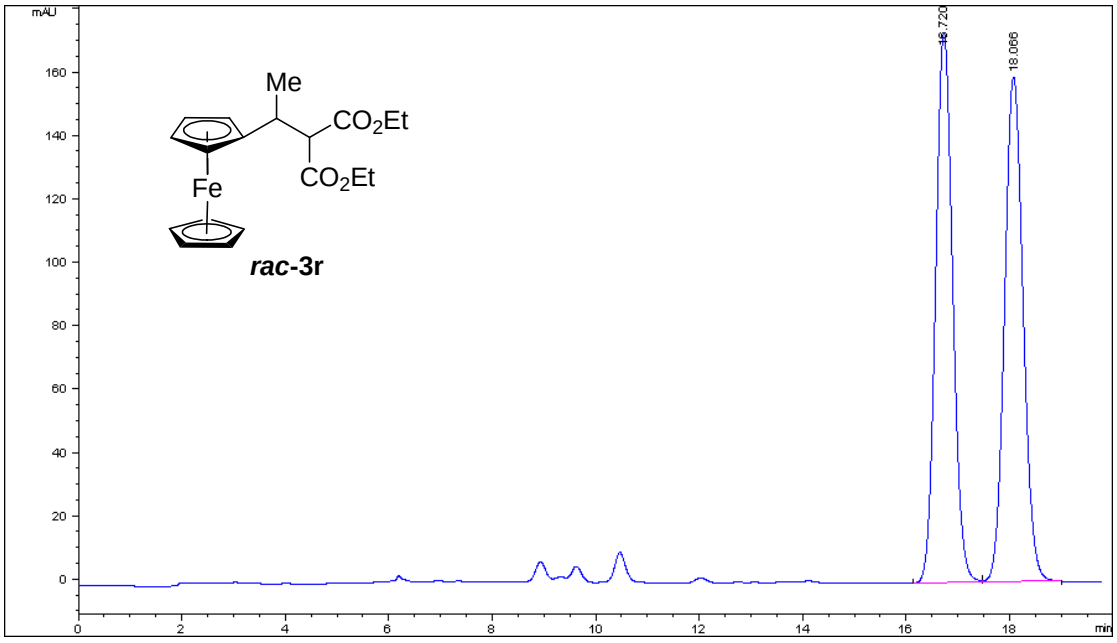
***rac*-3q**

Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	18.788	13646.2	298.3	0.7317	0.834	50.026
2	21.003	13632	234.1	0.9283	0.798	49.974

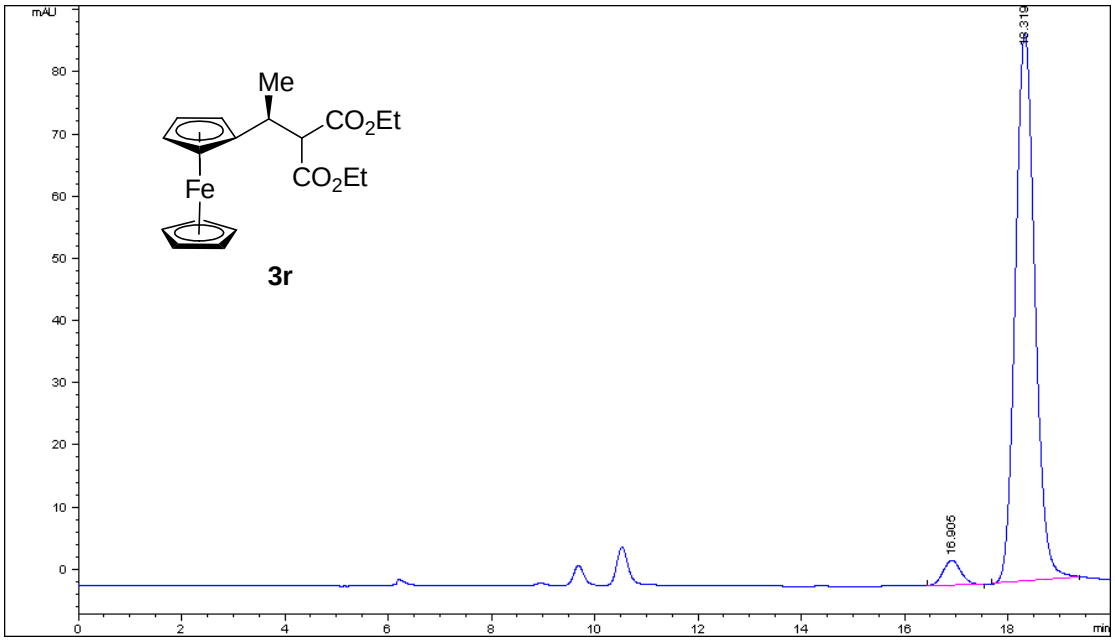


ent-3q

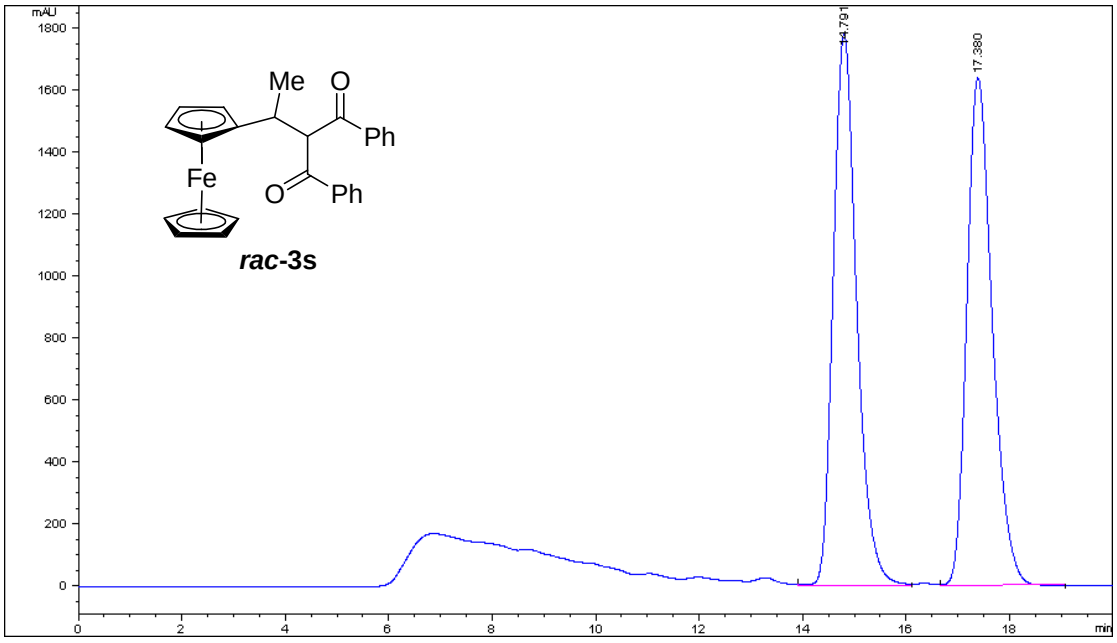
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	18.688	1643.4	35.3	0.7749	0.841	4.187
2	21.363	37609.2	605.5	1.0351	0.781	95.813



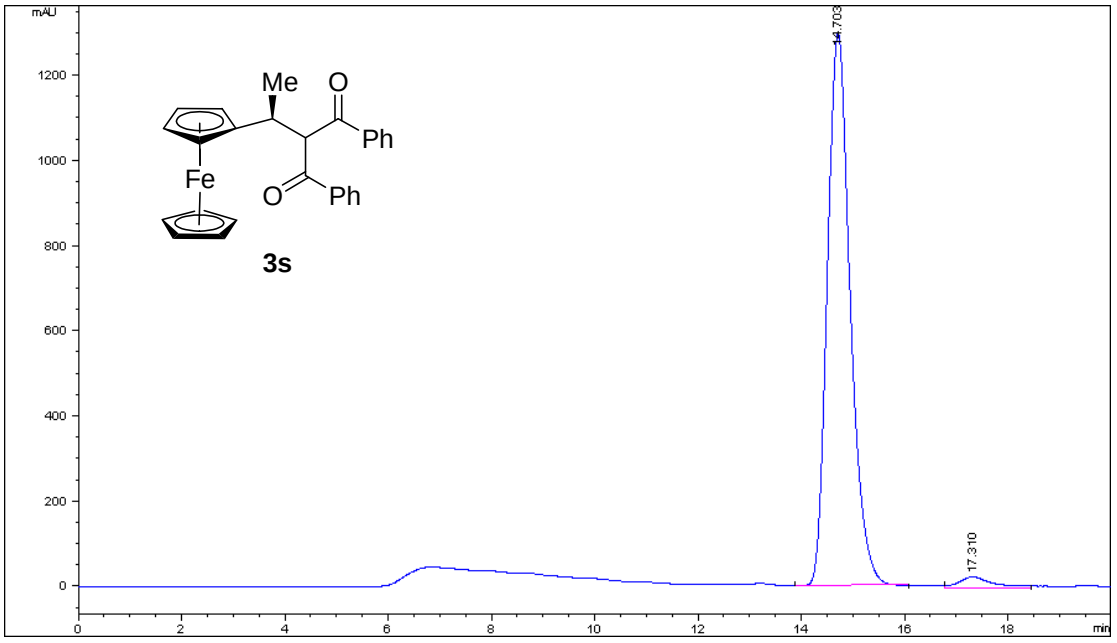
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	16.72	3978.9	173.4	0.3566	0.892	49.992
2	18.066	3980.2	159.3	0.389	0.894	50.008



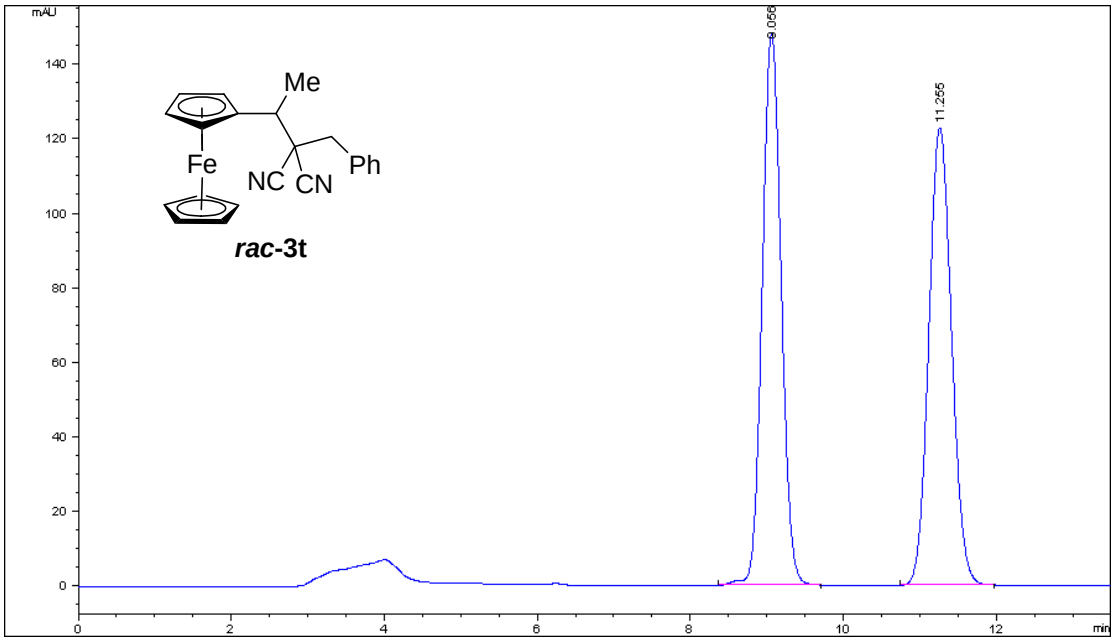
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	16.905	95.6	4	0.3723	0.895	3.957
2	18.319	2319.7	88.2	0.4087	0.867	96.043



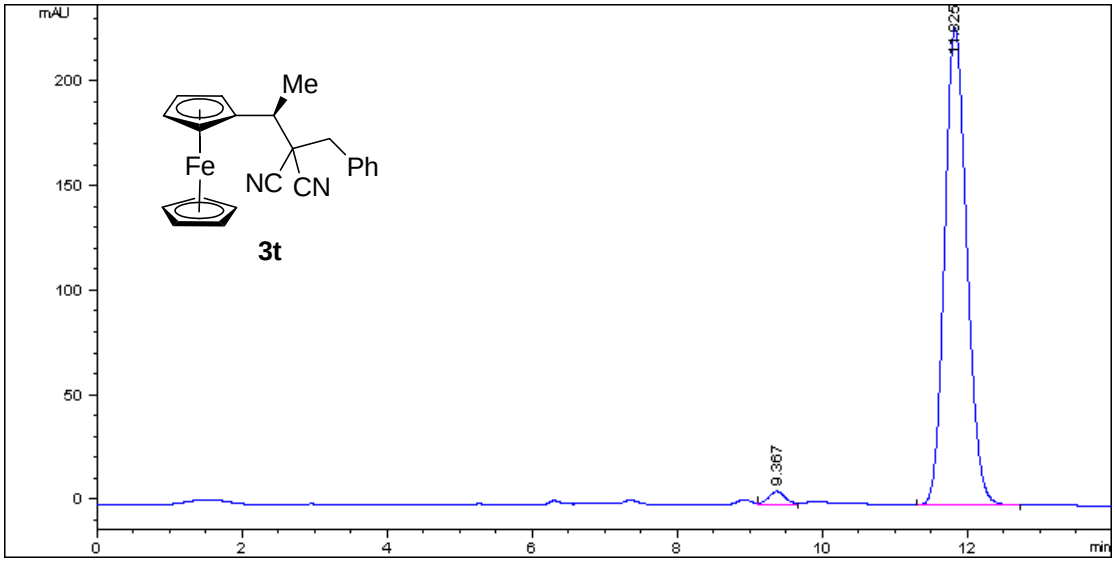
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	14.791	56242.6	1782.7	0.486	0.794	50.121
2	17.38	55970.4	1637.8	0.5254	0.727	49.879



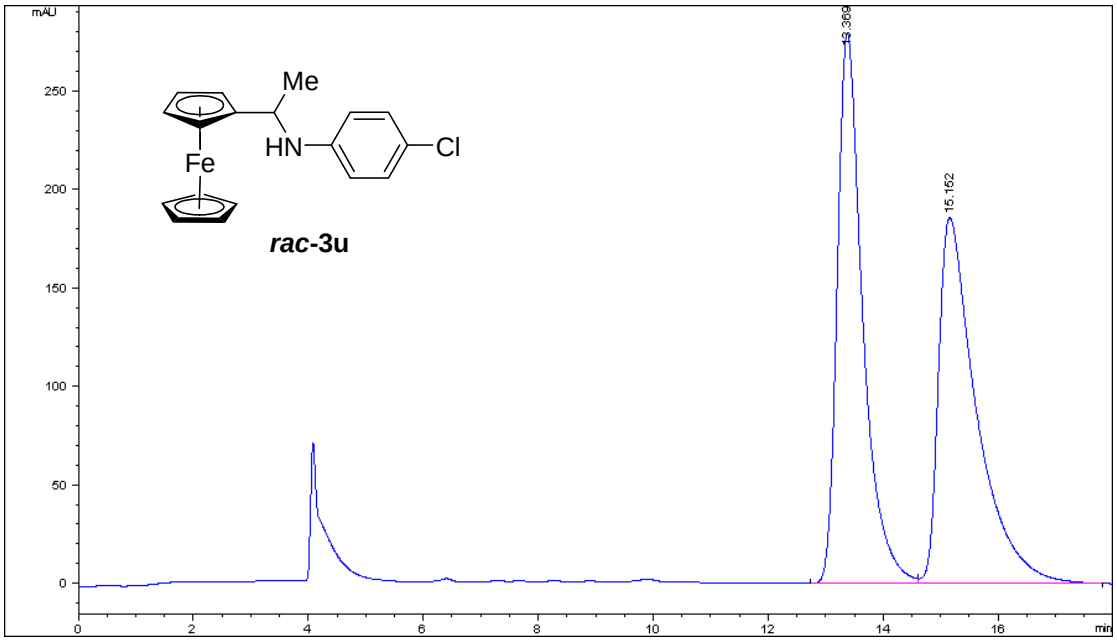
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	14.703	3986.2	1297.3	0.4735	0.809	96.898
2	17.31	1276.1	26.8	0.7943	0.632	3.102



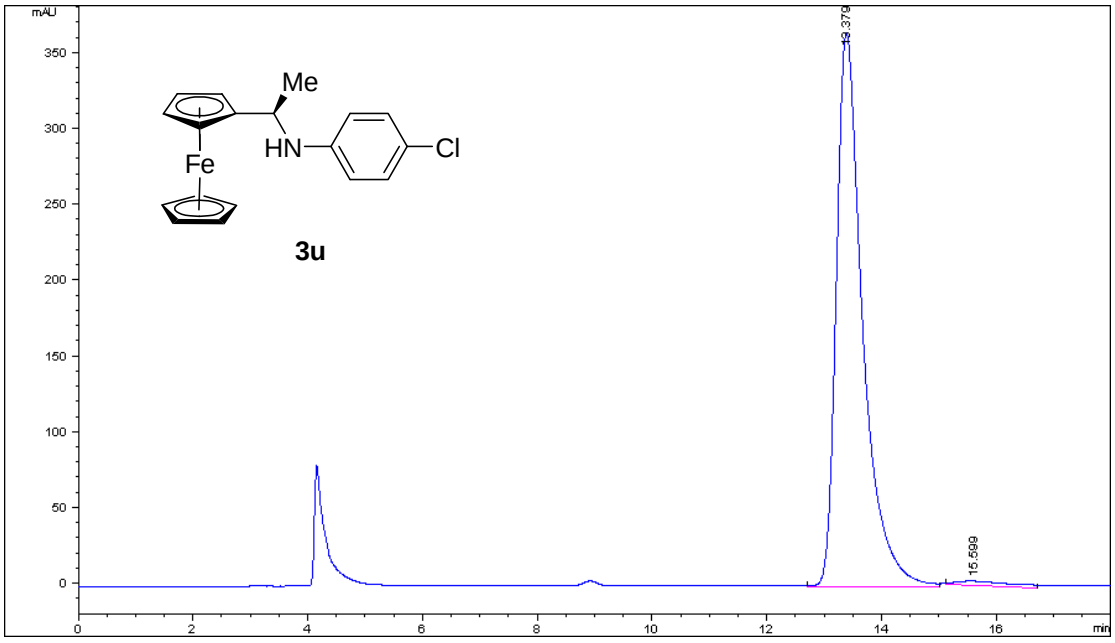
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	9.056	2559.1	148.2	0.2699	0.934	50.209
2	11.255	2537.7	122.8	0.3212	0.893	49.791



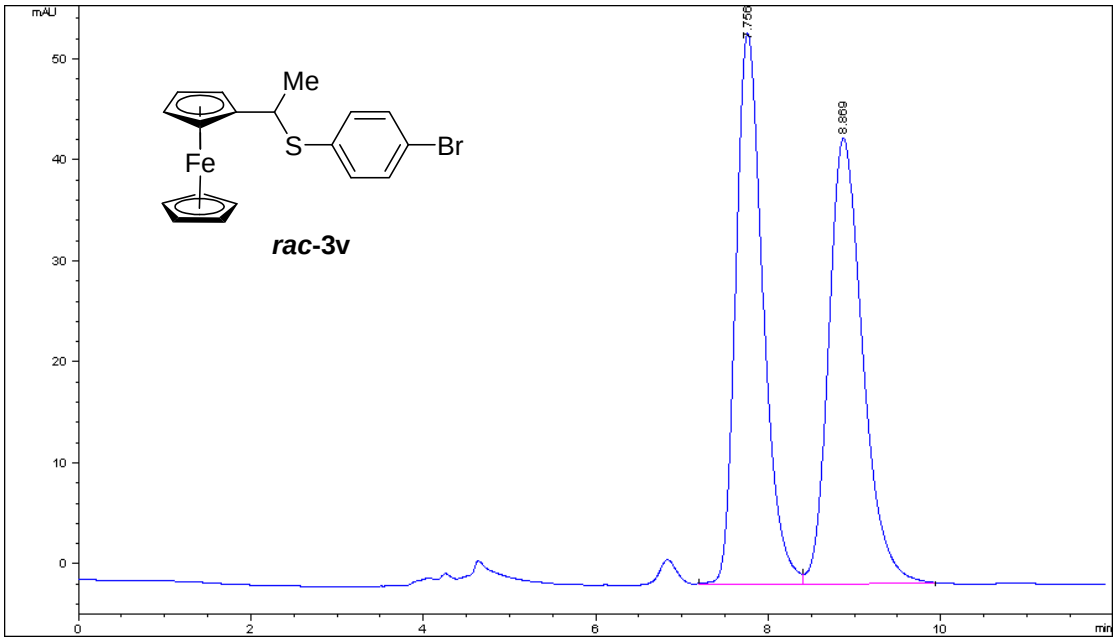
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	9.367	110.1	6.5	0.2605	0.908	2.218
2	11.825	4853.1	227.9	0.3314	0.826	97.782



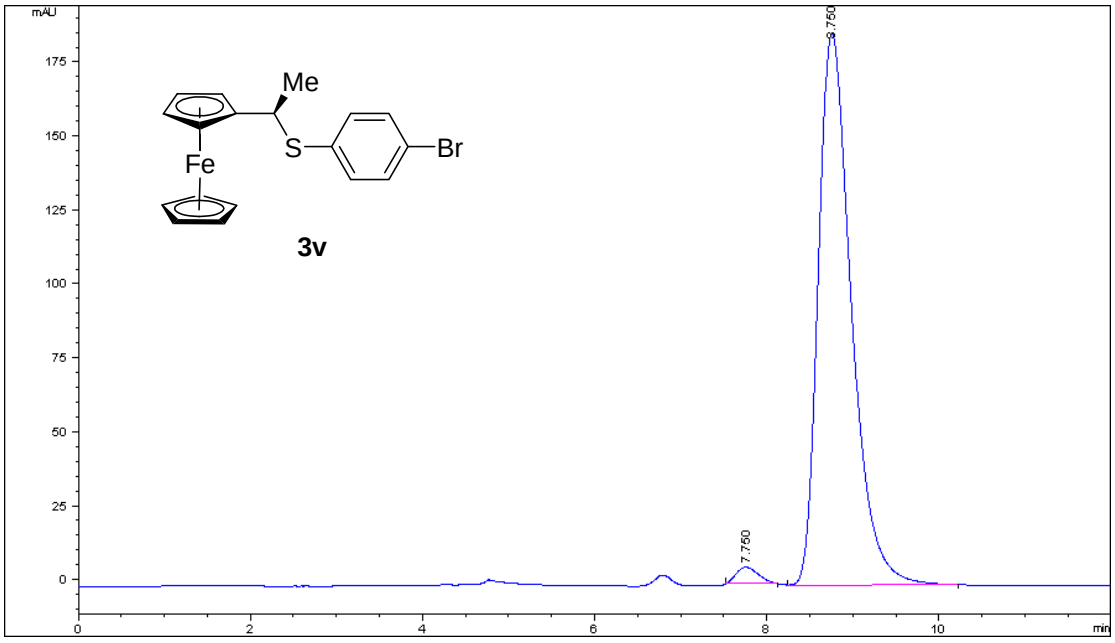
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	13.369	8642.3	279.6	0.4611	0.596	50.315
2	15.152	8534.1	185.8	0.6653	0.389	49.685



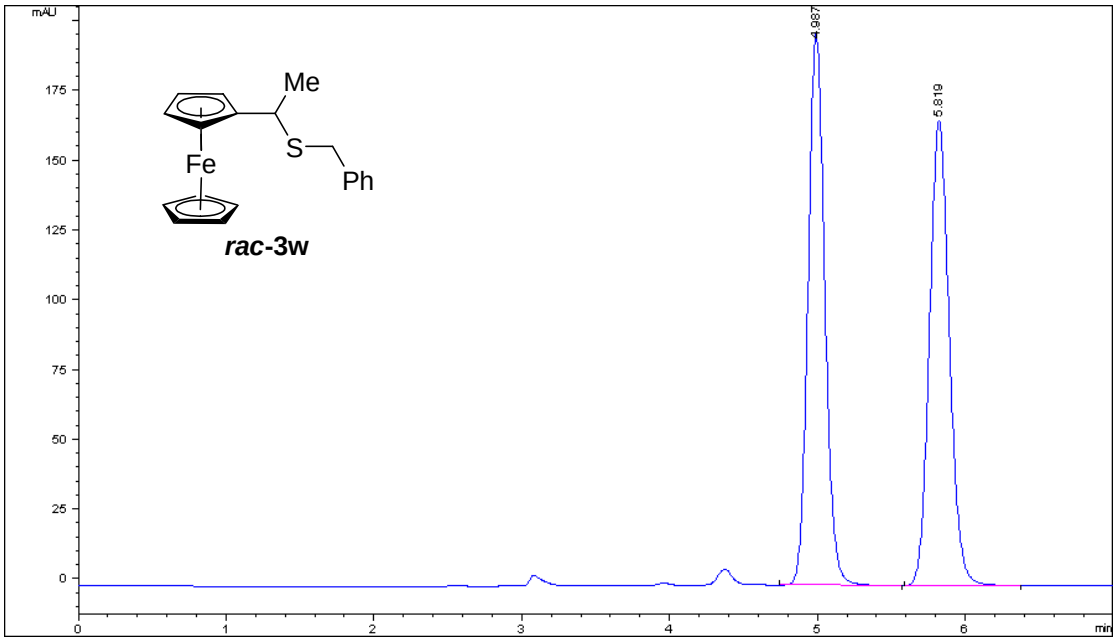
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	13.379	11668.9	365.1	0.5327	0.591	97.934
2	15.599	246.2	3.4	1.2091	0.328	2.066



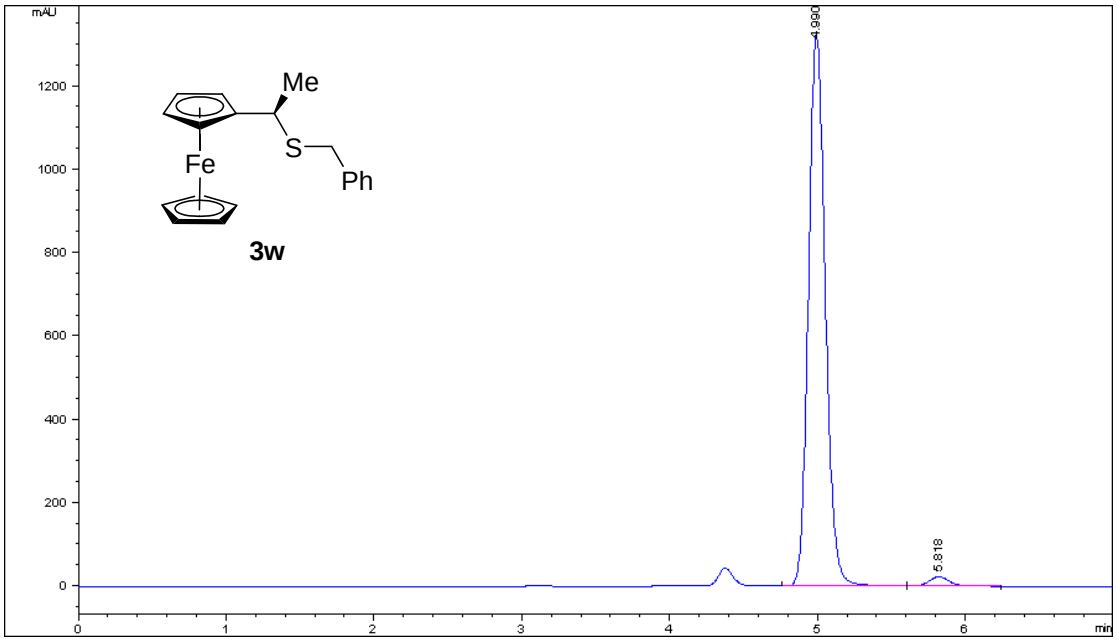
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	7.756	1204.1	54.6	0.3402	0.721	49.854
2	8.869	1211.1	44.1	0.4221	0.732	50.146



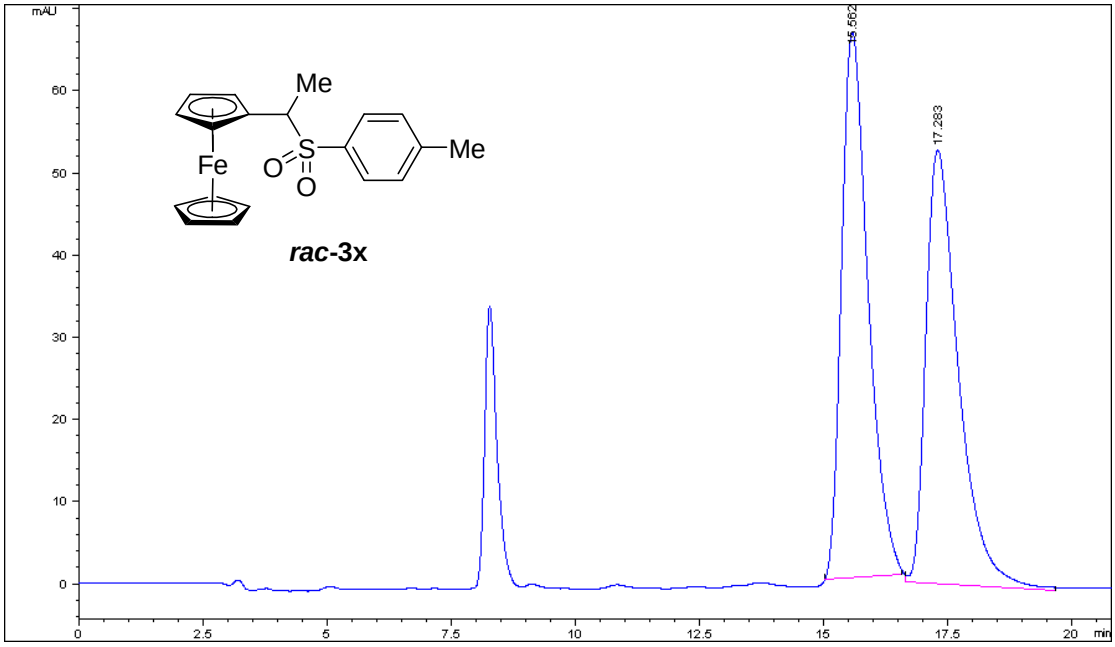
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	7.75	103.9	5.7	0.3055	0.745	2.036
2	8.75	4997	186.7	0.4098	0.641	97.964



Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	4.987	1565.6	198	0.1214	0.87	50.109
2	5.819	1558.7	166.6	0.1455	0.871	49.891

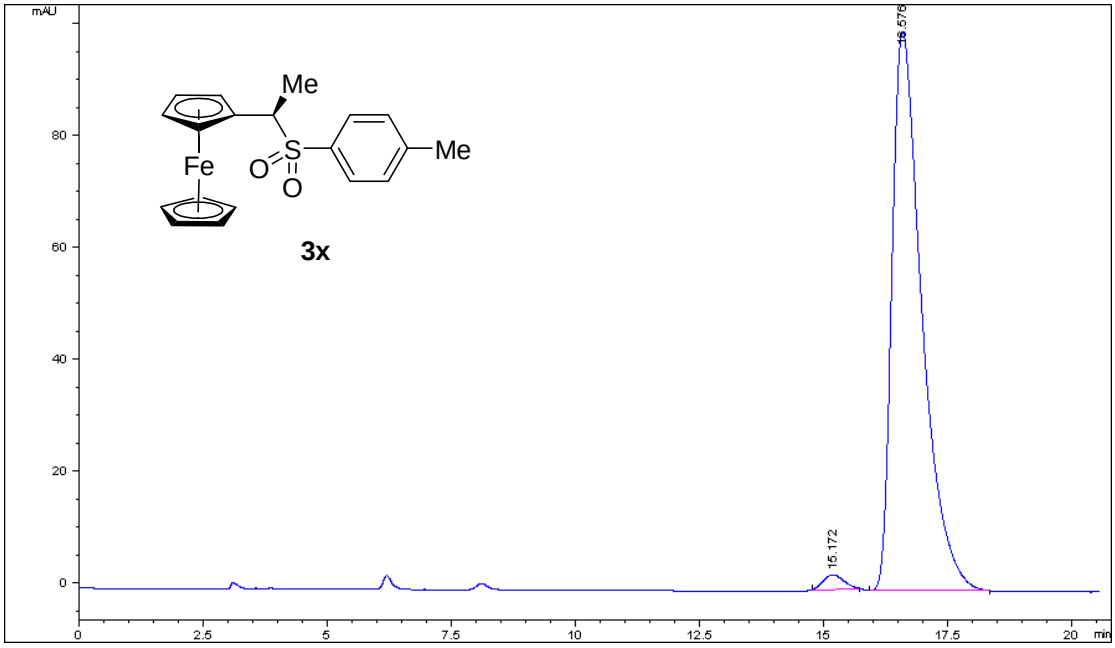


Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	4.99	10526.2	1327.3	0.1231	0.836	97.957
2	5.818	219.6	22.7	0.1476	0.877	2.043



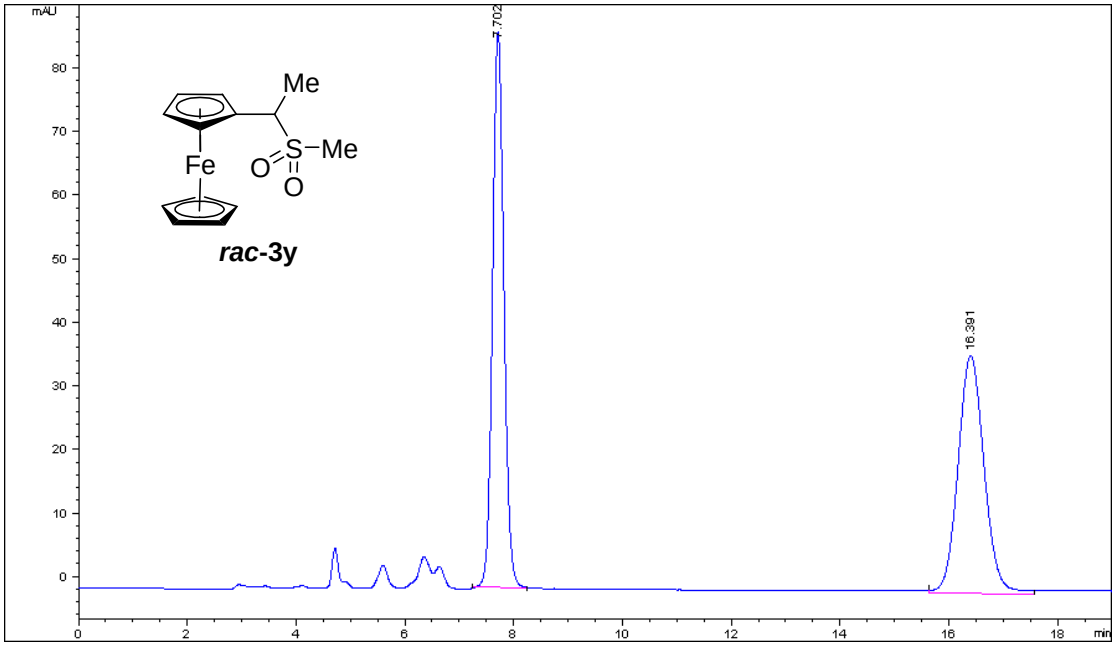
***rac*-3x**

Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	15.562	2478.7	66.4	0.6223	0.652	50.562
2	17.283	2423.6	52.8	0.7648	0.543	49.438

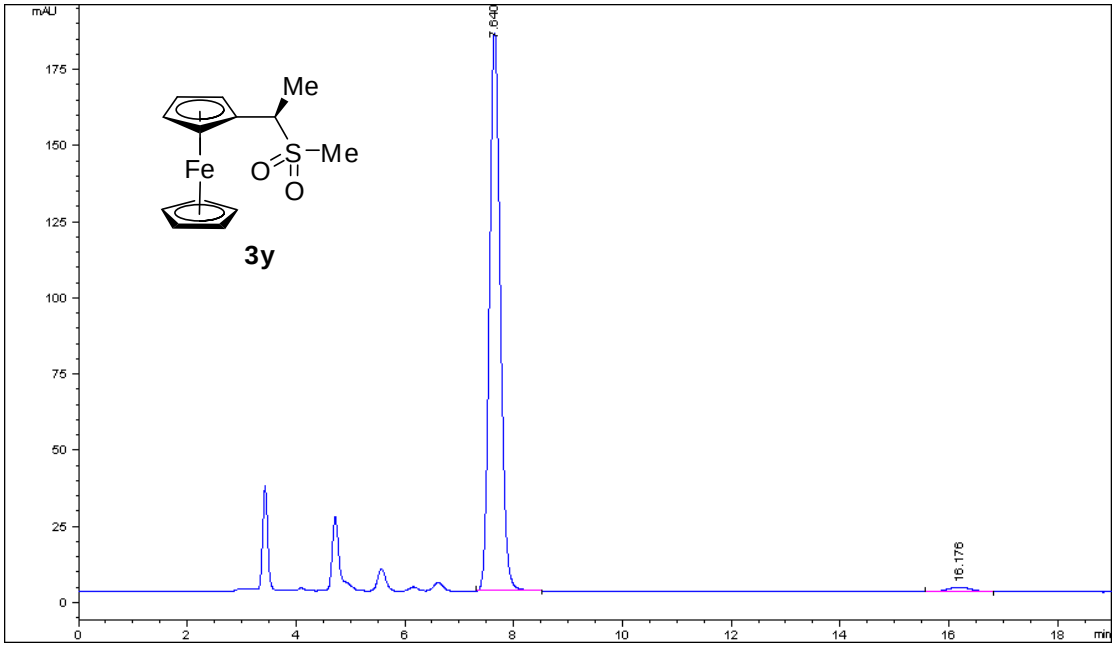


3x

Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	15.172	88.1	2.9	0.515	0.865	2.060
2	16.576	4188.1	99.9	0.6361	0.514	97.940



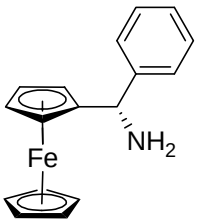
Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	7.702	1270.9	87.4	0.2423	0.894	50.235
2	16.391	1259	37.5	0.5598	0.894	49.765



Number	Time (min)	Area(mAU·s)	Height(mAU)	Width(min)	Symmetry factor	Area (%)
1	7.64	2545.9	183.4	0.2143	0.851	98.010
2	16.176	51.7	1.6	0.5422	0.968	1.990

Compound ent-1g

The crystal of compound **ent-1g** was obtained by leaving alone its solution in hexane and ether at room temperature in the open air for three days. The absolute configuration of compound **ent-1g** was assigned to be *S* by single crystal X-ray analysis. The crystal data of compound **ent-1g** have been deposited in CCDC with number 1000191.



ent-1g

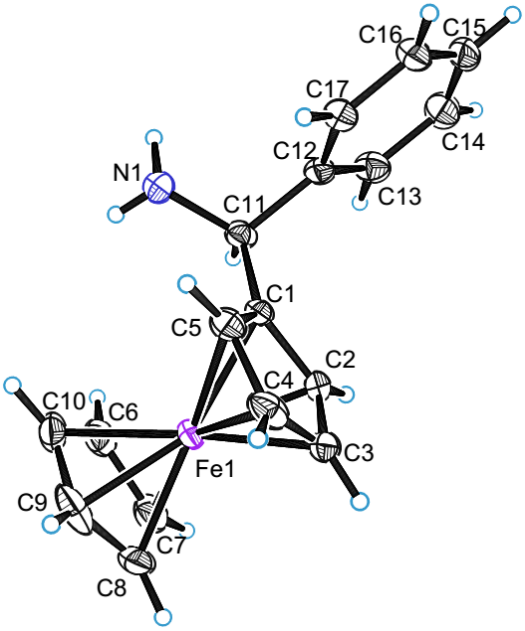


Table 1 Crystal data and structure refinement for **zmg-3**.

Identification code	**zmg-3**
Empirical formula	$C_{17}H_{17}FeN$
Formula weight	291.16
Temperature/K	291(2)
Crystal system	monoclinic
Space group	$P2_1$
a/Å	6.0146(3)
b/Å	23.0686(8)
c/Å	9.9522(3)
α/°	90
β/°	96.970(4)

γ/°	90
Volume/Å^3	1370.65(9)
Z	4
ρ_{calc}mg/mm^3	1.411
m/mm^{-1}	1.084
F(000)	608.0
Crystal size/mm^3	0.41 × 0.34 × 0.3
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection	6.714 to 57.924°
Index ranges	-7 ≤ h ≤ 8, -28 ≤ k ≤ 30, -13 ≤ l ≤ 13
Reflections collected	8058
Independent reflections	4966 [R_{int} = 0.0211, R_{sigma} = 0.0344]
Data/restraints/parameters	4966/1/360
Goodness-of-fit on F^2	1.042
Final R indexes [I>=2σ (I)]	R_1 = 0.0303, wR_2 = 0.0684
Final R indexes [all data]	R_1 = 0.0362, wR_2 = 0.0719
Largest diff. peak/hole / e Å^{-3}	0.24/-0.25
Flack parameter	-0.023(11)

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **zmg-3**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Fe1	2324.4(8)	7077.2(2)	9780.5(5)	36.06(13)
Fe2	8582.8(9)	3970.3(2)	4225.5(5)	37.02(14)
N2	11237(7)	5191(2)	6109(4)	57.5(10)
C29	8283(6)	5864.7(16)	5196(3)	38.3(8)
C28	8846(7)	5241.8(16)	5624(4)	41.5(8)
C12	4404(7)	5214.4(16)	9863(4)	38.3(8)
N1	4237(8)	5795.4(19)	11904(4)	60.3(11)
C17	2634(7)	4853.2(19)	10038(4)	46.7(10)
C19	6101(7)	4579.3(17)	4119(4)	46.5(10)
C18	8218(7)	4849.0(17)	4424(4)	34.6(8)
C22	9505(8)	4724.5(16)	3350(4)	44.7(9)
C34	6317(8)	6114.6(19)	5501(4)	50.7(10)
C1	2759(7)	6195.4(17)	9718(4)	33.9(8)
C11	4539(6)	5821.4(15)	10465(4)	39.9(8)
C4	-567(7)	6663.3(18)	9066(5)	54.5(11)
C30	9668(8)	6184.8(19)	4471(5)	52.9(11)
C33	5773(9)	6677(2)	5128(5)	59.5(12)
C2	2831(7)	6444.1(16)	8416(4)	41.5(9)

C31	9092(9)	6748(2)	4094(5)	63.9(14)
C13	6042(8)	5019.1(19)	9114(4)	52.4(10)
C32	7169(9)	6990.8(19)	4431(4)	59.0(12)
C5	631(7)	6331.1(17)	10104(4)	44.2(9)
C25	8206(12)	3097(2)	4280(6)	72.3(18)
C24	7903(9)	3327(2)	5525(6)	63.9(14)
C23	9857(9)	3620.0(19)	6048(4)	56.9(12)
C26	10336(11)	3233(2)	4012(5)	71.9(16)
C27	11382(8)	3560(2)	5104(6)	64.6(14)
C21	8158(10)	4380.8(18)	2403(4)	59.3(13)
C10	3201(8)	7485(2)	11586(4)	54.1(11)
C3	780(8)	6728.3(17)	8021(4)	52.5(11)
C20	6069(9)	4288.6(18)	2866(5)	62.4(14)
C15	4188(9)	4104.8(19)	8761(4)	62.3(13)
C7	4658(10)	7716(2)	9671(5)	63.3(13)
C6	5069(8)	7432.8(19)	10900(4)	54.2(11)
C9	1558(9)	7804(2)	10790(6)	73.2(17)
C14	5910(9)	4464(2)	8565(5)	63.0(13)
C16	2546(9)	4297(2)	9495(5)	59.3(13)
C8	2475(12)	7954(2)	9598(6)	73.7(19)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **zmg-3**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	$\mathbf{U_{11}}$	$\mathbf{U_{22}}$	$\mathbf{U_{33}}$	$\mathbf{U_{23}}$	$\mathbf{U_{13}}$	$\mathbf{U_{12}}$
Fe1	43.1(3)	28.7(2)	35.2(2)	-4.7(2)	-0.4(2)	0.0(2)
Fe2	44.5(3)	28.3(2)	36.4(3)	4.0(2)	-2.9(2)	1.9(2)
N2	57(2)	50(2)	59(2)	4.2(19)	-15.9(19)	-1.0(19)
C29	49(2)	32.0(19)	32.7(17)	-5.1(14)	1.6(16)	-6.8(17)
C28	50(2)	36(2)	38.0(18)	-0.8(15)	5.8(16)	-0.9(17)
C12	42(2)	32.2(19)	38.7(18)	5.4(15)	-1.6(15)	5.5(16)
N1	92(3)	43(2)	40.4(19)	-0.1(17)	-13.0(19)	4(2)
C17	52(3)	40(2)	48(2)	0.2(18)	5.5(18)	-4.3(19)
C19	39(2)	35(2)	64(3)	5.6(18)	-0.7(19)	2.4(17)
C18	39(2)	26.7(19)	37.9(18)	5.2(15)	2.0(16)	0.3(16)
C22	61(3)	33(2)	41(2)	6.4(16)	10.5(18)	0.2(18)
C34	61(3)	43(2)	51(2)	-4.0(18)	15(2)	0.4(19)
C1	39(2)	25.0(19)	36.6(19)	-1.5(14)	-0.4(16)	0.2(15)
C11	40(2)	31.6(19)	45.8(19)	1.4(15)	-2.7(16)	-4.0(16)
C4	41(2)	39(2)	80(3)	-9(2)	-9(2)	1.8(18)
C30	52(3)	47(2)	61(2)	3(2)	13(2)	-4(2)

C33	62(3)	49(3)	66(3)	-13(2)	0(2)	10(2)
C2	57(2)	33.4(19)	33.4(19)	-5.3(15)	2.6(17)	-0.3(18)
C31	77(3)	50(3)	64(3)	12(2)	4(3)	-18(3)
C13	53(3)	46(2)	59(2)	5.3(19)	9(2)	7.8(19)
C32	77(3)	32(2)	62(2)	-2(2)	-17(2)	0(2)
C5	43(2)	37(2)	53(2)	-1.0(17)	7.0(18)	-7.4(17)
C25	97(5)	30(3)	81(4)	9(2)	-30(3)	-7(3)
C24	61(3)	60(3)	69(3)	37(3)	6(2)	1(2)
C23	80(3)	46(2)	40(2)	9.8(18)	-9(2)	10(2)
C26	107(5)	45(3)	65(3)	2(2)	12(3)	38(3)
C27	45(3)	50(3)	96(4)	25(3)	-4(3)	8(2)
C21	106(4)	37(2)	31.8(19)	3.8(16)	-3(2)	7(2)
C10	71(3)	53(2)	39(2)	-14.9(18)	6(2)	-10(2)
C3	74(3)	34(2)	43(2)	-1.7(16)	-18(2)	0(2)
C20	74(3)	36(2)	67(3)	10(2)	-36(3)	-4(2)
C15	95(4)	38(3)	49(2)	-5.6(19)	-12(2)	19(2)
C7	86(4)	45(3)	63(3)	-10(2)	23(3)	-20(3)
C6	54(3)	46(2)	60(3)	-15(2)	-6(2)	-7(2)
C9	60(3)	56(3)	103(4)	-45(3)	6(3)	7(2)
C14	72(3)	55(3)	62(3)	-5(2)	9(2)	22(3)
C16	80(4)	38(2)	57(3)	1(2)	-6(2)	-10(2)
C8	120(6)	28(3)	64(3)	-1(2)	-27(3)	2(3)

Table 4 Bond Lengths for **zmg-3**.

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
Fe1	C1	2.053(4)	C17	C16	1.391(6)
Fe1	C4	2.035(4)	C19	C18	1.417(6)
Fe1	C2	2.042(4)	C19	C20	1.414(6)
Fe1	C5	2.045(4)	C18	C22	1.423(5)
Fe1	C10	2.040(4)	C22	C21	1.411(6)
Fe1	C3	2.045(4)	C34	C33	1.378(6)
Fe1	C7	2.046(5)	C1	C11	1.500(5)
Fe1	C6	2.048(4)	C1	C2	1.423(5)
Fe1	C9	2.036(5)	C1	C5	1.415(6)
Fe1	C8	2.035(5)	C4	C5	1.412(6)
Fe2	C19	2.043(4)	C4	C3	1.402(7)
Fe2	C18	2.051(4)	C30	C31	1.384(6)
Fe2	C22	2.052(4)	C33	C32	1.361(7)
Fe2	C25	2.029(5)	C2	C3	1.410(6)
Fe2	C24	2.042(5)	C31	C32	1.363(7)

Fe2	C23	2.048(4)	C13	C14	1.390(6)
Fe2	C26	2.026(5)	C25	C24	1.381(8)
Fe2	C27	2.034(4)	C25	C26	1.376(8)
Fe2	C21	2.035(4)	C24	C23	1.400(7)
Fe2	C20	2.040(4)	C23	C27	1.398(7)
N2	C28	1.465(5)	C26	C27	1.407(8)
C29	C28	1.525(5)	C21	C20	1.406(7)
C29	C34	1.382(6)	C10	C6	1.388(7)
C29	C30	1.380(6)	C10	C9	1.398(7)
C28	C18	1.510(5)	C15	C14	1.359(7)
C12	C17	1.379(6)	C15	C16	1.371(7)
C12	C11	1.521(5)	C7	C6	1.383(7)
C12	C13	1.381(6)	C7	C8	1.417(8)
N1	C11	1.467(5)	C9	C8	1.411(8)

Table 5 Bond Angles for **zmg-3**.

Atom	**Atom**	**Atom**	**Angle/˚**	**Atom**	**Atom**	**Atom**	**Angle/˚**
C4	Fe1	C1	68.35(16)	C20	Fe2	C23	153.8(2)
C4	Fe1	C2	67.80(18)	C34	C29	C28	119.9(3)
C4	Fe1	C5	40.48(16)	C30	C29	C28	121.5(4)
C4	Fe1	C10	130.0(2)	C30	C29	C34	118.6(4)
C4	Fe1	C3	40.18(19)	N2	C28	C29	110.1(3)
C4	Fe1	C7	151.8(2)	N2	C28	C18	110.7(3)
C4	Fe1	C6	167.5(2)	C18	C28	C29	108.6(3)
C4	Fe1	C9	108.9(2)	C17	C12	C11	120.8(4)
C2	Fe1	C1	40.65(14)	C17	C12	C13	118.9(4)
C2	Fe1	C5	67.67(16)	C13	C12	C11	120.3(4)
C2	Fe1	C3	40.36(17)	C12	C17	C16	120.1(4)
C2	Fe1	C7	108.68(19)	C18	C19	Fe2	70.0(2)
C2	Fe1	C6	118.22(18)	C20	C19	Fe2	69.6(2)
C5	Fe1	C1	40.41(16)	C20	C19	C18	108.2(4)
C5	Fe1	C3	67.69(18)	C28	C18	Fe2	130.5(3)
C5	Fe1	C7	166.4(2)	C19	C18	Fe2	69.5(2)
C5	Fe1	C6	129.45(18)	C19	C18	C28	124.4(4)
C10	Fe1	C1	117.61(17)	C19	C18	C22	107.9(4)
C10	Fe1	C2	150.69(18)	C22	C18	Fe2	69.8(2)
C10	Fe1	C5	109.27(18)	C22	C18	C28	127.5(4)
C10	Fe1	C3	167.9(2)	C18	C22	Fe2	69.7(2)
C10	Fe1	C7	67.02(19)	C21	C22	Fe2	69.1(2)
C10	Fe1	C6	39.71(19)	C21	C22	C18	107.1(4)

C3	Fe1	C1	68.31(15)	C33	C34	C29	121.0(4)
C3	Fe1	C7	118.72(19)	C11	C1	Fe1	129.9(3)
C3	Fe1	C6	151.2(2)	C2	C1	Fe1	69.3(2)
C7	Fe1	C1	128.4(2)	C2	C1	C11	125.8(4)
C7	Fe1	C6	39.48(19)	C5	C1	Fe1	69.5(2)
C6	Fe1	C1	108.43(17)	C5	C1	C11	127.4(3)
C9	Fe1	C1	150.2(2)	C5	C1	C2	106.6(3)
C9	Fe1	C2	168.0(2)	N1	C11	C12	109.9(3)
C9	Fe1	C5	117.9(2)	N1	C11	C1	110.0(3)
C9	Fe1	C10	40.1(2)	C1	C11	C12	109.5(3)
C9	Fe1	C3	129.8(2)	C5	C4	Fe1	70.1(2)
C9	Fe1	C7	68.4(2)	C3	C4	Fe1	70.3(3)
C9	Fe1	C6	67.5(2)	C3	C4	C5	108.2(4)
C8	Fe1	C1	167.3(2)	C29	C30	C31	119.8(4)
C8	Fe1	C4	118.7(2)	C32	C33	C34	119.8(5)
C8	Fe1	C2	129.8(2)	C1	C2	Fe1	70.1(2)
C8	Fe1	C5	151.6(2)	C3	C2	Fe1	69.9(2)
C8	Fe1	C10	67.1(2)	C3	C2	C1	108.6(4)
C8	Fe1	C3	109.60(18)	C32	C31	C30	120.7(5)
C8	Fe1	C7	40.6(2)	C12	C13	C14	120.1(5)
C8	Fe1	C6	67.0(2)	C33	C32	C31	120.1(4)
C8	Fe1	C9	40.6(2)	C1	C5	Fe1	70.1(2)
C19	Fe2	C18	40.49(16)	C4	C5	Fe1	69.4(2)
C19	Fe2	C22	68.20(17)	C4	C5	C1	108.6(4)
C19	Fe2	C23	120.64(19)	C24	C25	Fe2	70.7(3)
C18	Fe2	C22	40.57(15)	C26	C25	Fe2	70.0(3)
C25	Fe2	C19	126.9(2)	C26	C25	C24	108.3(5)
C25	Fe2	C18	164.9(2)	C25	C24	Fe2	69.7(3)
C25	Fe2	C22	152.9(2)	C25	C24	C23	108.9(5)
C25	Fe2	C24	39.6(2)	C23	C24	Fe2	70.2(3)
C25	Fe2	C23	67.40(19)	C24	C23	Fe2	69.8(3)
C25	Fe2	C27	67.4(2)	C27	C23	Fe2	69.4(3)
C25	Fe2	C21	118.9(2)	C27	C23	C24	107.0(4)
C25	Fe2	C20	107.4(2)	C25	C26	Fe2	70.3(3)
C24	Fe2	C19	109.3(2)	C25	C26	C27	108.2(5)
C24	Fe2	C18	128.7(2)	C27	C26	Fe2	70.0(3)
C24	Fe2	C22	166.0(2)	C23	C27	Fe2	70.5(3)
C24	Fe2	C23	40.0(2)	C23	C27	C26	107.7(5)
C23	Fe2	C18	109.73(17)	C26	C27	Fe2	69.4(3)
C23	Fe2	C22	128.25(18)	C22	C21	Fe2	70.5(2)

C26	Fe2	C19	163.4(2)	C20	C21	Fe2	70.0(2)
C26	Fe2	C18	154.5(2)	C20	C21	C22	109.3(4)
C26	Fe2	C22	119.7(2)	C6	C10	Fe1	70.4(2)
C26	Fe2	C25	39.7(2)	C6	C10	C9	109.0(4)
C26	Fe2	C24	66.6(2)	C9	C10	Fe1	69.8(2)
C26	Fe2	C23	67.56(19)	C4	C3	Fe1	69.5(2)
C26	Fe2	C27	40.6(2)	C4	C3	C2	108.0(3)
C26	Fe2	C21	107.9(2)	C2	C3	Fe1	69.7(2)
C26	Fe2	C20	125.9(2)	C19	C20	Fe2	69.9(2)
C27	Fe2	C19	154.6(2)	C21	C20	Fe2	69.6(2)
C27	Fe2	C18	120.73(19)	C21	C20	C19	107.5(4)
C27	Fe2	C22	108.93(19)	C14	C15	C16	119.3(4)
C27	Fe2	C24	67.0(2)	C6	C7	Fe1	70.3(3)
C27	Fe2	C23	40.0(2)	C6	C7	C8	107.1(5)
C27	Fe2	C21	127.4(2)	C8	C7	Fe1	69.2(3)
C27	Fe2	C20	163.9(2)	C10	C6	Fe1	69.8(2)
C21	Fe2	C19	67.78(19)	C7	C6	Fe1	70.2(3)
C21	Fe2	C18	67.82(16)	C7	C6	C10	109.0(5)
C21	Fe2	C22	40.38(17)	C10	C9	Fe1	70.1(3)
C21	Fe2	C24	152.8(2)	C10	C9	C8	106.5(5)
C21	Fe2	C23	165.1(2)	C8	C9	Fe1	69.7(3)
C21	Fe2	C20	40.4(2)	C15	C14	C13	120.9(5)
C20	Fe2	C19	40.53(18)	C15	C16	C17	120.6(5)
C20	Fe2	C18	68.21(15)	C7	C8	Fe1	70.1(3)
C20	Fe2	C22	68.29(18)	C9	C8	Fe1	69.8(3)
C20	Fe2	C24	119.5(2)	C9	C8	C7	108.4(5)

Table 6 Torsion Angles for **zmg-3**.

A	**B**	**C**	**D**	**Angle/˚**	**A**	**B**	**C**	**D**	**Angle/˚**
Fe1	C1	C11	C12	-168.6(3)	C1	C2	C3	Fe1	59.6(3)
Fe1	C1	C11	N1	70.6(4)	C1	C2	C3	C4	0.4(5)
Fe1	C1	C2	C3	-59.5(3)	C11	C12	C17	C16	-179.3(4)
Fe1	C1	C5	C4	58.8(3)	C11	C12	C13	C14	-180.0(4)
Fe1	C4	C5	C1	-59.3(3)	C11	C1	C2	Fe1	-124.9(4)
Fe1	C4	C3	C2	59.3(3)	C11	C1	C2	C3	175.6(4)
Fe1	C2	C3	C4	-59.2(3)	C11	C1	C5	Fe1	125.1(4)
Fe1	C10	C6	C7	59.5(3)	C11	C1	C5	C4	-176.0(4)
Fe1	C10	C9	C8	-60.5(3)	C30	C29	C28	N2	42.1(5)
Fe1	C7	C6	C10	-59.3(3)	C30	C29	C28	C18	-79.3(5)
Fe1	C7	C8	C9	59.5(4)	C30	C29	C34	C33	-1.9(6)

Fe1	C9	C8	C7	-59.7(4)	C30	C31	C32	C33	-1.0(7)
Fe2	C19	C18	C28	-125.8(4)	C2	C1	C11	C12	-76.7(5)
Fe2	C19	C18	C22	59.4(3)	C2	C1	C11	N1	162.5(4)
Fe2	C19	C20	C21	-59.7(3)	C2	C1	C5	Fe1	-59.6(3)
Fe2	C18	C22	C21	59.2(3)	C2	C1	C5	C4	-0.8(4)
Fe2	C22	C21	C20	59.4(3)	C13	C12	C17	C16	1.6(6)
Fe2	C25	C24	C23	-59.5(3)	C13	C12	C11	N1	-130.1(4)
Fe2	C25	C26	C27	60.0(3)	C13	C12	C11	C1	109.0(4)
Fe2	C24	C23	C27	-59.7(3)	C5	C1	C11	C12	97.8(5)
Fe2	C23	C27	C26	-59.7(3)	C5	C1	C11	N1	-23.1(6)
Fe2	C26	C27	C23	60.4(3)	C5	C1	C2	Fe1	59.7(3)
Fe2	C21	C20	C19	59.9(3)	C5	C1	C2	C3	0.2(4)
N2	C28	C18	Fe2	56.8(5)	C5	C4	C3	Fe1	-60.2(3)
N2	C28	C18	C19	148.3(4)	C5	C4	C3	C2	-0.9(5)
N2	C28	C18	C22	-37.9(5)	C25	C24	C23	Fe2	59.1(3)
C29	C28	C18	Fe2	177.7(3)	C25	C24	C23	C27	-0.6(5)
C29	C28	C18	C19	-90.8(4)	C25	C26	C27	Fe2	-60.2(3)
C29	C28	C18	C22	83.1(5)	C25	C26	C27	C23	0.2(5)
C29	C34	C33	C32	1.0(7)	C24	C25	C26	Fe2	-60.6(4)
C29	C30	C31	C32	0.0(7)	C24	C25	C26	C27	-0.6(6)
C28	C29	C34	C33	179.9(4)	C24	C23	C27	Fe2	59.9(3)
C28	C29	C30	C31	179.6(4)	C24	C23	C27	C26	0.3(5)
C28	C18	C22	Fe2	126.2(4)	C26	C25	C24	Fe2	60.2(4)
C28	C18	C22	C21	-174.6(4)	C26	C25	C24	C23	0.8(6)
C12	C17	C16	C15	-1.1(6)	C10	C9	C8	Fe1	60.8(3)
C12	C13	C14	C15	-0.5(7)	C10	C9	C8	C7	1.1(6)
C17	C12	C11	N1	50.8(5)	C3	C4	C5	Fe1	60.3(3)
C17	C12	C11	C1	-70.1(4)	C3	C4	C5	C1	1.0(5)
C17	C12	C13	C14	-0.8(6)	C20	C19	C18	Fe2	-59.3(3)
C19	C18	C22	Fe2	-59.2(3)	C20	C19	C18	C28	174.9(4)
C19	C18	C22	C21	0.1(4)	C20	C19	C18	C22	0.0(4)
C18	C19	C20	Fe2	59.6(3)	C6	C10	C9	Fe1	59.7(3)
C18	C19	C20	C21	-0.1(5)	C6	C10	C9	C8	-0.8(5)
C18	C22	C21	Fe2	-59.6(3)	C6	C7	C8	Fe1	-60.4(3)
C18	C22	C21	C20	-0.1(5)	C6	C7	C8	C9	-1.0(6)
C22	C21	C20	Fe2	-59.7(3)	C9	C10	C6	Fe1	-59.3(3)
C22	C21	C20	C19	0.2(5)	C9	C10	C6	C7	0.2(5)
C34	C29	C28	N2	-139.8(4)	C14	C15	C16	C17	-0.2(7)
C34	C29	C28	C18	98.8(4)	C16	C15	C14	C13	0.9(7)
C34	C29	C30	C31	1.4(6)	C8	C7	C6	Fe1	59.8(3)

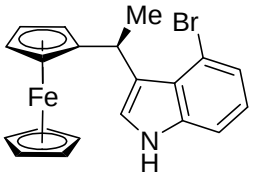
C34	C33	C32	C31	0.5(7)	C8	C7	C6	C10	0.5(5)

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **zmg-3**.

Atom	***x***	***y***	***z***	**U(eq)**
H28	7972	5133	6354	50
H17	1499	4982	10521	56
H19	4933	4591	4652	56
H22	10962	4847	3286	54
H34	5346	5900	5965	61
H11	6013	5987	10373	48
H4	-2001	6813	9074	65
H30	10983	6023	4237	63
H33	4455	6842	5352	71
H2	4031	6423	7909	50
H31	10028	6963	3606	77
H13	7236	5259	8977	63
H32	6811	7371	4183	71
H5	109	6220	10907	53
H25	7152	2886	3718	87
H24	6612	3293	5947	77
H23	10095	3817	6868	68
H26	10974	3127	3242	86
H27	12829	3709	5183	78
H21	8584	4238	1599	71
H10	3065	7332	12437	65
H3	390	6924	7210	63
H20	4883	4075	2428	75
H15	4125	3732	8402	75
H7	5630	7744	9015	76
H6	6384	7239	11217	65
H9	139	7898	11005	88
H14	7014	4337	8057	76
H16	1362	4053	9630	71
H8	1768	8173	8886	88
H1A	5100(90)	5530(20)	12320(50)	67(15)
H2A	11590(90)	4810(30)	6550(50)	86(17)
H1B	4380(80)	6080(20)	12280(50)	57(15)
H2B	11410(110)	5380(30)	6910(70)	120(30)

Compound 3d

The crystal of compound **3d** was obtained by leaving alone its solution in hexane and ether at room temperature in the open air for five days. The absolute configuration of compound **3d** was assigned to be *S* by single crystal X-ray analysis. The crystal data of compound **3d** have been deposited in CCDC with number 1000190.



3d

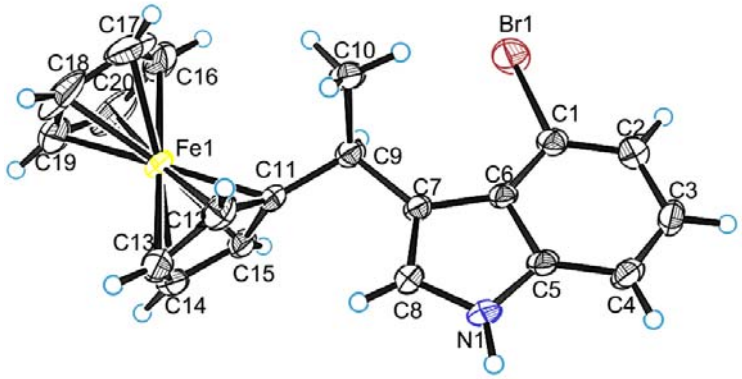


Table 1 Crystal data and structure refinement for **zmg-10**.

Identification code	**zmg-10**
Empirical formula	$C_{20}H_{18}BrFeN$
Formula weight	408.11
Temperature/K	291(2)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	6.0455(5)
b/Å	9.3540(8)
c/Å	29.031(3)
α/°	90.00
β/°	90.00
γ/°	90.00
Volume/Å^3	1641.7(2)
Z	4
ρ_{calc}mg/mm^3	1.651
m/mm^{-1}	3.350
F(000)	824.0

Crystal size/mm^3	0.46 × 0.41 × 0.38
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection	6.88 to 52.74°
Index ranges	-7 ≤ h ≤ 7, -11 ≤ k ≤ 11, -36 ≤ l ≤ 33
Reflections collected	7306
Independent reflections	3066[R(int) = 0.0361]
Data/restraints/parameters	3066/1/214
Goodness-of-fit on F^2	1.055
Final R indexes [I>=2σ (I)]	R_1 = 0.0362, wR_2 = 0.0756
Final R indexes [all data]	R_1 = 0.0441, wR_2 = 0.0801
Largest diff. peak/hole / e Å^{-3}	0.47/-0.52
Flack parameter	-0.018(12)

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **zmg-10**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Br1	2313.0(7)	708.8(4)	3744.52(16)	51.40(17)
Fe1	7644(1)	6433.6(5)	3290.30(16)	29.36(16)
C5	7340(7)	770(3)	4730.3(12)	31.1(8)
C11	7552(7)	4779(3)	3754.9(11)	29.8(7)
C6	6076(6)	1177(4)	4340.2(12)	27.3(8)
C13	10228(7)	6535(5)	3737.7(15)	45.1(10)
C2	3758(7)	-864(4)	4512.4(15)	40.9(10)
C9	6434(6)	3325(3)	3739.4(13)	30.4(8)
C17	7358(14)	5923(6)	2616.5(15)	76.9(19)
C10	7030(8)	2502(4)	3304.8(13)	45.5(11)
C4	6866(8)	-422(4)	5001.5(13)	40.4(11)
N1	8949(6)	1767(3)	4786.6(12)	39.8(9)
C7	7004(6)	2495(3)	4169.0(12)	25.9(8)
C3	5065(8)	-1222(4)	4890.8(15)	44.5(11)
C14	8323(7)	7118(4)	3939.2(14)	40.7(10)
C1	4245(7)	304(4)	4242.1(14)	32.6(9)
C19	7298(13)	8173(5)	2879.6(17)	72.0(17)
C18	8607(9)	7153(9)	2661.5(19)	83(2)
C12	9779(6)	5093(4)	3619.0(14)	38(1)
C8	8737(7)	2790(4)	4449.7(14)	37.5(10)
C16	5292(10)	6205(7)	2799(2)	72.0(18)
C20	5301(10)	7568(7)	2955(2)	73.7(19)
C15	6686(6)	6042(4)	3957.1(13)	32.1(9)

Table 3 Anisotropic Displacement Parameters (Å^2×10^3) for **zmg-10**. The Anisotropic displacement

factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka\times b\times U_{12}]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Br1	46.5(3)	51.3(2)	56.3(3)	3.5(2)	-21.9(3)	-2.5(2)
Fe1	36.4(3)	32.7(3)	19.0(2)	3.8(2)	0.8(3)	-0.6(3)
C5	44(2)	28.4(15)	20.9(16)	-4.5(15)	-3(2)	3(2)
C11	35.7(18)	33.7(16)	20.0(16)	6.2(15)	-4(2)	-1.8(16)
C6	37(2)	25.6(17)	19.1(19)	-3.2(16)	-0.4(16)	2.9(14)
C13	46(2)	52(2)	37(2)	12(2)	-8(2)	-16(2)
C2	52(2)	35(2)	36(2)	0(2)	0(2)	-6.6(19)
C9	35.6(19)	31.1(18)	24.5(19)	1.4(18)	-3.7(18)	2.0(15)
C17	139(6)	66(3)	26(2)	-4(2)	-17(4)	32(5)
C10	74(3)	35.9(19)	27(2)	-2.5(17)	-10(3)	0(2)
C4	67(3)	31.4(19)	22(2)	0.5(16)	-4(2)	11.6(19)
N1	53(2)	40.4(19)	26.0(19)	4.1(17)	-18.1(17)	-5.2(16)
C7	30.7(19)	26.4(16)	20.5(17)	0.3(15)	-2.9(17)	1.9(14)
C3	74(3)	28(2)	32(2)	7(2)	5(2)	-1(2)
C14	62(3)	35(2)	25(2)	-0.6(18)	-7(2)	-3.7(19)
C1	42(2)	29.0(18)	27(2)	-5.4(18)	-1.0(19)	4.2(15)
C19	127(5)	47(2)	42(3)	19(2)	-19(4)	-17(4)
C18	54(3)	161(6)	34(3)	40(4)	14(3)	-2(4)
C12	31(2)	48(2)	35(3)	8(2)	-0.5(19)	5.9(17)
C8	52(2)	33.0(19)	27(2)	5.8(19)	-7(2)	-7.7(18)
C16	80(4)	88(4)	48(3)	35(3)	-33(3)	-32(3)
C20	80(4)	98(5)	43(3)	29(4)	1(3)	46(4)
C15	40(2)	34.3(19)	21.8(19)	1.4(16)	3.7(17)	1.0(15)

Table 4 Bond Lengths for **zmg-10**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Br1	C1	1.896(4)	C6	C7	1.443(5)
Fe1	C11	2.054(3)	C6	C1	1.405(5)
Fe1	C13	2.034(4)	C13	C14	1.402(6)
Fe1	C17	2.021(4)	C13	C12	1.418(6)
Fe1	C14	2.032(4)	C2	C3	1.394(6)
Fe1	C19	2.028(4)	C2	C1	1.378(5)
Fe1	C18	2.031(5)	C9	C10	1.522(5)
Fe1	C12	2.037(4)	C9	C7	1.509(5)
Fe1	C16	2.026(5)	C17	C18	1.382(8)
Fe1	C20	2.019(5)	C17	C16	1.381(8)
Fe1	C15	2.054(4)	C4	C3	1.360(6)
C5	C6	1.418(5)	N1	C8	1.374(5)

C5	C4	1.395(5)	C7	C8	1.356(5)
C5	N1	1.357(5)	C14	C15	1.413(5)
C11	C9	1.519(4)	C19	C18	1.392(8)
C11	C12	1.434(6)	C19	C20	1.351(8)
C11	C15	1.419(5)	C16	C20	1.354(8)

Table 5 Bond Angles for **zmg-10**.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C13	Fe1	C11	68.69(16)	C12	C11	Fe1	68.9(2)
C13	Fe1	C12	40.78(17)	C12	C11	C9	126.4(3)
C13	Fe1	C15	67.85(16)	C15	C11	Fe1	69.77(19)
C17	Fe1	C11	117.07(18)	C15	C11	C9	126.4(4)
C17	Fe1	C13	134.0(3)	C15	C11	C12	106.8(3)
C17	Fe1	C14	171.6(3)	C5	C6	C7	107.1(3)
C17	Fe1	C19	67.2(2)	C1	C6	C5	115.5(3)
C17	Fe1	C18	39.9(2)	C1	C6	C7	137.1(3)
C17	Fe1	C12	111.2(2)	C14	C13	Fe1	69.7(2)
C17	Fe1	C16	39.9(2)	C14	C13	C12	108.3(4)
C17	Fe1	C15	147.8(2)	C12	C13	Fe1	69.7(2)
C14	Fe1	C11	68.54(14)	C1	C2	C3	121.2(4)
C14	Fe1	C13	40.35(16)	C11	C9	C10	111.9(3)
C14	Fe1	C12	68.38(17)	C7	C9	C11	109.6(3)
C14	Fe1	C15	40.47(14)	C7	C9	C10	111.8(3)
C19	Fe1	C11	171.1(3)	C18	C17	Fe1	70.4(3)
C19	Fe1	C13	114.7(2)	C16	C17	Fe1	70.3(3)
C19	Fe1	C14	108.24(18)	C16	C17	C18	107.4(5)
C19	Fe1	C18	40.1(2)	C3	C4	C5	118.1(4)
C19	Fe1	C12	146.6(3)	C5	N1	C8	109.0(3)
C19	Fe1	C15	131.9(2)	C6	C7	C9	129.5(3)
C18	Fe1	C11	148.0(3)	C8	C7	C6	105.5(3)
C18	Fe1	C13	109.8(2)	C8	C7	C9	124.6(3)
C18	Fe1	C14	132.2(3)	C4	C3	C2	120.5(4)
C18	Fe1	C12	116.3(2)	C13	C14	Fe1	69.9(2)
C18	Fe1	C15	170.9(3)	C13	C14	C15	108.3(4)
C12	Fe1	C11	41.03(16)	C15	C14	Fe1	70.6(2)
C12	Fe1	C15	68.12(15)	C6	C1	Br1	121.6(3)
C16	Fe1	C11	111.34(18)	C2	C1	Br1	117.4(3)
C16	Fe1	C13	173.7(3)	C2	C1	C6	120.9(4)
C16	Fe1	C14	145.9(3)	C18	C19	Fe1	70.0(3)
C16	Fe1	C19	66.3(2)	C20	C19	Fe1	70.1(3)

C16	Fe1	C18	66.6(2)	C20	C19	C18	107.1(5)
C16	Fe1	C12	135.2(2)	C17	C18	Fe1	69.7(3)
C16	Fe1	C15	116.6(2)	C17	C18	C19	107.6(5)
C20	Fe1	C11	133.9(2)	C19	C18	Fe1	69.8(3)
C20	Fe1	C13	145.3(3)	C11	C12	Fe1	70.1(2)
C20	Fe1	C17	66.3(2)	C13	C12	Fe1	69.5(2)
C20	Fe1	C14	115.0(2)	C13	C12	C11	107.9(4)
C20	Fe1	C19	39.0(2)	C7	C8	N1	111.0(3)
C20	Fe1	C18	66.1(2)	C17	C16	Fe1	69.8(3)
C20	Fe1	C12	173.5(3)	C20	C16	Fe1	70.2(3)
C20	Fe1	C16	39.1(2)	C20	C16	C17	107.7(5)
C20	Fe1	C15	110.5(2)	C19	C20	Fe1	70.9(3)
C15	Fe1	C11	40.44(14)	C19	C20	C16	110.1(5)
C4	C5	C6	123.7(4)	C16	C20	Fe1	70.7(3)
N1	C5	C6	107.3(3)	C11	C15	Fe1	69.8(2)
N1	C5	C4	128.9(3)	C14	C15	Fe1	68.9(2)
C9	C11	Fe1	131.9(3)	C14	C15	C11	108.6(3)

Table 6 Torsion Angles for **zmg-10**.

A	**B**	**C**	**D**	**Angle/˚**	**A**	**B**	**C**	**D**	**Angle/˚**
Fe1	C11	C9	C10	52.8(5)	C19	Fe1	C11	C15	-33.4(13)
Fe1	C11	C9	C7	177.3(3)	C19	Fe1	C13	C14	89.5(3)
Fe1	C11	C12	C13	59.4(3)	C19	Fe1	C13	C12	-150.9(3)
Fe1	C11	C15	C14	-58.1(3)	C19	Fe1	C17	C18	37.8(3)
Fe1	C13	C14	C15	60.4(3)	C19	Fe1	C17	C16	-79.9(4)
Fe1	C13	C12	C11	-59.8(3)	C19	Fe1	C14	C13	-106.9(3)
Fe1	C17	C18	C19	-59.8(4)	C19	Fe1	C14	C15	134.2(3)
Fe1	C17	C16	C20	60.2(4)	C19	Fe1	C18	C17	-118.7(5)
Fe1	C14	C15	C11	58.6(3)	C19	Fe1	C12	C11	172.3(3)
Fe1	C19	C18	C17	59.7(4)	C19	Fe1	C12	C13	53.3(5)
Fe1	C19	C20	C16	-60.1(4)	C19	Fe1	C16	C17	82.2(3)
Fe1	C16	C20	C19	60.2(4)	C19	Fe1	C16	C20	-36.3(4)
C5	C6	C7	C9	174.0(4)	C19	Fe1	C20	C16	120.4(5)
C5	C6	C7	C8	1.0(4)	C19	Fe1	C15	C11	173.4(3)
C5	C6	C1	Br1	178.2(3)	C19	Fe1	C15	C14	-66.1(4)
C5	C6	C1	C2	-0.3(5)	C18	Fe1	C11	C9	-64.8(6)
C5	C4	C3	C2	0.9(6)	C18	Fe1	C11	C12	55.7(5)
C5	N1	C8	C7	0.2(5)	C18	Fe1	C11	C15	174.0(4)
C11	Fe1	C13	C14	-81.5(3)	C18	Fe1	C13	C14	132.7(3)
C11	Fe1	C13	C12	38.0(2)	C18	Fe1	C13	C12	-107.7(4)

C11	Fe1	C17	C18	-150.8(4)	C18	Fe1	C17	C16	-117.7(5)
C11	Fe1	C17	C16	91.5(3)	C18	Fe1	C14	C13	-68.9(4)
C11	Fe1	C14	C13	81.9(3)	C18	Fe1	C14	C15	172.3(3)
C11	Fe1	C14	C15	-36.9(2)	C18	Fe1	C19	C20	117.7(5)
C11	Fe1	C19	C18	-157.7(11)	C18	Fe1	C12	C11	-150.7(3)
C11	Fe1	C19	C20	-40.1(13)	C18	Fe1	C12	C13	90.3(4)
C11	Fe1	C18	C17	54.9(5)	C18	Fe1	C16	C17	38.2(3)
C11	Fe1	C18	C19	173.7(4)	C18	Fe1	C16	C20	-80.3(4)
C11	Fe1	C12	C13	-119.0(4)	C18	Fe1	C20	C19	-38.6(4)
C11	Fe1	C16	C17	-107.1(3)	C18	Fe1	C20	C16	81.8(4)
C11	Fe1	C16	C20	134.4(4)	C18	Fe1	C15	C11	-159.4(12)
C11	Fe1	C20	C19	172.1(3)	C18	Fe1	C15	C14	-39.0(13)
C11	Fe1	C20	C16	-67.5(4)	C18	C17	C16	Fe1	-61.0(4)
C11	Fe1	C15	C14	120.4(3)	C18	C17	C16	C20	-0.8(6)
C11	C9	C7	C6	169.4(3)	C18	C19	C20	Fe1	60.6(4)
C11	C9	C7	C8	-18.8(5)	C18	C19	C20	C16	0.5(6)
C6	C5	C4	C3	-1.4(6)	C12	Fe1	C11	C9	-120.5(5)
C6	C5	N1	C8	0.5(4)	C12	Fe1	C11	C15	118.3(3)
C6	C7	C8	N1	-0.7(4)	C12	Fe1	C13	C14	-119.6(4)
C13	Fe1	C11	C9	-158.3(4)	C12	Fe1	C17	C18	-106.1(4)
C13	Fe1	C11	C12	-37.8(3)	C12	Fe1	C17	C16	136.2(3)
C13	Fe1	C11	C15	80.4(3)	C12	Fe1	C14	C13	37.7(3)
C13	Fe1	C17	C18	-65.0(4)	C12	Fe1	C14	C15	-81.2(2)
C13	Fe1	C17	C16	177.3(3)	C12	Fe1	C19	C18	56.7(5)
C13	Fe1	C14	C15	-118.9(3)	C12	Fe1	C19	C20	174.3(4)
C13	Fe1	C19	C18	91.9(4)	C12	Fe1	C18	C17	92.2(4)
C13	Fe1	C19	C20	-150.4(4)	C12	Fe1	C18	C19	-149.1(4)
C13	Fe1	C18	C17	136.1(4)	C12	Fe1	C16	C17	-66.2(4)
C13	Fe1	C18	C19	-105.1(4)	C12	Fe1	C16	C20	175.2(3)
C13	Fe1	C12	C11	119.0(4)	C12	Fe1	C20	C19	-151.4(17)
C13	Fe1	C16	C17	-18.1(19)	C12	Fe1	C20	C16	-31(2)
C13	Fe1	C16	C20	-136.6(17)	C12	Fe1	C15	C11	-38.5(2)
C13	Fe1	C20	C19	51.9(5)	C12	Fe1	C15	C14	81.9(3)
C13	Fe1	C20	C16	172.3(4)	C12	C11	C9	C10	-40.6(5)
C13	Fe1	C15	C11	-82.7(3)	C12	C11	C9	C7	84.0(4)
C13	Fe1	C15	C14	37.7(2)	C12	C11	C15	Fe1	59.1(2)
C13	C14	C15	Fe1	-60.0(3)	C12	C11	C15	C14	1.0(4)
C13	C14	C15	C11	-1.4(4)	C12	C13	C14	Fe1	-59.3(3)
C9	C11	C12	Fe1	127.1(3)	C12	C13	C14	C15	1.2(5)
C9	C11	C12	C13	-173.4(3)	C16	Fe1	C11	C9	14.9(5)

C9	C11	C15	Fe1	-127.7(4)	C16	Fe1	C11	C12	135.4(3)
C9	C11	C15	C14	174.2(3)	C16	Fe1	C11	C15	-106.4(3)
C9	C7	C8	N1	-174.2(4)	C16	Fe1	C13	C14	-173.1(17)
C17	Fe1	C11	C9	-28.6(5)	C16	Fe1	C13	C12	-53.5(18)
C17	Fe1	C11	C12	91.8(3)	C16	Fe1	C17	C18	117.7(5)
C17	Fe1	C11	C15	-149.9(3)	C16	Fe1	C14	C13	178.6(3)
C17	Fe1	C13	C14	170.9(3)	C16	Fe1	C14	C15	59.8(4)
C17	Fe1	C13	C12	-69.6(4)	C16	Fe1	C19	C18	-81.2(4)
C17	Fe1	C14	C13	-51.4(14)	C16	Fe1	C19	C20	36.4(4)
C17	Fe1	C14	C15	-170.2(13)	C16	Fe1	C18	C17	-38.2(4)
C17	Fe1	C19	C18	-37.6(4)	C16	Fe1	C18	C19	80.5(4)
C17	Fe1	C19	C20	80.0(4)	C16	Fe1	C12	C11	-68.2(4)
C17	Fe1	C18	C19	118.7(5)	C16	Fe1	C12	C13	172.8(3)
C17	Fe1	C12	C11	-107.3(3)	C16	Fe1	C20	C19	-120.4(5)
C17	Fe1	C12	C13	133.7(3)	C16	Fe1	C15	C11	92.3(3)
C17	Fe1	C16	C20	-118.5(5)	C16	Fe1	C15	C14	-147.2(3)
C17	Fe1	C20	C19	-82.4(4)	C16	C17	C18	Fe1	60.8(4)
C17	Fe1	C20	C16	38.0(4)	C16	C17	C18	C19	1.1(6)
C17	Fe1	C15	C11	56.9(5)	C20	Fe1	C11	C9	53.6(5)
C17	Fe1	C15	C14	177.3(4)	C20	Fe1	C11	C12	174.1(3)
C17	C16	C20	Fe1	-60.0(4)	C20	Fe1	C11	C15	-67.6(4)
C17	C16	C20	C19	0.2(6)	C20	Fe1	C13	C14	56.5(5)
C10	C9	C7	C6	-66.1(5)	C20	Fe1	C13	C12	176.1(4)
C10	C9	C7	C8	105.8(4)	C20	Fe1	C17	C18	80.4(4)
C4	C5	C6	C7	176.9(3)	C20	Fe1	C17	C16	-37.2(3)
C4	C5	C6	C1	1.1(5)	C20	Fe1	C14	C13	-148.4(3)
C4	C5	N1	C8	-177.2(4)	C20	Fe1	C14	C15	92.7(3)
N1	C5	C6	C7	-0.9(4)	C20	Fe1	C19	C18	-117.7(5)
N1	C5	C6	C1	-176.7(3)	C20	Fe1	C18	C17	-81.1(4)
N1	C5	C4	C3	175.9(4)	C20	Fe1	C18	C19	37.6(4)
C7	C6	C1	Br1	4.1(6)	C20	Fe1	C12	C11	-40.8(19)
C7	C6	C1	C2	-174.4(4)	C20	Fe1	C12	C13	-159.8(18)
C3	C2	C1	Br1	-178.7(3)	C20	Fe1	C16	C17	118.5(5)
C3	C2	C1	C6	-0.2(6)	C20	Fe1	C15	C11	134.6(3)
C14	Fe1	C11	C9	158.2(4)	C20	Fe1	C15	C14	-104.9(3)
C14	Fe1	C11	C12	-81.3(2)	C20	C19	C18	Fe1	-60.6(4)
C14	Fe1	C11	C15	37.0(2)	C20	C19	C18	C17	-1.0(6)
C14	Fe1	C13	C12	119.6(4)	C15	Fe1	C11	C9	121.3(5)
C14	Fe1	C17	C18	-20.4(16)	C15	Fe1	C11	C12	-118.3(3)
C14	Fe1	C17	C16	-138.0(14)	C15	Fe1	C13	C14	-37.9(2)

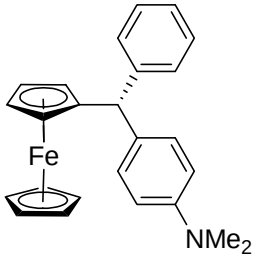
C14	Fe1	C19	C18	134.9(4)	C15	Fe1	C13	C12	81.7(3)
C14	Fe1	C19	C20	-107.5(4)	C15	Fe1	C17	C18	171.6(4)
C14	Fe1	C18	C17	176.1(4)	C15	Fe1	C17	C16	53.9(5)
C14	Fe1	C18	C19	-65.2(4)	C15	Fe1	C14	C13	118.9(3)
C14	Fe1	C12	C11	81.7(2)	C15	Fe1	C19	C18	173.6(3)
C14	Fe1	C12	C13	-37.3(3)	C15	Fe1	C19	C20	-68.8(4)
C14	Fe1	C16	C17	170.0(3)	C15	Fe1	C18	C17	-150.5(11)
C14	Fe1	C16	C20	51.4(5)	C15	Fe1	C18	C19	-31.8(14)
C14	Fe1	C20	C19	88.5(4)	C15	Fe1	C12	C11	38.0(2)
C14	Fe1	C20	C16	-151.1(4)	C15	Fe1	C12	C13	-81.0(3)
C14	Fe1	C15	C11	-120.4(3)	C15	Fe1	C16	C17	-151.2(3)
C14	C13	C12	Fe1	59.3(3)	C15	Fe1	C16	C20	90.3(4)
C14	C13	C12	C11	-0.6(5)	C15	Fe1	C20	C19	132.2(3)
C1	C6	C7	C9	-11.5(7)	C15	Fe1	C20	C16	-107.3(4)
C1	C6	C7	C8	175.5(4)	C15	C11	C9	C10	147.6(4)
C1	C2	C3	C4	-0.2(6)	C15	C11	C9	C7	-87.9(4)
C19	Fe1	C11	C9	87.8(12)	C15	C11	C12	Fe1	-59.7(2)
C19	Fe1	C11	C12	-151.7(12)	C15	C11	C12	C13	-0.3(4)

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **zmg-10**.

Atom	***x***	***y***	***z***	**U(eq)**
H13	11558	7012	3690	54
H2	2534	-1425	4441	49
H9	4831	3482	3738	36
H17	7823	5064	2487	92
H10A	6410	2977	3042	68
H10B	6445	1549	3325	68
H10C	8610	2459	3274	68
H4	7757	-664	5251	48
H3	4702	-2015	5069	53
H14	8165	8053	4043	49
H19	7718	9098	2958	86
H18	10059	7277	2564	100
H12	10757	4463	3478	46
H8	9660	3579	4418	45
H16	4108	5571	2811	86
H20	4108	8021	3095	88
H15	5275	6144	4081	39
H1	9870(60)	1800(40)	5027(11)	62(15)

Compound ent-3q

The crystal of compound **ent-3q** was obtained by leaving alone its solution in hexane and ether at room temperature in the open air for two days. The absolute configuration of compound **ent-3q** was assigned to be *R* by single crystal X-ray analysis. The crystal data of compound **ent-3q** have been deposited in CCDC with number 1000193.



ent-3q

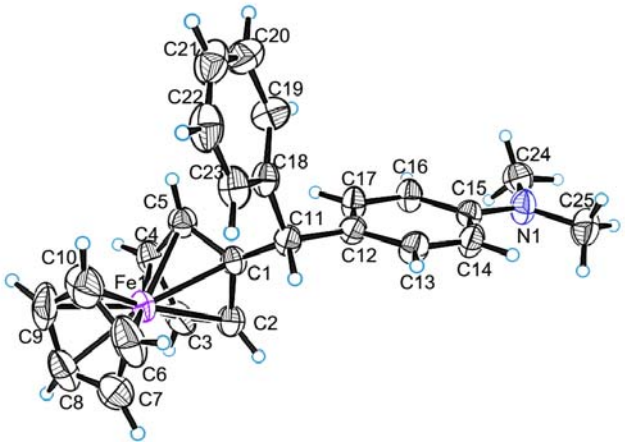


Table 1 Crystal data and structure refinement for **zmg14-3**.

Identification code	**zmg14-3**
Empirical formula	$C_{25}H_{25}FeN$
Formula weight	395.31
Temperature/K	291(2)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	6.0693(3)
b/Å	17.2089(11)
c/Å	19.2688(9)
α/°	90.00
β/°	90.00
γ/°	90.00
Volume/Å^3	2012.55(19)
Z	4
ρ_{calc}mg/mm^3	1.305

m/mm^{-1}	0.758
F(000)	832.0
Crystal size/mm^3	0.45 × 0.4 × 0.32
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection	6.78 to 52.74°
Index ranges	$-7 \le h \le 7$, $-21 \le k \le 21$, $-24 \le l \le 23$
Reflections collected	9551
Independent reflections	4126 [R_{int} = 0.0266, R_{sigma} = 0.0388]
Data/restraints/parameters	4126/0/247
Goodness-of-fit on F^2	1.036
Final R indexes [I>=2σ (I)]	R_1 = 0.0393, wR_2 = 0.0791
Final R indexes [all data]	R_1 = 0.0586, wR_2 = 0.0872
Largest diff. peak/hole / e $Å^{-3}$	0.14/-0.17
Flack parameter	-0.020(16)

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters ($Å^2$×10^3) for **zmg14-3**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Fe1	5263.7(6)	3771.9(2)	6592.29(18)	62.04(15)
N1	6426(4)	1268.1(17)	10334.2(11)	71.4(6)
C18	4504(4)	1615.4(15)	7013.6(13)	54.8(7)
C15	6271(4)	1478.4(14)	9643.7(13)	52.1(6)
C17	4437(4)	2160.6(16)	8711.8(13)	59.6(7)
C14	7816(4)	1245.6(19)	9155.6(13)	63.9(7)
C12	5960(4)	1923.5(15)	8227.6(13)	50.4(6)
C13	7635(4)	1452.6(16)	8464.0(14)	61.2(7)
C11	5855(4)	2162.9(15)	7463.8(12)	53.2(7)
C16	4552(4)	1941.2(15)	9402.1(13)	59.3(7)
C20	1201(6)	867(2)	6795.2(18)	84.1(10)
C1	5042(5)	2992.3(15)	7397.3(12)	53.6(6)
C19	2509(4)	1316.6(19)	7231.7(16)	71.4(8)
C24	4746(5)	1485.6(19)	10820.2(13)	77.1(9)
C5	2915(5)	3257.9(17)	7197.4(14)	59.7(7)
C23	5204(5)	1432.9(17)	6346.3(14)	71.5(8)
C25	8231(6)	812(2)	10581.8(17)	86.4(10)
C4	2826(6)	4074.3(19)	7275.6(17)	72.9(9)
C21	1899(7)	714(2)	6135(2)	89.7(11)
C22	3860(7)	984(2)	5910.6(17)	85.9(10)
C2	6243(5)	3660(2)	7594.3(13)	72.1(9)
C3	4882(7)	4323.8(18)	7515.9(15)	79.8(10)

C7	7894(7)	4085(3)	6000(2)	105.2(15)
C6	7269(9)	3349(3)	5833(2)	111.2(15)
C8	6141(8)	4585(3)	5877(2)	99.1(12)
C9	4407(8)	4147(4)	5634.6(19)	108.8(15)
C10	5104(10)	3370(3)	5606.8(17)	108.7(13)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for **zmg14-3**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
Fe1	68.8(2)	71.6(3)	45.7(2)	12.9(2)	-2.01(18)	-2.01(19)
N1	76.5(15)	86.7(17)	50.9(13)	14.7(15)	-3.9(11)	14.0(15)
C18	59.6(17)	58.3(15)	46.4(14)	1.9(12)	0.3(12)	16.7(13)
C15	54.9(14)	53.4(16)	48.1(15)	2.4(12)	-4.3(12)	-2.0(12)
C17	62.6(16)	69.7(18)	46.6(14)	8.0(13)	3.6(12)	23.0(13)
C14	52.9(14)	80(2)	58.8(17)	12.4(18)	-5.3(12)	14.6(15)
C12	47.2(14)	57.3(15)	46.7(15)	1.8(12)	1.3(11)	2.0(11)
C13	48.7(13)	83(2)	52.2(16)	1.8(16)	8.8(12)	12.2(12)
C11	45.4(14)	69.4(18)	44.9(15)	6.6(13)	6.7(10)	6.7(11)
C16	64.5(16)	69.5(17)	43.9(13)	2.6(13)	7.7(13)	15.4(14)
C20	77(2)	86(2)	89(3)	-14(2)	-16.3(18)	-3.3(17)
C1	59.8(16)	63.9(16)	37.2(12)	8.9(12)	-0.3(14)	-4.6(14)
C19	67.0(18)	83(2)	63.9(18)	-20.2(18)	5.6(15)	-2.3(16)
C24	83(2)	99(2)	48.9(15)	11.1(15)	2.3(16)	-10.4(18)
C5	61.4(17)	64(2)	53.5(17)	3.7(15)	3.1(14)	3.5(13)
C23	88(2)	74.2(19)	52.0(14)	1.4(14)	9.8(16)	20.3(17)
C25	97(3)	96(3)	66(2)	11.1(19)	-19.9(19)	10(2)
C4	90(2)	69(2)	60.2(19)	3.9(17)	10.3(18)	12.2(16)
C21	114(3)	78(2)	77(3)	-14(2)	-32(2)	16(2)
C22	129(3)	80(2)	48.7(18)	-10.8(17)	-10.3(19)	24(2)
C2	80.1(19)	92(3)	44.3(15)	13.1(18)	-12.0(13)	-16.3(18)
C3	122(3)	59.8(18)	57.5(18)	3.6(14)	1(2)	-17(2)
C7	84(3)	159(4)	73(3)	40(3)	15(2)	-19(3)
C6	141(4)	116(4)	77(3)	38(3)	43(3)	37(3)
C8	125(3)	98(3)	74(3)	37(2)	15(2)	1(3)
C9	102(3)	169(5)	55(2)	45(3)	-4(2)	29(3)
C10	151(4)	127(4)	47.1(18)	1(2)	1(3)	-30(4)

Table 4 Bond Lengths for **zmg14-3**.

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
Fe1	C1	2.055(2)	C17	C16	1.384(3)
Fe1	C5	2.043(3)	C14	C13	1.384(3)

Fe1	C4	2.048(3)	C12	C13	1.378(3)
Fe1	C2	2.029(3)	C12	C11	1.530(3)
Fe1	C3	2.031(3)	C11	C1	1.516(4)
Fe1	C7	2.035(3)	C20	C19	1.392(4)
Fe1	C6	2.037(4)	C20	C21	1.367(5)
Fe1	C8	2.035(3)	C1	C5	1.423(4)
Fe1	C9	2.023(3)	C1	C2	1.413(4)
Fe1	C10	2.024(4)	C5	C4	1.414(4)
N1	C15	1.382(3)	C23	C22	1.403(5)
N1	C24	1.434(3)	C4	C3	1.398(5)
N1	C25	1.430(4)	C21	C22	1.348(5)
C18	C11	1.521(4)	C2	C3	1.418(5)
C18	C19	1.381(4)	C7	C6	1.361(6)
C18	C23	1.390(3)	C7	C8	1.389(5)
C15	C14	1.387(3)	C6	C10	1.385(6)
C15	C16	1.393(3)	C8	C9	1.376(5)
C17	C12	1.375(3)	C9	C10	1.405(6)

Table 5 Bond Angles for **zmg14-3**.

Atom	**Atom**	**Atom**	**Angle/˚**	**Atom**	**Atom**	**Atom**	**Angle/˚**
C5	Fe1	C1	40.63(11)	N1	C15	C14	122.1(2)
C5	Fe1	C4	40.45(11)	N1	C15	C16	121.5(2)
C4	Fe1	C1	68.49(12)	C14	C15	C16	116.4(2)
C2	Fe1	C1	40.46(11)	C12	C17	C16	122.5(2)
C2	Fe1	C5	67.69(12)	C13	C14	C15	121.7(2)
C2	Fe1	C4	67.92(14)	C17	C12	C13	116.5(2)
C2	Fe1	C3	40.88(13)	C17	C12	C11	123.0(2)
C2	Fe1	C7	109.22(15)	C13	C12	C11	120.5(2)
C2	Fe1	C6	118.30(19)	C12	C13	C14	121.9(2)
C2	Fe1	C8	129.26(17)	C18	C11	C12	113.9(2)
C3	Fe1	C1	68.67(11)	C1	C11	C18	111.1(2)
C3	Fe1	C5	67.83(13)	C1	C11	C12	110.4(2)
C3	Fe1	C4	40.10(14)	C17	C16	C15	121.0(2)
C3	Fe1	C7	117.23(18)	C21	C20	C19	119.5(4)
C3	Fe1	C6	149.8(2)	C11	C1	Fe1	131.09(18)
C3	Fe1	C8	107.55(16)	C5	C1	Fe1	69.23(14)
C7	Fe1	C1	130.36(17)	C5	C1	C11	128.4(2)
C7	Fe1	C5	169.13(18)	C2	C1	Fe1	68.78(14)
C7	Fe1	C4	149.3(2)	C2	C1	C11	125.1(3)
C7	Fe1	C6	39.04(16)	C2	C1	C5	106.2(3)

C6	Fe1	C1	110.34(14)	C18	C19	C20	121.6(3)
C6	Fe1	C5	132.20(18)	C1	C5	Fe1	70.15(15)
C6	Fe1	C4	169.8(2)	C4	C5	Fe1	69.95(18)
C8	Fe1	C1	167.72(17)	C4	C5	C1	109.0(3)
C8	Fe1	C5	150.08(16)	C18	C23	C22	120.0(3)
C8	Fe1	C4	116.71(15)	C5	C4	Fe1	69.61(18)
C8	Fe1	C7	39.91(15)	C3	C4	Fe1	69.30(19)
C8	Fe1	C6	66.64(17)	C3	C4	C5	107.8(3)
C9	Fe1	C1	151.65(19)	C22	C21	C20	120.4(4)
C9	Fe1	C5	118.65(16)	C21	C22	C23	120.8(3)
C9	Fe1	C4	108.65(16)	C1	C2	Fe1	70.75(14)
C9	Fe1	C2	166.8(2)	C1	C2	C3	109.0(3)
C9	Fe1	C3	128.37(18)	C3	C2	Fe1	69.60(16)
C9	Fe1	C7	66.75(17)	C4	C3	Fe1	70.61(18)
C9	Fe1	C6	67.22(17)	C4	C3	C2	107.9(3)
C9	Fe1	C8	39.65(15)	C2	C3	Fe1	69.52(17)
C9	Fe1	C10	40.63(17)	C6	C7	Fe1	70.6(2)
C10	Fe1	C1	118.80(16)	C6	C7	C8	108.9(4)
C10	Fe1	C5	110.74(16)	C8	C7	Fe1	70.0(2)
C10	Fe1	C4	131.0(2)	C7	C6	Fe1	70.4(2)
C10	Fe1	C2	150.96(19)	C7	C6	C10	108.3(4)
C10	Fe1	C3	167.7(2)	C10	C6	Fe1	69.5(2)
C10	Fe1	C7	66.51(18)	C7	C8	Fe1	70.1(2)
C10	Fe1	C6	39.87(18)	C9	C8	Fe1	69.7(2)
C10	Fe1	C8	67.20(17)	C9	C8	C7	107.7(4)
C15	N1	C24	120.8(2)	C8	C9	Fe1	70.6(2)
C15	N1	C25	121.2(2)	C8	C9	C10	107.7(4)
C25	N1	C24	118.0(2)	C10	C9	Fe1	69.7(2)
C19	C18	C11	122.0(2)	C6	C10	Fe1	70.6(2)
C19	C18	C23	117.7(3)	C6	C10	C9	107.4(4)
C23	C18	C11	120.2(3)	C9	C10	Fe1	69.7(2)

Table 6 Torsion Angles for **zmg14-3**.

A	**B**	**C**	**D**	**Angle/˚**	**A**	**B**	**C**	**D**	**Angle/˚**
Fe1	C1	C5	C4	-59.4(2)	C2	Fe1	C8	C9	-169.7(2)
Fe1	C1	C2	C3	59.3(2)	C2	Fe1	C9	C8	37.0(8)
Fe1	C5	C4	C3	-58.9(2)	C2	Fe1	C9	C10	155.3(6)
Fe1	C4	C3	C2	-59.7(2)	C2	Fe1	C10	C6	-50.7(5)
Fe1	C2	C3	C4	60.4(2)	C2	Fe1	C10	C9	-168.6(3)
Fe1	C7	C6	C10	59.4(3)	C2	C1	C5	Fe1	59.09(18)

Fe1	C7	C8	C9	-59.8(3)	C2	C1	C5	C4	-0.3(3)
Fe1	C6	C10	C9	60.3(3)	C3	Fe1	C1	C11	-156.2(3)
Fe1	C8	C9	C10	-60.1(3)	C3	Fe1	C1	C5	80.4(2)
Fe1	C9	C10	C6	-60.9(3)	C3	Fe1	C1	C2	-37.5(2)
N1	C15	C14	C13	179.4(3)	C3	Fe1	C5	C1	-82.64(19)
N1	C15	C16	C17	178.7(3)	C3	Fe1	C5	C4	37.3(2)
C18	C11	C1	Fe1	-71.1(3)	C3	Fe1	C4	C5	-119.3(3)
C18	C11	C1	C5	24.0(4)	C3	Fe1	C2	C1	119.9(3)
C18	C11	C1	C2	-162.6(2)	C3	Fe1	C7	C6	155.4(3)
C18	C23	C22	C21	-1.0(5)	C3	Fe1	C7	C8	-85.0(3)
C15	C14	C13	C12	2.4(5)	C3	Fe1	C6	C7	-47.4(4)
C17	C12	C13	C14	-1.7(4)	C3	Fe1	C6	C10	-166.7(3)
C17	C12	C11	C18	-89.1(3)	C3	Fe1	C8	C7	111.7(3)
C17	C12	C11	C1	36.6(3)	C3	Fe1	C8	C9	-129.7(3)
C14	C15	C16	C17	-0.9(4)	C3	Fe1	C9	C8	69.4(3)
C12	C17	C16	C15	1.6(4)	C3	Fe1	C9	C10	-172.4(3)
C12	C11	C1	Fe1	161.6(2)	C3	Fe1	C10	C6	147.2(8)
C12	C11	C1	C5	-103.2(3)	C3	Fe1	C10	C9	29.3(10)
C12	C11	C1	C2	70.1(3)	C7	Fe1	C1	C11	-48.0(4)
C13	C12	C11	C18	91.2(3)	C7	Fe1	C1	C5	-171.4(2)
C13	C12	C11	C1	-143.0(3)	C7	Fe1	C1	C2	70.7(3)
C11	C18	C19	C20	174.7(3)	C7	Fe1	C5	C1	37.2(9)
C11	C18	C23	C22	-174.3(2)	C7	Fe1	C5	C4	157.2(8)
C11	C12	C13	C14	177.9(3)	C7	Fe1	C4	C5	-171.8(3)
C11	C1	C5	Fe1	-126.6(3)	C7	Fe1	C4	C3	-52.4(4)
C11	C1	C5	C4	174.0(3)	C7	Fe1	C2	C1	-130.4(2)
C11	C1	C2	Fe1	126.1(3)	C7	Fe1	C2	C3	109.7(3)
C11	C1	C2	C3	-174.6(2)	C7	Fe1	C3	C4	153.0(2)
C16	C15	C14	C13	-1.0(4)	C7	Fe1	C3	C2	-88.3(2)
C16	C17	C12	C13	-0.2(4)	C7	Fe1	C6	C10	-119.3(4)
C16	C17	C12	C11	-179.9(3)	C7	Fe1	C8	C9	118.6(4)
C20	C21	C22	C23	-0.8(5)	C7	Fe1	C9	C8	-37.8(3)
C1	Fe1	C5	C4	120.0(3)	C7	Fe1	C9	C10	80.5(3)
C1	Fe1	C4	C5	-37.33(19)	C7	Fe1	C10	C6	36.8(3)
C1	Fe1	C4	C3	82.02(19)	C7	Fe1	C10	C9	-81.1(3)
C1	Fe1	C2	C3	-119.9(3)	C7	C6	C10	Fe1	-59.9(3)
C1	Fe1	C3	C4	-81.5(2)	C7	C6	C10	C9	0.3(5)
C1	Fe1	C3	C2	37.17(19)	C7	C8	C9	Fe1	60.0(3)
C1	Fe1	C7	C6	71.1(3)	C7	C8	C9	C10	-0.1(5)
C1	Fe1	C7	C8	-169.3(2)	C6	Fe1	C1	C11	-8.6(3)

C1	Fe1	C6	C7	-129.7(3)	C6	Fe1	C1	C5	-131.9(2)
C1	Fe1	C6	C10	111.0(3)	C6	Fe1	C1	C2	110.1(3)
C1	Fe1	C8	C7	41.6(9)	C6	Fe1	C5	C1	70.3(3)
C1	Fe1	C8	C9	160.2(6)	C6	Fe1	C5	C4	-169.7(3)
C1	Fe1	C9	C8	-171.3(3)	C6	Fe1	C4	C5	48.1(9)
C1	Fe1	C9	C10	-53.0(5)	C6	Fe1	C4	C3	167.4(8)
C1	Fe1	C10	C6	-87.7(3)	C6	Fe1	C2	C1	-88.7(3)
C1	Fe1	C10	C9	154.4(3)	C6	Fe1	C2	C3	151.4(3)
C1	C5	C4	Fe1	59.50(19)	C6	Fe1	C3	C4	-175.6(3)
C1	C5	C4	C3	0.6(3)	C6	Fe1	C3	C2	-56.9(4)
C1	C2	C3	Fe1	-59.99(19)	C6	Fe1	C7	C8	119.6(4)
C1	C2	C3	C4	0.4(3)	C6	Fe1	C8	C7	-36.6(3)
C19	C18	C11	C12	42.6(3)	C6	Fe1	C8	C9	82.0(3)
C19	C18	C11	C1	-82.8(3)	C6	Fe1	C9	C8	-80.4(3)
C19	C18	C23	C22	2.3(4)	C6	Fe1	C9	C10	37.9(3)
C19	C20	C21	C22	1.3(5)	C6	Fe1	C10	C9	-117.9(4)
C24	N1	C15	C14	-176.9(3)	C6	C7	C8	Fe1	60.1(3)
C24	N1	C15	C16	3.5(4)	C6	C7	C8	C9	0.3(5)
C5	Fe1	C1	C11	123.4(3)	C8	Fe1	C1	C11	-82.0(7)
C5	Fe1	C1	C2	-117.9(3)	C8	Fe1	C1	C5	154.6(7)
C5	Fe1	C4	C3	119.3(3)	C8	Fe1	C1	C2	36.7(8)
C5	Fe1	C2	C1	38.45(18)	C8	Fe1	C5	C1	-169.5(3)
C5	Fe1	C2	C3	-81.4(2)	C8	Fe1	C5	C4	-49.5(4)
C5	Fe1	C3	C4	-37.64(18)	C8	Fe1	C4	C5	154.9(2)
C5	Fe1	C3	C2	81.1(2)	C8	Fe1	C4	C3	-85.8(2)
C5	Fe1	C7	C6	40.0(9)	C8	Fe1	C2	C1	-170.6(2)
C5	Fe1	C7	C8	159.6(7)	C8	Fe1	C2	C3	69.6(3)
C5	Fe1	C6	C7	-170.6(2)	C8	Fe1	C3	C4	110.9(2)
C5	Fe1	C6	C10	70.1(3)	C8	Fe1	C3	C2	-130.4(2)
C5	Fe1	C8	C7	-172.4(3)	C8	Fe1	C7	C6	-119.6(4)
C5	Fe1	C8	C9	-53.8(4)	C8	Fe1	C6	C7	37.4(3)
C5	Fe1	C9	C8	152.7(2)	C8	Fe1	C6	C10	-81.9(3)
C5	Fe1	C9	C10	-89.0(3)	C8	Fe1	C9	C10	118.3(4)
C5	Fe1	C10	C6	-131.8(3)	C8	Fe1	C10	C6	80.4(3)
C5	Fe1	C10	C9	110.2(3)	C8	Fe1	C10	C9	-37.6(3)
C5	C1	C2	Fe1	-59.37(18)	C8	C7	C6	Fe1	-59.8(3)
C5	C1	C2	C3	-0.1(3)	C8	C7	C6	C10	-0.4(5)
C5	C4	C3	Fe1	59.1(2)	C8	C9	C10	Fe1	60.7(3)
C5	C4	C3	C2	-0.6(4)	C8	C9	C10	C6	-0.1(5)
C23	C18	C11	C12	-140.8(2)	C9	Fe1	C1	C11	70.9(4)

C23	C18	C11	C1	93.8(3)	C9	Fe1	C1	C5	-52.4(4)
C23	C18	C19	C20	-1.9(4)	C9	Fe1	C1	C2	-170.4(3)
C25	N1	C15	C14	1.5(4)	C9	Fe1	C5	C1	154.6(2)
C25	N1	C15	C16	-178.1(3)	C9	Fe1	C5	C4	-85.4(3)
C4	Fe1	C1	C11	160.5(3)	C9	Fe1	C4	C5	112.6(3)
C4	Fe1	C1	C5	37.17(18)	C9	Fe1	C4	C3	-128.1(3)
C4	Fe1	C1	C2	-80.8(2)	C9	Fe1	C2	C1	159.7(6)
C4	Fe1	C5	C1	-120.0(3)	C9	Fe1	C2	C3	39.8(8)
C4	Fe1	C2	C1	82.29(19)	C9	Fe1	C3	C4	72.1(3)
C4	Fe1	C2	C3	-37.6(2)	C9	Fe1	C3	C2	-169.2(2)
C4	Fe1	C3	C2	118.7(3)	C9	Fe1	C7	C6	-82.0(3)
C4	Fe1	C7	C6	-169.6(3)	C9	Fe1	C7	C8	37.6(3)
C4	Fe1	C7	C8	-50.0(4)	C9	Fe1	C6	C7	80.7(3)
C4	Fe1	C6	C7	148.8(8)	C9	Fe1	C6	C10	-38.6(3)
C4	Fe1	C6	C10	29.5(10)	C9	Fe1	C8	C7	-118.6(4)
C4	Fe1	C8	C7	154.1(3)	C9	Fe1	C10	C6	117.9(4)
C4	Fe1	C8	C9	-87.3(3)	C10	Fe1	C1	C11	34.5(3)
C4	Fe1	C9	C8	109.7(3)	C10	Fe1	C1	C5	-88.8(3)
C4	Fe1	C9	C10	-132.1(3)	C10	Fe1	C1	C2	153.2(3)
C4	Fe1	C10	C6	-173.3(3)	C10	Fe1	C5	C1	110.5(2)
C4	Fe1	C10	C9	68.8(3)	C10	Fe1	C5	C4	-129.6(3)
C21	C20	C19	C18	0.1(5)	C10	Fe1	C4	C5	72.8(3)
C2	Fe1	C1	C11	-118.7(3)	C10	Fe1	C4	C3	-167.9(2)
C2	Fe1	C1	C5	117.9(3)	C10	Fe1	C2	C1	-54.4(4)
C2	Fe1	C5	C1	-38.30(17)	C10	Fe1	C2	C3	-174.2(4)
C2	Fe1	C5	C4	81.7(2)	C10	Fe1	C3	C4	48.1(8)
C2	Fe1	C4	C5	-81.1(2)	C10	Fe1	C3	C2	166.8(7)
C2	Fe1	C4	C3	38.29(18)	C10	Fe1	C7	C6	-37.6(3)
C2	Fe1	C3	C4	-118.7(3)	C10	Fe1	C7	C8	82.0(3)
C2	Fe1	C7	C6	111.5(3)	C10	Fe1	C6	C7	119.3(4)
C2	Fe1	C7	C8	-128.9(3)	C10	Fe1	C8	C7	-80.1(3)
C2	Fe1	C6	C7	-86.0(3)	C10	Fe1	C8	C9	38.5(3)
C2	Fe1	C6	C10	154.7(3)	C10	Fe1	C9	C8	-118.3(4)
C2	Fe1	C8	C7	71.7(3)					

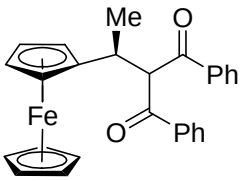
Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **zmg14-3**.

Atom	***x***	***y***	***z***	**U(eq)**
H17	3286	2480	8570	72
H14	9002	943	9297	77

H13	8675	1269	8150	73
H11	7367	2152	7286	64
H16	3465	2105	9709	71
H20	-139	672	6952	101
H19	2029	1418	7681	86
H24A	4577	2040	10818	116
H24B	5159	1316	11277	116
H24C	3378	1246	10691	116
H5	1768	2945	7041	72
H23	6564	1609	6189	86
H25A	8107	292	10405	130
H25B	8207	800	11080	130
H25C	9592	1037	10427	130
H4	1616	4389	7184	88
H21	1016	423	5838	108
H22	4326	871	5462	103
H2	7694	3664	7750	86
H3	5285	4835	7608	96
H7	9270	4229	6168	126
H6	8146	2907	5866	133
H8	6139	5120	5947	119
H9	3022	4333	5511	131
H10	4267	2947	5463	130

Compound 3s

The crystal of compound **3s** was obtained by leaving alone its solution in hexane and ether at room temperature in the open air for seven days. The absolute configuration of compound **3s** was assigned to be *S* by single crystal X-ray analysis. The crystal data of compound **3s** have been deposited in CCDC with number 1000192.



3s

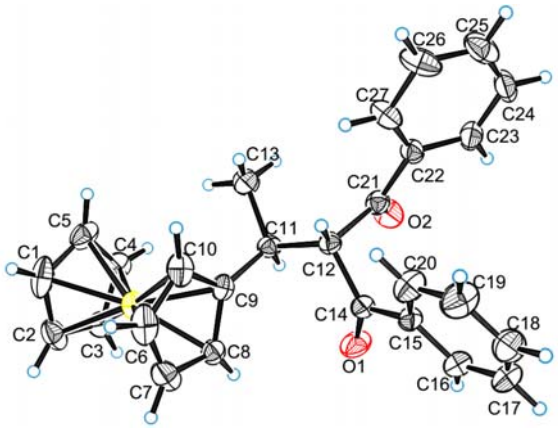


Table 1 Crystal data and structure refinement for **zmg-2**.

Identification code	**zmg-2**
Empirical formula	$C_{27}H_{24}FeO_2$
Formula weight	436.31
Temperature/K	290(2)
Crystal system	monoclinic
Space group	$P2_1$
a/Å	5.8706(2)
b/Å	24.6518(7)
c/Å	14.8502(6)
α/°	90
β/°	90.859(3)
γ/°	90
Volume/Å^3	2148.89(13)
Z	4
ρ_{calc}mg/mm^3	1.349
m/mm^{-1}	0.722

F(000)	912.0
Crystal size/mm^3	0.46 × 0.42 × 0.39
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection	6.406 to 52.742°
Index ranges	-7 ≤ h ≤ 7, -30 ≤ k ≤ 30, -18 ≤ l ≤ 15
Reflections collected	10642
Independent reflections	7298[R(int) = 0.0205]
Data/restraints/parameters	7298/2/543
Goodness-of-fit on F^2	1.055
Final R indexes [I>=2σ (I)]	R_1 = 0.0381, wR_2 = 0.0764
Final R indexes [all data]	R_1 = 0.0464, wR_2 = 0.0813
Largest diff. peak/hole / e Å^{-3}	0.33/-0.18
Flack parameter	-0.019(10)

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **zmg-2**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Fe2	-7389.1(9)	5048.4(2)	-425.9(4)	41.06(15)
Fe1	-2878.3(9)	7228.1(2)	2732.1(4)	43.26(15)
O2	2309(5)	5339.7(15)	4425(2)	66.8(9)
O1	473(6)	5410.0(14)	2408(2)	68.6(10)
O3	-5421(6)	6402.4(15)	-3684(2)	79.0(11)
O4	-3442(5)	6709.0(13)	-1775(2)	64.6(9)
C42	-7673(6)	7184.3(19)	-3549(2)	44.0(9)
C39	-7215(6)	6490.1(16)	-2258(2)	37.8(9)
C49	-6233(6)	7204.1(17)	-1002(3)	42.8(9)
C27	-2750(7)	5007(2)	5599(3)	59.9(12)
C48	-5464(6)	6794.0(16)	-1670(3)	42.5(9)
C22	-658(7)	4918.9(16)	5207(3)	42.8(10)
C12	-1342(6)	5557.1(16)	3811(3)	37.6(9)
C15	-2159(7)	4721.7(17)	2774(3)	43.0(9)
C33	-9636(7)	5573.7(18)	147(3)	51.0(11)
C11	-815(6)	6169.4(16)	3739(3)	39.4(9)
C37	-7377(8)	5701.8(18)	410(3)	51.2(11)
C47	-6520(9)	7472(2)	-4204(3)	59.3(12)
C14	-939(7)	5250.3(17)	2931(3)	43.8(10)
C9	-2425(6)	6422.2(16)	3063(3)	40.8(9)
C54	-8322(7)	7175(2)	-583(3)	57.1(12)
C38	-7064(7)	5870.7(15)	-2106(3)	41.9(9)
C41	-6689(7)	6665.1(18)	-3222(3)	46.7(10)

C34	-9798(7)	5607.0(16)	-797(3)	44(1)
C50	-4793(8)	7626.1(19)	-776(3)	58.4(12)
C35	-7621(7)	5756.2(15)	-1137(3)	36.3(9)
C16	-1171(9)	4352(2)	2198(3)	57.5(12)
C36	-6140(7)	5818.3(16)	-371(3)	42.5(9)
C26	-3461(8)	4680(3)	6304(4)	76.3(17)
C21	273(6)	5279.1(17)	4489(3)	43.0(9)
C46	-7335(10)	7958(2)	-4522(4)	76.3(16)
C8	-2038(7)	6507.5(17)	2132(3)	45.5(10)
C45	-9337(11)	8163(2)	-4204(4)	75.1(15)
C3	-485(8)	7801.9(18)	2446(3)	54.0(12)
C44	-10519(10)	7881(2)	-3587(4)	77.9(17)
C43	-9704(8)	7391(2)	-3251(3)	59.9(13)
C25	-2126(11)	4258(2)	6598(4)	77.7(16)
C53	-8931(9)	7554(2)	44(4)	72.7(15)
C20	-4186(8)	4589(2)	3177(4)	62.9(13)
C4	-412(7)	7679.3(17)	3363(3)	48.9(11)
C28	-8255(10)	4277.8(19)	-61(4)	66.2(14)
C13	-913(9)	6428(2)	4673(3)	63.1(13)
C52	-7467(11)	7975(2)	246(4)	75.4(16)
C51	-5403(11)	8014(2)	-170(4)	72.6(15)
C40	-8673(10)	5576(2)	-2757(3)	69.8(14)
C17	-2178(11)	3855(2)	2046(4)	74.6(16)
C19	-5185(9)	4091(2)	3009(4)	78.1(16)
C7	-4047(9)	6720.9(19)	1733(4)	67.4(15)
C5	-2524(9)	7791.2(19)	3722(4)	62.5(14)
C24	-52(11)	4166(2)	6213(4)	74.7(16)
C23	707(9)	4496.1(19)	5530(3)	58.6(12)
C10	-4715(7)	6588.4(17)	3231(4)	55.0(12)
C6	-5672(8)	6775(2)	2415(4)	68.6(15)
C29	-8144(11)	4317(2)	-981(5)	78.1(17)
C18	-4168(11)	3727(2)	2454(4)	78.0(16)
C32	-6172(10)	4414(2)	312(4)	72.1(16)
C1	-3968(9)	7989.0(19)	3036(5)	73.9(17)
C2	-2670(10)	7995(2)	2224(4)	67.6(15)
C30	-5940(15)	4476(2)	-1197(5)	98(2)
C31	-4696(9)	4535(2)	-383(6)	91(2)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **zmg-2**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka \times b \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe2	45.4(3)	33.7(3)	44.2(3)	5.2(3)	3.0(2)	4.1(3)
Fe1	39.4(3)	34.0(3)	56.2(4)	-0.8(3)	-5.0(2)	-4.2(3)
O2	36.8(15)	90(3)	74(2)	17.6(19)	6.0(15)	7.1(16)
O1	86(2)	62(2)	59(2)	-6.3(16)	36.8(19)	-9.7(18)
O3	105(3)	76(2)	57(2)	13.9(18)	35(2)	34(2)
O4	40.5(16)	66(2)	87(3)	-3.0(19)	10.4(15)	-4.4(15)
C42	52(2)	48(2)	32(2)	1(2)	-0.2(16)	-3(2)
C39	39.7(19)	42(2)	32(2)	0.5(17)	6.6(16)	0.8(17)
C49	46(2)	37(2)	45(2)	2(2)	-8.5(16)	2(2)
C27	52(2)	72(3)	56(3)	24(3)	-1(2)	-1(3)
C48	41(2)	37(2)	50(3)	9.4(18)	7.0(17)	-2.0(18)
C22	49(2)	40(2)	40(2)	0.4(17)	-6.0(17)	1.2(18)
C12	37.5(19)	38(2)	37(2)	-0.1(17)	5.3(16)	0.9(17)
C15	50(2)	42(2)	37(2)	-3.8(17)	-5.0(17)	7.4(19)
C33	54(2)	46(3)	53(3)	4(2)	18(2)	10(2)
C11	42(2)	40(2)	37(2)	-0.4(17)	5.4(16)	-4.4(17)
C37	74(3)	44(2)	36(2)	-0.5(19)	-5(2)	7(2)
C47	78(3)	56(3)	44(3)	7(2)	8(2)	-1(2)
C14	48(2)	45(2)	39(2)	-0.4(18)	4.3(19)	7.4(19)
C9	39(2)	31(2)	52(3)	-3.9(18)	-0.4(18)	-6.8(17)
C54	51(2)	65(3)	55(3)	-19(2)	0.7(19)	0(2)
C38	53(2)	34(2)	39(2)	-2.9(17)	4.5(18)	5.7(18)
C41	48(2)	53(3)	39(2)	1(2)	10.1(19)	5(2)
C34	41(2)	41(2)	49(3)	2.0(19)	-3.5(18)	5.5(19)
C50	72(3)	48(3)	55(3)	8(2)	-9(2)	-16(2)
C35	44(2)	29(2)	35(2)	1.1(16)	0.0(16)	1.4(17)
C16	71(3)	55(3)	46(3)	-8(2)	5(2)	6(3)
C36	42(2)	36(2)	49(3)	1.2(19)	-2.3(18)	-3.1(18)
C26	60(3)	114(5)	55(3)	26(3)	0(2)	-23(3)
C21	39(2)	46(2)	45(2)	-2.0(19)	2.7(17)	4.9(18)
C46	106(4)	71(4)	52(3)	16(3)	8(3)	-12(3)
C8	51(2)	38(2)	48(3)	-3.5(19)	-5(2)	-3(2)
C45	111(5)	54(3)	60(3)	16(3)	-14(3)	11(3)
C3	61(3)	45(3)	57(3)	-1(2)	5(2)	-16(2)
C44	76(3)	78(4)	80(4)	18(3)	-1(3)	25(3)
C43	57(3)	61(3)	62(3)	18(2)	5(2)	3(2)
C25	106(4)	64(4)	63(4)	21(3)	-7(3)	-34(3)
C53	72(3)	85(4)	61(3)	-24(3)	1(3)	14(3)
C20	55(3)	62(3)	72(3)	-15(3)	6(2)	-4(2)

C4	52(2)	42(2)	53(3)	-5(2)	-8(2)	-12(2)
C28	80(4)	35(3)	84(4)	8(2)	17(3)	1(3)
C13	91(3)	48(3)	50(3)	-6(2)	-6(2)	-1(3)
C52	115(5)	56(3)	54(3)	-14(3)	-11(3)	18(3)
C51	113(5)	43(3)	61(3)	-4(2)	-22(3)	-16(3)
C40	112(4)	52(3)	45(3)	-7(2)	-8(3)	-13(3)
C17	111(5)	58(3)	55(3)	-20(3)	-2(3)	9(3)
C19	76(3)	74(4)	85(4)	-16(3)	8(3)	-27(3)
C7	90(4)	48(3)	63(3)	0(2)	-36(3)	-16(3)
C5	78(3)	41(3)	69(3)	-15(2)	21(3)	-15(2)
C24	125(5)	35(3)	64(4)	8(2)	-25(3)	5(3)
C23	75(3)	42(3)	59(3)	-5(2)	-6(2)	11(2)
C10	40(2)	42(3)	83(4)	4(2)	4(2)	-12(2)
C6	42(2)	47(3)	115(5)	-2(3)	-22(3)	-7(2)
C29	106(5)	41(3)	86(5)	-14(3)	-16(4)	9(3)
C18	108(5)	55(3)	70(4)	-10(3)	-14(3)	-17(3)
C32	81(4)	51(3)	84(4)	18(3)	-16(3)	19(3)
C1	49(3)	37(3)	136(6)	-11(3)	-3(3)	2(2)
C2	87(4)	42(3)	73(4)	11(2)	-24(3)	-7(3)
C30	166(7)	44(3)	87(4)	12(3)	70(4)	46(4)
C31	51(3)	49(3)	172(6)	24(4)	20(4)	18(3)

Table 4 Bond Lengths for **zmg-2**.

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
Fe2	C33	2.043(4)	C15	C16	1.384(6)
Fe2	C37	2.034(4)	C15	C20	1.379(6)
Fe2	C34	2.044(4)	C33	C37	1.413(6)
Fe2	C35	2.043(4)	C33	C34	1.406(6)
Fe2	C36	2.036(4)	C11	C9	1.503(6)
Fe2	C28	2.042(5)	C11	C13	1.528(6)
Fe2	C29	2.029(5)	C37	C36	1.407(6)
Fe2	C32	2.033(5)	C47	C46	1.373(7)
Fe2	C30	2.013(5)	C9	C8	1.421(6)
Fe2	C31	2.025(5)	C9	C10	1.431(5)
Fe1	C9	2.063(4)	C54	C53	1.372(6)
Fe1	C8	2.051(4)	C38	C35	1.508(5)
Fe1	C3	2.043(4)	C38	C40	1.525(6)
Fe1	C4	2.042(4)	C34	C35	1.429(5)
Fe1	C7	2.050(5)	C50	C51	1.364(7)
Fe1	C5	2.030(5)	C35	C36	1.430(5)

Fe1	C10	2.055(4)	C16	C17	1.377(7)
Fe1	C6	2.034(4)	C26	C25	1.370(8)
Fe1	C1	2.035(5)	C46	C45	1.369(7)
Fe1	C2	2.040(5)	C8	C7	1.413(6)
O2	C21	1.210(4)	C45	C44	1.350(7)
O1	C14	1.210(5)	C3	C4	1.394(6)
O3	C41	1.208(5)	C3	C2	1.403(7)
O4	C48	1.218(4)	C44	C43	1.389(7)
C42	C47	1.388(6)	C25	C24	1.372(7)
C42	C41	1.483(6)	C53	C52	1.378(8)
C42	C43	1.376(6)	C20	C19	1.382(7)
C39	C48	1.534(6)	C4	C5	1.385(6)
C39	C38	1.546(5)	C28	C29	1.372(8)
C39	C41	1.530(5)	C28	C32	1.376(7)
C49	C48	1.491(6)	C52	C51	1.372(8)
C49	C54	1.385(5)	C17	C18	1.361(7)
C49	C50	1.379(6)	C19	C18	1.363(8)
C27	C22	1.384(5)	C7	C6	1.408(7)
C27	C26	1.390(6)	C5	C1	1.402(8)
C22	C21	1.497(5)	C24	C23	1.380(7)
C22	C23	1.395(6)	C10	C6	1.406(7)
C12	C11	1.545(5)	C29	C30	1.394(9)
C12	C14	1.531(5)	C32	C31	1.390(8)
C12	C21	1.534(5)	C1	C2	1.437(8)
C15	C14	1.504(6)	C30	C31	1.411(9)

Table 5 Bond Angles for **zmg-2**.

Atom	**Atom**	**Atom**	**Angle/˚**	**Atom**	**Atom**	**Atom**	**Angle/˚**
C33	Fe2	C34	40.25(17)	C14	C12	C11	112.9(3)
C37	Fe2	C33	40.56(17)	C14	C12	C21	103.8(3)
C37	Fe2	C34	68.11(17)	C21	C12	C11	111.1(3)
C37	Fe2	C35	68.81(17)	C16	C15	C14	117.7(4)
C37	Fe2	C36	40.44(16)	C20	C15	C14	123.4(4)
C37	Fe2	C28	125.0(2)	C20	C15	C16	119.0(4)
C35	Fe2	C33	68.61(16)	C37	C33	Fe2	69.4(2)
C35	Fe2	C34	40.93(15)	C34	C33	Fe2	69.9(2)
C36	Fe2	C33	68.08(17)	C34	C33	C37	108.2(4)
C36	Fe2	C34	68.29(16)	C9	C11	C12	109.1(3)
C36	Fe2	C35	41.05(15)	C9	C11	C13	113.6(4)
C36	Fe2	C28	161.4(2)	C13	C11	C12	109.5(3)

C28	Fe2	C33	108.3(2)	C33	C37	Fe2	70.1(3)
C28	Fe2	C34	121.6(2)	C36	C37	Fe2	69.9(2)
C28	Fe2	C35	156.5(2)	C36	C37	C33	108.2(4)
C29	Fe2	C33	126.4(2)	C46	C47	C42	121.1(5)
C29	Fe2	C37	161.9(2)	O1	C14	C12	120.2(4)
C29	Fe2	C34	110.1(2)	O1	C14	C15	120.8(4)
C29	Fe2	C35	122.5(2)	C15	C14	C12	118.8(3)
C29	Fe2	C36	157.1(2)	C11	C9	Fe1	129.5(3)
C29	Fe2	C28	39.4(2)	C8	C9	Fe1	69.3(2)
C29	Fe2	C32	66.9(2)	C8	C9	C11	127.1(3)
C32	Fe2	C33	119.2(2)	C8	C9	C10	106.9(4)
C32	Fe2	C37	106.4(2)	C10	C9	Fe1	69.4(2)
C32	Fe2	C34	154.1(2)	C10	C9	C11	125.8(4)
C32	Fe2	C35	162.9(2)	C53	C54	C49	120.7(5)
C32	Fe2	C36	124.9(2)	C35	C38	C39	108.2(3)
C32	Fe2	C28	39.5(2)	C35	C38	C40	112.0(4)
C30	Fe2	C33	164.1(3)	C40	C38	C39	110.2(3)
C30	Fe2	C37	154.8(3)	O3	C41	C42	121.1(4)
C30	Fe2	C34	127.9(3)	O3	C41	C39	121.0(4)
C30	Fe2	C35	109.2(2)	C42	C41	C39	117.8(3)
C30	Fe2	C36	121.4(2)	C33	C34	Fe2	69.8(2)
C30	Fe2	C28	67.0(2)	C33	C34	C35	108.6(4)
C30	Fe2	C29	40.3(3)	C35	C34	Fe2	69.5(2)
C30	Fe2	C32	67.6(3)	C51	C50	C49	121.6(5)
C30	Fe2	C31	40.9(3)	C38	C35	Fe2	129.8(3)
C31	Fe2	C33	153.1(3)	C34	C35	Fe2	69.6(2)
C31	Fe2	C37	118.7(3)	C34	C35	C38	126.4(4)
C31	Fe2	C34	165.0(2)	C34	C35	C36	106.4(3)
C31	Fe2	C35	126.6(2)	C36	C35	Fe2	69.2(2)
C31	Fe2	C36	107.5(2)	C36	C35	C38	127.0(4)
C31	Fe2	C28	66.9(2)	C17	C16	C15	120.3(5)
C31	Fe2	C29	67.9(3)	C37	C36	Fe2	69.7(2)
C31	Fe2	C32	40.1(2)	C37	C36	C35	108.6(4)
C8	Fe1	C9	40.41(16)	C35	C36	Fe2	69.7(2)
C8	Fe1	C10	67.85(18)	C25	C26	C27	120.2(5)
C3	Fe1	C9	129.02(17)	O2	C21	C22	120.1(4)
C3	Fe1	C8	109.81(19)	O2	C21	C12	119.6(4)
C3	Fe1	C7	119.7(2)	C22	C21	C12	120.3(3)
C3	Fe1	C10	166.54(19)	C45	C46	C47	120.0(5)
C4	Fe1	C9	109.10(17)	C9	C8	Fe1	70.2(2)

C4	Fe1	C8	119.85(18)	C7	C8	Fe1	69.8(3)
C4	Fe1	C3	39.90(17)	C7	C8	C9	108.6(4)
C4	Fe1	C7	153.0(2)	C44	C45	C46	119.8(5)
C4	Fe1	C10	128.7(2)	C4	C3	Fe1	70.0(2)
C7	Fe1	C9	68.02(18)	C4	C3	C2	108.6(4)
C7	Fe1	C8	40.30(18)	C2	C3	Fe1	69.8(3)
C7	Fe1	C10	67.7(2)	C45	C44	C43	120.9(5)
C5	Fe1	C9	118.3(2)	C42	C43	C44	120.1(4)
C5	Fe1	C8	152.2(2)	C26	C25	C24	120.0(5)
C5	Fe1	C3	67.27(19)	C54	C53	C52	119.6(5)
C5	Fe1	C4	39.77(18)	C15	C20	C19	119.9(5)
C5	Fe1	C7	166.0(2)	C3	C4	Fe1	70.1(2)
C5	Fe1	C10	108.2(2)	C5	C4	Fe1	69.7(3)
C5	Fe1	C6	128.1(2)	C5	C4	C3	108.6(4)
C5	Fe1	C1	40.4(2)	C29	C28	Fe2	69.8(3)
C5	Fe1	C2	68.2(2)	C29	C28	C32	109.1(5)
C10	Fe1	C9	40.66(15)	C32	C28	Fe2	69.9(3)
C6	Fe1	C9	68.09(18)	C51	C52	C53	120.4(5)
C6	Fe1	C8	67.78(19)	C50	C51	C52	119.4(5)
C6	Fe1	C3	152.5(2)	C18	C17	C16	120.1(5)
C6	Fe1	C4	165.7(2)	C18	C19	C20	120.4(5)
C6	Fe1	C7	40.3(2)	C8	C7	Fe1	69.9(3)
C6	Fe1	C10	40.2(2)	C6	C7	Fe1	69.2(3)
C6	Fe1	C1	107.6(2)	C6	C7	C8	107.7(5)
C6	Fe1	C2	118.4(2)	C4	C5	Fe1	70.6(3)
C1	Fe1	C9	151.0(2)	C4	C5	C1	108.9(5)
C1	Fe1	C8	166.7(2)	C1	C5	Fe1	70.0(3)
C1	Fe1	C3	68.11(19)	C25	C24	C23	120.5(5)
C1	Fe1	C4	67.6(2)	C24	C23	C22	120.2(5)
C1	Fe1	C7	128.3(2)	C9	C10	Fe1	70.0(2)
C1	Fe1	C10	117.3(2)	C6	C10	Fe1	69.1(3)
C1	Fe1	C2	41.3(2)	C6	C10	C9	107.9(4)
C2	Fe1	C9	166.5(2)	C7	C6	Fe1	70.5(3)
C2	Fe1	C8	128.7(2)	C10	C6	Fe1	70.7(2)
C2	Fe1	C3	40.20(19)	C10	C6	C7	108.8(4)
C2	Fe1	C4	67.6(2)	C28	C29	Fe2	70.8(3)
C2	Fe1	C7	108.6(2)	C28	C29	C30	107.9(6)
C2	Fe1	C10	151.6(2)	C30	C29	Fe2	69.2(3)
C47	C42	C41	118.6(4)	C17	C18	C19	120.3(5)
C43	C42	C47	118.0(4)	C28	C32	Fe2	70.6(3)

C43	C42	C41	123.4(4)	C28	C32	C31	108.3(6)
C48	C39	C38	111.3(3)	C31	C32	Fe2	69.7(3)
C41	C39	C48	104.6(3)	C5	C1	Fe1	69.6(3)
C41	C39	C38	113.8(3)	C5	C1	C2	106.9(4)
C54	C49	C48	122.8(4)	C2	C1	Fe1	69.6(3)
C50	C49	C48	118.9(4)	C3	C2	Fe1	70.0(3)
C50	C49	C54	118.3(4)	C3	C2	C1	107.0(5)
C22	C27	C26	120.2(5)	C1	C2	Fe1	69.2(3)
O4	C48	C39	119.3(4)	C29	C30	Fe2	70.4(3)
O4	C48	C49	120.4(4)	C29	C30	C31	107.5(5)
C49	C48	C39	120.2(3)	C31	C30	Fe2	70.0(3)
C27	C22	C21	122.8(4)	C32	C31	Fe2	70.3(3)
C27	C22	C23	118.8(4)	C32	C31	C30	107.1(5)
C23	C22	C21	118.3(4)	C30	C31	Fe2	69.1(3)

Table 6 Torsion Angles for **zmg-2**.

A	**B**	**C**	**D**	**Angle/˚**	**A**	**B**	**C**	**D**	**Angle/˚**
Fe2	C33	C37	C36	59.7(3)	C38	C39	C48	O4	61.9(5)
Fe2	C33	C34	C35	-58.8(3)	C38	C39	C48	C49	-120.3(4)
Fe2	C37	C36	C35	59.1(3)	C38	C39	C41	O3	-28.7(6)
Fe2	C34	C35	C38	125.0(4)	C38	C39	C41	C42	155.0(4)
Fe2	C34	C35	C36	-59.7(3)	C38	C35	C36	Fe2	-124.8(4)
Fe2	C35	C36	C37	-59.0(3)	C38	C35	C36	C37	176.2(4)
Fe2	C28	C29	C30	59.5(4)	C41	C42	C47	C46	-179.1(4)
Fe2	C28	C32	C31	-59.7(4)	C41	C42	C43	C44	179.9(5)
Fe2	C29	C30	C31	60.5(4)	C41	C39	C48	O4	-61.4(5)
Fe2	C32	C31	C30	-59.6(4)	C41	C39	C48	C49	116.4(4)
Fe2	C30	C31	C32	60.3(4)	C41	C39	C38	C35	-179.9(3)
Fe1	C9	C8	C7	-59.5(3)	C41	C39	C38	C40	-57.2(5)
Fe1	C9	C10	C6	58.9(3)	C34	C33	C37	Fe2	-59.3(3)
Fe1	C8	C7	C6	-59.1(3)	C34	C33	C37	C36	0.4(5)
Fe1	C3	C4	C5	-59.2(3)	C34	C35	C36	Fe2	59.9(3)
Fe1	C3	C2	C1	59.5(3)	C34	C35	C36	C37	0.9(5)
Fe1	C4	C5	C1	-59.7(3)	C50	C49	C48	O4	25.9(6)
Fe1	C7	C6	C10	-60.6(3)	C50	C49	C48	C39	-151.8(4)
Fe1	C5	C1	C2	-59.8(3)	C50	C49	C54	C53	-0.5(7)
Fe1	C10	C6	C7	60.4(3)	C16	C15	C14	O1	19.6(6)
Fe1	C1	C2	C3	-60.0(3)	C16	C15	C14	C12	-154.6(4)
C42	C47	C46	C45	-1.1(8)	C16	C15	C20	C19	0.7(7)
C39	C38	C35	Fe2	-171.8(3)	C16	C17	C18	C19	0.4(9)

C39	C38	C35	C34	95.4(5)	C26	C27	C22	C21	-175.8(5)
C39	C38	C35	C36	-79.0(5)	C26	C27	C22	C23	0.3(7)
C49	C54	C53	C52	1.4(8)	C26	C25	C24	C23	0.1(9)
C49	C50	C51	C52	2.0(7)	C21	C22	C23	C24	177.8(4)
C27	C22	C21	O2	149.5(5)	C21	C12	C11	C9	179.6(3)
C27	C22	C21	C12	-32.7(6)	C21	C12	C11	C13	-55.5(4)
C27	C22	C23	C24	1.5(7)	C21	C12	C14	O1	-91.7(5)
C27	C26	C25	C24	1.7(9)	C21	C12	C14	C15	82.5(4)
C48	C39	C38	C35	62.2(4)	C46	C45	C44	C43	1.7(9)
C48	C39	C38	C40	-175.1(3)	C8	C9	C10	Fe1	-59.4(3)
C48	C39	C41	O3	92.9(5)	C8	C9	C10	C6	-0.6(5)
C48	C39	C41	C42	-83.4(4)	C8	C7	C6	Fe1	59.5(3)
C48	C49	C54	C53	178.3(4)	C8	C7	C6	C10	-1.0(6)
C48	C49	C50	C51	179.9(4)	C45	C44	C43	C42	-0.4(9)
C22	C27	C26	C25	-1.9(8)	C3	C4	C5	Fe1	59.5(3)
C12	C11	C9	Fe1	173.3(3)	C3	C4	C5	C1	-0.2(5)
C12	C11	C9	C8	-93.8(4)	C43	C42	C47	C46	2.4(7)
C12	C11	C9	C10	81.5(5)	C43	C42	C41	O3	153.8(5)
C15	C16	C17	C18	0.8(8)	C43	C42	C41	C39	-29.9(6)
C15	C20	C19	C18	0.6(9)	C25	C24	C23	C22	-1.7(8)
C33	C37	C36	Fe2	-59.9(3)	C53	C52	C51	C50	-1.0(8)
C33	C37	C36	C35	-0.8(5)	C20	C15	C14	O1	-160.8(5)
C33	C34	C35	Fe2	59.1(3)	C20	C15	C14	C12	25.1(6)
C33	C34	C35	C38	-176.0(4)	C20	C15	C16	C17	-1.4(7)
C33	C34	C35	C36	-0.6(4)	C20	C19	C18	C17	-1.1(9)
C11	C12	C14	O1	28.7(6)	C4	C3	C2	Fe1	-59.5(3)
C11	C12	C14	C15	-157.2(3)	C4	C3	C2	C1	0.0(5)
C11	C12	C21	O2	-51.7(5)	C4	C5	C1	Fe1	60.1(3)
C11	C12	C21	C22	130.5(4)	C4	C5	C1	C2	0.2(6)
C11	C9	C8	Fe1	-124.5(4)	C28	C29	C30	Fe2	-60.5(4)
C11	C9	C8	C7	176.0(4)	C28	C29	C30	C31	-0.1(6)
C11	C9	C10	Fe1	124.5(4)	C28	C32	C31	Fe2	60.3(4)
C11	C9	C10	C6	-176.7(4)	C28	C32	C31	C30	0.7(6)
C37	C33	C34	Fe2	59.0(3)	C13	C11	C9	Fe1	50.8(5)
C37	C33	C34	C35	0.1(5)	C13	C11	C9	C8	143.7(4)
C47	C42	C41	O3	-24.7(6)	C13	C11	C9	C10	-41.0(6)
C47	C42	C41	C39	151.6(4)	C40	C38	C35	Fe2	66.6(5)
C47	C42	C43	C44	-1.6(7)	C40	C38	C35	C34	-26.2(6)
C47	C46	C45	C44	-1.0(9)	C40	C38	C35	C36	159.4(4)
C14	C12	C11	C9	63.5(4)	C5	C1	C2	Fe1	59.9(3)

C14	C12	C11	C13	-171.6(3)	C5	C1	C2	C3	-0.2(5)
C14	C12	C21	O2	69.9(5)	C23	C22	C21	O2	-26.7(6)
C14	C12	C21	C22	-107.9(4)	C23	C22	C21	C12	151.2(4)
C14	C15	C16	C17	178.3(4)	C10	C9	C8	Fe1	59.4(3)
C14	C15	C20	C19	-179.0(5)	C10	C9	C8	C7	-0.1(5)
C9	C8	C7	Fe1	59.8(3)	C29	C28	C32	Fe2	58.9(4)
C9	C8	C7	C6	0.7(5)	C29	C28	C32	C31	-0.8(6)
C9	C10	C6	Fe1	-59.4(3)	C29	C30	C31	Fe2	-60.7(4)
C9	C10	C6	C7	1.0(5)	C29	C30	C31	C32	-0.4(6)
C54	C49	C48	O4	-152.9(4)	C32	C28	C29	Fe2	-59.0(4)
C54	C49	C48	C39	29.4(6)	C32	C28	C29	C30	0.5(6)
C54	C49	C50	C51	-1.3(7)	C2	C3	C4	Fe1	59.3(3)
C54	C53	C52	C51	-0.7(8)	C2	C3	C4	C5	0.1(5)

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **zmg-2**.

Atom	***x***	***y***	***z***	**U(eq)**
H39	-8747	6614	-2107	45
H27	-3683	5286	5390	72
H12	-2922	5506	3997	45
H33	-10813	5483	531	61
H11	739	6210	3517	47
H37	-6806	5708	998	61
H47	-5173	7333	-4431	71
H54	-9323	6895	-730	69
H38	-5501	5752	-2218	50
H34	-11104	5543	-1143	53
H50	-3373	7647	-1043	70
H16	179	4439	1912	69
H36	-4614	5919	-386	51
H26	-4848	4748	6576	92
H46	-6529	8149	-4953	92
H8	-690	6435	1834	55
H45	-9880	8495	-4412	90
H3	714	7762	2049	65
H44	-11898	8017	-3385	93
H43	-10533	7203	-2823	72
H25	-2626	4035	7059	93
H53	-10322	7527	332	87
H20	-4880	4835	3561	76

H4	845	7545	3679	59
H28	-9534	4176	260	79
H13B	-2378	6360	4929	95
H13C	-677	6812	4623	95
H13A	254	6274	5054	95
H52	-7882	8235	667	90
H51	-4428	8301	-40	87
H40C	-10193	5712	-2687	105
H40A	-8646	5194	-2629	105
H40B	-8194	5636	-3364	105
H17	-1496	3606	1664	90
H19	-6559	4004	3277	94
H7	-4257	6810	1129	81
H5	-2921	7743	4320	75
H24	849	3879	6414	90
H23	2132	4436	5283	70
H10	-5441	6575	3783	66
H6	-7138	6911	2338	82
H29	-9329	4249	-1388	94
H18	-4838	3390	2352	94
H32	-5813	4423	924	86
H1	-5477	8096	3096	89
H2	-3182	8106	1657	81
H30	-5391	4534	-1774	118
H31	-3175	4636	-323	109