Supporting Information File……

Construction of Planar Chiral Ferrocenes Diketone Derivatives *via* Cascade Pd-Catalyzed Asymmetric C-H Arylation/α-Arylation Reaction

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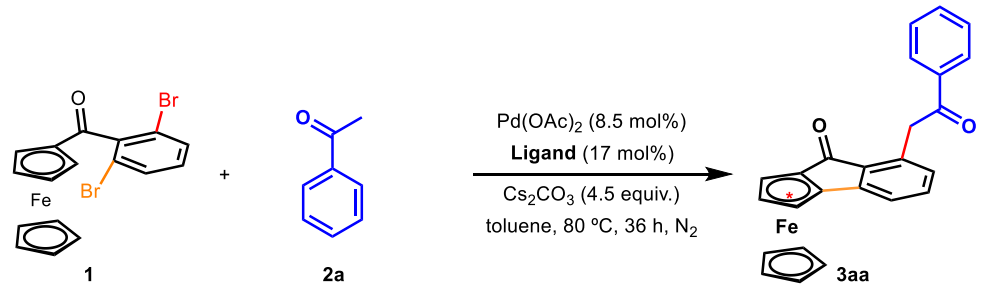
1. General information

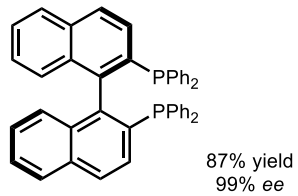
All manipulations of air- and moisture-sensitive compounds were performed under a nitrogen atmosphere by using standard Schlenk techniques or a nitrogen atmosphere in a MBRAUN LabMaster PRS314/10-164-2 glovebox. All ^{1}H NMR, ^{13}C NMR, ^{19}F NMR and ^{31}P NMR spectra were recorded on a Bruker Avance (600 MHz) instrument. The ^{1}H NMR chemical shifts were given using $CDCl_3$ as the internal standard ($CDCl_3$: δ = 7.26 ppm). The ^{13}C NMR chemical shifts were given using $CDCl_3$ as the internal standard ($CDCl_3$: δ = 77.00 ppm). The ^{31}P NMR chemical shifts were measured relative to 85% H_3PO_4 as external standard (85% H_3PO_4: δ = 0 ppm). High-resolution mass spectra (HRMS) were obtained on a Bruker QTOF mass spectrometer. Optical rotation was measured on a Anton Paar MCP100 polarimeter. Enantiomeric excess was determined by a Shimadzu LC-20A liquid chromatograph, using chiralpak® OD-H column, chiralpak® AD-H column, or chiralpak® OJ-H column with hexane and i-PrOH as solvent.

Unless otherwise noted, all reagents were obtained from commercial suppliers and used without further purification.

2. Complete optimization data

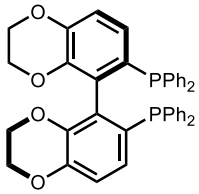
Table S2.1 Examination of ligand [a,b,c]





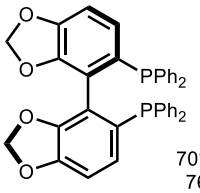
87% yield
99% *ee*

(R_a) - **L1**



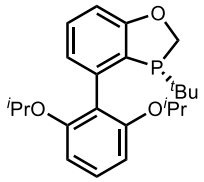
65% yield
88% *ee*

(R_a) - **L2**



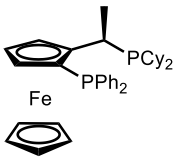
70% yield
76% *ee*

(R_a) - **L3**



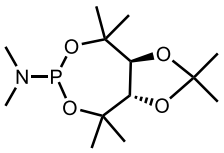
N.R.

(*R*) - **L4**



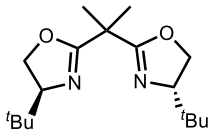
42% yield
54% *ee*

(*R*, *R*) - **L5**



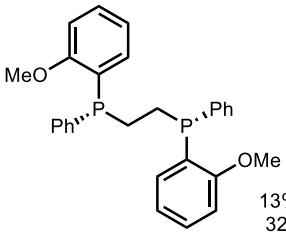
N.R.

(*R*, S_p) - **L6**



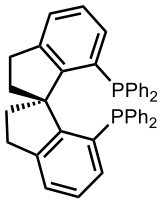
N.R.

(*S*, *S*) - **L7**



13%yield
32% *ee*

(*R*, *R*) - **L8**

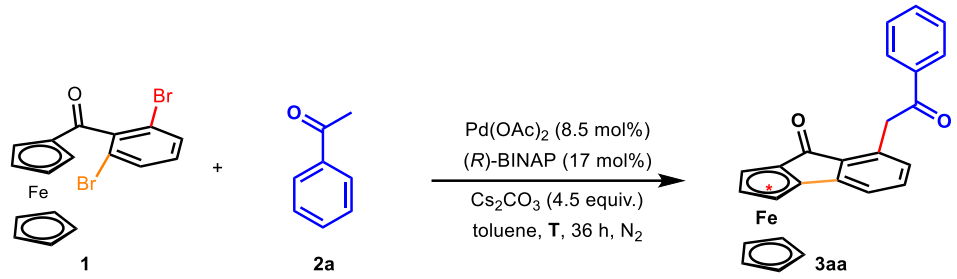


45% yield
46% *ee*

(*R*) - **L9**

[a] Reaction conditions: **1** (0.2 mmol), **2a** (0.24 mmol), $Pd(OAc)_2$ (8.5 mol%), **Ligand** (17 mol%), Cs_2CO_3 (4.5 equiv.) in toluene at 80 °C. [b] Isolated yield. [c] Determined by HPLC analysis.

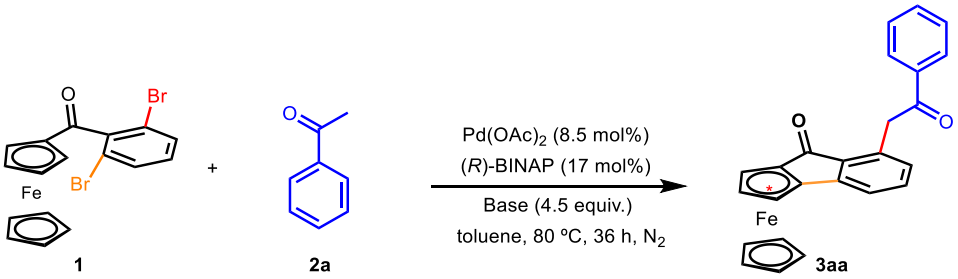
Table S2.2 Examination of reaction temperature [a]



Entry	T (ºC)	Yield[b] (%)	e.e.[c] (%)
1	40	0	-
2	60	33	99
3	80	87	99
4	100	88	88
5[d]	120	64	70
6[d]	140	24	55

[a] Reaction conditions: **1** (0.2 mmol), **2a** (0.24 mmol), $Pd(OAc)_2$ (8.5 mol%), (*R*)-BINAP (17 mol%), Cs_2CO_3 (4.5 equiv.) in toluene at T ºC. [b] Isolated yield. [c] Determined by HPLC analysis.[d] In *p*-xylene.

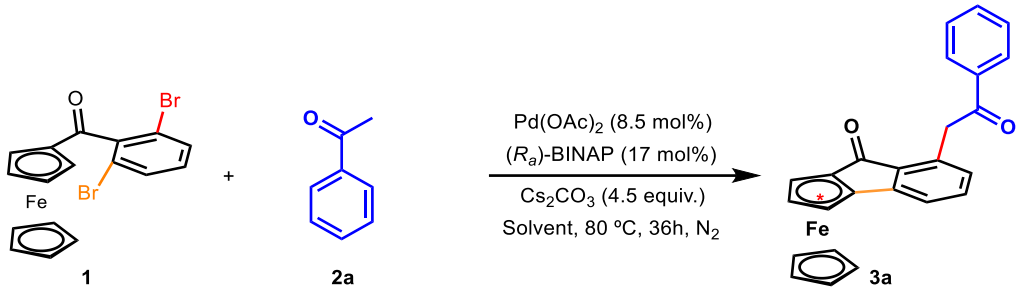
Table S2.3 Examination of base [a]



Entry	Base	Yield[b] (%)	e.e.[c] (%)
1	Cs_2CO_3	87	99
2	K_2CO_3	71	97
3	Na_2CO_3	54	98
4	K_3PO_4	66	98
5	CH_3CH_2ONa	45	95
6	$NH_2CH_2CH_2NH_2$	0	-
7	Et_3N	0	-

[a] Reaction conditions: **1** (0.2 mmol), **2a** (0.24 mmol), $Pd(OAc)_2$ (8.5 mol%), (*R*)-BINAP (17 mol%), Base (4.5 equiv.) in toluene at 80 ºC. [b] Isolated yield. [c] Determined by HPLC analysis.

Table S2.4 Examination of solvent [a]

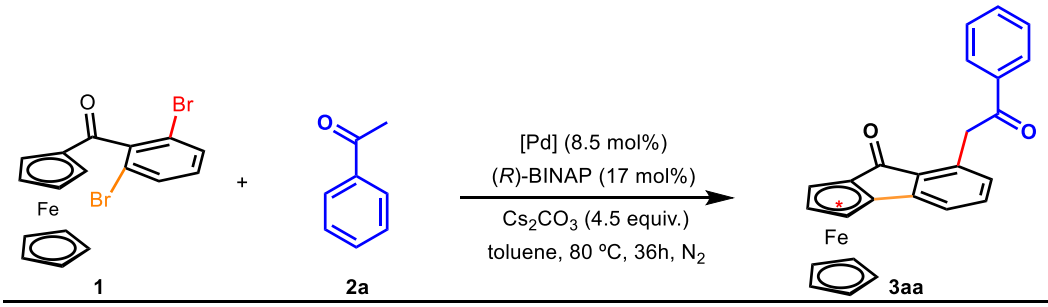


1 **2a** **3a**

Entry	Solvent	Yield[b] (%)	e.e.[c] (%)
1	toluene	87	99
2	*p*-xylene	72	97
3	DCM	46	85
4	DCE	15	70
5	MeCN	0	-

[a] Reaction conditions: **1** (0.2 mmol), **2a** (0.24 mmol), $Pd(OAc)_2$ (8.5 mol %), (R_a)-BINAP (17 mol %), Cs_2CO_3 (4.5 equiv.) in solvent at 80 °C. [b] Isolated yield. [c] Determined by HPLC analysis.

Table S2.5 Examination of palladium precursor [a]



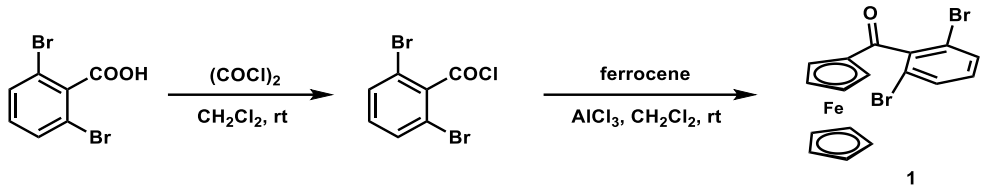
1 **2a** **3aa**

Entry	[Pd]	Yield[b] (%)	e.e.[c] (%)
1	$Pd(OAc)_2$	87	99
2	$[Pd(allyl)Cl]_2$	22	95
3	$Pd(TFA)_2$	0	-
4	$Pd_2(dba)_3$	0	-

[a] Reaction conditions: **1** (0.2 mmol), **2a** (0.24 mmol), [Pd] (8.5 mol%), (*R*)-BINAP (17 mol%), Cs_2CO_3 (4.5 equiv.) in toluene at 80 °C. [b] Isolated yield. [c] Determined by HPLC analysis.

S

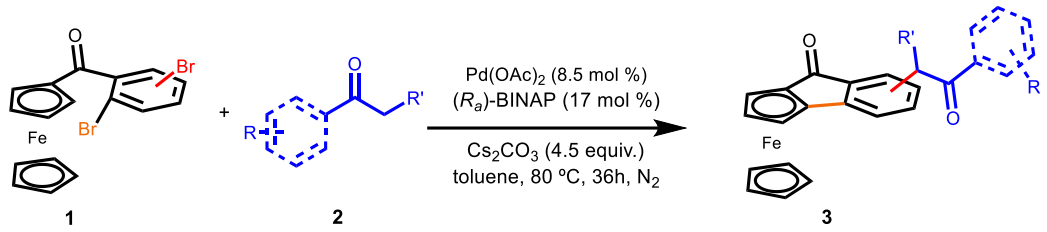
3. General procedure for preparation of substrate (1)



1

To a solution of the substituted 2,6-dibromobenzoic acid (10 mmol, 1.0 equiv.) in CH_2Cl_2 (30 mL) was added oxalyl chloride (1.7 mL, 20 mmol) and a drop of *N*,*N*-dimethylformamide. The reaction mixture was stirred at room temperature for 6-12 h. Then the solvent was removed under reduced pressure. The resulting substituted 2,6-dibromobenzoyl chloride was directly used without purification in the next step. A solution of aluminum chloride (1.40 g, 10.5 mmol) in CH_2Cl_2 (30 mL) was added dropwise to a solution of ferrocene (9.5 mmol, 0.95 equiv.) and the substituted 2,6-dibromobenzoyl chloride in CH_2Cl_2 (30 mL) at 0 ℃. The mixture was warmed to room temperature and stirred for 2 h. Then the reaction mixture was quenched with ice-cold water and extracted with CH_2Cl_2. The combined organic layers were washed with brine, dried over Na_2SO_4 and filtered. After the solvent was removed under reduced pressure, the residue was purified by silica gel column chromatography (petroleum ether/ethyl acetate = 15:1) to give **1** as a solid.

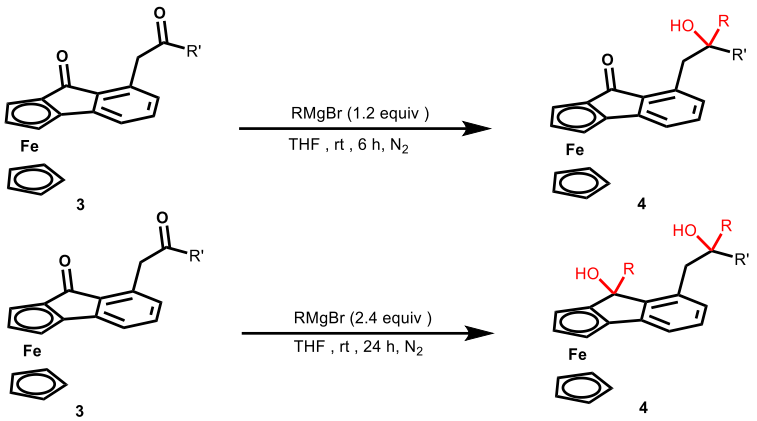
3. General procedure for preparation of substrates (3aa-3bh)



To a 10 mL Schlenk-type sealed tube, substrate **1** (0.2 mmol), **2** (0.24 mmol, 1.2 equiv.), $Pd(OAc)_2$ (3.8 mg, 0.017 mmol, 8.5 mol %), (*R*)-BINAP (21.2 mg, 0.034 mmol, 17.0 mol %), Cs_2CO_3 (293.2 mg, 0.9 mmol, 4.5 equiv.) were dissolved in toluene (5 mL) under argon and dissolved. The tube was sealed with a Teflon-lined cap, and the reaction mixture was stirred at 80 °C. After the reaction was complete (monitored by TLC), the mixture was cooled to room temperature. The reaction mixture was concentrated under reduced pressure, and the residue was purified by silica gel column chromatography (eluent: petroleum ether/ethyl acetate = 10:1) to afford the desired product **3**.

The synthesis procedure for the racemic substrate remains identical to that described above, except that (*R*)-BINAP is replaced with (*rac*)-BINAP in the experiment.

4. Synthetic applications (4aa-4ae)



At 0 °C, a solution of **3** (0.2 mmol) in THF (5 mL) was added phenylmagnesium bromide (0.24 or 0.48 mmol in 5 mL THF, prepared in situ from 1-bromobenzene and magnesium turnings). The mixture was stirred at 0 °C for 6 h, with progress monitored by thin layer chromatography (TLC). The reaction was then quenched with saturated NH_4Cl solution (30 mL). The layers were separated, and the aqueous layer was extracted with ethyl acetate (EtOAc, 3×40 mL). The combined organic layers were dried over anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (4% EtOAc in hexanes) to afford the desired oxetane **4** as a yellow solid.

5. *In-situ* ^{31}P NMR spectroscopy.

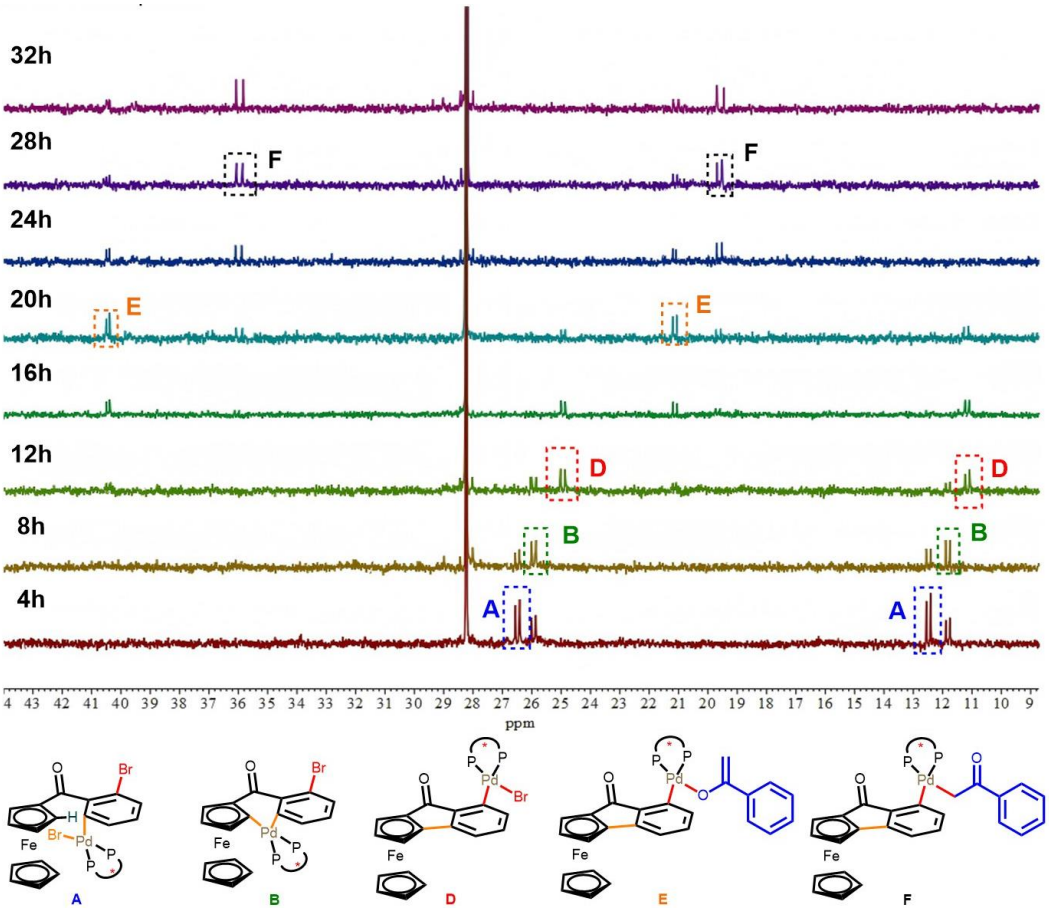


Figure S5.1. ^{31}P NMR of the mixture system (243 MHz, $CDCl_3$).

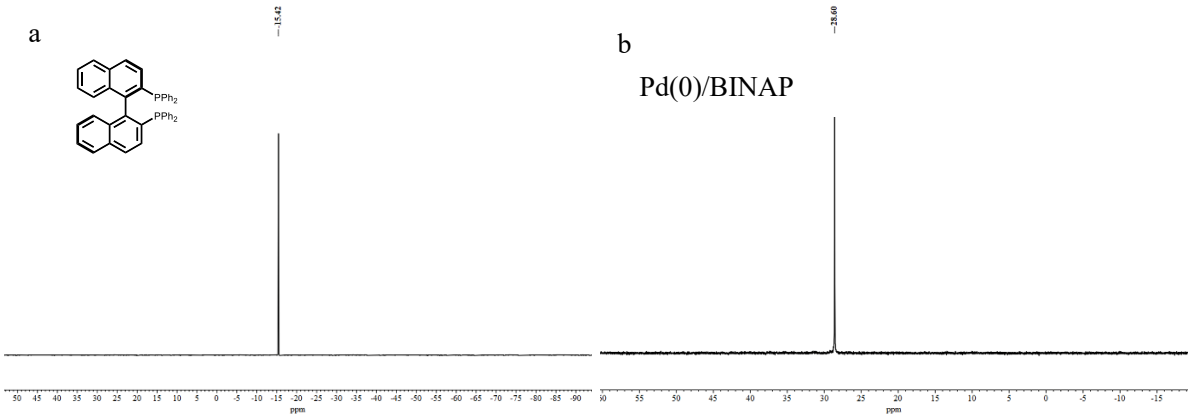
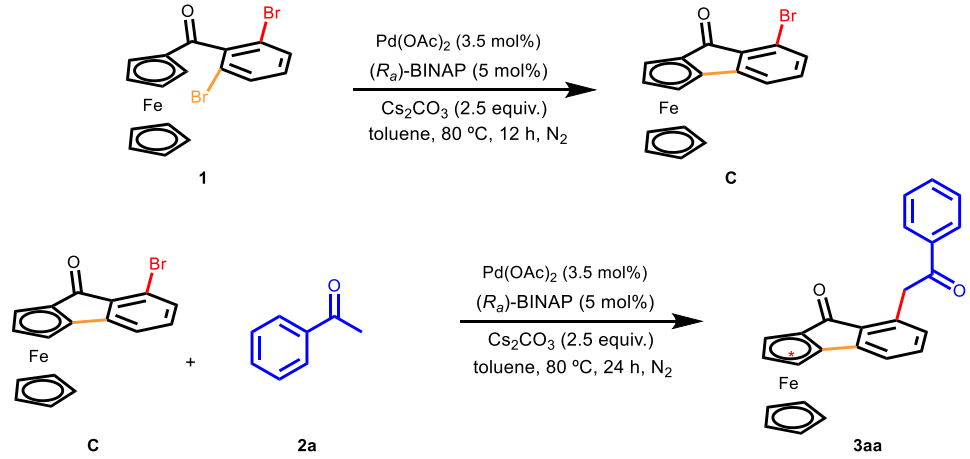


Figure S5.2. ^{31}P NMR of the intermediate of each step (243 MHz, $CDCl_3$).



We carried out *in-situ* ^{31}P NMR experiments to determine the specific peak signal of the intermediate:

(a) ^{31}P NMR of BINAP.

(b) ^{31}P NMR of Pd(0)/BINAP.

(c) The intermediates were trapped in the asymmetric C-H arylation of compound **1**, to determine intermediates **A** and **B**.

(d) The intermediates were trapped in the α-arylation of cyclization compound, to determine intermediates **D**, **E** and **F**.

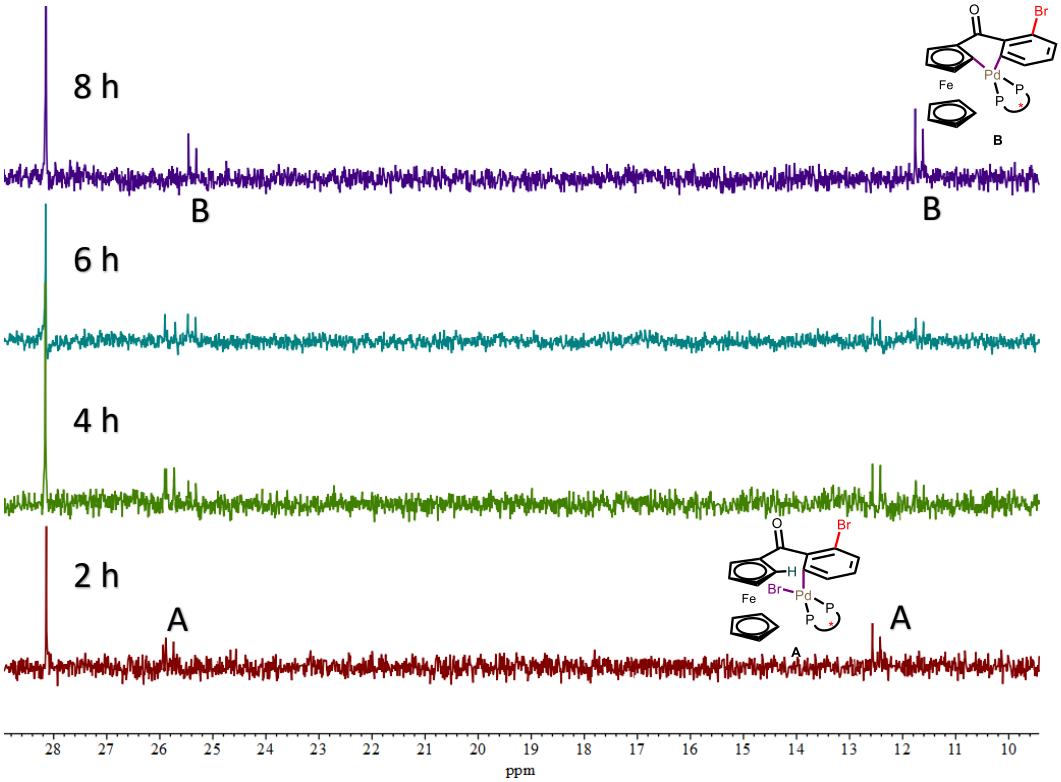


Figure S5.3. ^{31}P NMR of reaction c (243 MHz, $CDCl_3$).

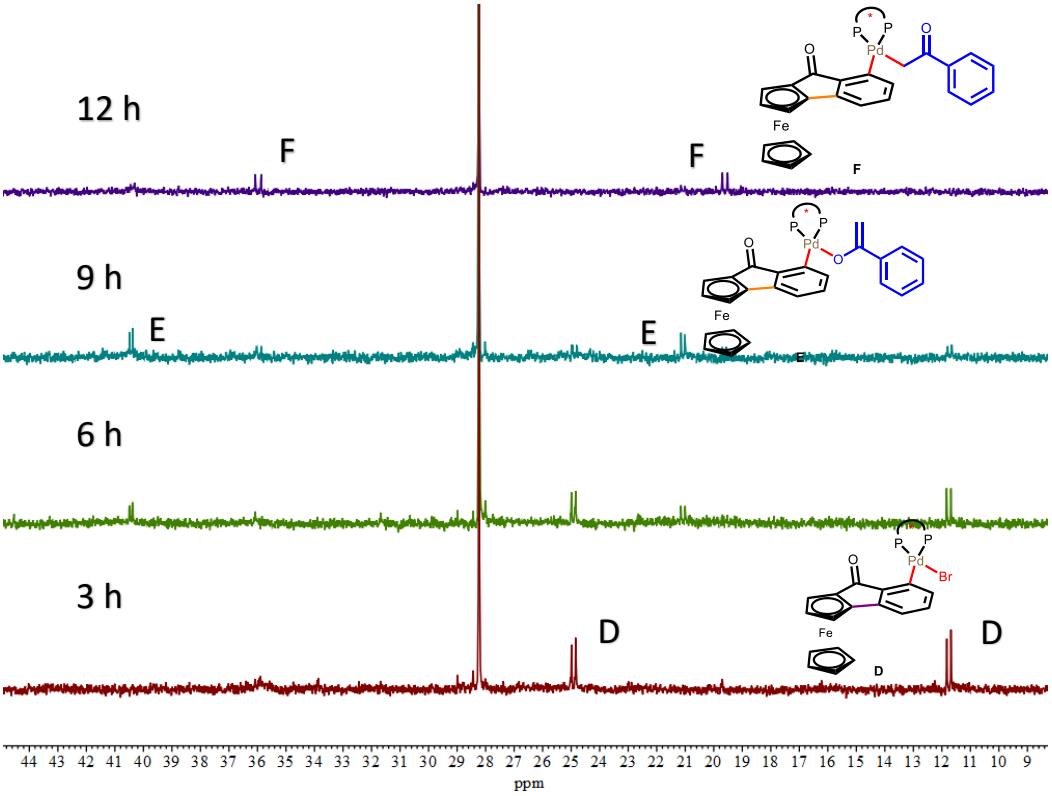
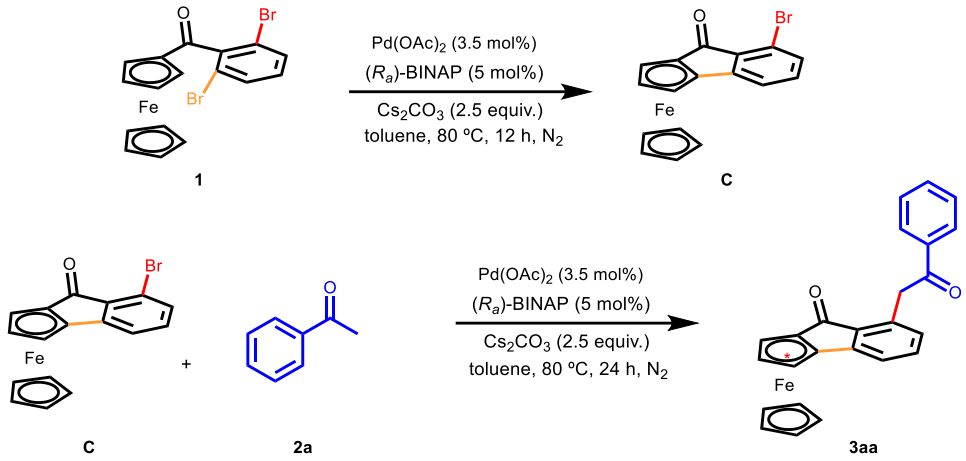


Figure S5.4. ^{31}P NMR of reaction d (243 MHz, $CDCl_3$).

6. Kinetic experiments



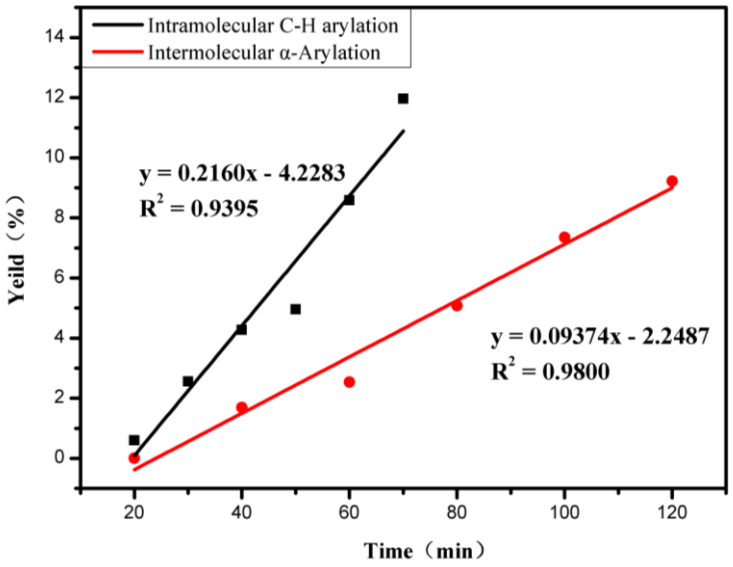
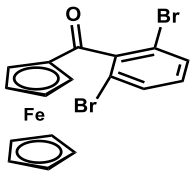


Figure S6.1. Kinetic experiment.

This cascade reaction was carried out step by step. After the appropriate time the mixture was filtered through silica gel column chromatography and concentrated in vacuo. The product yield based on ^{1}H NMR analysis of the crude reaction mixture using dibromomethane as internal standard. The yields of intramolecular C-H arylation products and intermolecular α-Arylation products over time were plotted respectively, and the corresponding slopes (K values) were obtained. As shown in the figure, K_1 is 2.30 times that of K_2, suggesting that in this cascade reaction, the rate of intramolecular C-H arylation reaction is higher than that of intermolecular α-Arylation reaction. In other words, C-H arylation happens first followed by coupling.

7. Characterization data

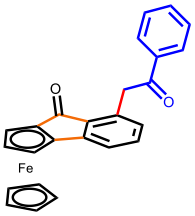
Compound 1



The resultant residue was purified by flash silica gel column chromatography to afford **1** as a red solid; 2.93 g, 69% yield; (eluent: petroleum ether/ethyl acetate: 15:1) m.p. = 149.9-151.7 ℃.

^{1}H NMR (600 MHz, DMSO-d_6) δ 7.72 (d, J = 7.6 Hz, 2H), 7.31 (t, J = 7.9 Hz, 1H), 4.74 – 4.64 (m, 2H), 4.59 – 4.49 (m, 2H), 4.34 (s, 5H). **^{13}C NMR** (151 MHz, DMSO-d_6) δ 198.2, 141.0, 132.1, 131. 9, 119.4, 78.6, 72.3, 70.1. **HRMS** (ESI-TOF) m/z: $[M]^+$ calcd for $C_{17}H_{12}Br_2FeO$ 445.8599; Found: 445.8591.

Compound 3aa



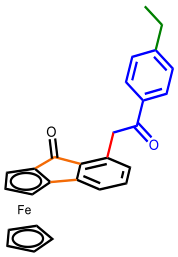
The resultant residue was purified by flash silica gel column chromatography to afford **3aa** as a red solid; 55.1 mg, 87% yield; (eluent: petroleum ether/ethyl acetate: 30:1); 99% *e.e.*.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.12 – 8.07 (m, 2H), 7.56 (t, J = 7.4 Hz, 1H), 7.48 (t, J = 7.6 Hz, 2H), 7.27 – 7.21 (m, 1H), 7.08 (d, J = 7.4 Hz, 1H), 6.90 (d, J = 7.7 Hz, 1H), 4.96 (d, J = 16.4 Hz, 1H), 4.90 (d, J = 2.3 Hz, 1H), 4.86 (d, J = 2.3 Hz, 1H), 4.80 (t, J

= 2.4 Hz, 1H), 4.43 (d, *J* = 16.4 Hz, 1H), 4.14 (s, 5H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 197.2, 195.8, 144.1, 137.3, 137.3, 134.0, 132.9, 132.84, 129.5, 128.6, 128.4, 119.1, 89.7, 78.4, 77.2, 77.0, 76.8, 75.0, 73.0, 66.2, 66.2, 40.9. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{25}H_{18}FeO_2Na$ 429.0548; Found: 429.0549.

The e.e. value was determined by the chiral HPLC analysis (chiralpak® AD-H, Hexane / IPA = 90 / 10, 1.0 mL / min, λ= 254 nm, $t_{(minor)}$ = 5.807 min, $t_{(major)}$ = 6.988 min).

Compound 3ab

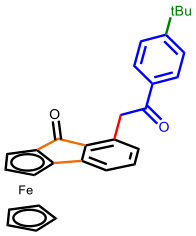


The resultant residue was purified by flash silica gel column chromatography to afford **3ab** as a red solid; 57.6 mg, 85% yield; (eluent: petroleum ether/ethyl acetate: 30:1); 97% *e.e.*.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.3 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 7.27 – 7.20 (m, 1H), 7.09 – 7.05 (m, 1H), 6.91 (d, *J* = 7.7 Hz, 1H), 4.94 (d, *J* = 16.3 Hz, 1H), 4.90 (d, *J* = 2.4 Hz, 1H), 4.86 (d, *J* = 2.4 Hz, 1H), 4.80 (t, *J* = 2.4 Hz, 1H), 4.43 (d, *J* = 16.3 Hz, 1H), 4.15 (s, 5H), 2.71 (q, *J* = 7.6 Hz, 2H), 1.25 (t, *J* = 7.6 Hz, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 196.9, 195.9, 149.8, 144.1, 137.2, 135.0, 134.2, 132.8, 129.5, 128.7, 128.1, 119.0, 89.8, 78.4, 77.3, 77.1, 76.9, 75.0, 73.5, 73.0, 66.2, 66.1, 40.8, 29.0, 15.3. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{27}H_{23}FeO_2$ 435.1042; Found: 435.1041.

The e.e. value was determined by the chiral HPLC analysis (chiralpak® AD-H, Hexane / IPA = 90 / 10, 1.0 mL / min, λ= 254 nm, $t_{(minor)}$ = 5.211 min, $t_{(major)}$ = 9.005 min).

Compound 3ac

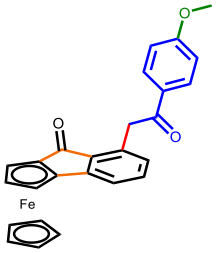


The resultant residue was purified by flash silica gel column chromatography to afford **3ac** as a red solid; 67.8 mg, 87% yield; (eluent: petroleum ether/ethyl acetate: 30:1); 98% *e.e.*.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.05 (d, *J* = 8.5 Hz, 2H), 7.52 – 7.48 (m, 2H), 7.27 – 7.21 (m, 1H), 7.07 (dd, *J* = 7.4, 1.0 Hz, 1H), 6.91 (dd, *J* = 7.7, 0.9 Hz, 1H), 4.94 (d, *J* = 16.2 Hz, 1H), 4.90 (dd, *J* = 2.4, 0.7 Hz, 1H), 4.86 (dd, *J* = 2.4, 0.7 Hz, 1H), 4.80 (t, *J* = 2.4 Hz, 1H), 4.43 (d, *J* = 16.3 Hz, 1H), 4.14 (s, 5H), 1.34 (s, 9H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 196.9, 195.8, 156.6, 144.1, 137.2, 134.7, 134.2, 132.8, 129.5, 128.4, 125.5, 119.0, 89.8, 77.3, 77.1, 76.8, 75.0, 73.5, 73.0, 66.2, 66.1, 40.8, 35.1, 31.1. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{29}H_{27}FeO_2$ 463.1355; Found: 463.1355.

The e.e. value was determined by the chiral HPLC analysis (chiralpak® AD-H, Hexane / IPA = 90 / 10, 1.0 mL / min, λ= 254 nm, $t_{(minor)}$ = 4.738 min, $t_{(major)}$ = 6.618 min).

Compound 3ad

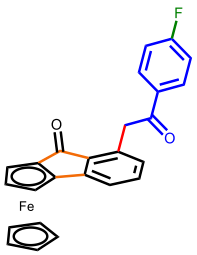


The resultant residue was purified by flash silica gel column chromatography to afford **3ad** as a red solid; 59.9 mg, 88% yield; (eluent: petroleum ether/ethyl acetate: 30:1); 99% *e.e.*.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.09 (d, *J* = 8.9 Hz, 2H), 7.27 – 7.20 (m, 1H), 7.06 (dd, *J* = 7.4, 1.0 Hz, 1H), 6.97 – 6.93 (m, 2H), 6.94 – 6.90 (m, 1H), 4.93 – 4.88 (m, 2H), 4.86 (dd, *J* = 2.3, 0.7 Hz, 1H), 4.80 (d, *J* = 2.4 Hz, 1H), 4.44 (d, *J* = 16.1 Hz, 1H), 4.14 (s, 5H), 3.86 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 195.9, 195.8, 163.4, 144.1, 137.1, 134.4, 132.8, 130.8, 130.3, 129.5, 119.0, 113.7, 89.8, 78.4, 77.3, 77.0, 76.8, 75.0, 73.5, 73.0, 66.2, 66.1, 55.5, 40.4. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{26}H_{21}FeO_3$ 456.0654; Found: 456.0657.

The e.e. value was determined by the chiral HPLC analysis (chiralpak® AD-H, Hexane / IPA = 90 / 10, 1.0 mL / min, λ= 254 nm, $t_{(minor)}$ = 8.291 min, $t_{(major)}$ = 9.225 min).

Compound 3ae



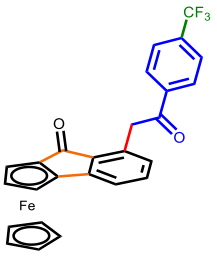
The resultant residue was purified by flash silica gel column chromatography to afford

3ae as a red solid; 43.7 mg, 66% yield; (eluent: petroleum ether/ethyl acetate: 30:1); 93% *e.e.*.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.13 (dd, *J* = 8.6, 5.6 Hz, 2H), 7.24 (d, *J* = 7.5 Hz, 1H), 7.15 (t, *J* = 8.6 Hz, 2H), 7.09 (d, *J* = 7.4 Hz, 1H), 6.90 (d, *J* = 7.6 Hz, 1H), 4.90 (d, *J* = 3.1 Hz, 1H), 4.87 (d, *J* = 2.7 Hz, 1H), 4.81 (d, *J* = 2.4 Hz, 1H), 4.42 (d, *J* = 16.3 Hz, 1H), 4.15 (s, 5H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 195.9, 195.6, 165.7 (d, *J* = 254.1 Hz), 144.1, 137.2, 133.2 (d, *J* = 9.5 Hz), 131.1 (d, *J* = 9.2 Hz), 129.5, 119.2, 115.6 (d, *J* = 21.9 Hz) 89.7, 77.3, 77.1, 76.9, 75.2, 73.6, 73.1, 66.3, 66.2, 40.8. **^{19}F NMR** (565 MHz, CDCl3) δ -105.75. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{25}H_{18}FFeO_2$ 425.0635; Found: 425.0636.

The e.e. value was determined by the chiral HPLC analysis (chiralpak® AD-H, Hexane / IPA = 90 / 10, 1.0 mL / min, λ= 254 nm, $t_{(minor)}$ = 7.387 min, $t_{(major)}$ = 9.648 min).

Compound 3af



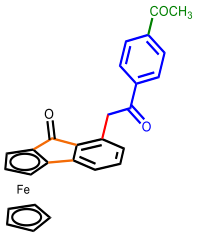
The resultant residue was purified by flash silica gel column chromatography to afford **3af** as a red solid; 46.6 mg, 63% yield; (eluent: petroleum ether/ethyl acetate: 30:1); 95% *e.e.*.

^{1}H NMR (600 MHz, $CDCl_3$)δ 8.20 (d, *J* = 8.0 Hz, 2H), 7.76 (d, *J* = 8.1 Hz, 2H), 7.27 – 7.24 (m, 1H), 7.10 (dd, *J* = 7.4, 1.0 Hz, 1H), 6.92 – 6.87 (m, 1H), 4.92 – 4.89 (m, 1H),

4.88 (d, J = 2.4 Hz, 1H), 4.83 (d, J = 2.4 Hz, 1H), 4.42 (d, J = 16.7 Hz, 1H), 4.21 (s, 0.5H), 4.15 (s, 5H), 4.11 (s, 0.5H). **^{13}C NMR** (151 MHz, $CDCl_3$)δ 196.3, 195.9, 144.2, 140.1, 137.2, 134.3, 134.1, 133.5, 133.2, 133.1, 133.0, 130.8, 129.5, 129.2, 128.7, 125.7 (q, J = 3.7 Hz), 126.5, 125.7, 125.7, 124.6, 124.1, 123.0, 122.8, 119.4, 89.6, 78.3, 77.3, 77.0, 76.8, 75.3, 73.7, 73.1, 73.0, 72.8, 66.5, 66.3, 41.4. **^{19}F NMR** (565 MHz, CDCl3) δ -63.10. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{26}H_{17}F_3FeO_2Na$ 497.0422; Found: 497.0424.

The e.e. value was determined by the chiral HPLC analysis (chiralpak® AD-H, Hexane / IPA = 90 / 10, 1.0 mL / min, λ= 254 nm, $t_{(minor)}$ = 11.797 min, $t_{(major)}$ = 17.609 min).

Compound 3ag



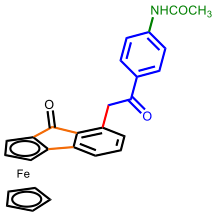
The resultant residue was purified by flash silica gel column chromatography to afford **3ag** as a red solid; 51.1 mg, 73% yield; (eluent: petroleum ether/ethyl acetate: 30:1); 99% *e.e.*.

^{1}H NMR (600 MHz, $CDCl_3$)δ 8.19 – 8.14 (m, 2H), 8.10 – 8.03 (m, 2H), 7.28 – 7.23 (m, 1H), 7.10 (dd, J = 7.4, 1.0 Hz, 1H), 6.90 (dd, J = 7.7, 0.9 Hz, 1H), 4.93 (s, 1H), 4.91 – 4.89 (m, 1H), 4.87 (dd, J = 2.4, 0.7 Hz, 1H), 4.82 (s, 1H), 4.45 (d, J = 16.6 Hz, 1H), 4.15 (s, 5H), 2.64 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 197.5, 196.7, 195.8, 144.2, 140.7, 140.1, 137.3, 133.3, 133.0, 129.5, 128.6, 128.5, 119.3, 89.7, 78.3, 77.2,

77.0, 76.8, 75.2, 73.6, 73.1, 66.4, 66.2, 41.4, 26.9. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{27}H_{21}FeO_3$ 471.0654; Found: 471.0657.

The e.e. value was determined by the chiral HPLC analysis (chiralpak® AD-H, Hexane / IPA = 90 / 10, 1.0 mL / min, λ= 254 nm, $t_{(minor)}$ = 11.163 min, $t_{(major)}$ = 12.444 min).

Compound 3ah

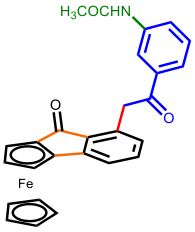


The resultant residue was purified by flash silica gel column chromatography to afford **3ah** as a red solid; 54.2 mg, 75% yield; (eluent: petroleum ether/ethyl acetate: 5:1); 95% *e.e.*.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.05 (d, *J* = 8.4 Hz, 1H), 7.61 (d, *J* = 8.3 Hz, 1H), 7.27 – 7.21 (m, 1H), 7.08 (d, *J* = 7.3 Hz, 0H), 6.90 (d, *J* = 7.6 Hz, 0H), 4.96 – 4.85 (m, 2H), 4.82 (t, *J* = 2.4 Hz, 0H), 4.44 (dd, *J* = 16.3, 1.7 Hz, 0H), 4.15 (s, 2H), 2.19 (s, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 196.1, 195.9, 168.4, 144.1, 142.2, 137.3, 134.1, 132.9, 129.8, 129.5, 119.1, 118.8, 89.7, 78.3, 77.2, 77.0, 76.8, 75.1, 73.5, 73.1, 66.3, 66.2, 40.7, 29.7, 24.8. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{27}H_{21}FeNO_3Na$ 486.0763; Found: 486.0764.

The e.e. value was determined by the chiral HPLC analysis (chiralpak® AD-H, Hexane / IPA = 90 / 10, 1.0 mL / min, λ= 254 nm, $t_{(minor)}$ = 25.932 min, $t_{(major)}$ = 35.853 min).

Compound 3ai

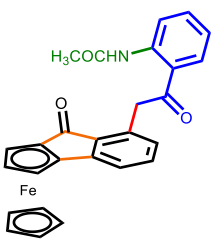


The resultant residue was purified by flash silica gel column chromatography to afford **3ai** as a red solid; 50.6 mg, 70% yield; (eluent: petroleum ether/ethyl acetate: 10:1); 95% *e.e.*.

^{1}H NMR (600 MHz, $CDCl_3$) δ 11.58 (s, 1H), 8.75 (d, *J* = 8.5 Hz, 1H), 8.17 (d, *J* = 7.8 Hz, 1H), 7.57 (t, *J* = 7.9 Hz, 1H), 7.28 (dd, *J* = 15.7, 8.2 Hz, 2H), 7.17 (t, *J* = 7.7 Hz, 1H), 7.13 (d, *J* = 7.4 Hz, 1H), 6.88 (d, *J* = 7.7 Hz, 1H), 4.99 – 4.87 (m, 3H), 4.84 (t, *J* = 2.6 Hz, 1H), 4.52 (d, *J* = 16.7 Hz, 1H), 4.17 (s, 5H), 2.15 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 201.6, 195.7, 169.3, 144.2, 141.1, 137.4, 134.9, 133.4, 133.0, 130.8, 129.4, 122.4, 121.9, 120.8, 119.4, 89.7, 78.3, 75.2, 73.0, 66.4, 66.2, 53.4, 42.4, 29.7, 25.5. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{27}H_{21}FeNO_3Na$ 486.0763; Found: 486.0764.

The e.e. value was determined by the chiral HPLC analysis (chiralpak® AD-H, Hexane / IPA = 80 / 20, 1.0 mL / min, λ= 254 nm, $t_{(minor)}$ = 10.488 min, $t_{(major)}$ = 14.875 min).

Compound 3aj

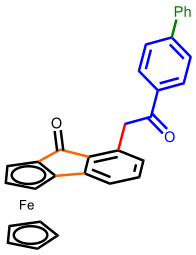


The resultant residue was purified by flash silica gel column chromatography to afford **3aj** as a red solid; 52.1 mg, 72% yield; (eluent: petroleum ether/ethyl acetate: 5:1); 99% *e.e.*.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.99 (s, 1H), 7.94 (d, *J* = 8.3 Hz, 1H), 7.84 (s, 1H), 7.80 (d, *J* = 7.7 Hz, 1H), 7.42 (t, *J* = 8.0 Hz, 1H), 7.25 (dd, *J* = 12.5, 5.2 Hz, 1H), 7.08 (d, *J* = 7.4 Hz, 1H), 6.87 (d, *J* = 7.7 Hz, 1H), 4.89 – 4.80 (m, 4H), 4.43 (d, *J* = 16.7 Hz, 1H), 4.15 (s, 5H), 2.14 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 196.8, 196.1, 168.9, 144.1, 138.7, 137.7, 137.4, 133.8, 133.0, 129.7, 129.2, 124.4, 123.7, 119.2, 119.2, 89.7, 78.2, 77.3, 77.1, 76.9, 75.3, 73.6, 73.1, 66.5, 66.2, 60.4, 41.4, 24.5. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{27}H_{21}FeNO_3Na$ 486.0763; Found: 486.0764.

The e.e. value was determined by the chiral HPLC analysis (chiralpak® AD-H, Hexane / IPA = 80 / 20, 1.0 mL / min, λ= 254 nm, $t_{(minor)}$ = 16.819 min, $t_{(major)}$ = 18.591 min).

Compound 3ak



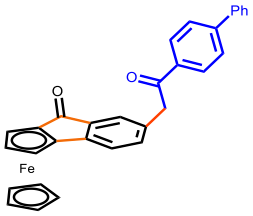
The resultant residue was purified by flash silica gel column chromatography to afford **3ak** as a red solid; 51.9 mg, 69% yield; (eluent: petroleum ether/ethyl acetate: 20:1); 90% *e.e.*.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.19 (m, 1H), 7.76 – 7.69 (m, 1H), 7.71 – 7.64 (m, 1H), 7.43 (d, *J* = 7.4 Hz, 0H), 7.31 – 7.24 (m, 1H), 7.12 (dd, *J* = 7.4, 1.0 Hz, 1H), 6.96 (dd,

J = 7.6, 0.9 Hz, 1H), 5.01 (d, J = 16.3 Hz, 1H), 4.94 (dd, J = 2.4, 0.7 Hz, 1H), 4.90 (dd, J = 2.4, 0.7 Hz, 1H), 4.84 (d, J = 2.4 Hz, 0H), 4.51 (d, J = 16.3 Hz, 1H), 4.19 (s, 5H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 196.8, 195.9, 145.7, 144.1, 140.2, 137.3, 136.1, 134.0, 132.9, 129.5, 129.0, 128.9, 128.1, 127.3, 127.3, 119.1, 89.7, 77.3, 77.0, 76.8, 75.1, 73.1, 66.3, 66.2, 40.9. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{31}H_{22}FeO_2Na$ 505.0861; Found: 505.0863.

The e.e. value was determined by the chiral HPLC analysis (chiralpak® AD-H, Hexane / IPA = 90 / 10, 1.0 mL / min, λ= 254 nm, $t_{(minor)}$ = 13.053 min, $t_{(major)}$ = 24.895 min).

Compound 3al



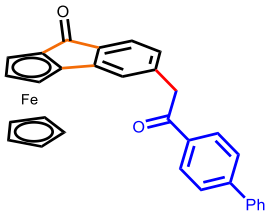
The resultant residue was purified by flash silica gel column chromatography to afford **3al** as a red solid; 60.9 mg, 81% yield; (eluent: petroleum ether/ethyl acetate: 10:1); 97% *e.e.*.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.05 (dd, J = 17.6, 7.1 Hz, 4H), 7.74 (d, J = 8.4 Hz, 2H), 7.63 (d, J = 7.2 Hz, 2H), 7.48 (t, J = 7.6 Hz, 2H), 7.42 (d, J = 6.6 Hz, 1H), 7.29 (d, J = 8.4 Hz, 1H), 5.12 (s, 1H), 4.99 (s, 2H), 4.84 (s, 0.5H), 4.26 (s, 0.5H), 4.16 (s, 5H), 4.11 (s, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 193.8, 193.1, 150.8, 147.7, 140.9, 139.6, 135.1, 131.6, 131.4, 130.6, 129.1, 128.7, 127.7, 127.4, 124.1, 120.4, 88.2, 79.5, 77.3, 77.0, 76.9, 76.8, 73.5, 73.0, 67.7, 67.7, 30.9. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ calcd for

$C_{31}H_{22}FeO_2Na$ 505.0861; Found: 505.0863.

The e.e. value was determined by the chiral HPLC analysis (chiralpak® AD-H, Hexane / IPA = 90 / 10, 1.0 mL / min, λ= 254 nm, $t_{(minor)}$ = 14.809 min, $t_{(major)}$ = 16.548 min).

Compound 3am

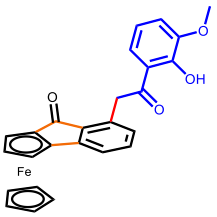


The resultant residue was purified by flash silica gel column chromatography to afford **3am** as a red solid; 59.4 mg, 79% yield; (eluent: petroleum ether/ethyl acetate: 10:1); 95% *e.e.*

^{1}H NMR (600 MHz, $CDCl_3$)δ 8.09 (d, *J* = 8.4 Hz, 2H), 7.70 (d, *J* = 8.4 Hz, 2H), 7.62 (dd, *J* = 8.3, 1.3 Hz, 2H), 7.50 – 7.44 (m, 3H), 7.41 (d, *J* = 7.3 Hz, 1H), 7.10 (s, 1H), 7.03 (d, *J* = 9.1 Hz, 1H), 4.96 (d, *J* = 3.1 Hz, 1H), 4.86 – 4.78 (m, 2H), 4.29 (s, 2H), 4.10 (s, 5H). **^{13}C NMR** (151 MHz, $CDCl_3$) 197.7, 193.9, 146.2, 144.1, 140.2, 139.7, 139.3, 135.1, 129.2, 129.0, 128.4, 127.7, 127.4, 127.3, 123.3, 121.4, 89.9, 78.6, 77.2, 77.0, 76.8, 75.3, 73.0, 66.4, 66.4, 45.9. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{31}H_{22}FeO_2Na$ 505.0861; Found: 505.0863.

The e.e. value was determined by the chiral HPLC analysis (chiralpak® AD-H, Hexane / IPA = 90 / 10, 1.0 mL / min, λ= 254 nm, $t_{(minor)}$ = 12.723 min, $t_{(major)}$ = 15.349 min).

Compound 3an



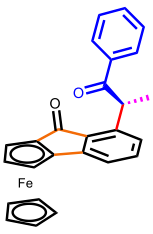
The resultant residue was purified by flash silica gel column chromatography to afford **3an** as a red solid; 52.2 mg, 74% yield; (eluent: petroleum ether/ethyl acetate: 10:1); 98% *e.e.*.

^{1}H NMR (600 MHz, $CDCl_3$) δ 12.48 (s, 1H), 7.62 (dd, *J* = 8.2, 1.3 Hz, 1H), 7.11 (d, *J* = 7.4 Hz, 1H), 7.07 (d, *J* = 8.0 Hz, 1H), 6.93 – 6.87 (m, 2H), 5.01 (d, *J* = 16.5 Hz, 1H), 4.92 (d, *J* = 2.4 Hz, 1H), 4.88 (d, *J* = 2.3 Hz, 1H), 4.83 (t, *J* = 2.4 Hz, 1H), 4.47 (d, *J* = 16.6 Hz, 1H), 4.15 (s, 5H), 3.91 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) ^{13}C NMR (151 MHz, $CDCl_3$) δ 203.9, 195.7, 153.0, 149.0, 144.2, 137.3, 133.0, 132.9, 129.4, 121.6, 119.6, 119.4, 118.3, 117.1, 89.6, 78.4, 77.3, 77.0, 76.8, 75.2, 73.1, 66.4, 66.3, 56.3, 40.8

HRMS (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{26}H_{20}FeO_4Na$ 475.0603; Found: 475.0603.

The e.e. value was determined by the chiral HPLC analysis (chiralpak® AD-H, Hexane / IPA = 80 / 20, 1.0 mL / min, λ= 254 nm, $t_{(minor)}$ = 19.500 min, $t_{(major)}$ = 21.697 min).

Compound (R_p, *R*)-3ao



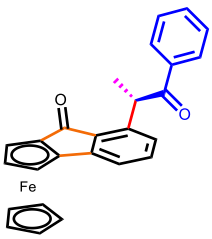
The resultant residue was purified by flash silica gel column chromatography to afford

(R_p, *R*)-3ao as a red solid; 29.3 mg, 45% yield; (eluent: petroleum ether/ethyl acetate: 30:1); 99% *e.e.*; *d.r.* = 2.7: 1 (obtained from the crude ^{1}H NMR spectrum).

^{1}H NMR (600 MHz, $CDCl_3$)δ 8.01 – 7.96 (m, 1H), 7.87 – 7.83 (m, 1H), 7.35 (d, *J* = 7.2 Hz, 1H), 7.30 (t, *J* = 7.4 Hz, 2H), 7.21 (t, *J* = 7.7 Hz, 1H), 7.02 (q, *J* = 7.1 Hz, 1H), 6.85 (dd, *J* = 7.7, 2.5 Hz, 1H), 6.75 (t, *J* = 8.1 Hz, 1H), 6.07 (dd, *J* = 30.7, 6.8 Hz, 1H), 4.87 (s, 1H), 4.73 (dd, *J* = 5.4, 3.0 Hz, 2H), 3.98 (d, *J* = 23.3 Hz, 5H), 1.38 (dd, *J* = 64.2, 6.8 Hz, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 200.8, 196.3, 144.5, 141.4, 136.5, 135.0, 133.5, 133.5, 132.8, 132.7, 128.8, 128.8, 128.5, 128.4, 127.7, 126.1, 126.1, 118.9, 118.8, 89.6, 89.5, 78.6, 78.3, 77.2, 77.0, 76.8, 75.2, 75.2, 73.2, 73.0, 72.9, 72.8, 66.4, 66.3, 66.3, 40.4, 40.3, 18.8.**HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{26}H_{20}FeO_2$ 421.0885; Found: 421.0885.

The e.e. value was determined by the chiral HPLC analysis (chiralpak® AD-H, Hexane / IPA = 90 / 10, 1.0 mL / min, λ= 254 nm, $t_{(minor)}$ = 7.654 min, $t_{(major)}$ = 9.785 min).

Compound (R_p, *S*)-3ao



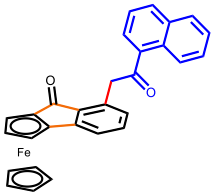
The resultant residue was purified by flash silica gel column chromatography to afford **(R_p, *S*)-3ao** as a red solid; 10.8 mg, 16% yield; (eluent: petroleum ether/ethyl acetate: 30:1); 99% *e.e.*; *d.r.* = 2.7: 1 (obtained from the crude ^{1}H NMR spectrum).

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.11 (d, *J* = 7.4 Hz, 1H), 7.98 (d, *J* = 7.2 Hz, 1H), 7.48 (t, *J* = 7.5 Hz, 1H), 7.43 (t, *J* = 7.6 Hz, 1H), 7.33 (t, *J* = 7.7 Hz, 1H), 7.15 (td, *J* = 7.6,

5.7 Hz, 1H), 6.98 (dd, *J* = 7.3, 2.7 Hz, 1H), 6.87 (t, *J* = 8.0 Hz, 1H), 6.20 (dq, *J* = 30.8, 6.8 Hz, 1H), 4.99 (t, *J* = 2.9 Hz, 1H), 4.87 – 4.83 (m, 2H), 4.10 (d, *J* = 22.8 Hz, 5H), 1.50 (dd, *J* = 64.5, 6.8 Hz, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 200.9, 196.5, 144.5, 144.4, 141.4, 140.9, 136.9, 136.6, 135.1, 135.0, 133.5, 133.5, 132.8, 132.7, 128.8, 128.8, 128.5, 128.4, 126.1, 126.1, 118.9, 118.8, 89.6, 89.5, 78.6, 78.3, 77.2, 77.0, 76.8, 75.2, 75.2, 73.0, 72.9, 66.4, 66.3, 66.3, 40.4, 40.3, 18.8, 17.9. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{26}H_{20}FeO_2$ 421.0885; Found: 421.0885.

The e.e. value was determined by the chiral HPLC analysis (chiralpak® AD-H, Hexane / IPA = 90 / 10, 1.0 mL / min, λ= 254 nm, $t_{(minor)}$ = 7.439 min, $t_{(major)}$ = 9.683 min).

Compound 3ap



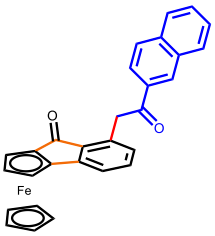
The resultant residue was purified by flash silica gel column chromatography to afford **3ap** as a red solid; 48.4 mg, 66% yield; (eluent: petroleum ether/ethyl acetate: 20:1); 95% *e.e.*.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.57 (d, *J* = 7.5 Hz, 1H), 8.25 (d, *J* = 8.4 Hz, 1H), 7.99 (s, 1H), 7.87 (d, *J* = 9.8 Hz, 1H), 7.58 (s, 1H), 7.52 (t, *J* = 7.5 Hz, 1H), 7.28 (t, *J* = 7.5 Hz, 2H), 7.10 (d, *J* = 8.3 Hz, 1H), 6.97 (d, *J* = 8.5 Hz, 1H), 5.08 (d, *J* = 16.8 Hz, 1H), 4.93 (d, *J* = 2.4 Hz, 1H), 4.87 (d, *J* = 1.7 Hz, 1H), 4.82 (t, *J* = 2.4 Hz, 1H), 4.44 (d, *J* = 16.8 Hz, 1H), 4.11 (s, 5H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 201.1, 195.8, 144.2, 137.4, 136.4, 134.0, 133.8, 132.9, 132.3, 130.3, 129.6, 128.3, 127.7, 126.3, 125.9, 124.5, 119.2,

89.7, 78.4, 75.1, 73.5, 73.3, 73.0, 66.3, 66.2, 44.8. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{29}H_{20}FeO_2Na$ 479.0705; Found: 479.0706.

The e.e. value was determined by the chiral HPLC analysis (chiralpak® AD-H, Hexane / IPA = 90 / 10, 1.0 mL / min, λ= 254 nm, $t_{(minor)}$ = 11.875 min, $t_{(major)}$ = 19.500 min).

Compound 3aq



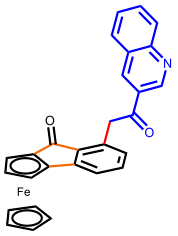
The resultant residue was purified by flash silica gel column chromatography to afford **3aq** as a red solid; 45.5 mg, 64% yield; (eluent: petroleum ether/ethyl acetate: 20:1); 99% *e.e.*.

^{1}H NMR (600 MHz, $CDCl_3$)δ 8.69 (s, 1H), 8.12 (d, *J* = 10.3 Hz, 1H), 8.00 (d, *J* = 8.0 Hz, 1H), 7.91 (d, *J* = 8.6 Hz, 1H), 7.87 (d, *J* = 8.1 Hz, 1H), 7.58 (t, *J* = 6.8 Hz, 1H), 7.54 (t, *J* = 7.5 Hz, 1H), 7.27 – 7.24 (m, 1H), 7.09 (d, *J* = 7.4 Hz, 1H), 6.95 (d, *J* = 7.7 Hz, 1H), 5.08 (d, *J* = 16.3 Hz, 1H), 4.91 (d, *J* = 2.5 Hz, 1H), 4.86 (d, *J* = 2.4 Hz, 1H), 4.81 (d, *J* = 2.4 Hz, 1H), 4.59 (d, *J* = 16.3 Hz, 1H), 4.15 (s, 5H). **^{13}C NMR** (151 MHz, $CDCl_3$)δ 197.2, 195.9, 144.1, 137.3, 135.7, 134.6, 134.0, 132.9, 132.7, 130.1, 129.7, 129.5, 128.4, 128.3, 127.8, 126.6, 124.3, 119.1, 89.7, 78.4, 77.3, 77.0, 76.8, 75.1, 73.1, 66.3, 66.2, 41.0, 29.7. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{29}H_{20}FeO_2Na$ 457.0885; Found: 457.0883.

The e.e. value was determined by the chiral HPLC analysis (chiralpak® AD-H, Hexane

/ IPA = 80 / 20, 1.0 mL / min, λ= 254 nm, $t_{(minor)}$ = 9.975 min, $t_{(major)}$ = 21.542 min).

Compound 3ar

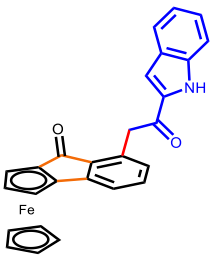


The resultant residue was purified by flash silica gel column chromatography to afford **3ar** as a red solid; 39.2 mg, 55% yield; (eluent: petroleum ether/ethyl acetate: 20:1); 97% *e.e.*.

^{1}H NMR (600 MHz, $CDCl_3$)δ 9.52 (d, *J* = 2.2 Hz, 1H), 8.93 (d, *J* = 2.4 Hz, 1H), 8.17 (d, *J* = 8.5 Hz, 1H), 7.99 (dd, *J* = 8.2, 1.4 Hz, 1H), 7.83 (d, *J* = 1.5 Hz, 1H), 7.65 – 7.60 (m, 1H), 7.30 – 7.24 (m, 1H), 7.13 – 7.08 (m, 1H), 6.95 (d, *J* = 7.7 Hz, 1H), 5.03 (d, *J* = 16.4 Hz, 1H), 4.92 – 4.90 (m, 1H), 4.88 (d, *J* = 2.2 Hz, 1H), 4.82 (s, 1H), 4.55 (d, *J* = 16.4 Hz, 1H), 4.15 (s, 5H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 196.1, 195.9, 149.9, 149.4, 144.2, 137.4, 137.3, 133.0, 133.0, 131.8, 129.6, 129.5, 129.5, 129.5, 127.4, 127.0, 119.4, 89.7, 78.3, 77.3, 77.0, 76.8, 75.2, 73.1, 66.4, 66.3, 41.3. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{28}H_{20}FeNO_2$ 458.0838; Found: 458.0838.

The e.e. value was determined by the chiral HPLC analysis (chiralpak® AD-H, Hexane / IPA = 80 / 20, 1.0 mL / min, λ= 254 nm, $t_{(minor)}$ = 24.041 min, $t_{(major)}$ = 30.196 min).

Compound 3as

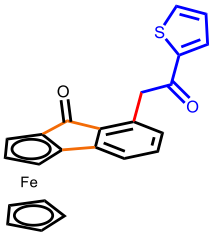


The resultant residue was purified by flash silica gel column chromatography to afford **3as** as a red solid; 22.3 mg, 32% yield; (eluent: petroleum ether/ethyl acetate: 15:1); 95% *e.e.*.

^{1}H NMR (600 MHz, $CDCl_3$)δ 9.16 (s, 1H), 7.73 (d, *J* = 8.1 Hz, 1H), 7.47 – 7.43 (m, 1H), 7.41 (d, *J* = 8.4 Hz, 1H), 7.32 (t, *J* = 7.6 Hz, 1H), 7.28 – 7.22 (m, 3H), 7.13 (t, *J* = 7.5 Hz, 1H), 7.08 (d, *J* = 7.4 Hz, 1H), 4.96 – 4.91 (m, 2H), 4.87 (d, *J* = 2.3 Hz, 1H), 4.83 (t, *J* = 2.4 Hz, 1H), 4.50 (d, *J* = 15.4 Hz, 1H), 4.14 (s, 5H). **^{13}C NMR** (151 MHz, $CDCl_3$)δ 196.2, 189.7, 144.2, 137.3, 137.1, 135.1, 133.6, 133.0, 129.4, 127.8, 126.2, 123.2, 120.9, 119.2, 112.1, 109.8, 89.7, 78.5, 77.2, 77.0, 76.8, 75.2, 73.0, 70.2, 66.3, 66.3, 40.0. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{27}H_{20}FeNO_2$ 446.0838; Found: 446.0839.

The e.e. value was determined by the chiral HPLC analysis (chiralpak® AD-H, Hexane / IPA = 80 / 20, 1.0 mL / min, λ= 254 nm, $t_{(minor)}$ = 13.241 min, $t_{(major)}$ = 14.681 min).

Compound 3at

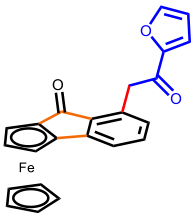


The resultant residue was purified by flash silica gel column chromatography to afford **3at** as a red solid; 46.3 mg, 72% yield; (eluent: petroleum ether/ethyl acetate: 30:1); 99% *e.e.*.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.96 (dd, *J* = 3.8, 1.1 Hz, 1H), 7.63 (dd, *J* = 5.0, 1.1 Hz, 1H), 7.24 (t, *J* = 7.6 Hz, 1H), 7.15 (dd, *J* = 5.0, 3.8 Hz, 1H), 7.07 (dd, *J* = 7.4, 1.0 Hz, 1H), 6.97 (dd, *J* = 7.7, 0.9 Hz, 1H), 4.92 (dd, *J* = 2.4, 0.8 Hz, 1H), 4.89 (s, 1H), 4.88 – 4.85 (m, 2H), 4.82 (d, *J* = 2.4 Hz, 1H), 4.14 (s, 5H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 196.0, 190.0, 144.3, 144.1, 137.1, 133.6, 133.5, 132.9, 132.6, 129.4, 128.1, 119.2, 89.7, 78.4, 77.2, 77.0, 76.8, 75.1, 73.0, 73.0, 66.3, 66.2, 41.0. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{23}H_{17}FeO_2S$ 413.0293; Found: 413.0295.

The e.e. value was determined by the chiral HPLC analysis (chiralpak® AD-H, Hexane / IPA = 90 / 10, 1.0 mL / min, λ= 254 nm, $t_{(minor)}$ = 9.706 min, $t_{(major)}$ = 11.025 min).

Compound 3au



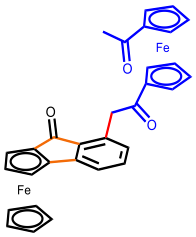
The resultant residue was purified by flash silica gel column chromatography to afford **3au** as a red solid; 47.0 mg, 76% yield; (eluent: petroleum ether/ethyl acetate: 30:1);

99% *e.e.*.

^{1}H NMR (600 MHz, $CDCl_3$)δ 7.61 (d, *J* = 1.7 Hz, 1H), 7.37 (d, *J* = 3.6 Hz, 1H), 7.24 (dd, *J* = 14.3, 6.8 Hz, 1H), 7.08 (d, *J* = 7.4 Hz, 1H), 6.94 (d, *J* = 7.7 Hz, 1H), 6.55 (dd, *J* = 3.6, 1.7 Hz, 1H), 4.91 (d, *J* = 2.4 Hz, 1H), 4.86 (d, *J* = 2.3 Hz, 1H), 4.81 (s, 1H), 4.77 (d, *J* = 16.2 Hz, 1H), 4.35 (d, *J* = 16.2 Hz, 1H), 4.14 (s, 5H). **^{13}C NMR** (151 MHz, $CDCl_3$)δ 195.8, 185.8, 152.6, 146.4, 144.1, 137.3, 133.1, 132.9, 129.5, 119.2 117.7, 112.2, 89.6, 78.4, 77.3, 77.1, 76.8, 75.1, 73.6, 73.1, 73.0, 66.3, 66.2, 40.4. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{23}H_{17}FeO_3$ 419.0341; Found: 419.0349.

The e.e. value was determined by the chiral HPLC analysis (chiralpak® AD-H, Hexane / IPA = 90 / 10, 1.0 mL / min, λ= 254 nm, $t_{(minor)}$ = 8.631 min, $t_{(major)}$ = 10.133 min).

Compound 3av



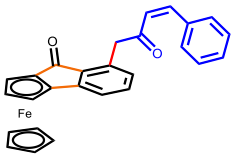
The resultant residue was purified by flash silica gel column chromatography to afford **3av** as a red solid; 38.9 mg, 44% yield; (eluent: petroleum ether/ethyl acetate: 20:1); 94% *e.e.*

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.29 – 7.27 (m, 1H), 7.10 (d, *J* = 7.4 Hz, 1H), 6.99 (d, *J* = 7.7 Hz, 1H), 4.98 – 4.95 (m, 3H), 4.91 (dd, *J* = 10.8, 2.5 Hz, 2H), 4.88 – 4.84 (m, 2H), 4.64 (d, *J* = 16.5 Hz, 1H), 4.58 (d, *J* = 16.1 Hz, 2H), 4.54 (d, *J* = 6.8 Hz, 1H), 4.18 (s, 5H), 2.41 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 201.6, 200.0, 196.3, 144.0, 137.3,

133.7, 132.8, 129.6, 119.1, 89.7, 80.6, 80.2, 78.4, 77.3, 77.0, 76.8, 75.1, 74.0, 73.9, 73.6, 73.6, 73.0, 73.0, 71.3, 71.3, 71.1, 70.9, 66.3, 66.2, 41.5, 27.7. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{31}H_{24}Fe_2O_3Na$ 579.0317; Found: 579.0319.

The e.e. value was determined by the chiral HPLC analysis (chiralpak® AD-H, Hexane / IPA = 90 / 10, 1.0 mL / min, λ= 254 nm, $t_{(minor)}$ = 11.265 min, $t_{(major)}$ = 14.482 min).

Compound 3aw

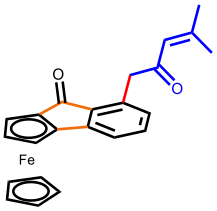


The resultant residue was purified by flash silica gel column chromatography to afford **3aw** as a red solid; 22.7 mg, 34% yield; (eluent: petroleum ether/ethyl acetate: 20:1); 96% *e.e.*.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.73 (d, *J* = 16.2 Hz, 1H), 7.58 (dd, *J* = 6.6, 2.8 Hz, 2H), 7.38 (dd, *J* = 5.3, 1.9 Hz, 3H), 7.26 – 7.22 (t, 1H), 7.08 (d, *J* = 7.4 Hz, 1H), 6.93 (s, 1H), 6.91 (d, *J* = 6.8 Hz, 1H), 4.93 (d, *J* = 2.4 Hz, 1H), 4.87 (d, *J* = 2.3 Hz, 1H), 4.82 (d, *J* = 2.5 Hz, 1H), 4.59 (d, *J* = 15.7 Hz, 1H), 4.22 (d, *J* = 14.7 Hz, 1H), 4.13 (s, 5H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 196.9, 196.0, 144.1, 143.0, 137.2, 134.7, 133.7, 132.9, 130.4, 129.6, 128.9, 128.9, 128.9, 128.4, 126.2, 119.1, 89.7, 78.4, 77.2, 77.0, 76.8, 75.1, 73.5, 73.0, 66.2, 66.2, 43.0, 29.7. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{27}H_{21}FeO_2$ 433.0885; Found: 433.0885.

The e.e. value was determined by the chiral HPLC analysis (chiralpak® AD-H, Hexane / IPA = 80 / 20, 1.0 mL / min, λ= 254 nm, $t_{(minor)}$ = 9.932 min, $t_{(major)}$ = 15.849 min).

Compound 3ax

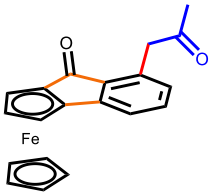


The resultant residue was purified by flash silica gel column chromatography to afford **3ax** as a red solid; 20.4 mg, 34% yield; (eluent: petroleum ether/ethyl acetate: 20:1); 99% *e.e.*.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.22 (t, J = 7.6 Hz, 1H), 7.06 (d, J = 7.3 Hz, 1H), 6.85 (d, J = 7.6 Hz, 1H), 6.26 (s, 1H), 4.92 (d, J = 2.4 Hz, 1H), 4.85 (d, J = 2.2 Hz, 1H), 4.82 – 4.79 (m, 1H), 4.31 (d, J = 15.8 Hz, 1H), 4.14 (s, 5H), 3.97 (d, J = 15.8 Hz, 1H), 2.14 (s, 3H), 1.90 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 197.0, 195.8, 155.5, 144.0, 137.2, 134.4, 132.8, 129.6, 123.8, 118.9, 89.8, 78.5, 77.2, 77.0, 76.8, 74.9, 73.0, 66.1, 46.1, 30.9, 27.7, 20.8. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{23}H_{20}FeO_2Na$ 407.0705; Found: 407.0712.

The e.e. value was determined by the chiral HPLC analysis (chiralpak® AD-H, Hexane / IPA = 90 / 10, 1.0 mL / min, λ= 254 nm, $t_{(minor)}$ = 8.254 min, $t_{(major)}$ = 9.954 min).

Compound 3ay



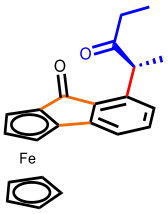
The resultant residue was purified by flash silica gel column chromatography to afford **3ay** as a red solid; 48.4 mg, 90% yield; (eluent: petroleum ether/ethyl acetate: 50:1);

97% *e.e.*.

^{1}H NMR (600 MHz, $CDCl_3$)δ 7.22 (t, *J* = 7.5 Hz, 1H), 7.07 (d, *J* = 7.4 Hz, 1H), 6.79 (d, *J* = 7.6 Hz, 1H), 4.91 (d, *J* = 2.4 Hz, 1H), 4.86 (d, *J* = 2.4 Hz, 1H), 4.81 (d, *J* = 2.4 Hz, 1H), 4.26 (d, *J* = 16.6 Hz, 1H), 4.14 (s, 5H), 3.89 (d, *J* = 16.6 Hz, 1H), 2.32 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 205.2, 195.8, 144.1, 137.3, 133.6, 132.9, 129.5, 119.2, 89.7, 78.3, 77.3, 77.0, 76.8, 75.1, 73.0, 66.3, 66.1, 46.1, 30.0. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{20}H_{17}FeO_2$ 345.0572; Found: 345.0573.

The e.e. value was determined by the chiral HPLC analysis (chiralpak® AD-H, Hexane / IPA = 90 / 10, 1.0 mL / min, λ= 254 nm, $t_{(minor)}$ = 8.213 min, $t_{(major)}$ = 12.772 min).

Compound (*R_p*, *R*)-3az



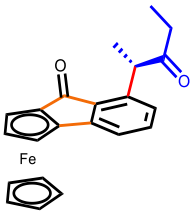
The resultant residue was purified by flash silica gel column chromatography to afford **(*R_p*, *R*)-3az** as a red solid; 27.2 mg, 47% yield; (eluent: petroleum ether/ethyl acetate: 30:1); 95% *e.e.*; *d.r.* = 1.6: 1 (obtained from the crude ^{1}H NMR spectrum).

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.28 – 7.19 (m, 1H), 7.04 (dd, *J* = 7.2, 5.7 Hz, 1H), 6.87 (dd, *J* = 23.2, 7.9 Hz, 1H), 5.29 – 5.23 (m, 1H), 4.98 – 4.94 (m, 1H), 4.87 (t, *J* = 3.7 Hz, 1H), 4.86 – 4.82 (m, 1H), 4.11 (s, 5H), 2.58 (dt, *J* = 7.2, 3.6 Hz, 1H), 2.49 – 2.33 (m, 1H), 1.39 (ddd, *J* = 40.7, 7.0, 1.1 Hz, 3H), 1.01 (dtd, *J* = 64.0, 7.3, 1.1 Hz, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$)δ 211.4, 196.3, 144.5 (d, *J* = 37.2 Hz), 140.9 (d, *J* = 46.0 Hz), 135.9, 133.3, 126.0 (d, *J* = 28.6 Hz), 119.2, 89.5 (d, *J* = 5.4 Hz), 78.7 (d, *J* = 21.7 Hz),

75.2 (d, J = 3.2 Hz), 72.9 (d, J = 7.0 Hz), 66.0 (d, J = 52.4 Hz), 44.7 (d, J = 11.9 Hz), 34.7, 16.9, 16.0, 8.1 (d, J = 34.7 Hz). **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{22}H_{20}FeO_2Na$ 395.0705; Found: 395.0715.

The e.e. value was determined by the chiral HPLC analysis (chiralpak® AD-H, Hexane / IPA = 90 / 10, 1.0 mL / min, λ= 254 nm, $t_{(minor)}$ = 8.764 min, $t_{(major)}$ = 11.105 min).

Compound (*R_p*, *S*)-3az



The resultant residue was purified by flash silica gel column chromatography to afford **(*R_p*, *S*)-3az** as a red solid; 17.0 mg, 29% yield; (eluent: petroleum ether/ethyl acetate: 30:1); 95% *e.e.*; *d.r.* = 1.6: 1 (obtained from the crude ^{1}H NMR spectrum).

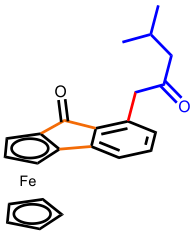
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.22 – 7.16 (m, 1H), 7.09 – 7.00 (m, 2H), 6.90 (dd, J = 22.9, 7.8 Hz, 1H), 5.29 (p, J = 7.1 Hz, 1H), 4.99 (dd, J = 5.6, 2.3 Hz, 1H), 4.97 (s, 1H), 4.86 (dt, J = 4.7, 2.3 Hz, 1H), 4.14 (d, J = 2.3 Hz, 5H), 2.61 (qd, J = 7.3, 2.8 Hz, 1H), 2.52 – 2.36 (m, 1H), 1.42 (dd, J = 40.7, 7.0 Hz, 3H), 1.04 (dt, J = 63.7, 7.3 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 211.5,, 196.3, 144.4, 144.3, 140.8, 140.4, 136.1, 135.9, 133.3, 126.0, 125.9, 119.0, 118.9, 89.5, 89.4, 78.6, 78.3, 77.2, 77.0, 76.8, 75.2, 75.2, 73.0, 72.9, 66.3, 66.2, 66.2, 66.2, 44.7, 44.7, 34.7, 34.6, 29.7, 16.9, 16.0, 8.2, 7.9.

HRMS (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{22}H_{20}FeO_2$ 395.0705; Found: 395.0715.

The e.e. value was determined by the chiral HPLC analysis (chiralpak® AD-H, Hexane / IPA = 90 / 10, 1.0 mL / min, λ= 254 nm, $t_{(minor)}$ = 8.683 min, $t_{(major)}$ = 11.249 min).

Compound 3ba

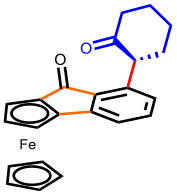


The resultant residue was purified by flash silica gel column chromatography to afford **3ba** as a red solid; 49.4 mg, 82% yield; (eluent: petroleum ether/ethyl acetate: 40:1); 99% *e.e.*

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.22 (t, *J* = 7.5 Hz, 1H), 7.06 (d, *J* = 7.3 Hz, 1H), 6.79 (d, *J* = 7.6 Hz, 1H), 4.92 (d, *J* = 2.4 Hz, 1H), 4.85 (d, *J* = 2.4 Hz, 1H), 4.80 (t, *J* = 2.4 Hz, 1H), 4.27 (d, *J* = 16.3 Hz, 1H), 4.14 (d, *J* = 1.2 Hz, 5H), 3.86 (d, *J* = 16.4 Hz, 1H), 2.50 (t, *J* = 7.2 Hz, 2H), 2.23 (dt, *J* = 13.4, 6.7 Hz, 1H), 0.96 (dd, *J* = 6.7, 5.0 Hz, 6H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 207.0, 195.9, 144.0, 137.3, 133.7, 132.8, 129.6, 119.0, 89.7, 78.3, 77.3, 77.0, 76.8, 75.0, 73.0, 72.8, 66.2, 66.1, 51.8, 45.6, 24.5, 22.7. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{23}H_{23}FeO_2$ 387.1042; Found: 387.1042.

The e.e. value was determined by the chiral HPLC analysis (chiralpak® AD-H, Hexane / IPA = 90 / 10, 1.0 mL / min, λ= 254 nm, $t_{(minor)}$ = 8.336 min, $t_{(major)}$ = 10.003 min).

Compound (*R_p*, *R*)-3bb



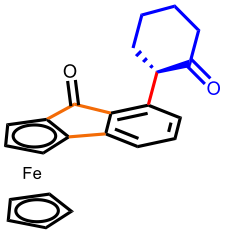
The resultant residue was purified by flash silica gel column chromatography to afford ***(R_p*, *R)*-3bb** as a red solid; 28.0 mg, 46% yield; (eluent: petroleum ether/ethyl acetate:

30:1); 99% *e.e.* ; *d.r.* = 2.5: 1 (obtained from the crude ^{1}H NMR spectrum).

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.29 – 7.21 (m, 1H), 7.05 (dd, *J* = 7.4, 2.5 Hz, 1H), 6.88 (dd, *J* = 24.7, 7.8 Hz, 1H), 4.89 (d, *J* = 2.4 Hz, 1H), 4.84 (s, 1H), 4.79 (d, *J* = 3.2 Hz, 1H), 4.17 (d, *J* = 2.9 Hz, 5H), 2.70 – 2.47 (m, 2H), 2.32 – 1.97 (m, 5H), 1.92 – 1.82 (m, 2H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 209.7, 195.9, 144.3, 143.8, 139.2, 138.5, 137.1, 136.7, 132.9, 132.9, 128.0, 125.8, 118.9, 118.7, 89.8, 89.6, 78.4, 78.2, 77.2, 77.0, 76.8, 74.9, 74.9, 73.1, 73.0, 66.1, 66.0, 66.0, 51.7, 42.4, 41.9, 33.3, 32.4, 29.7, 27.6, 25.6, 25.4. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{23}H_{21}FeO_2$ 385.0885; Found: 385.0884.

The e.e. value was determined by the chiral HPLC analysis (chiralpak® AD-H, Hexane / IPA = 90 / 10, 1.0 mL / min, λ= 254 nm, $t_{(minor)}$ = 8.314 min, $t_{(major)}$ = 9.491 min).

Compound (*R_p*, *S*)-3bb



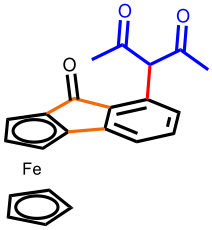
The resultant residue was purified by flash silica gel column chromatography to afford **(*R_p*, *S*)-3bb** as a red solid; 11.2 mg, 19% yield; (eluent: petroleum ether/ethyl acetate: 30:1); 99% *e.e.*; *d.r.* = 2.5: 1 (obtained from the crude ^{1}H NMR spectrum).

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.33 – 7.16 (m, 1H), 7.05 (ddd, *J* = 7.4, 2.5, 1.0 Hz, 1H), 6.88 (dd, *J* = 24.9, 7.7 Hz, 1H), 4.89 (dd, *J* = 2.4, 0.7 Hz, 1H), 4.85 – 4.83 (m, 1H), 4.79 (dt, *J* = 3.9, 2.4 Hz, 1H), 4.17 (d, *J* = 3.0 Hz, 5H), 2.71 – 2.61 (m, 1H), 2.58 – 2.45 (m, 1H), 2.24 (dddd, *J* = 44.4, 11.6, 5.3, 2.8 Hz, 2H), 2.14 – 1.99 (m, 3H), 1.90 – 1.78 (m,

2H).**^{13}C NMR** (151 MHz, $CDCl_3$) δ 209.3, 196.5, 144.3, 143.8, 139.2, 138.5, 137.1, 136.6, 133.0, 132.9, 119.0, 118.8, 89.8, 89.6, 78.4, 77.2, 77.0, 76.8, 75.0, 74.9, 73.1, 73.0, 73.0, 72.8, 66.2, 66.1, 66.0, 42.4, 41.9, 33.3, 32.4, 29.7, 25.6, 25.4.**HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{23}H_{20}FeO_2$ 385.0885; Found: 385.0884.

The e.e. value was determined by the chiral HPLC analysis (chiralpak® AD-H, Hexane / IPA = 90 / 10, 1.0 mL / min, λ= 254 nm, $t_{(minor)}$ = 8.455 min, $t_{(major)}$ = 9.328 min).

Compound 3bc

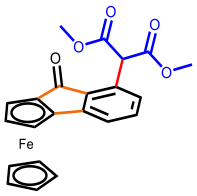


The resultant residue was purified by flash silica gel column chromatography to afford **3bc** as a red solid; 38.3 mg, 65% yield; (eluent: petroleum ether/ethyl acetate: 10:1); 98% *e.e.*.

^{1}H NMR (600 MHz, DMSO-d6) δ 7.42 (t, *J* = 7.5 Hz, 1H), 7.33 (d, *J* = 7.3 Hz, 1H), 6.95 (d, *J* = 7.6 Hz, 1H), 5.19 (d, *J* = 2.3 Hz, 1H), 4.98 (d, *J* = 2.4 Hz, 1H), 4.97 (d, *J* = 2.4 Hz, 1H), 4.15 (s, 5H), 1.95 (s, 3H), 1.73 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 194.5, 189.9, 189.3, 144.7, 138.1, 134.7, 133.2, 130.9, 119.9, 111.1, 89.5, 78.6, 77.2, 77.0, 76.8, 75.2, 73.0, 72.6, 66.3, 66.1, 46.1, 29.7, 23.7, 23.7. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{22}H_{18}FeO_3Na$ 409.0498; Found: 409.0500.

The e.e. value was determined by the chiral HPLC analysis (chiralpak® AD-H, Hexane / IPA = 80 / 20, 1.0 mL / min, λ= 254 nm, $t_{(minor)}$ = 7.903 min, $t_{(major)}$ = 16.555 min).

Compound 3bd

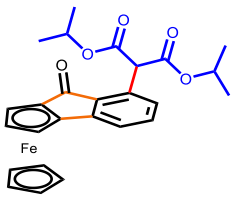


The resultant residue was purified by flash silica gel column chromatography to afford **3bd** as a red solid; 34.6 mg, 53% yield; (eluent: petroleum ether/ethyl acetate: 20:1); 97% *e.e.*.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.28 (t, *J* = 7.6 Hz, 1H), 7.12 (d, *J* = 7.5 Hz, 1H), 7.08 (d, *J* = 7.9 Hz, 1H), 6.13 (s, 1H), 4.95 (d, *J* = 1.8 Hz, 1H), 4.88 (d, *J* = 2.4 Hz, 1H), 4.84 (t, *J* = 2.4 Hz, 1H), 4.12 (s, 5H), 3.81 (s, 3H), 3.77 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 195.3, 168.6, 168.6, 144.1, 136.8, 133.1, 131.4, 127.1, 120.0, 89.3, 78.2, 77.2, 77.0, 76.8, 75.4, 73.2, 66.5, 66.5, 52.8, 52.7, 52.7, 50.9. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{22}H_{18}FeO_5Na$ 419.0576; Found: 419.0576.

The e.e. value was determined by the chiral HPLC analysis (chiralpak® AD-H, Hexane / IPA = 90 / 10, 1.0 mL / min, λ= 254 nm, $t_{(minor)}$ = 9.886 min, $t_{(major)}$ = 12.886 min).

Compound 3be



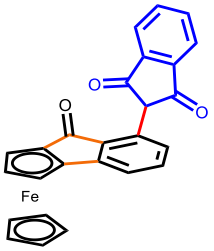
The resultant residue was purified by flash silica gel column chromatography to afford **3be** as a red solid; 38.5 mg, 52% yield; (eluent: petroleum ether/ethyl acetate: 20:1); 90% *e.e.*.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.28 (t, *J* = 7.6 Hz, 1H), 7.12 (d, *J* = 7.5 Hz, 1H), 7.08

(d, J = 7.9 Hz, 1H), 6.13 (s, 1H), 4.95 (d, J = 1.8 Hz, 1H), 4.88 (d, J = 2.4 Hz, 1H), 4.84 (t, J = 2.4 Hz, 1H), 4.12 (s, 5H), 3.81 (s, 3H), 3.77 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 195.3, 168.6, 168.6, 144.1, 136.8, 133.1, 131.4, 127.1, 120.0, 89.3, 78.2, 77.2, 77.0, 76.8, 75.4, 73.2, 66.5, 66.5, 52.8, 52.7, 52.7, 50.9. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{22}H_{18}FeO_5Na$ 419.0576; Found: 419.0576.

The e.e. value was determined by the chiral HPLC analysis (chiralpak® AD-H, Hexane / IPA = 80 / 20, 1.0 mL / min, λ= 254 nm, $t_{(minor)}$ = 7.108 min, $t_{(major)}$ = 9.106 min).

Compound 3bf

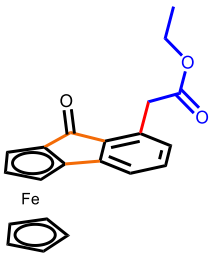


The resultant residue was purified by flash silica gel column chromatography to afford **3bf** as a red solid; 14.2 mg, 21% yield; (eluent: petroleum ether/ethyl acetate: 5:1); 99% *e.e.*.

^{1}H NMR (600 MHz, DMSO-d_6) δ 8.07 (s, 1H), 7.99 (s, 3H), 7.61 (s, 1H), 7.52 (s, 2H), 7.33 (s, 1H), 5.19 (s, 1H), 4.95 (s, 1H), 4.81 (s, 1H), 4.09 (s, 5H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 197.4, 196.9, 141.4, 140.9, 136.3, 134.2, 134.1, 133.2, 128.9, 128.9, 125.6, 124.4, 124.3, 120.5, 89.6, 79.3, 77.2, 77.0, 76.8, 76.3, 73.8, 67.5, 67.4, 29.7. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{26}H_{17}FeO_3$ 433.0522; Found: 433.0522.

The e.e. value was determined by the chiral HPLC analysis (chiralpak® AD-H, Hexane / IPA = 80 / 20, 1.0 mL / min, λ= 254 nm, $t_{(minor)}$ = 17.773 min, $t_{(major)}$ = 19.157 min).

Compound 3bg

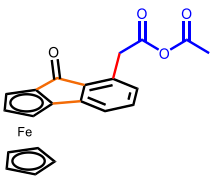


The resultant residue was purified by flash silica gel column chromatography to afford **3bg** as a red solid; 19.3 mg, 33% yield; (eluent: petroleum ether/ethyl acetate: 20:1); 95% *e.e.*.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.23 (t, *J* = 7.5 Hz, 1H), 7.08 (d, *J* = 7.4 Hz, 1H), 6.88 (d, *J* = 7.7 Hz, 1H), 4.93 (s, 1H), 4.85 (s, 1H), 4.81 (d, *J* = 2.6 Hz, 1H), 4.23 – 4.17 (m, 3H), 4.13 (s, 5H), 3.85 (d, *J* = 16.5 Hz, 1H), 1.30 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 195.5, 171.1, 144.1, 137.5, 133.3, 132.8, 129.2, 119.2, 89.7, 78.4, 77.2, 77.0, 76.8, 75.0, 73.0, 66.2, 66.1, 60.7, 36.6, 29.7, 14.3. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{21}H_{19}FeO_3$ 375.0678; Found: 375.0678.

The e.e. value was determined by the chiral HPLC analysis (chiralpak® AD-H, Hexane / IPA = 90 / 10, 1.0 mL / min, λ= 254 nm, $t_{(minor)}$ = 11.163 min, $t_{(major)}$ = 12.444 min).

Compound 3bh



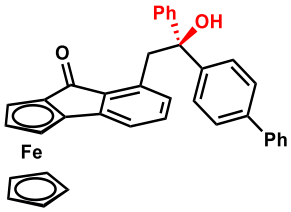
The resultant residue was purified by flash silica gel column chromatography to afford

3bh as a red solid; 41.2 mg, 65% yield; (eluent: petroleum ether/ethyl acetate: 20:1); 99% *e.e.*

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.23 (t, *J* = 7.5 Hz, 1H), 7.08 (d, *J* = 7.4 Hz, 1H), 6.80 (d, *J* = 8.6 Hz, 1H), 4.92 (d, *J* = 2.4 Hz, 0H), 4.86 (d, *J* = 1.7 Hz, 1H), 4.82 (t, *J* = 2.4 Hz, 1H), 4.27 (d, *J* = 16.5 Hz, 1H), 4.15 (s, 5H), 3.90 (d, *J* = 16.5 Hz, 1H), 2.33 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 205.3, 195.9, 144.1, 137.3, 133.6, 132.9, 129.5, 119.2, 89.7, 78.3, 77.2, 77.0, 76.8, 75.1, 73.0, 66.3, 66.1, 46.1, 30.0. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{21}H_{27}FeO_4$ 399.1253; Found: 399.1253.

The e.e. value was determined by the chiral HPLC analysis (chiralpak® AD-H, Hexane / IPA = 90 / 10, 1.0 mL / min, λ= 254 nm, $t_{(minor)}$ = 9.493 min, $t_{(major)}$ = 17.859 min).

Compound (R_p, *S*)-4aa

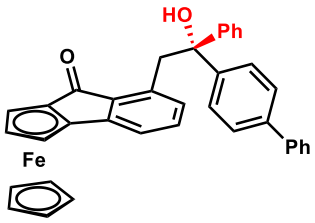


The resultant residue was purified by flash silica gel column chromatography to afford **(R_p, *S*)-4aa** as a red solid; 31.3 mg, 46% yield; (eluent: petroleum ether/ethyl acetate: 15:1); *d.r.* = 1.3: 1 (obtained from the crude ^{1}H NMR spectrum).

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.83 (d, *J* = 8.1 Hz, 2H), 7.55 (dd, *J* = 7.9, 1.4 Hz, 4H), 7.40 (t, *J* = 7.6 Hz, 2H), 7.33 (d, *J* = 7.0 Hz, 1H), 7.27 – 7.21 (m, 3H), 7.18 – 7.13 (m, 1H), 7.11 (t, *J* = 7.1 Hz, 2H), 7.07 (d, *J* = 6.9 Hz, 1H), 6.86 (d, *J* = 7.6 Hz, 1H), 4.58 (d, *J* = 2.3 Hz, 1H), 4.25 (d, *J* = 16.4 Hz, 1H), 4.20 (t, *J* = 2.4 Hz, 1H), 4.12 (d, *J* = 2.2 Hz,

2H), 4.09 (s, 5H), 4.03 (d, J = 16.5 Hz, 1H), 3.34 (s, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 198.3, 151.7, 145.6, 143.2, 140.4, 140.0, 135.7, 132.4, 129.1, 129.0, 128.9, 128.5, 128.2, 127.3, 127.1, 126.9, 126.9, 125.9, 125.3, 119.0, 104.7, 89.3, 79.9, 77.2, 77.0, 76.8, 70.4, 69.8, 61.6, 60.2, 41.1. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{37}H_{28}FeO_2Na$ 583.1331; Found: 583.1334.

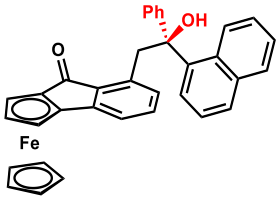
Compound (*R_p*, *R*)-4aa



The resultant residue was purified by flash silica gel column chromatography to afford **(*R_p*, *R*)-4aa** as a red solid; 24.1 mg, 36% yield; (eluent: petroleum ether/ethyl acetate: 15:1); *d.r.* = 1.3: 1 (obtained from the crude ^{1}H NMR spectrum).

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.90 (d, J = 8.1 Hz, 2H), 7.64 – 7.60 (m, 4H), 7.47 (t, J = 7.6 Hz, 2H), 7.43 – 7.37 (m, 1H), 7.30 (dd, J = 16.2, 7.4 Hz, 3H), 7.23 (t, J = 7.6 Hz, 1H), 7.18 (t, J = 7.3 Hz, 2H), 7.15 – 7.11 (m, 1H), 6.92 (d, J = 7.6 Hz, 1H), 4.66 (d, J = 2.3 Hz, 1H), 4.33 – 4.26 (m, 2H), 4.18 (d, J = 2.3 Hz, 1H), 4.16 (s, 5H), 4.10 (d, J = 16.5 Hz, 1H), 3.40 (s, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 198.3, 151.7, 145.6, 143.1, 140.4, 140.0, 135.6, 132.3, 129.1, 129.0, 128.9, 128.4, 128.2, 128.2, 127.3, 127.1, 127.0, 126.9, 125.8, 125.3, 119.0, 104.6, 89.2, 79.9, 77.2, 77.0, 76.8, 70.6, 70.4, 69.8, 61.6, 60.2, 41.1. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{37}H_{28}FeO_2$ 583.1331; Found: 583.1334.

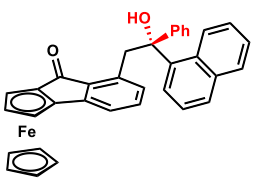
Compound (R_p, *S*)-4ab



The resultant residue was purified by flash silica gel column chromatography to afford **(R_p, *S*)-4ab** as a red solid; 36.3 mg, 51% yield; (eluent: petroleum ether/ethyl acetate: 15:1); *d.r.* = 2.1: 1 (obtained from the crude ^{1}H NMR spectrum).

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.54 (d, *J* = 8.6 Hz, 1H), 7.91 (d, *J* = 8.3 Hz, 1H), 7.82 (d, *J* = 8.1 Hz, 1H), 7.70 (d, *J* = 7.2 Hz, 1H), 7.54 (t, *J* = 7.8 Hz, 1H), 7.48 (t, *J* = 7.5 Hz, 1H), 7.39 (t, *J* = 7.7 Hz, 1H), 7.29 (d, *J* = 7.6 Hz, 3H), 7.23 (t, *J* = 7.6 Hz, 1H), 7.14 (t, *J* = 7.6 Hz, 2H), 7.09 (d, *J* = 7.3 Hz, 1H), 6.99 (d, *J* = 7.6 Hz, 1H), 4.63 – 4.60 (m, 1H), 4.40 (d, *J* = 16.9 Hz, 1H), 4.22 (s, 2H), 4.15 (s, 1H), 4.08 (s, 6H), 3.32 (s, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 198.6, 156.8, 148.2, 144.5, 144.5, 135.8, 135.3, 134.0, 130.9, 129.6, 129.5, 129.2, 129.0, 128.8, 128.2, 128.1, 128.0, 127.5, 127.1, 127.0, 126.9, 126.2, 125.8, 125.8, 125.3, 124.8, 124.4, 102.0, 81.0, 77.2, 77.0, 76.8, 70.8, 70.6, 70.2, 62.6, 59.5, 30.9. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{35}H_{26}FeO_2Na$ 557.1174; Found: 557.1180.

Compound (R_p, *R*)-4ab

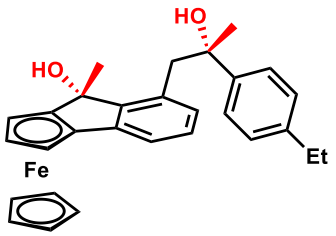


The resultant residue was purified by flash silica gel column chromatography to afford **(R_p, *R*)- 4ab** as a red solid; 17.3 mg, 25% yield; (eluent: petroleum ether/ethyl acetate:

15:1); *d.r.* = 2.1: 1 (obtained from the crude ^{1}H NMR spectrum).

^{1}H NMR (600 MHz, $CDCl_3$) δ 9.28 (d, *J* = 8.6 Hz, 1H).7.97 (d, *J* = 8.2 Hz, 1H), 7.86 (d, *J* = 8.2 Hz, 1H), 7.71 (ddd, *J* = 8.5, 6.9, 1.4 Hz, 1H), 7.66 (dd, *J* = 7.5, 1.1 Hz, 1H), 7.61 – 7.57 (m, 2H), 7.32 (t, *J* = 7.7 Hz, 2H), 7.27 (d, *J* = 2.1 Hz, 1H), 7.24 (dd, *J* = 5.1, 2.0 Hz, 2H), 7.07 (t, *J* = 7.7 Hz, 1H), 6.66 (dd, *J* = 7.3, 1.2 Hz, 1H), 6.43 (s, 1H), 4.60 (d, *J* = 2.2 Hz, 1H), 4.32 (dd, *J* = 10.1, 2.3 Hz, 3H), 4.24 (s, 6H), 4.16 (s, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 202.5, 151.8, 143.2, 140.5, 135.9, 134.0, 132.4, 132.3, 130.4, 129.1, 128.8, 128.4, 128.2, 127.8, 127.8, 127.0, 126.4, 126.0, 125.3, 125.3, 124.3, 119.1, 104.6, 89.2, 80.0, 77.3, 77.1, 76.9, 70.7, 70.4, 69.8, 61.6, 60.3, 44.8. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{35}H_{26}FeO_2$ 557.1174; Found: 557.1180.

Compound (*R_p*, *S*, *S*)-4ac

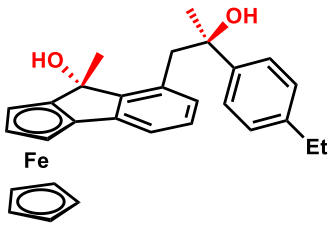


The resultant residue was purified by flash silica gel column chromatography to afford **(*R_p*, *S*, *S*)-4ac** as a red solid; 25.2 mg, 31% yield; (eluent: petroleum ether/ethyl acetate: 15:1); *d.r.* = 1.4: 1 (obtained from the crude ^{1}H NMR spectrum).

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.54 (d, *J* = 8.0 Hz, 2H), 7.23 (d, *J* = 7.9 Hz, 2H), 7.20 – 7.15 (m, 2H), 7.06 (dd, *J* = 6.0, 2.8 Hz, 1H), 4.60 (s, 1H), 4.38 (s, 1H), 4.30 (s, 1H), 4.07 (d, *J* = 6.4 Hz, 6H), 3.88 (s, 1H), 3.59 (d, *J* = 14.0 Hz, 1H), 3.02 (d, *J* = 14.0 Hz, 1H), 2.67 (q, *J* = 7.6 Hz, 2H), 1.65 (s, 3H), 1.62 (s, 3H), 1.26 (t, *J* = 7.6 Hz, 3H).**^{13}C NMR** (151 MHz, $CDCl_3$) δ 152.2, 147.6, 142.4, 139.6, 134.0, 129.7, 127.7, 124.8,

118.7, 102.3, 77.2, 77.0, 77.0, 76.8, 73.9, 69.8, 69.7, 60.3, 60.0, 45.3, 28.7, 28.4, 28.2, 15.4. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{29}H_{30}FeO_2Na$ 489.1487; Found: 489.1490.

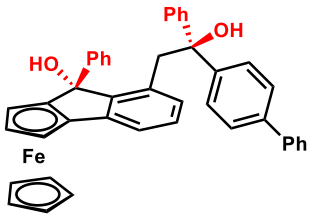
Compound (*R_p*, *S*, *R*)-4ac



The resultant residue was purified by flash silica gel column chromatography to afford **(*R_p*, *S*, *R*)-4ac** as a red solid; 18.0 mg, 22% yield; (eluent: petroleum ether/ethyl acetate: 15:1); *d.r.* = 1.4: 1 (obtained from the crude ^{1}H NMR spectrum).

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.65 – 7.62 (m, 2H), 7.33 (d, *J* = 7.8 Hz, 2H), 7.30 – 7.24 (m, 2H), 7.17 (d, *J* = 7.3 Hz, 1H), 4.65 (d, *J* = 2.2 Hz, 1H), 4.45 (d, *J* = 2.0 Hz, 1H), 4.36 (d, *J* = 2.2 Hz, 1H), 4.14 (s, 5H), 3.99 (s, 1H), 3.70 (d, *J* = 14.0 Hz, 1H), 3.13 (d, *J* = 13.9 Hz, 1H), 2.77 (q, *J* = 7.6 Hz, 2H), 1.74 (s, 3H), 1.72 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 152.2, 147.6, 142.4, 139.6, 134.0, 129.7, 127.7, 124.8, 118.7, 102.3, 77.2, 77.0, 77.0, 76.8, 73.9, 69.8, 70.0, 60.3, 60.0, 45.3, 28.7, 28.4, 28.2, 15.4. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{29}H_{30}FeO_2$ 489.1487; Found: 489.1490.

Compound (*R_p*, *S*, *S*)-4ad

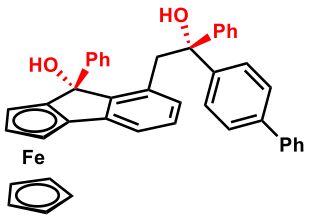


The resultant residue was purified by flash silica gel column chromatography to afford

(R_p, *S*, *S*)-4ad as a red solid; 24.9 mg, 28% yield; (eluent: petroleum ether/ethyl acetate: 15:1); *d.r.* = 1.2: 1 (obtained from the crude ^{1}H NMR spectrum).

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.59 – 7.55 (m, 2H), 7.46 (dd, *J* = 8.4, 1.9 Hz, 2H), 7.44 – 7.40 (m, 2H), 7.37 (t, *J* = 7.9 Hz, 2H), 7.33 – 7.30 (m, 2H), 7.27 (t, *J* = 7.5 Hz, 3H), 7.21 – 7.18 (m, 3H), 7.13 (dd, *J* = 5.2, 2.6 Hz, 4H), 6.80 (td, *J* = 7.6, 1.8 Hz, 1H), 5.96 (d, *J* = 7.8 Hz, 1H), 5.04 (s, 1H), 4.59 (d, *J* = 2.3 Hz, 1H), 4.20 (t, *J* = 2.3 Hz, 1H), 4.13 (d, *J* = 1.8 Hz, 6H), 4.11 (d, *J* = 2.2 Hz, 1H), 3.62 (d, *J* = 13.8 Hz, 1H), 3.23 (d, *J* = 13.7 Hz, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 152.1, 151.4, 149.6, 148.0, 145.2, 140.9, 129.8, 129.6, 128.7, 128.2, 128.1, 127.9, 127.4, 127.1, 127.0, 126.8, 126.5, 126.2, 125.2, 118.5, 104.7, 89.7, 79.9, 77.2, 77.0, 76.8, 70.3, 69.9, 61.1, 60.3, 42.8. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{43}H_{34}FeO_2Na$ 661.1800; Found: 661.1803.

Compound (R_p, *S*, *R*)-4ad

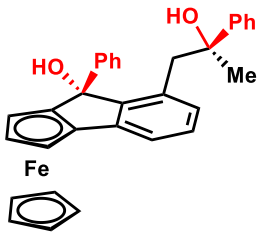


The resultant residue was purified by flash silica gel column chromatography to afford **(R_p, *S*, *R*)-4ad** as a red solid; 20.7 mg, 23% yield; (eluent: petroleum ether/ethyl acetate: 15:1); *d.r.* = 1.2: 1 (obtained from the crude ^{1}H NMR spectrum).

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.65 – 7.61 (m, 2H), 7.54 – 7.49 (m, 2H), 7.49 – 7.46 (m, 2H), 7.43 (t, *J* = 7.7 Hz, 2H), 7.38 – 7.31 (m, 5H), 7.27 – 7.23 (m, 4H), 7.19 (td, *J* = 4.7, 4.0, 2.0 Hz, 4H), 6.85 (t, *J* = 7.6 Hz, 1H), 5.98 (d, *J* = 7.7 Hz, 1H), 5.20 (s, 1H), 4.65 (d, *J* = 2.3 Hz, 1H), 4.26 (t, *J* = 2.3 Hz, 1H), 4.21 (s, 1H), 4.19 (s, 5H), 4.17 (d, *J*

= 2.4 Hz, 1H), 3.66 (d, *J* = 13.8 Hz, 1H), 3.28 (d, *J* = 13.7 Hz, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 152.7, 149.4, 145.9, 143.7, 141.0, 139.4, 139.0, 134.1, 129.6, 128.7, 128.2, 128.1, 128.0, 127.4, 127.1, 127.0 126.8, 126.5, 126.2, 125.2, 118.5, 104.7, 89.8, 79.9, 77.2, 77.1, 77.0, 76.8, 70.3, 69.9, 61.1, 60.3, 42.8. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{43}H_{34}FeO_2$ 661.1800; Found: 661.1803.

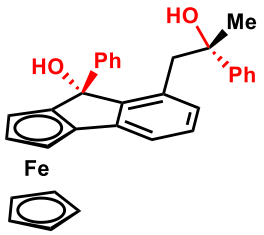
Compound (*R_p*, *S*, *R*)-4ae



The resultant residue was purified by flash silica gel column chromatography to afford **(*R_p*, *S*, *R*)-4ae** as a red solid; 27.0 mg, 36% yield; (eluent: petroleum ether/ethyl acetate: 15:1); *d.r.* = 1.4: 1 (obtained from the crude ^{1}H NMR spectrum).

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.50 (d, *J* = 7.7 Hz, 2H), 7.32 (t, *J* = 7.5 Hz, 2H), 7.25 (d, *J* = 7.4 Hz, 1H), 7.22 – 7.19 (m, 2H), 7.17 (d, *J* = 7.6 Hz, 2H), 7.08 (dt, *J* = 13.3, 7.3 Hz, 3H), 7.00 (d, *J* = 7.6 Hz, 1H), 4.62 (s, 1H), 4.45 (s, 1H), 4.24 (s, 1H), 4.15 (s, 7H), 2.97 (d, *J* = 14.3 Hz, 1H), 2.65 (d, *J* = 14.3 Hz, 1H), 1.51 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 152.6, 150.2, 143.8, 140.2, 134.8, 130.2, 128.4, 128.2, 128.1, 128.1, 127.8, 126.8, 126.4, 125.6, 125.1, 125.1, 124.7, 118.7, 79.7, 77.2, 77.0, 76.8, 73.7, 70.3, 69.9, 69.8, 61.3, 60.0, 45.1, 28.5. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{32}H_{28}FeO_2Na$ 523.1331; Found: 523.1333.

Compound (R_p, *S*, *S*)-4ae



The resultant residue was purified by flash silica gel column chromatography to afford **(R_p, *S*, *S*)-4ae** as a red solid; 19.3 mg, 26% yield; (eluent: petroleum ether/ethyl acetate: 15:1); *d.r.* = 1.4: 1 (obtained from the crude ^{1}H NMR spectrum).

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.57 – 7.51 (d, 2H), 7.35 (t, *J* = 7.8 Hz, 3H), 7.31 – 7.27 (d, 1H), 7.24 (t, *J* = 7.5 Hz, 2H), 7.22 – 7.17 (m, 2H), 7.13 – 7.08 (m, 2H), 7.03 (d, *J* = 7.6 Hz, 1H), 4.66 – 4.63 (m, 1H), 4.54 (s, 1H), 4.29 – 4.25 (m, 2H), 4.20 – 4.14 (m, 6H), 2.99 (d, *J* = 14.3 Hz, 1H), 2.67 (d, *J* = 14.4 Hz, 1H), 1.55 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 152.7, 150.2, 143.8, 140.2, 134.8, 130.2, 128.4, 128.1, 128.0, 126.8, 126.4, 125.1, 124.7, 118.7, 105.0, 89.6, 79.8, 77.2, 77.0, 76.8, 73.8, 70.3, 70.0, 61.3, 60.0, 45.1, 28.6. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ calcd for $C_{32}H_{28}FeO_2$ 523.1331; Found: 523.1333.

8. NMR spectroscopic and HPLC data

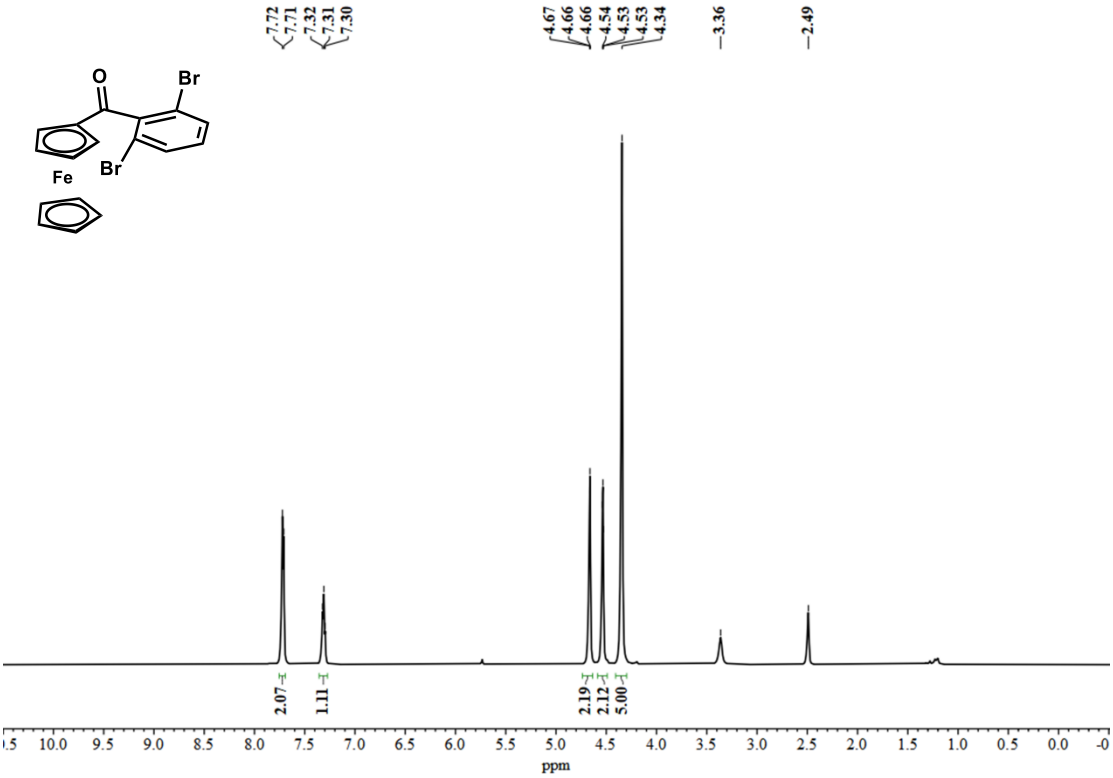


Figure S8.1 ^{1}H NMR of **1** (600 MHz, DMSO-d_6)

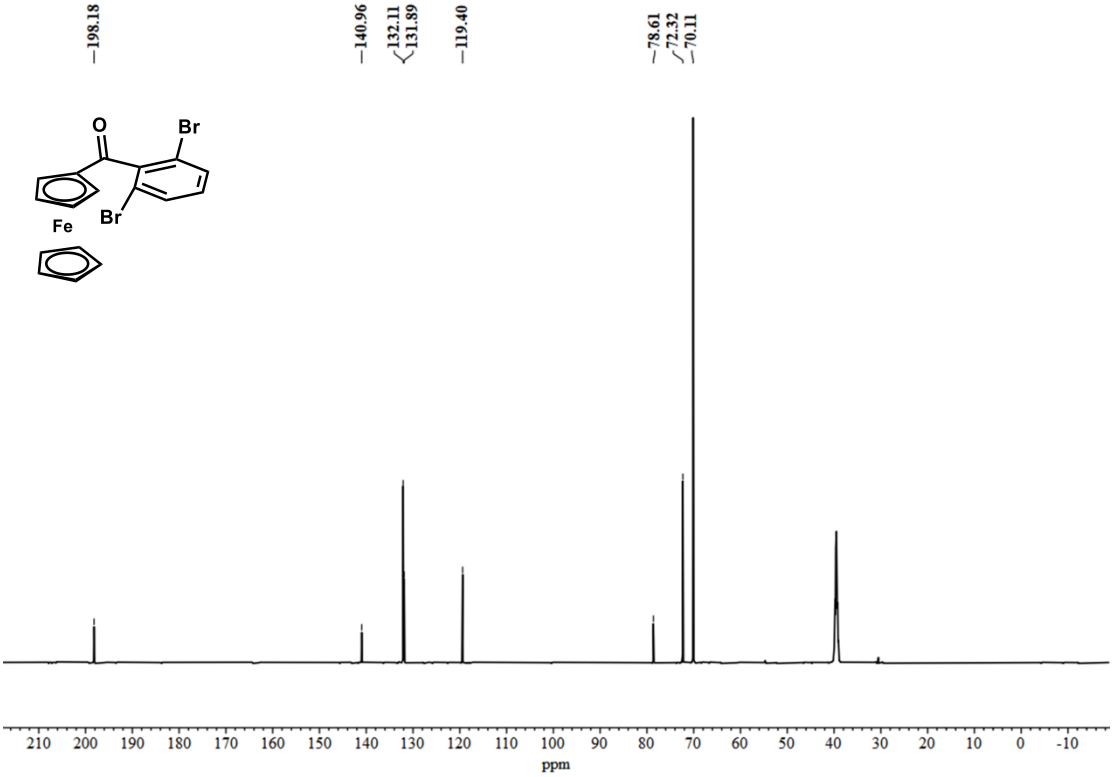


Figure S8.2 ^{13}C NMR of **1** (151 MHz, DMSO-d_6)

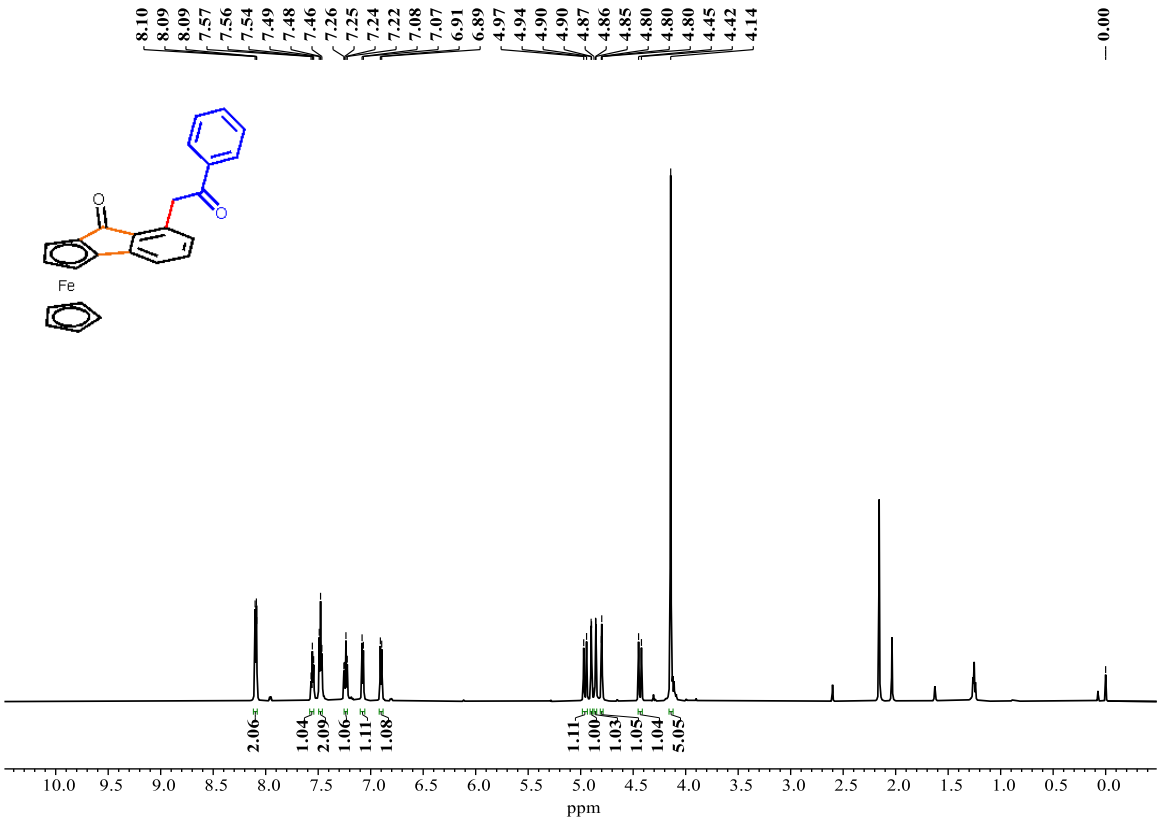


Figure S8.3 ^{1}H NMR of **3aa** (600 MHz, $CDCl_3$)

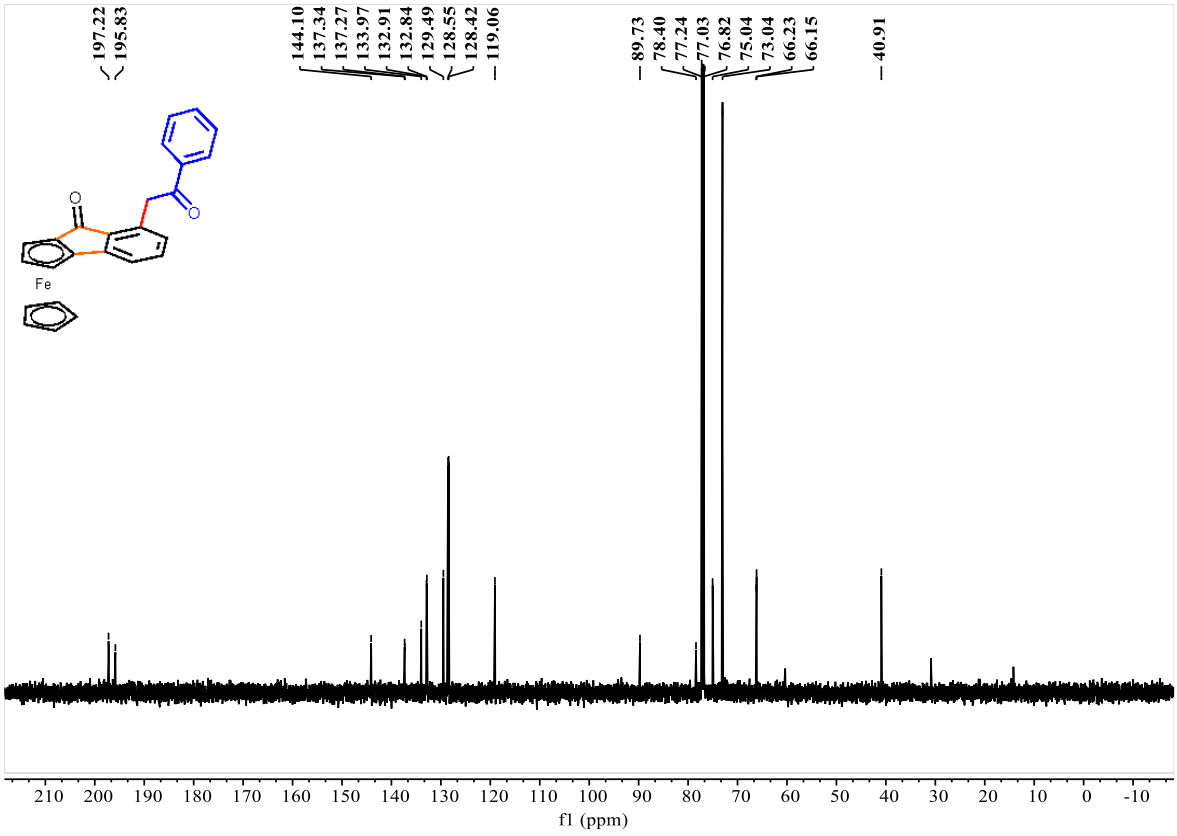


Figure S8.4 ^{13}C NMR of **3aa** (151 MHz, $CDCl_3$)

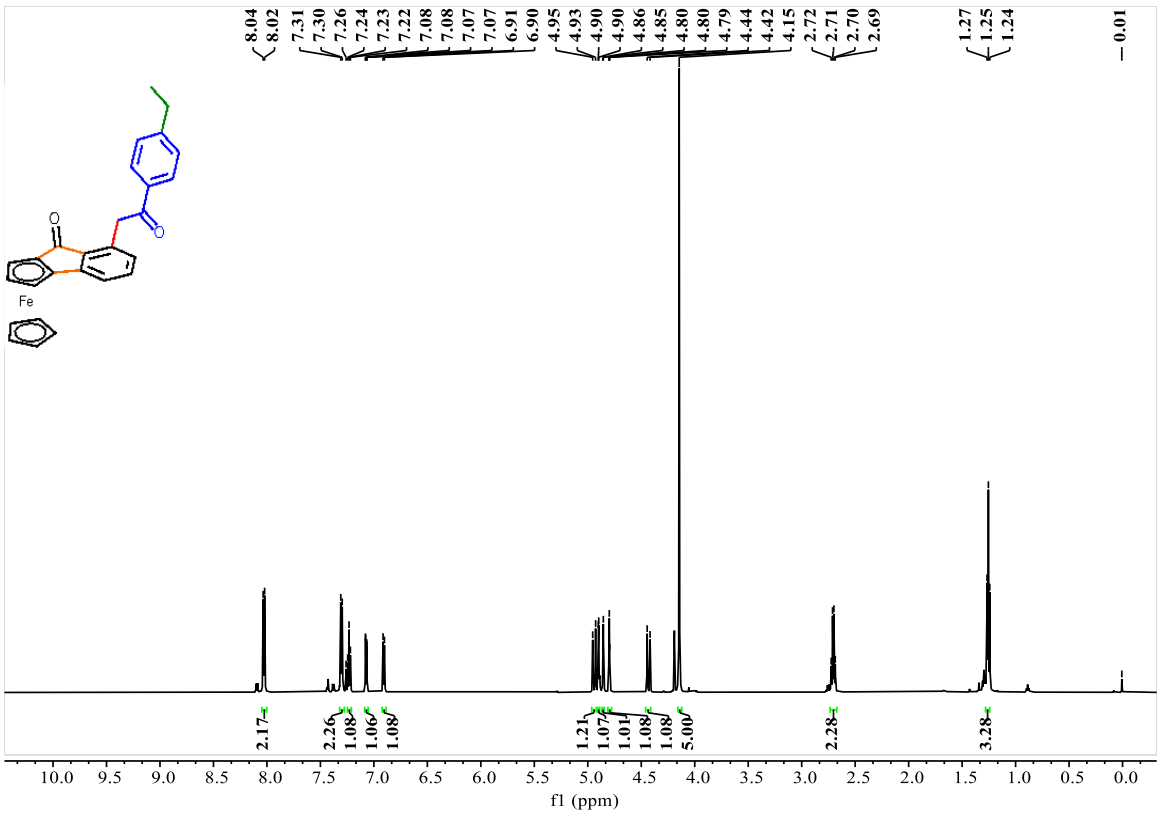


Figure S8.5 ^{1}H NMR of **3ab** (600 MHz, $CDCl_3$)

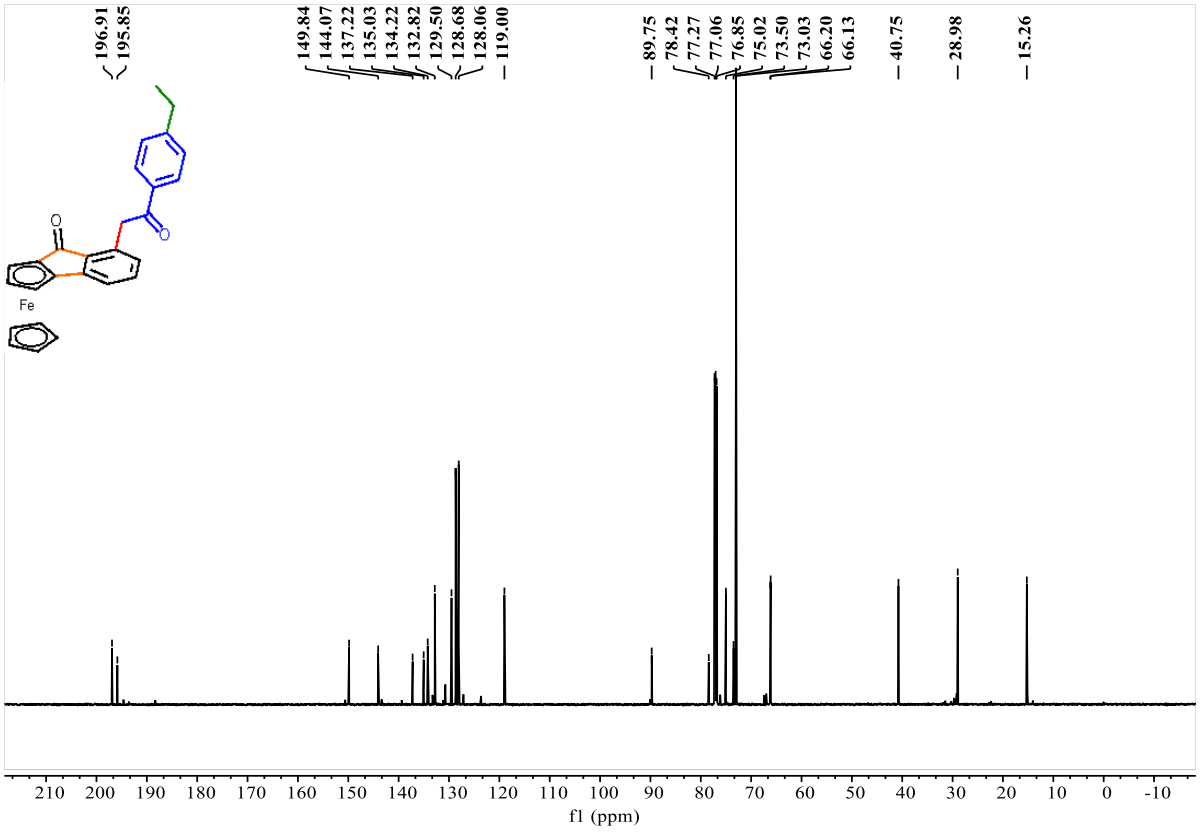


Figure S8.6 ^{13}C NMR of **3ab** (151 MHz, $CDCl_3$)

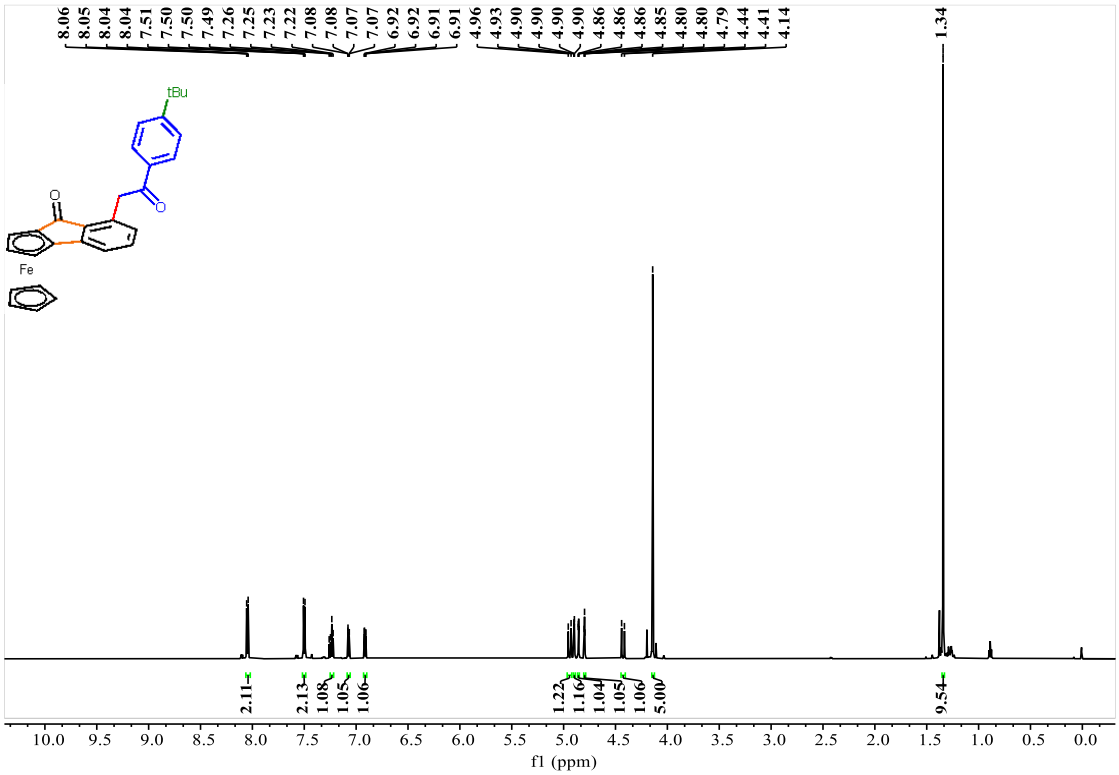


Figure S8.7 ^{1}H NMR of **3ac** (600 MHz, $CDCl_3$)

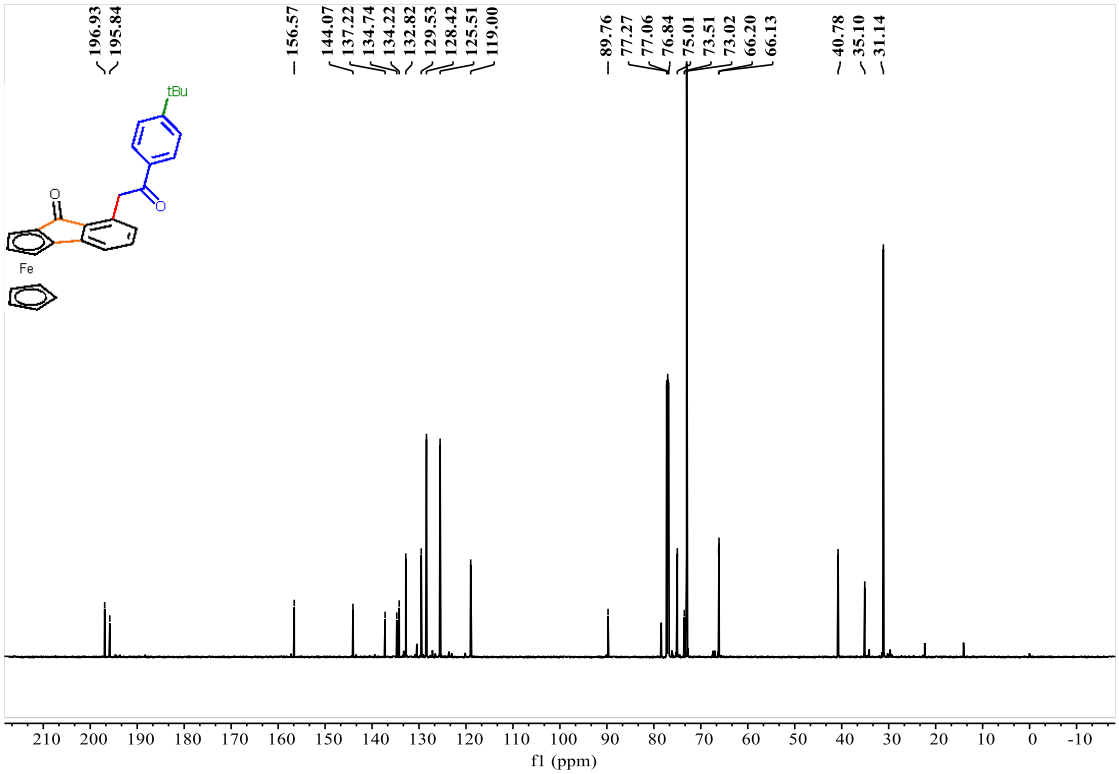


Figure S8.8 ^{13}C NMR of **3ac** (151 MHz, $CDCl_3$)

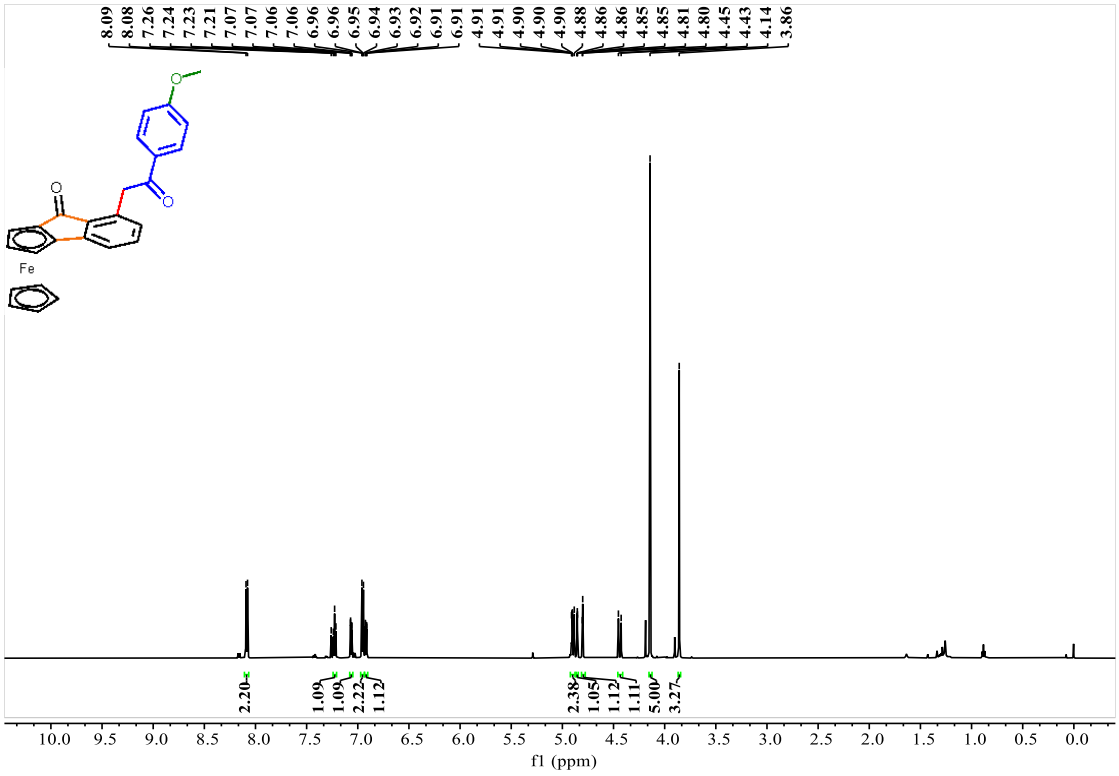


Figure S8.9 ^{1}H NMR of **3ad** (600 MHz, $CDCl_3$)

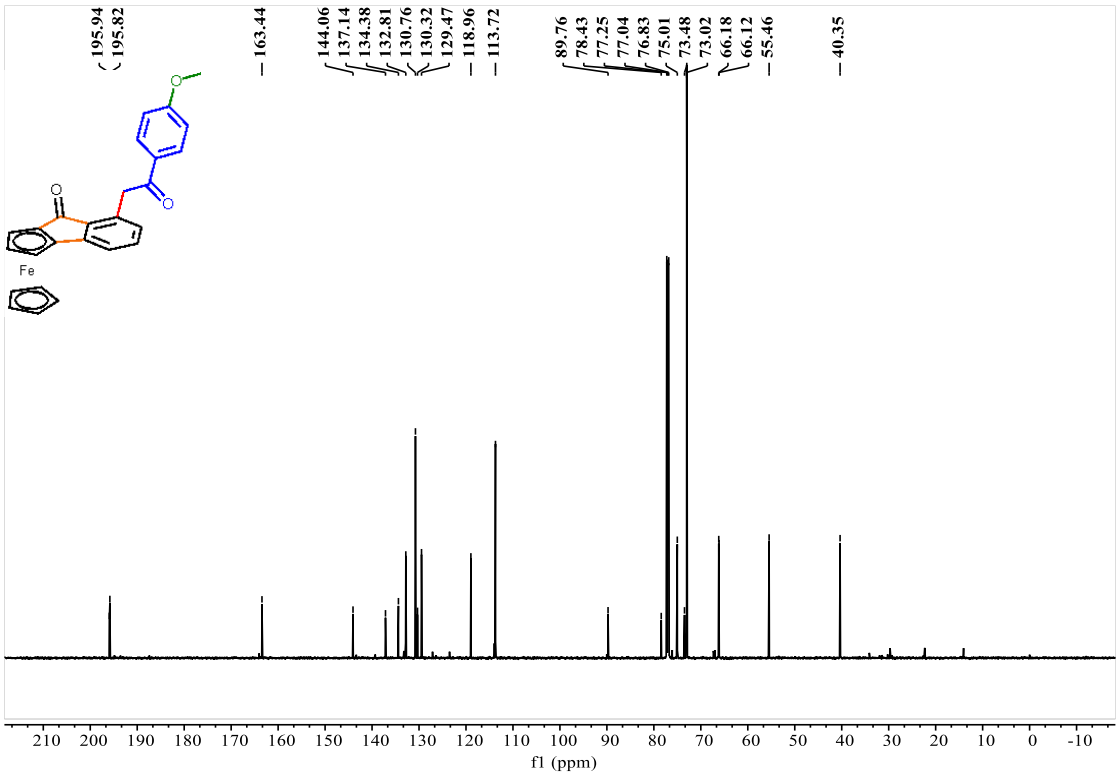


Figure S8.10 ^{13}C NMR of **3ad** (151 MHz, $CDCl_3$)

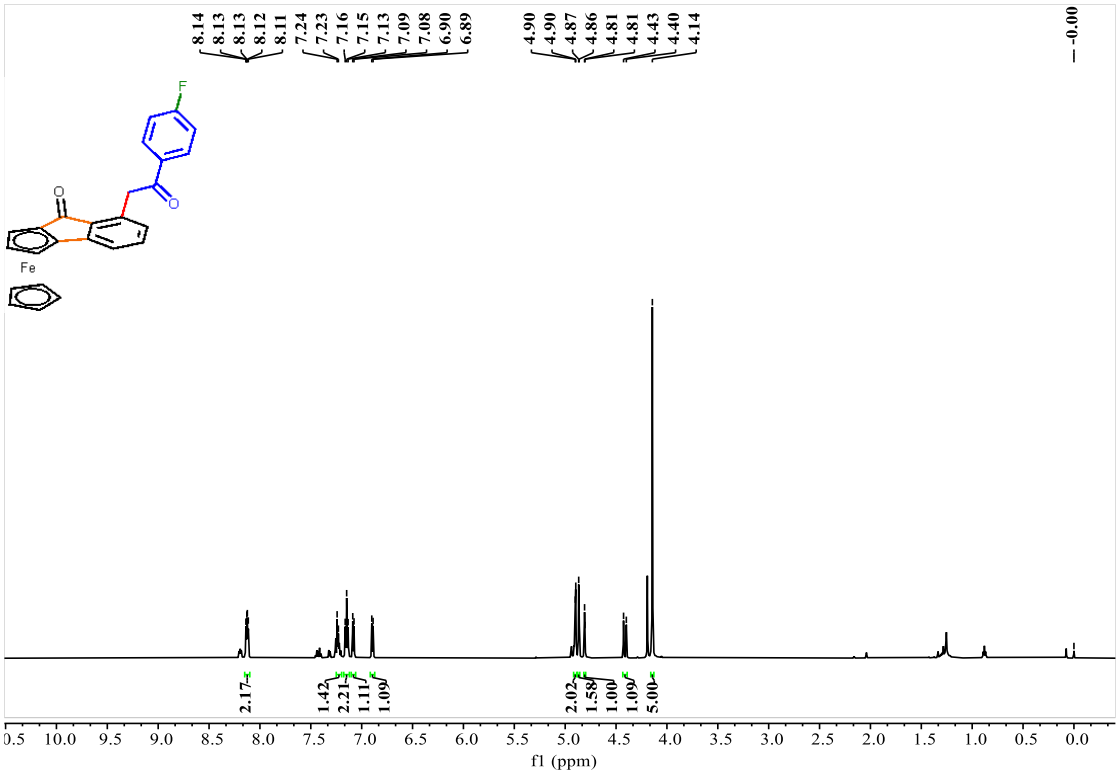


Figure S8.11 ^{1}H NMR of **3ae** (600 MHz, $CDCl_3$)

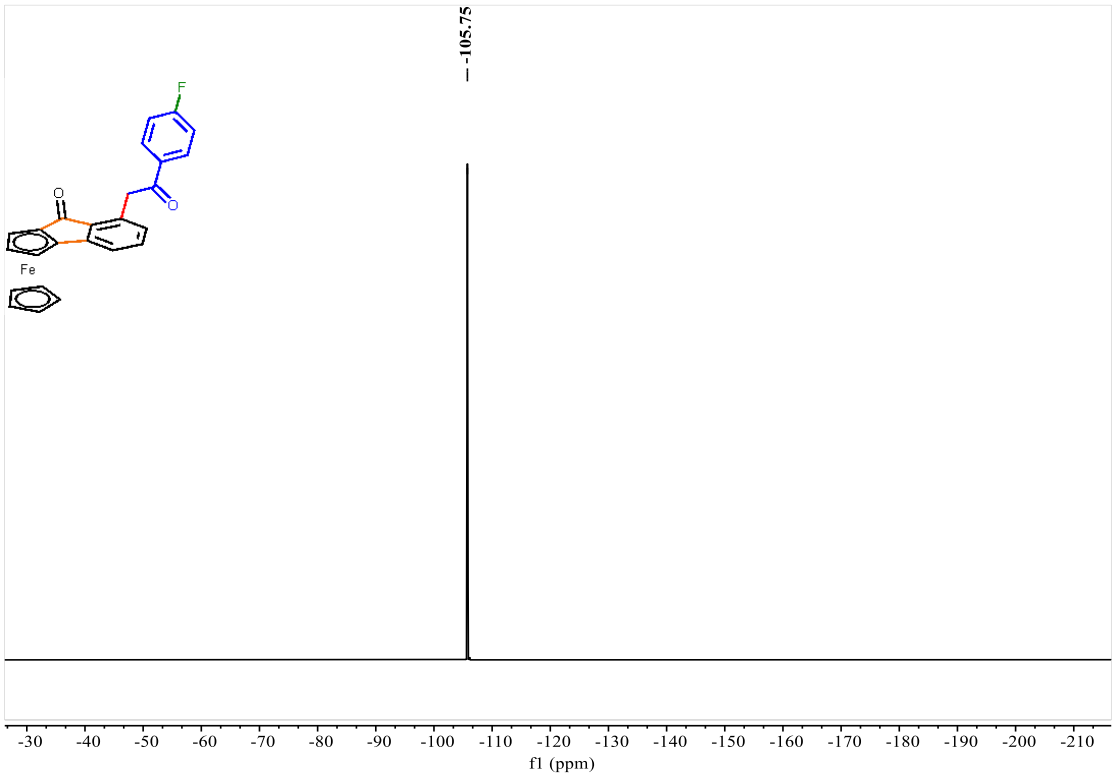


Figure S8.12 ^{19}F NMR of **3ae** (565 MHz, $CDCl_3$)

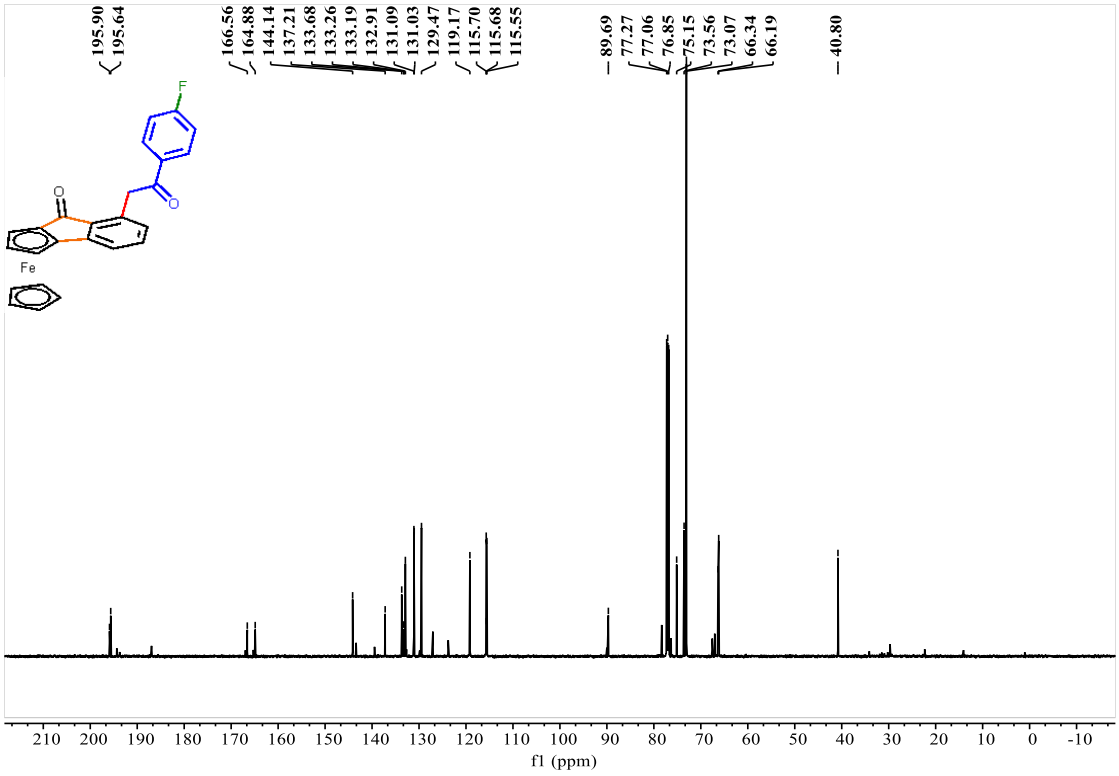


Figure S8.13 ^{13}C NMR of **3ae** (151 MHz, $CDCl_3$)

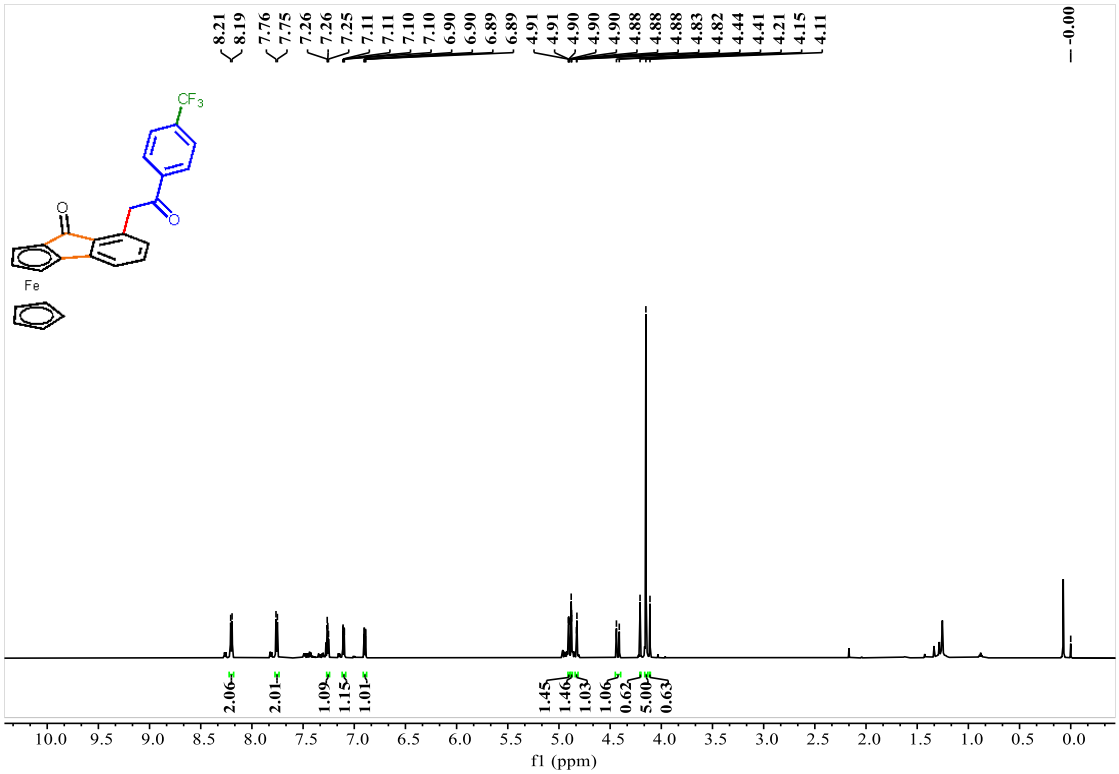


Figure S8.14 ^{1}H NMR of **3af** (600 MHz, $CDCl_3$)

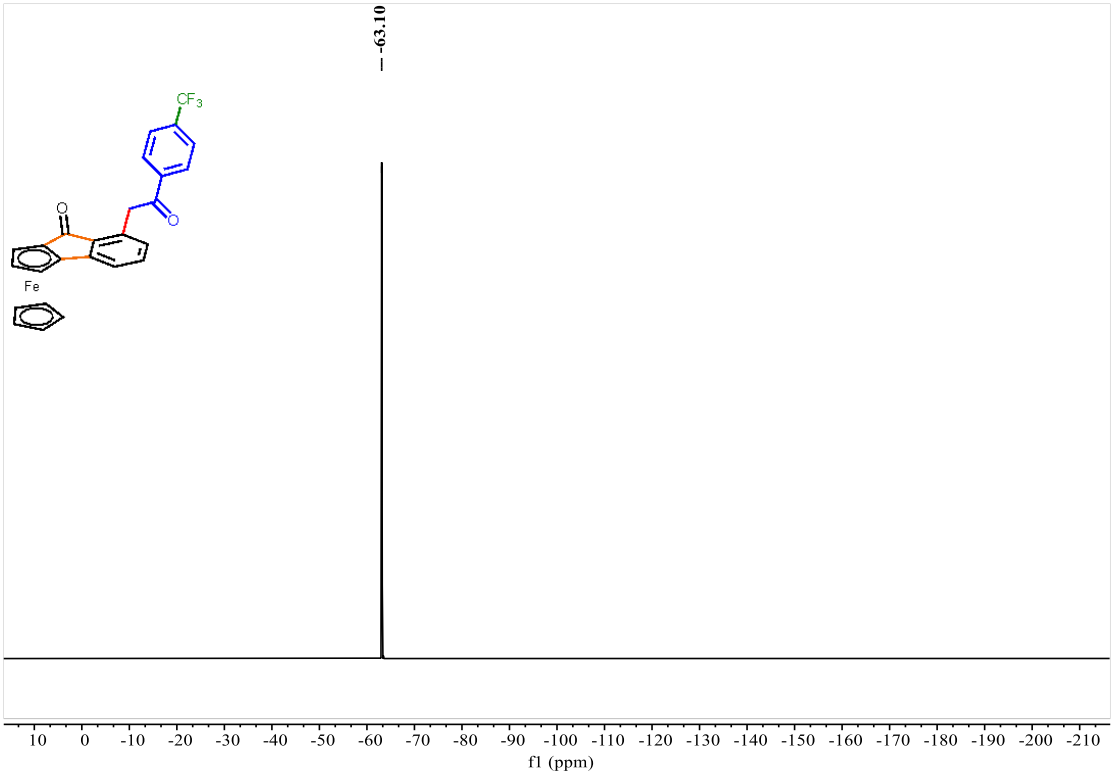


Figure S8.15 ^{19}F NMR of **3af** (565 MHz, $CDCl_3$)

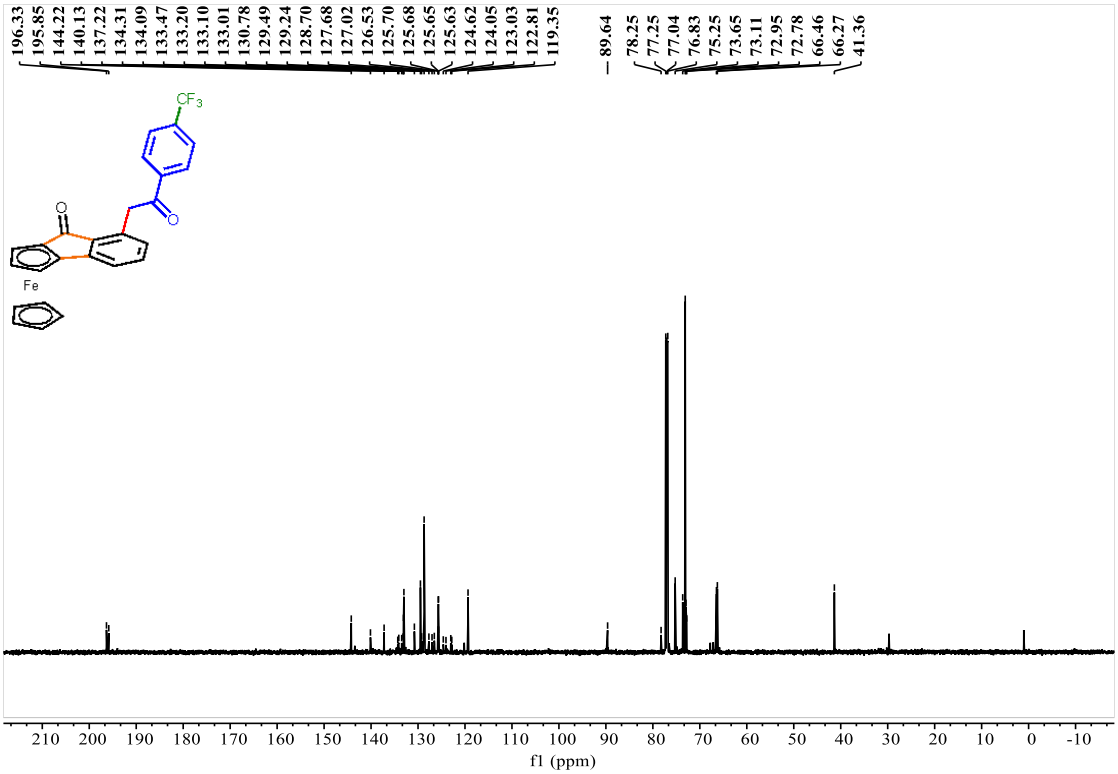


Figure S8.16 ^{13}C NMR of **3af** (151 MHz, $CDCl_3$)

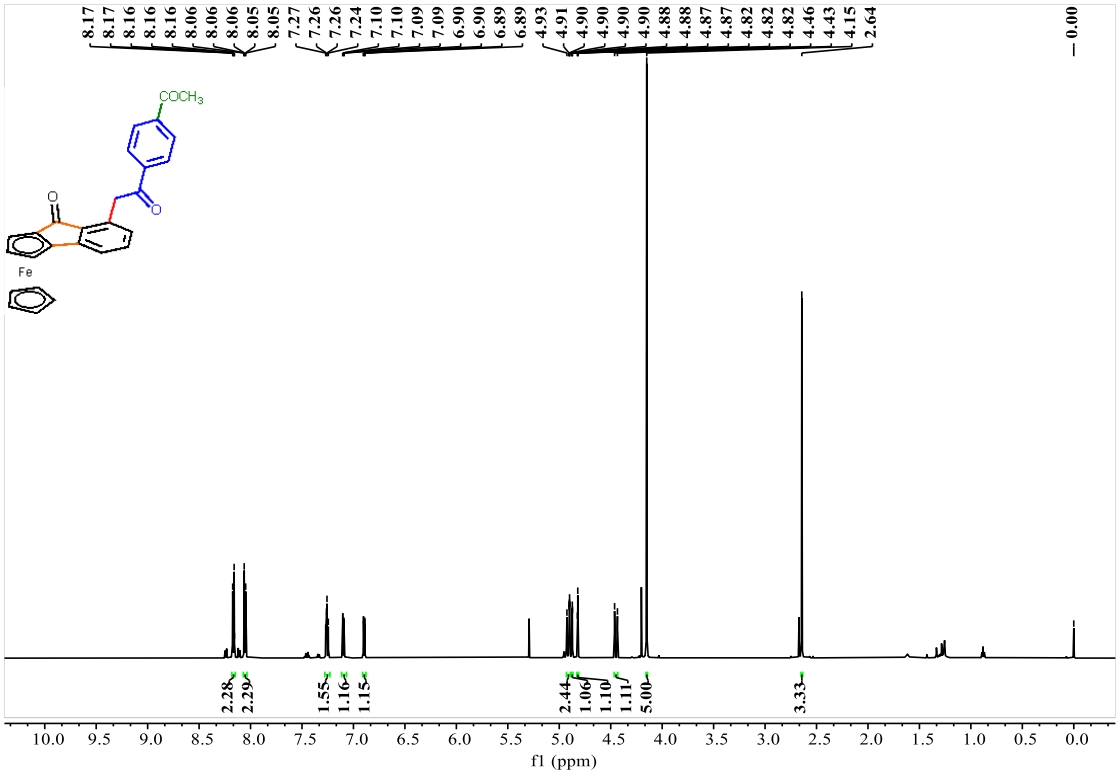


Figure S8.17 ^{1}H NMR of **3ag** (600 MHz, $CDCl_3$)

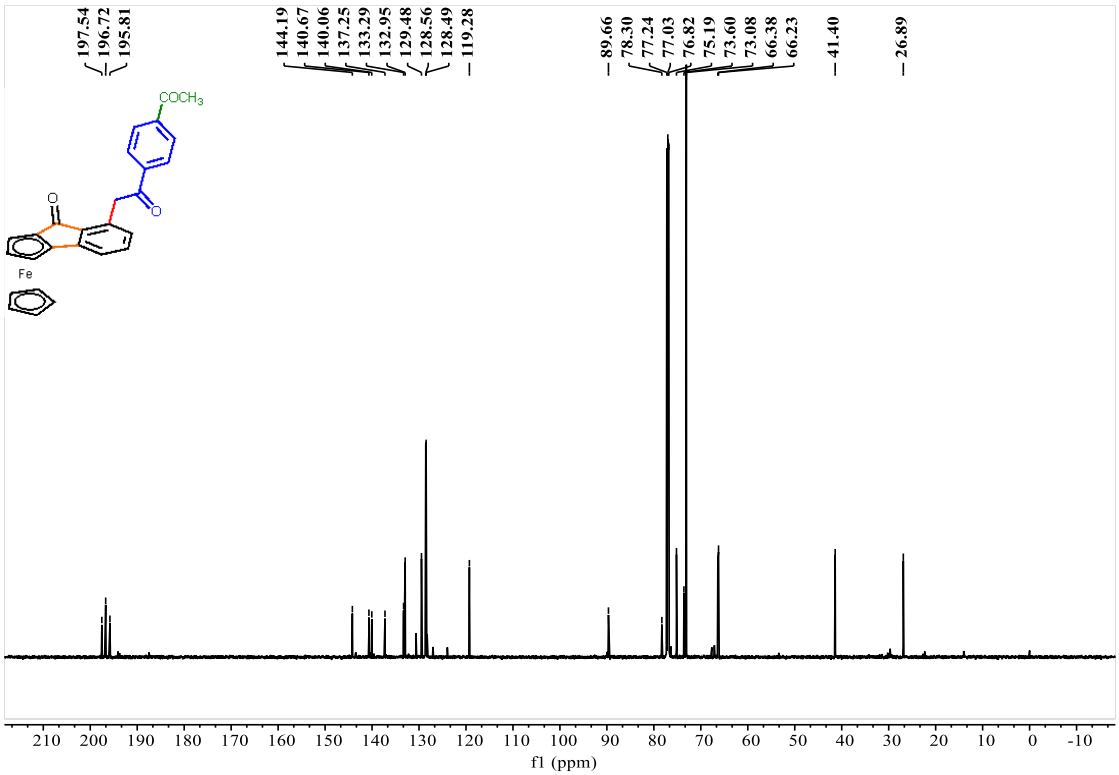


Figure S8.18 ^{13}C NMR of **3ag** (151 MHz, $CDCl_3$)

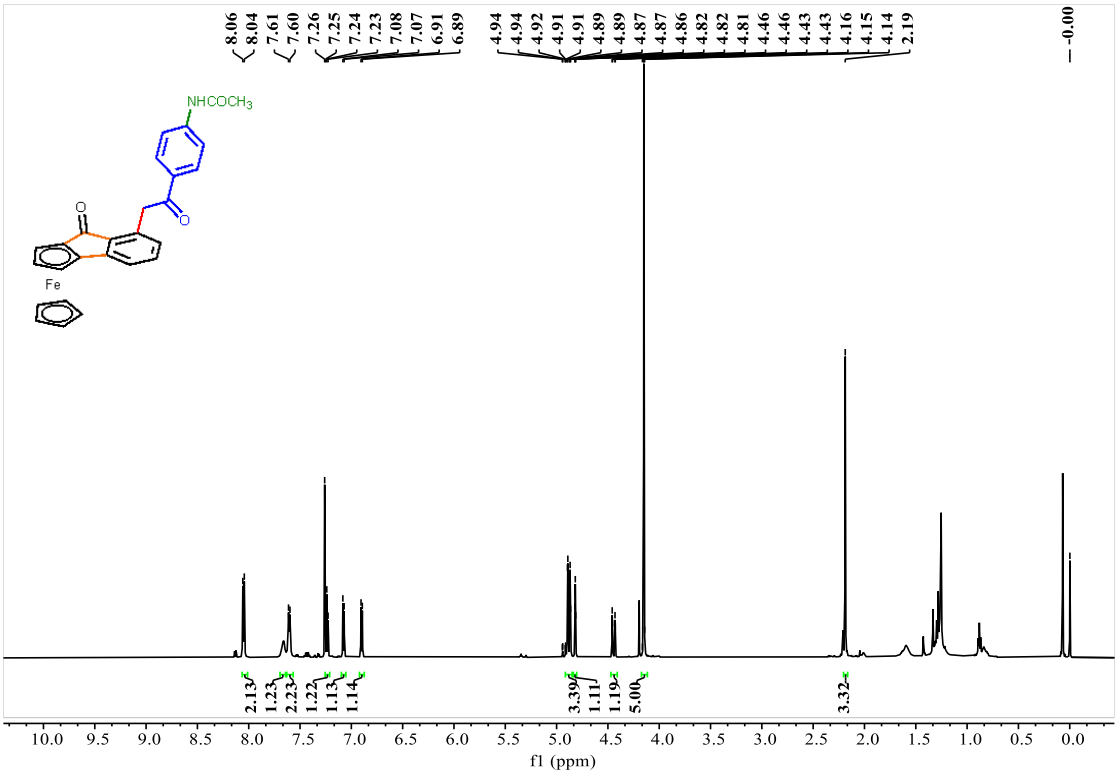


Figure S8.19 ^{1}H NMR of **3ah** (600 MHz, $CDCl_3$)

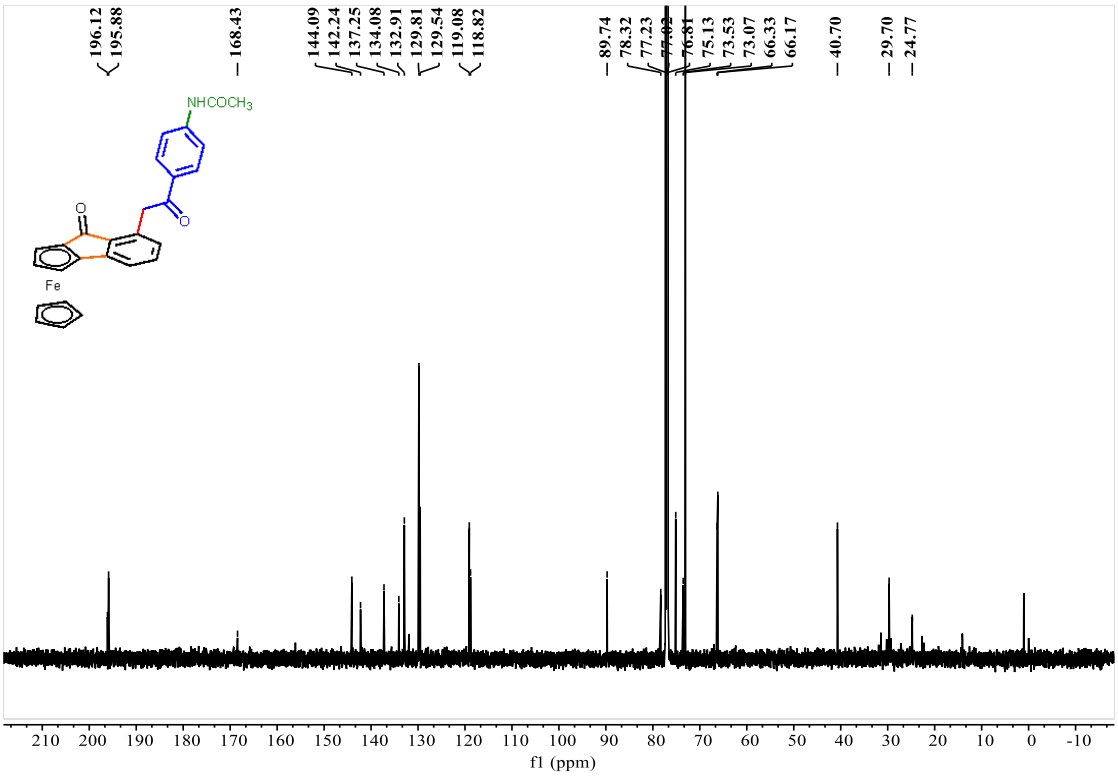


Figure S8.20 ^{13}C NMR of **3ah** (151 MHz, $CDCl_3$)

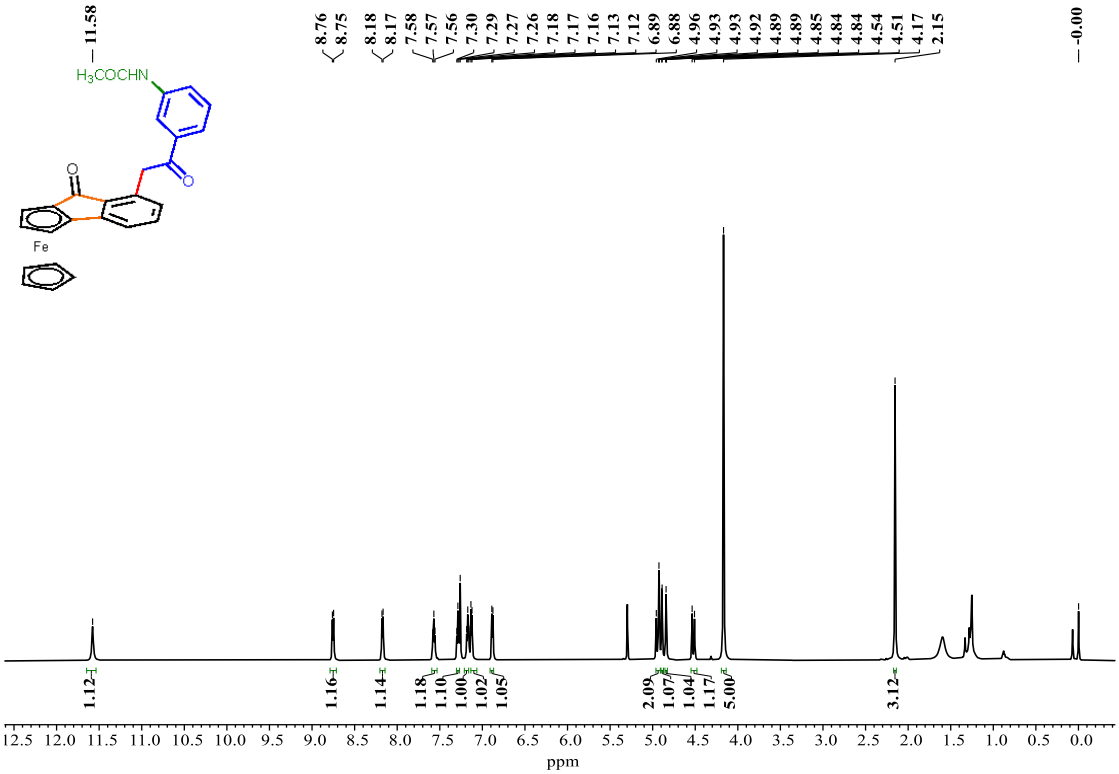


Figure S8.21 ^{1}H NMR of **3ai** (600 MHz, $CDCl_3$)

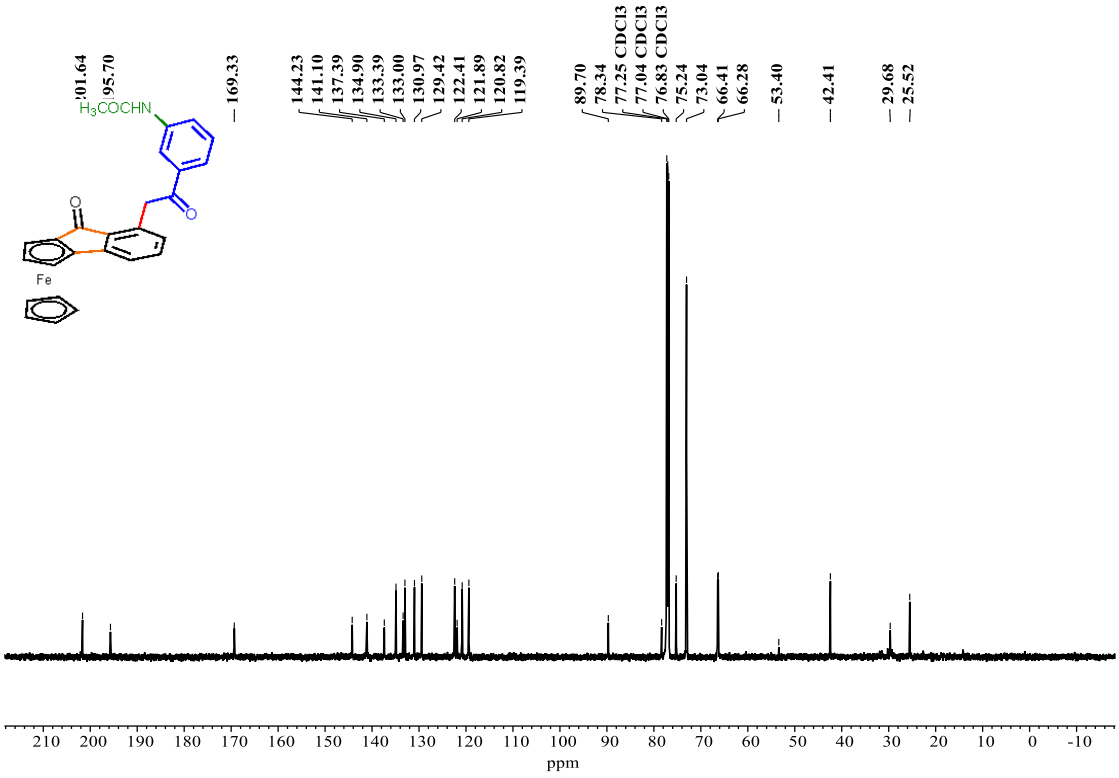


Figure S8.22 ^{13}C NMR of **3ai** (151 MHz, $CDCl_3$)

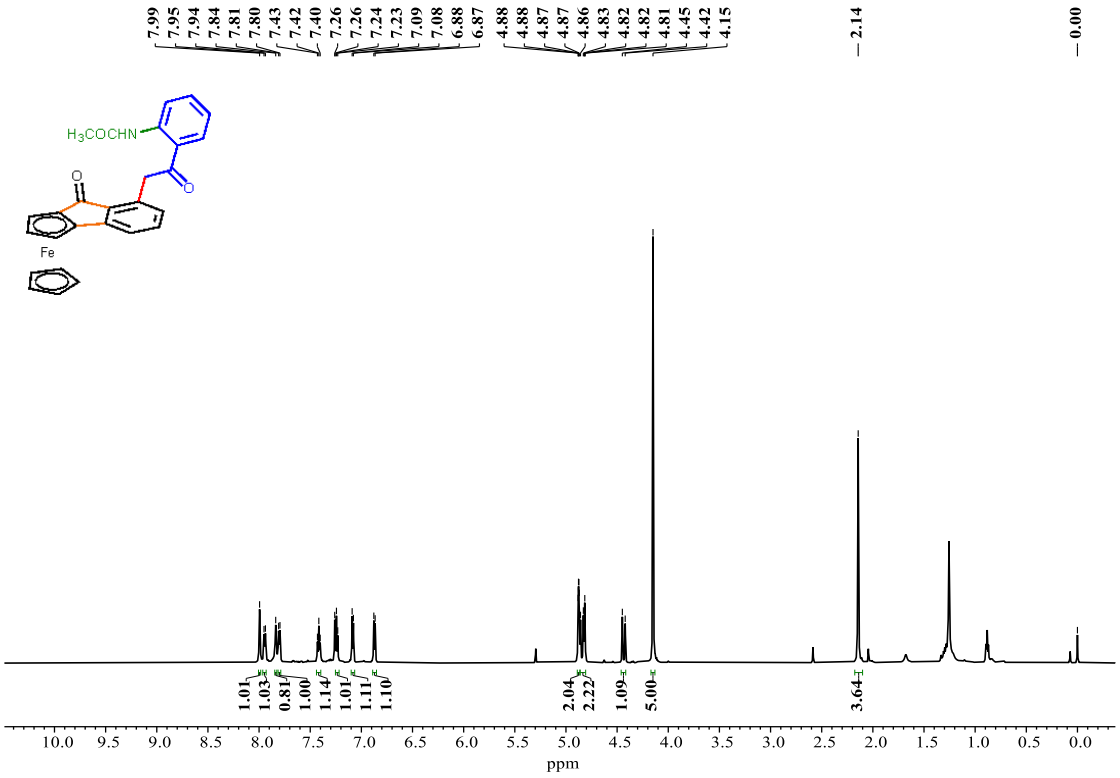


Figure S8.23 ^{1}H NMR of **3aj** (600 MHz, $CDCl_3$)

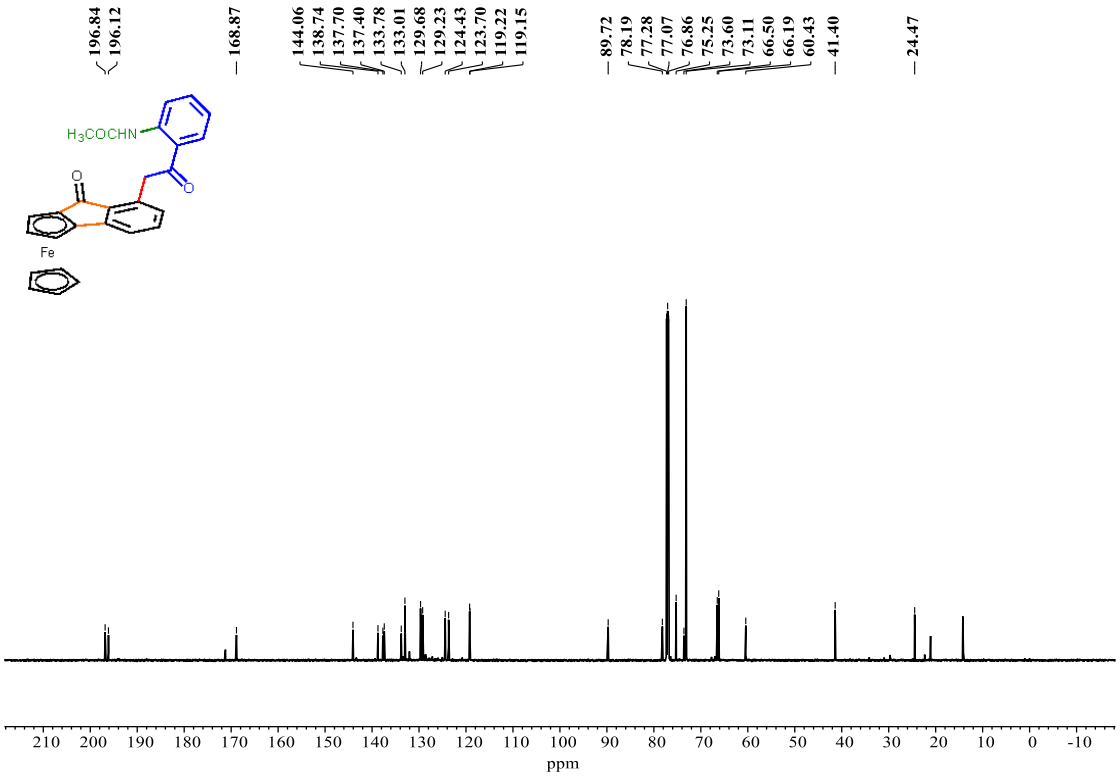


Figure S8.24 ^{13}C NMR of **3aj** (151 MHz, $CDCl_3$)

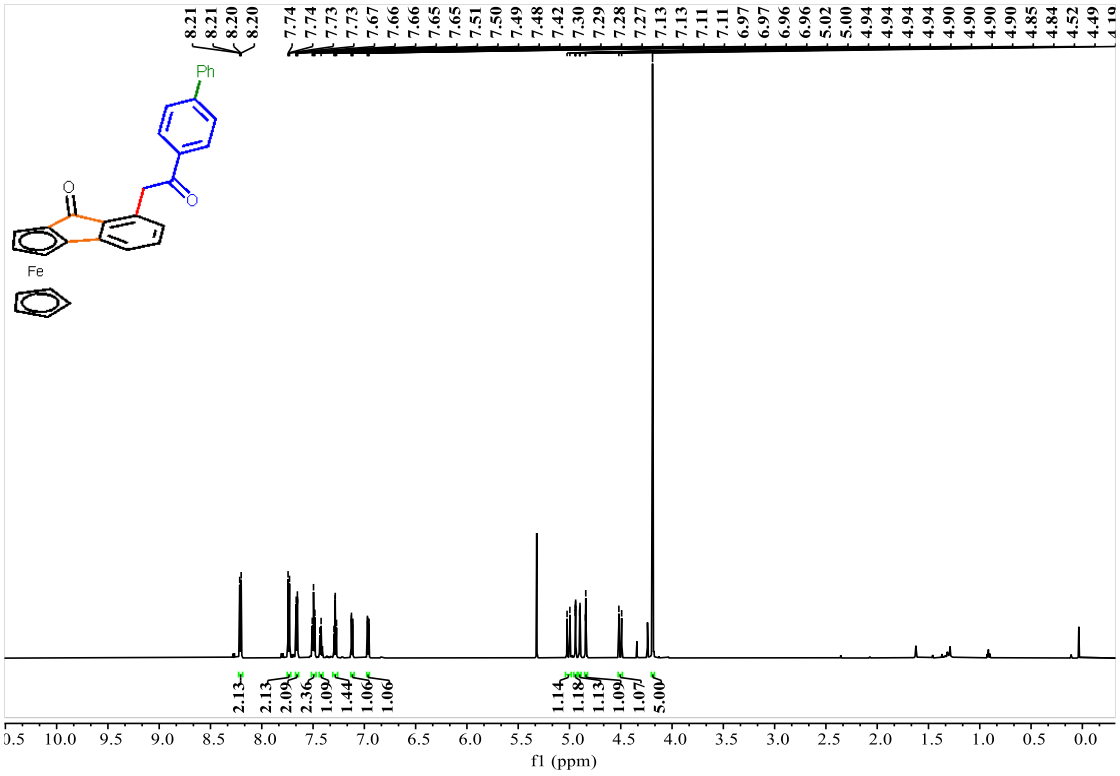


Figure S8.25 ^{1}H NMR of **3ak** (600 MHz, $CDCl_3$)

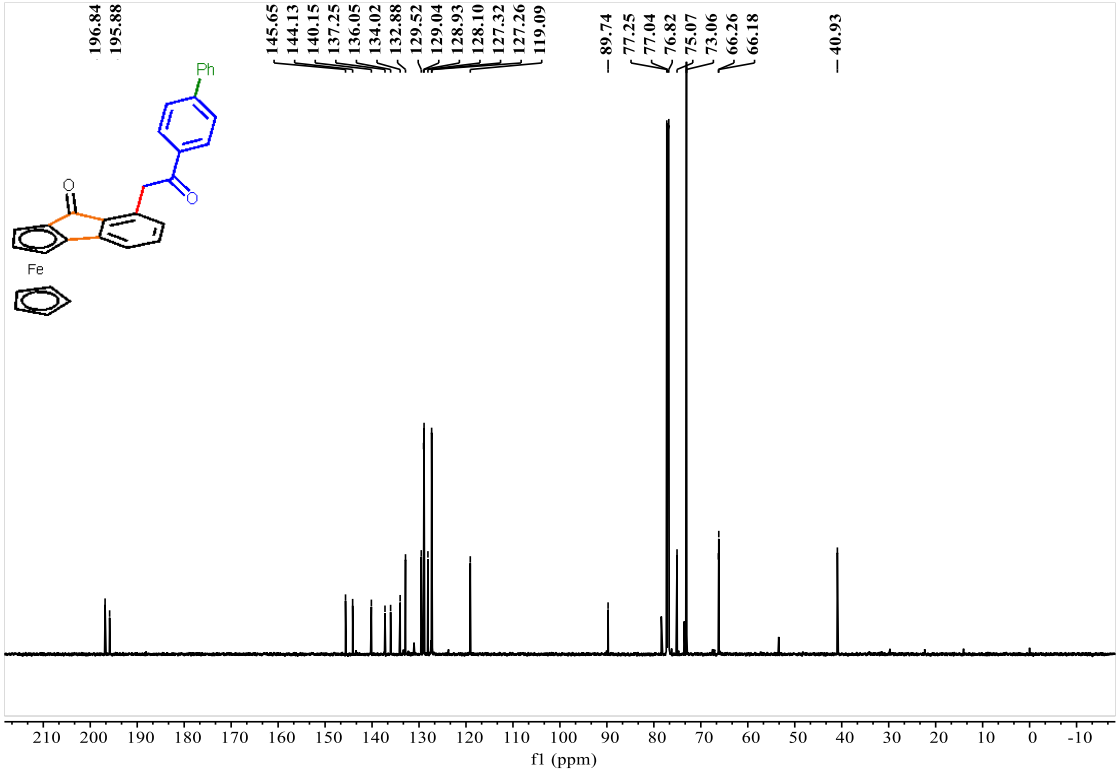


Figure S8.26 ^{13}C NMR of **3ak** (151 MHz, $CDCl_3$)

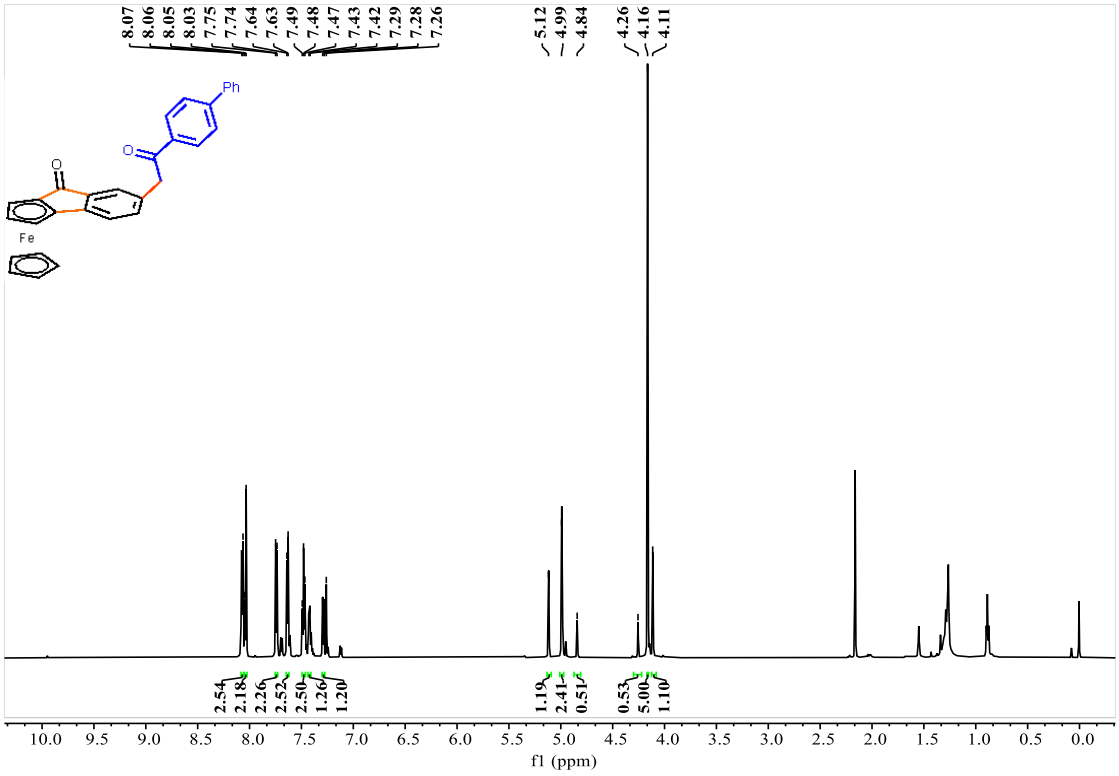


Figure S8.27 ^{1}H NMR of **3al** (600 MHz, $CDCl_3$)

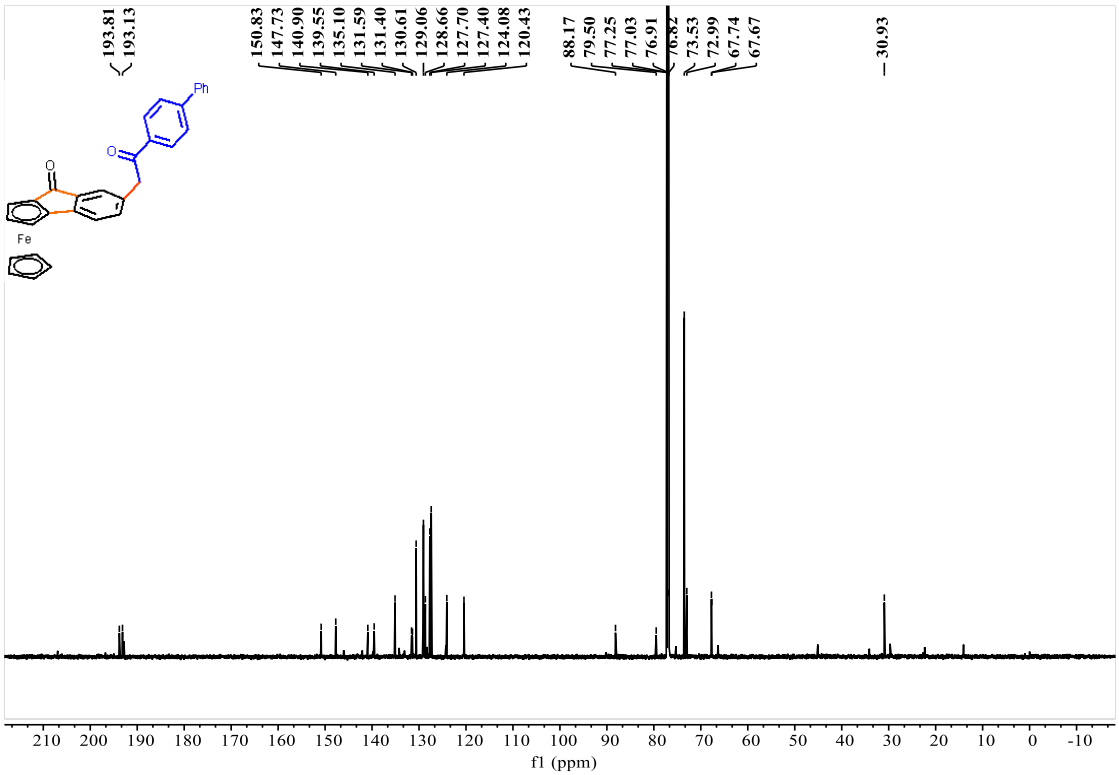


Figure S8.28 ^{13}C NMR of **3al** (151 MHz, $CDCl_3$)

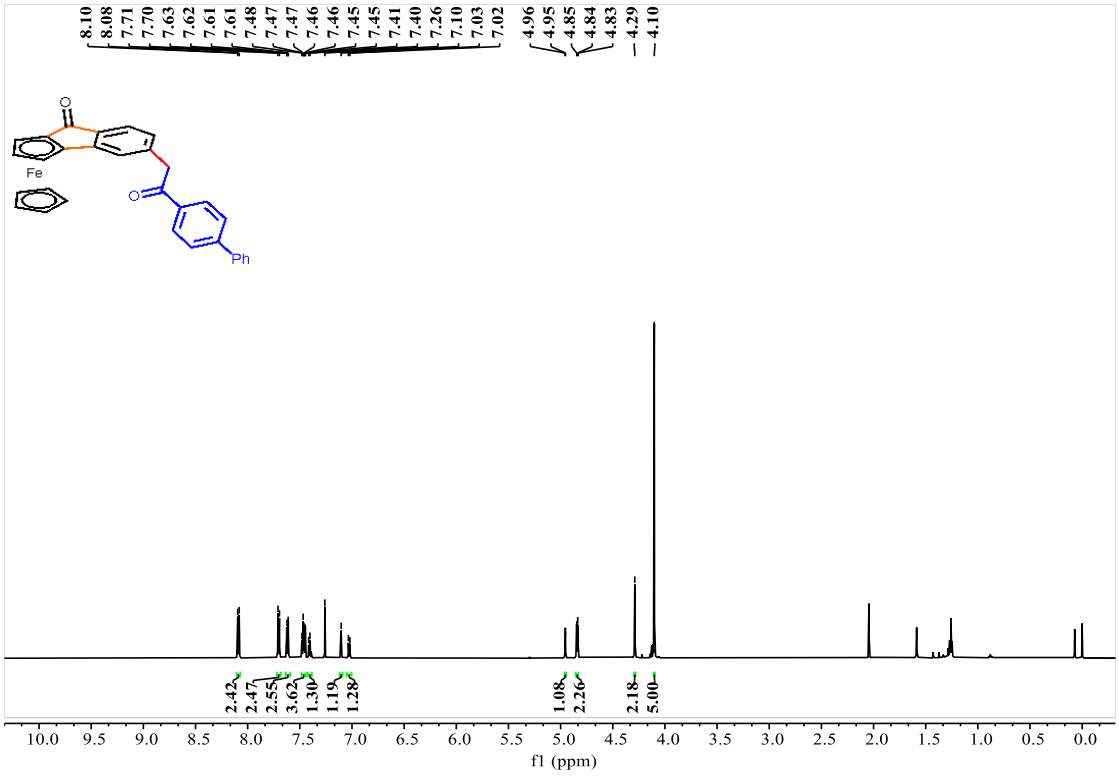


Figure S8.29 ^{1}H NMR of **3am** (600 MHz, $CDCl_3$)

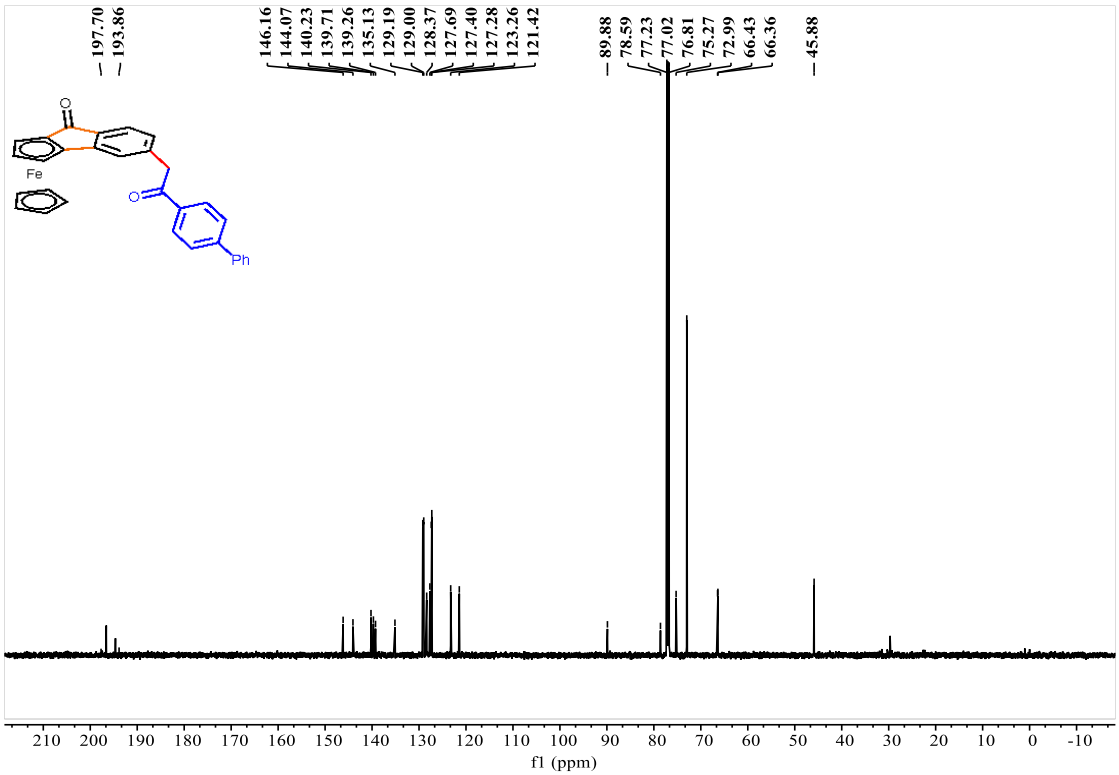


Figure S8.30 ^{13}C NMR of **3am** (151 MHz, $CDCl_3$)

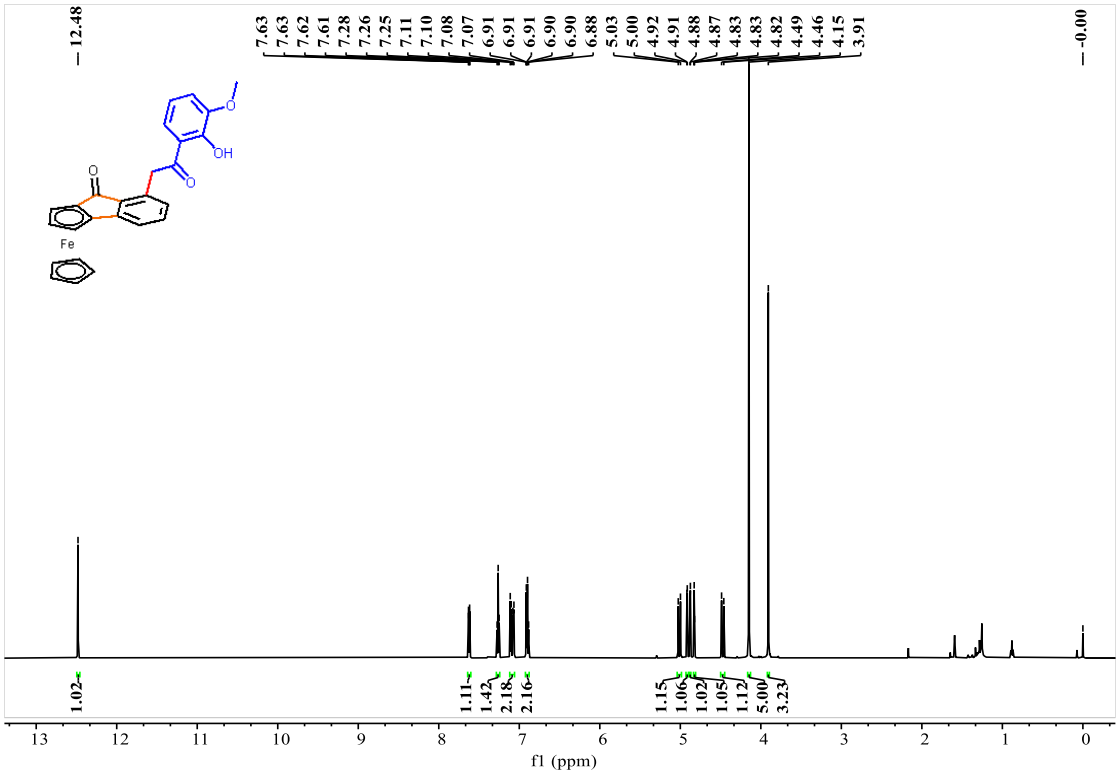


Figure S8.31 ^{1}H NMR of **3an**(600 MHz, $CDCl_3$)

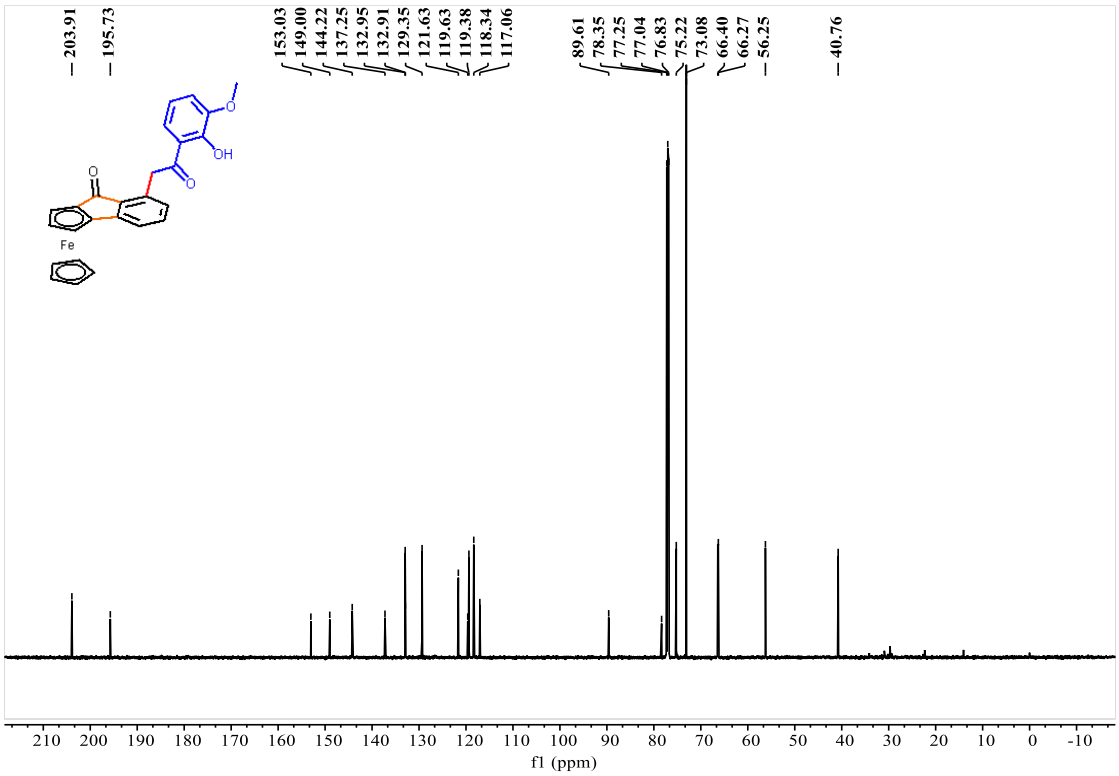


Figure S8.32 ^{13}C NMR of **3an** (151 MHz, $CDCl_3$)

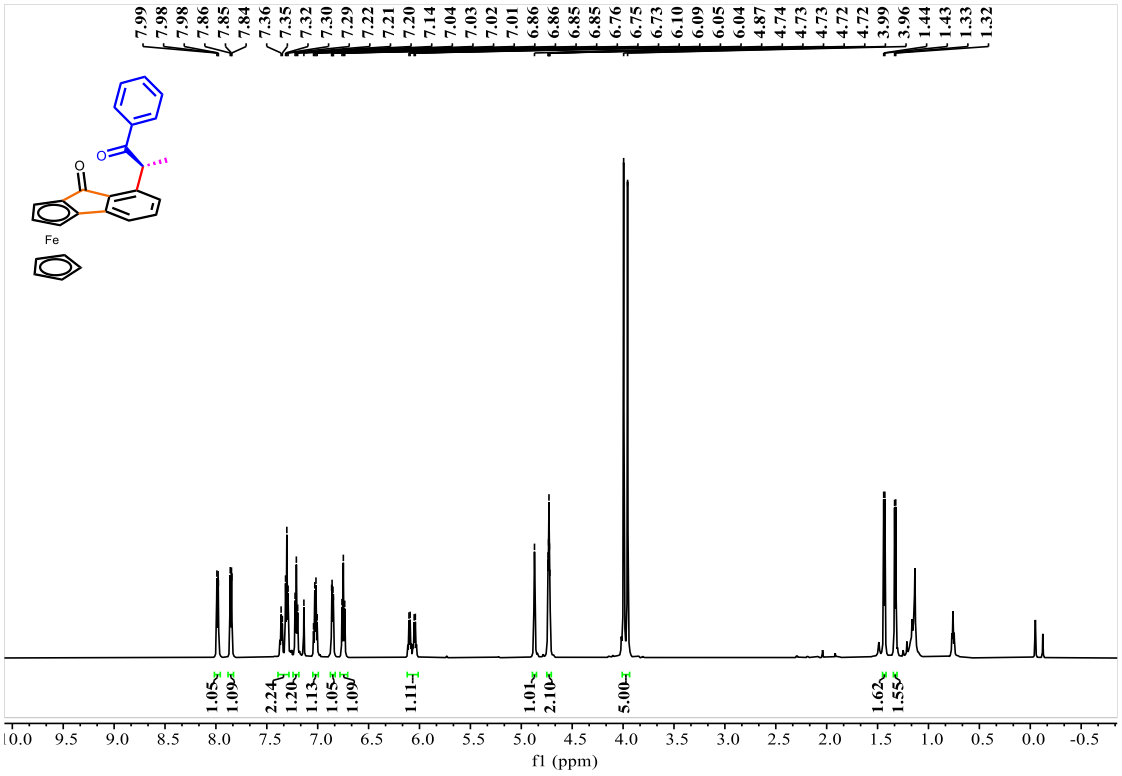


Figure S8.33 ^{1}H NMR of **(R_p, *R*)-3ao** (600 MHz, $CDCl_3$)

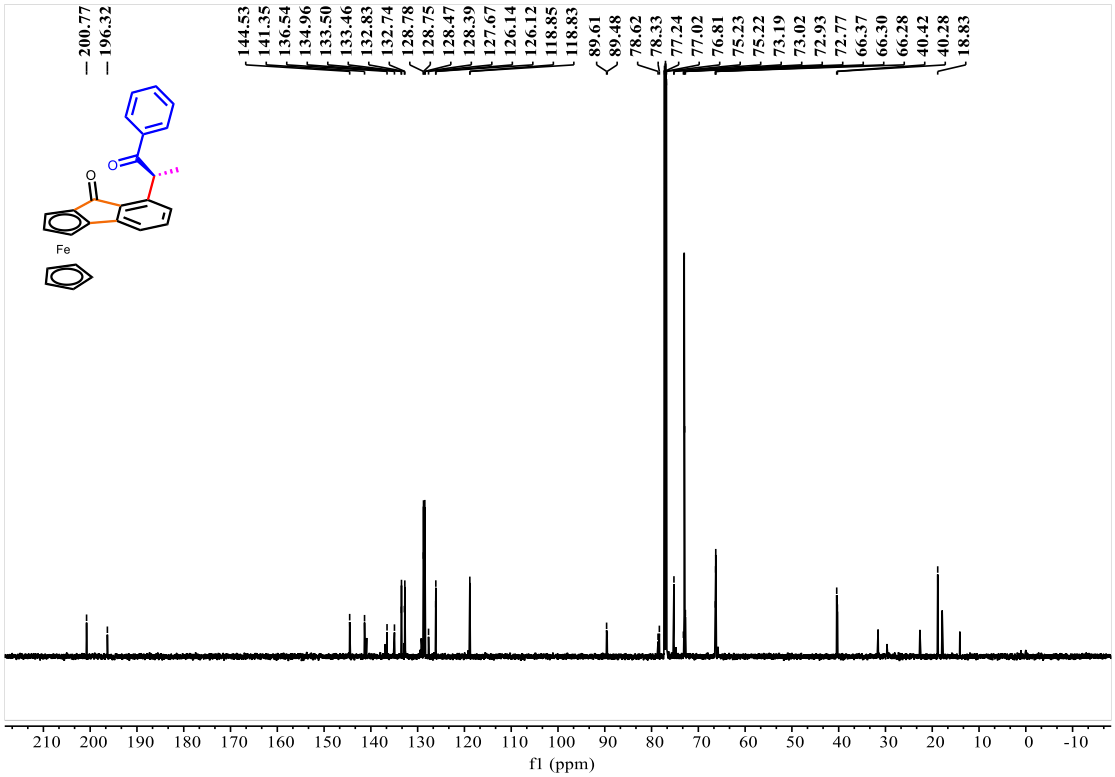


Figure S8.34 ^{13}C NMR of **(R_p, *R*)-3ao** (151 MHz, $CDCl_3$)

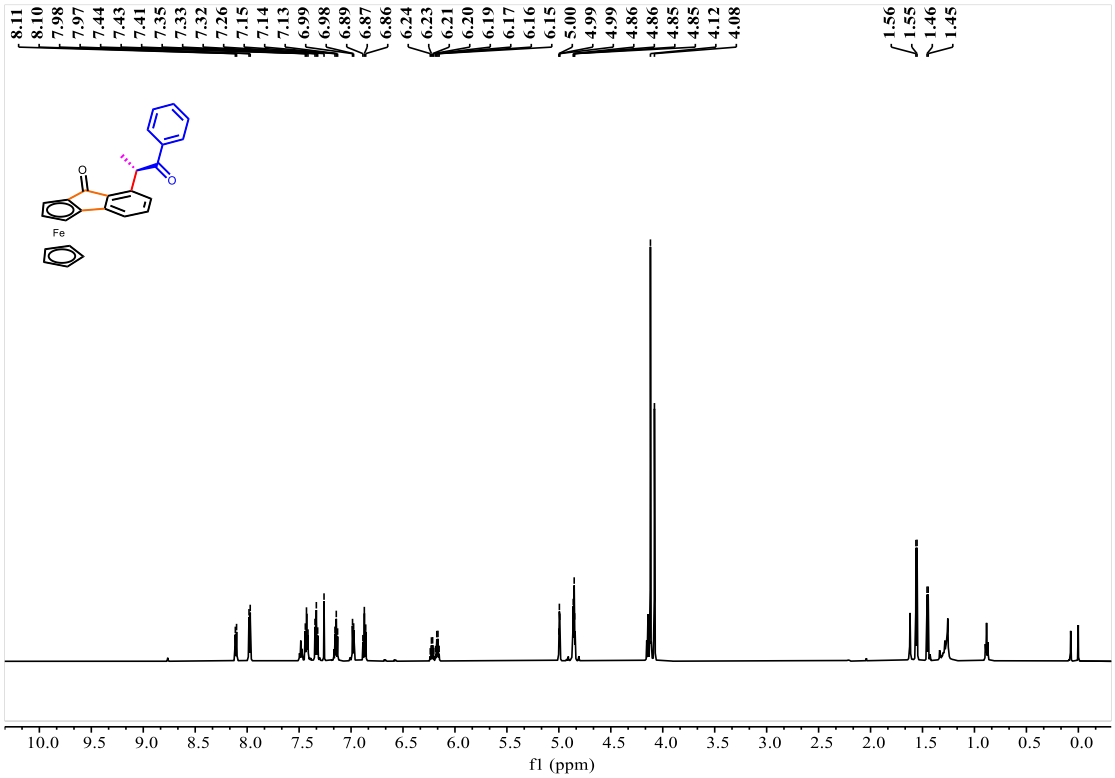


Figure S8.35 ^{1}H NMR of **(R_p, *S*)-3ao** (600 MHz, $CDCl_3$)

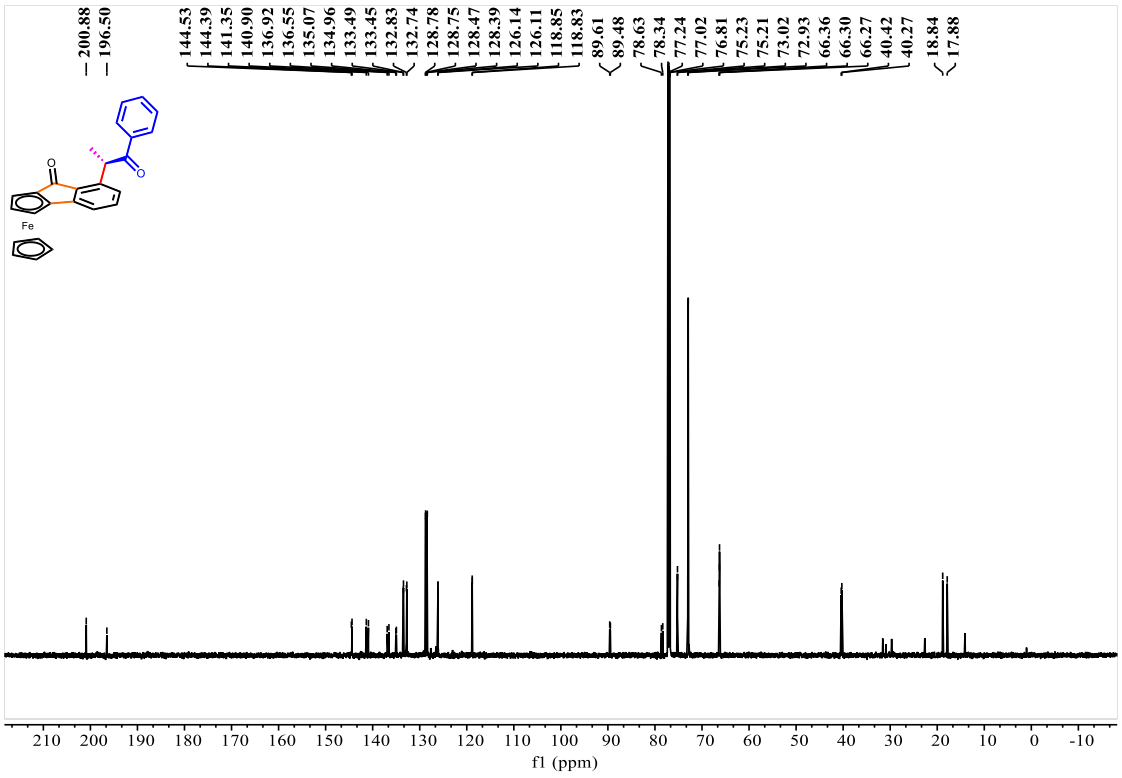


Figure S8.36 ^{13}C NMR of **(R_p, *S*)-3ao** (151 MHz, $CDCl_3$)

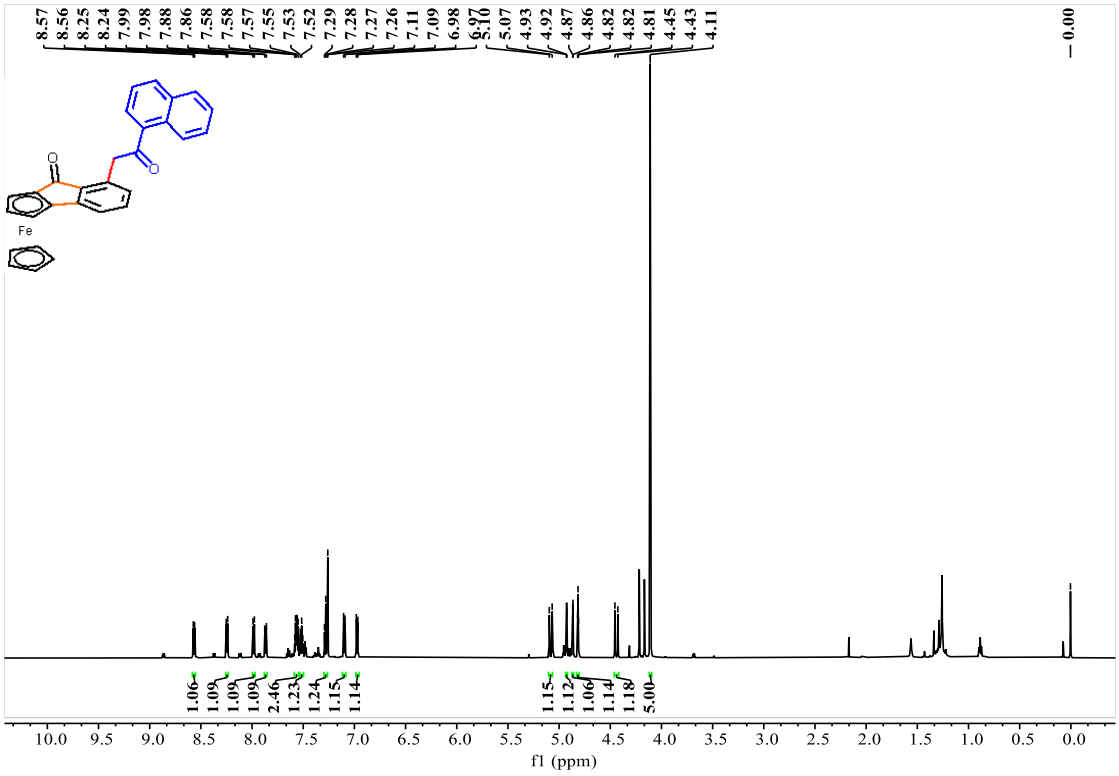


Figure S8.37 ^{1}H NMR of **3ap** (600 MHz, $CDCl_3$)

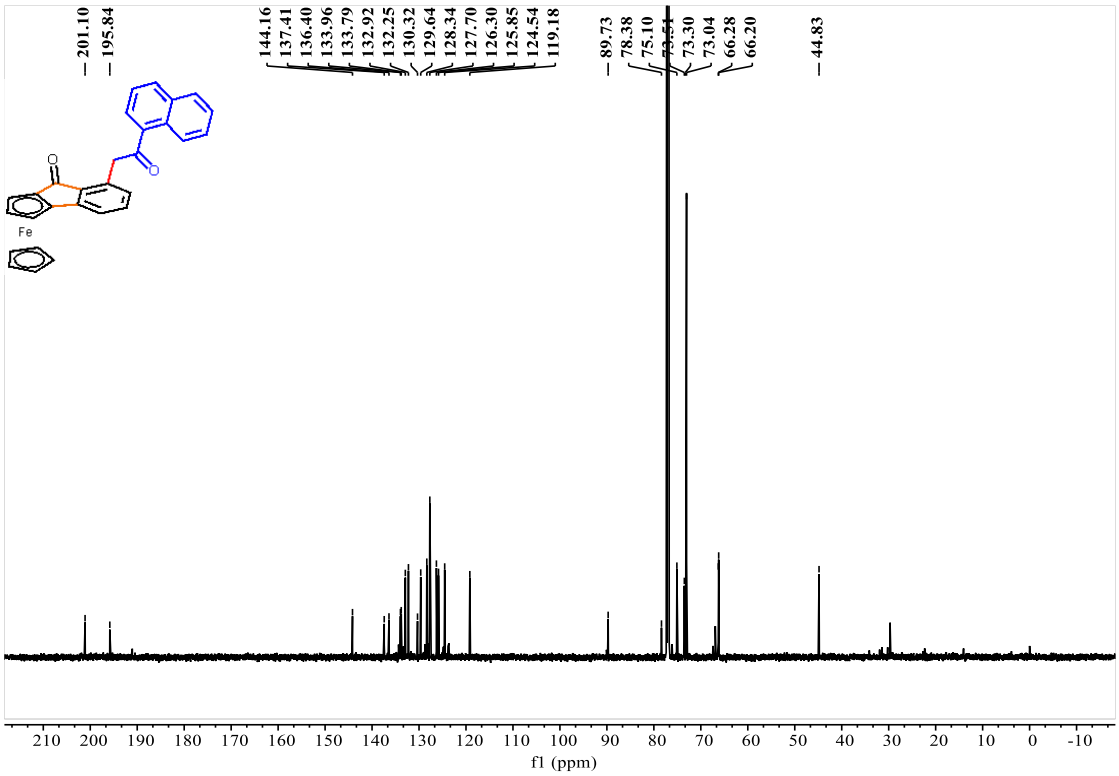


Figure S8.38 ^{13}C NMR of **3ap** (151 MHz, $CDCl_3$)

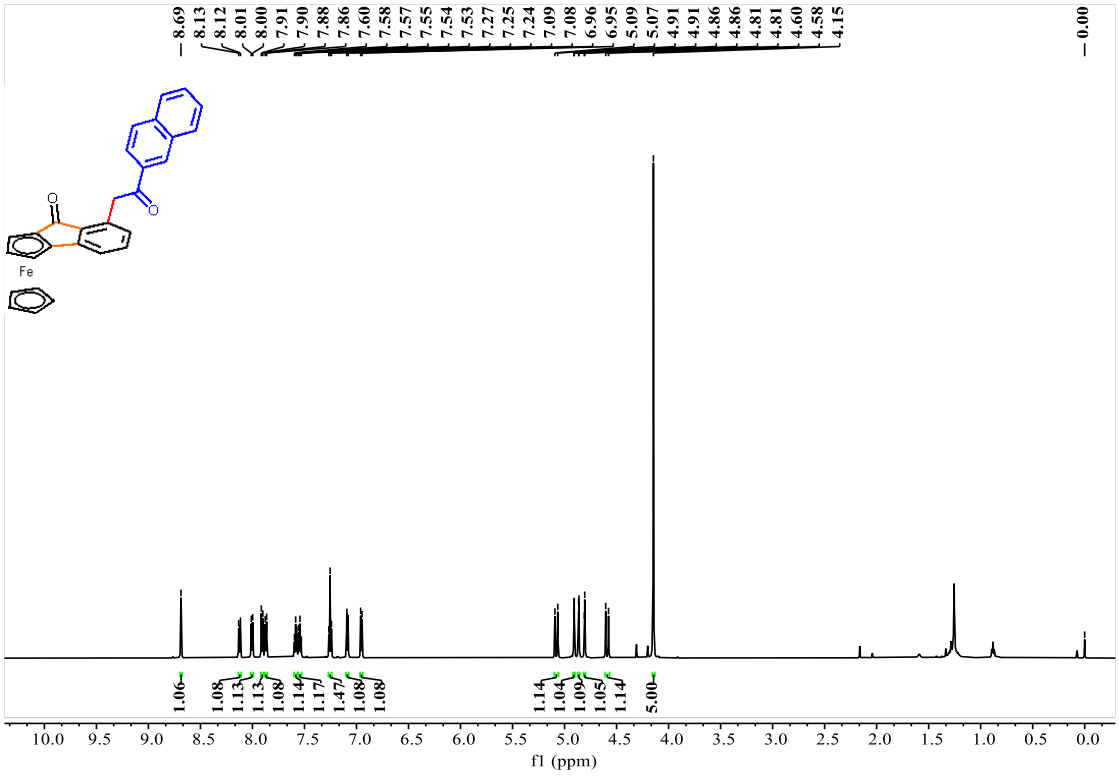


Figure S8.39 ^{1}H NMR of **3aq** (600 MHz, $CDCl_3$)

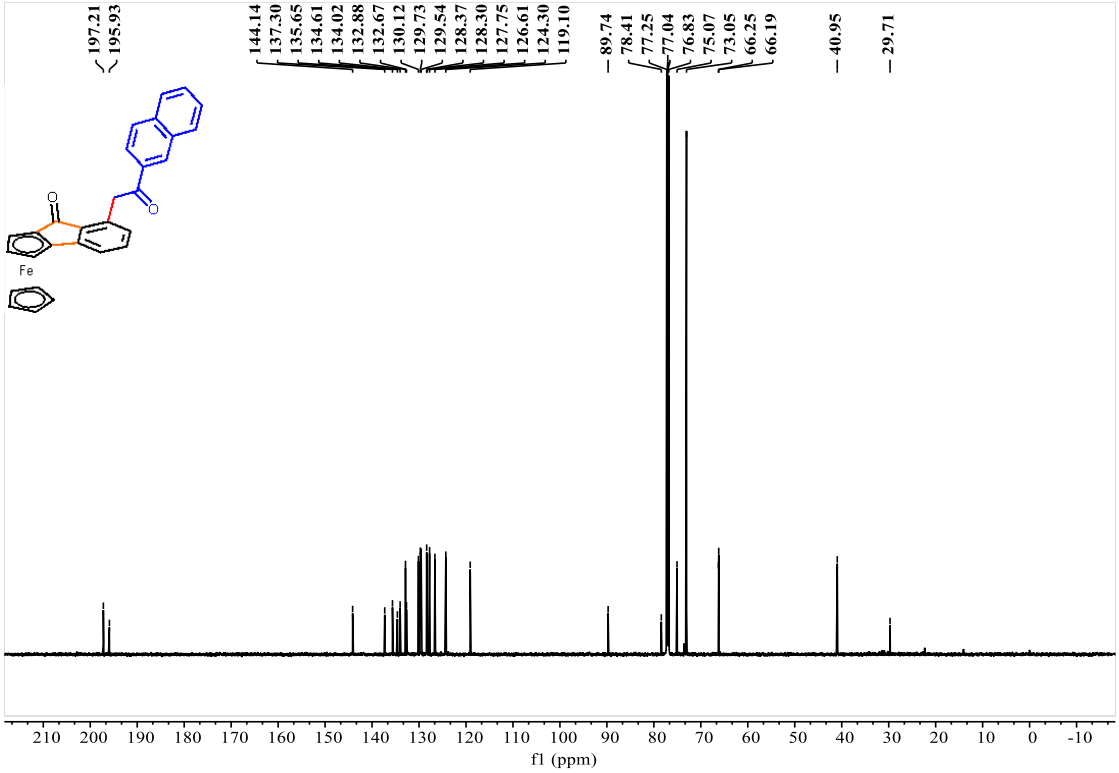


Figure S8.40 ^{13}C NMR of **3aq** (151 MHz, $CDCl_3$)

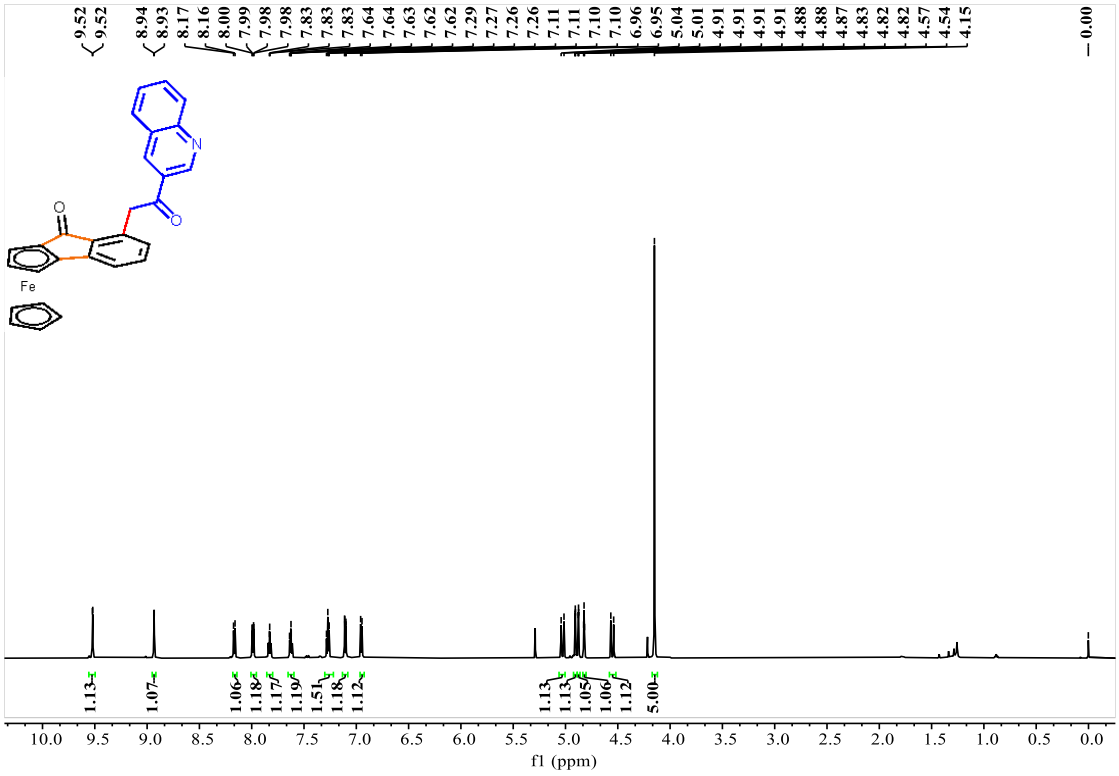


Figure S8.41 ^{1}H NMR of **3ar** (600 MHz, $CDCl_3$)

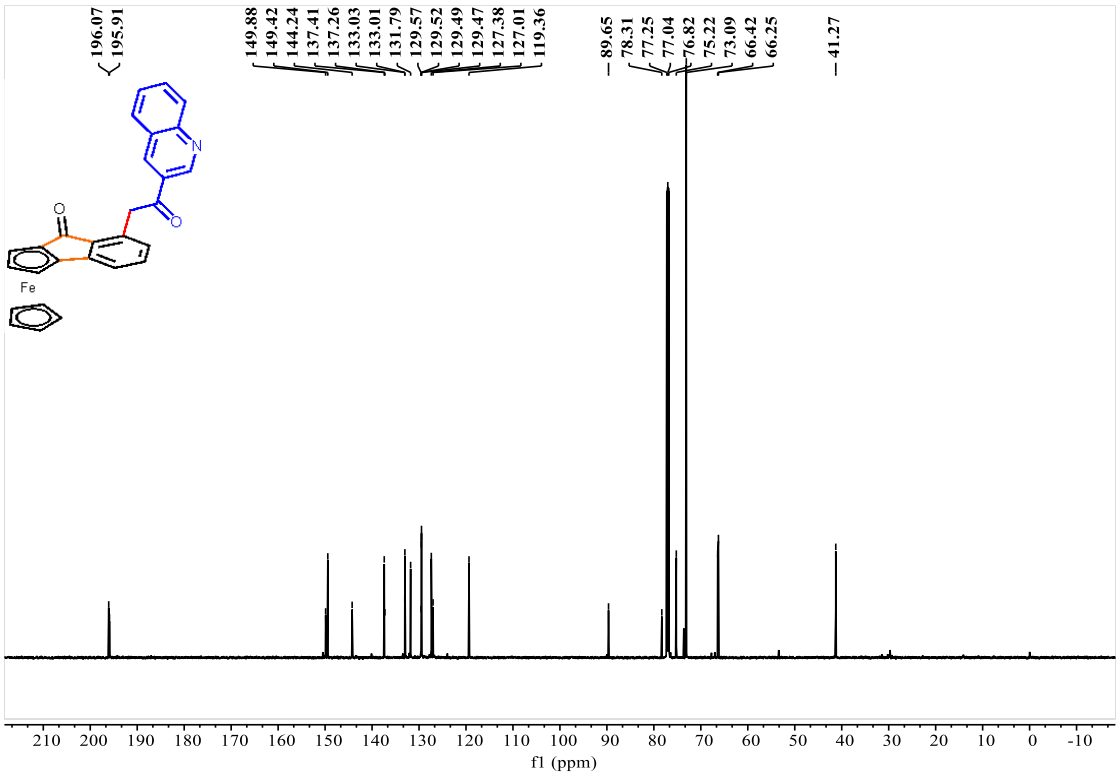


Figure S8.42 ^{13}C NMR of **3ar** (151 MHz, $CDCl_3$)

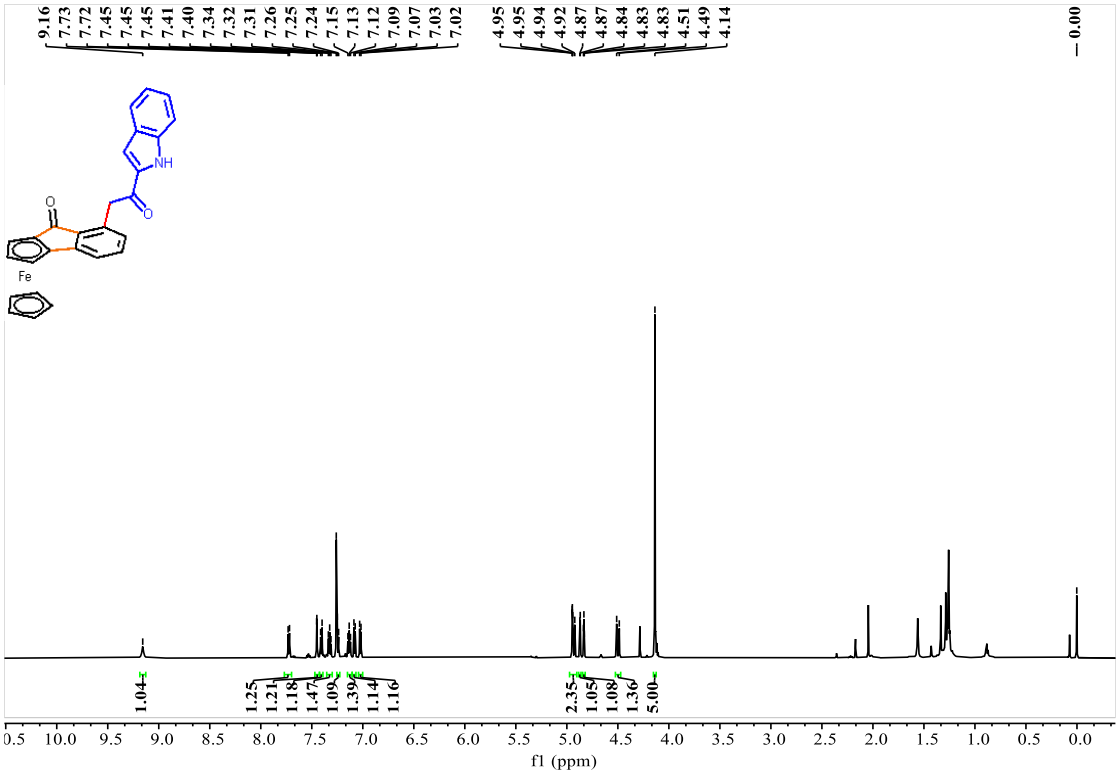


Figure S8.43 ^{1}H NMR of **3as** (600 MHz, $CDCl_3$)

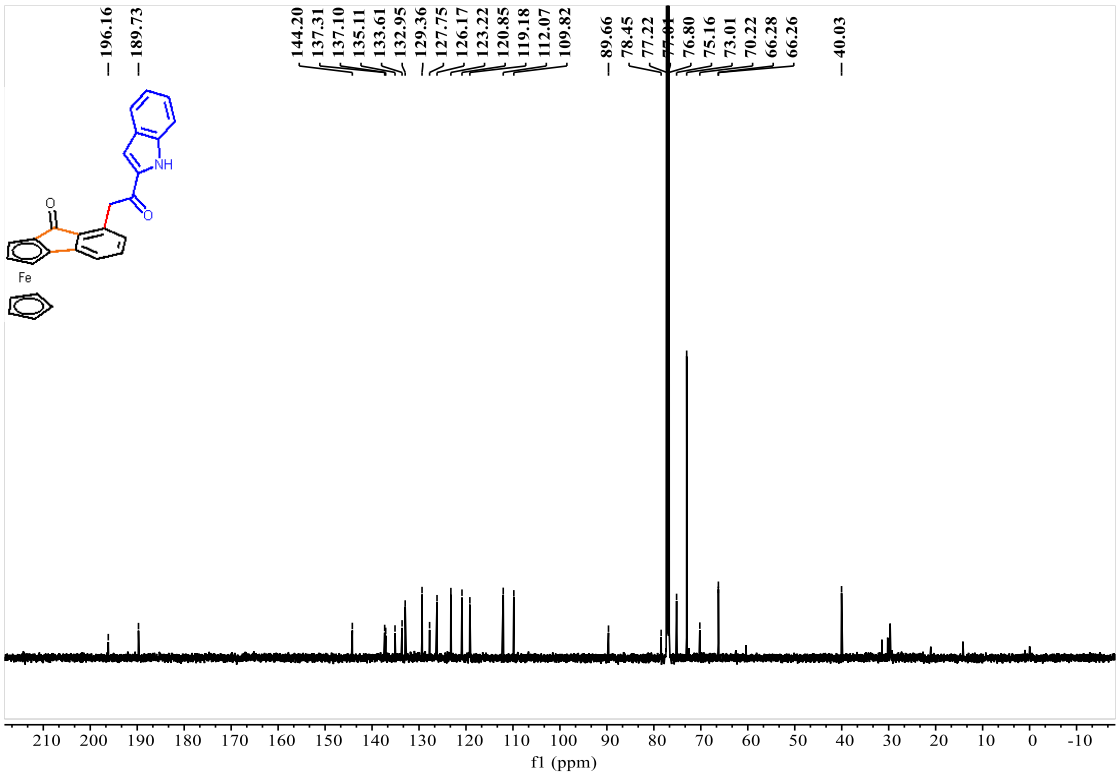


Figure S8.44 ^{13}C NMR of **3as** (151 MHz, $CDCl_3$)

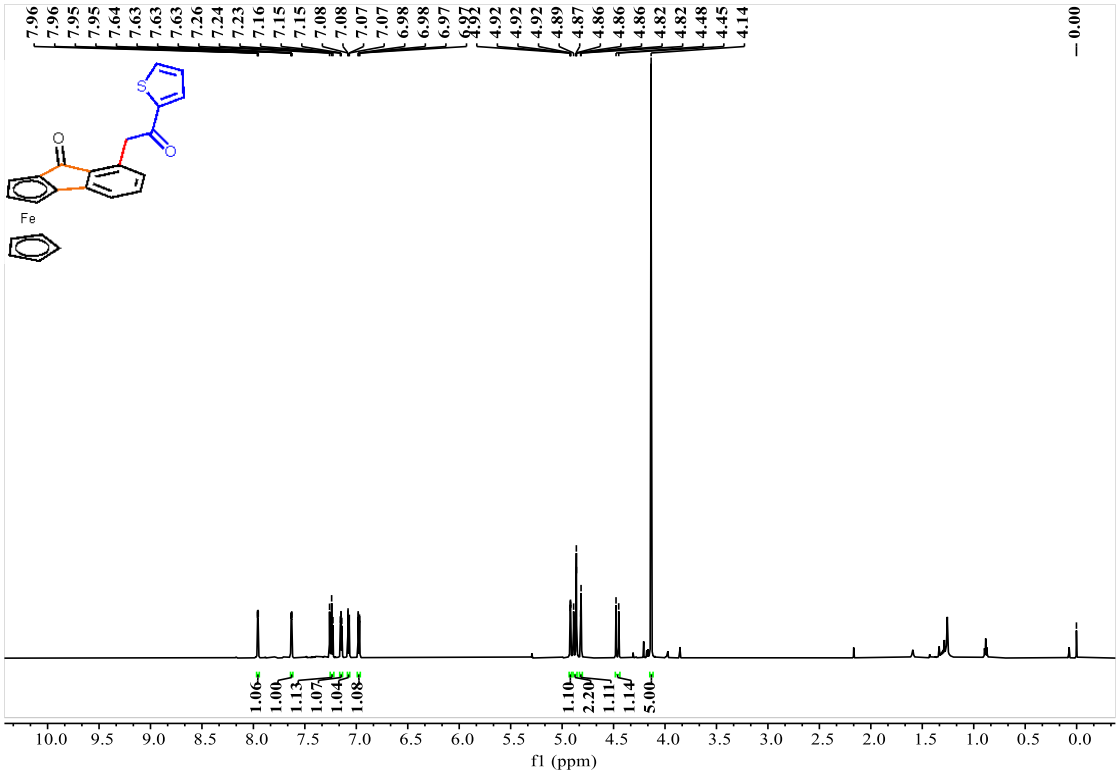


Figure S8.45 ^{1}H NMR of **3at** (600 MHz, $CDCl_3$)

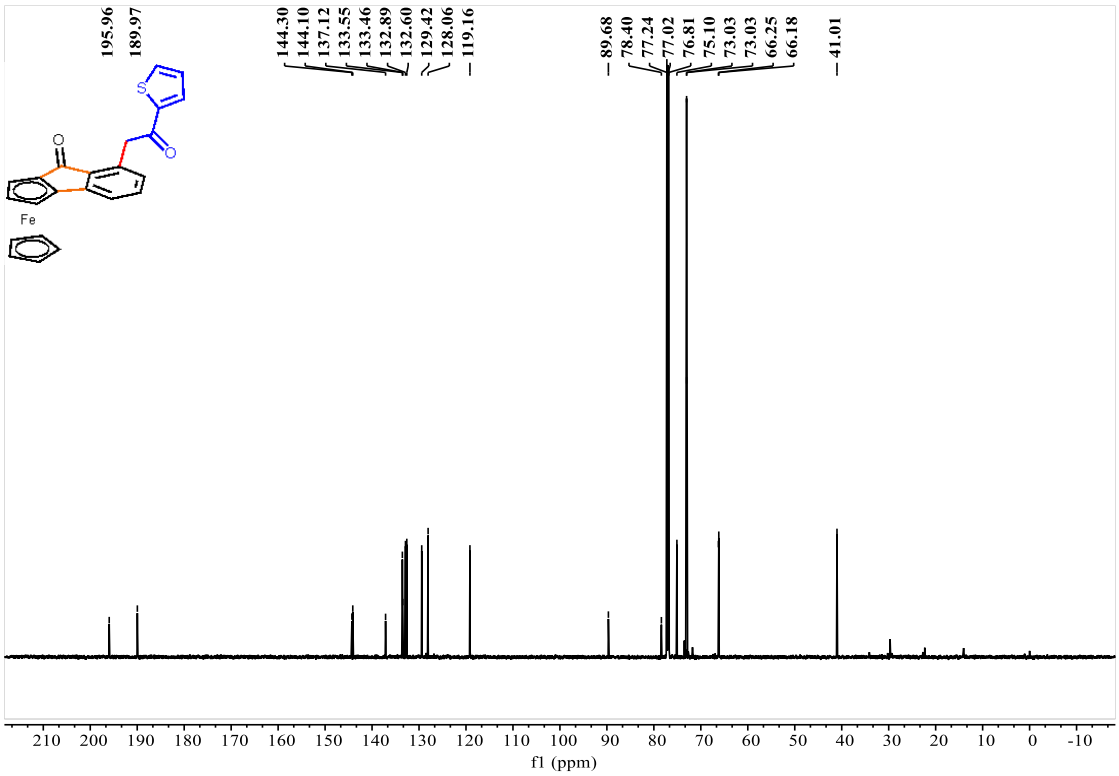


Figure S8.46^{13}C NMR of **3at** (151 MHz, $CDCl_3$)

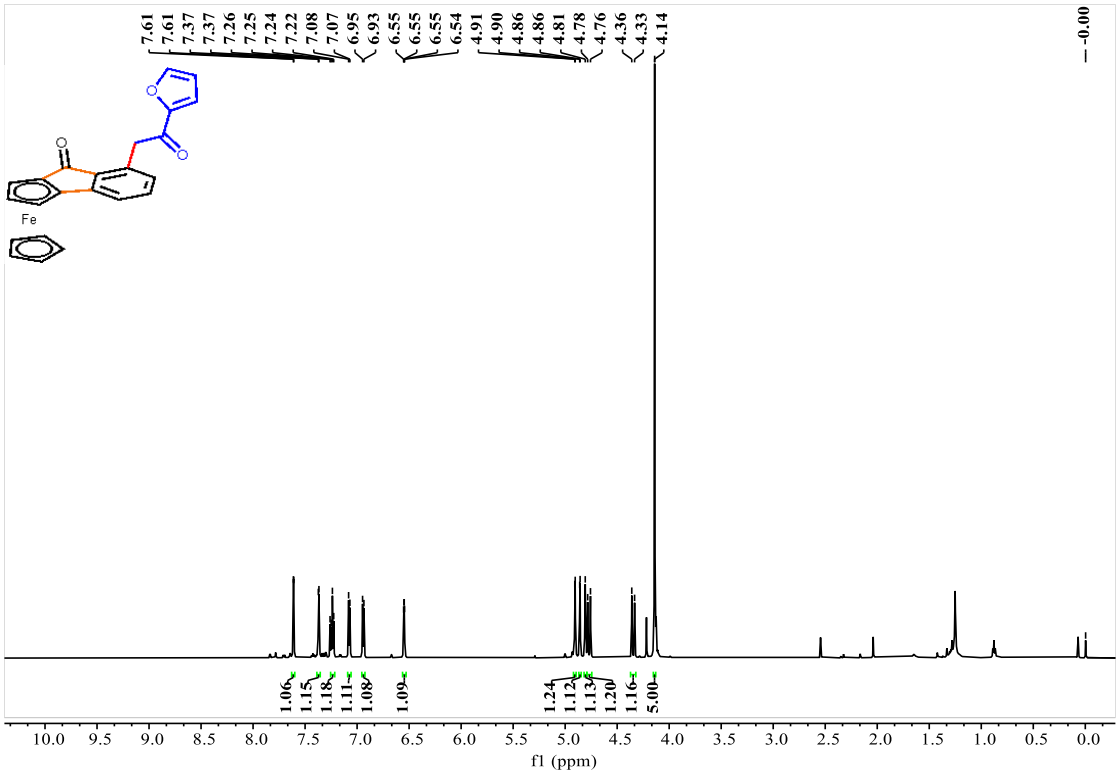


Figure S8.47 ^{1}H NMR of **3au** (600 MHz, $CDCl_3$)

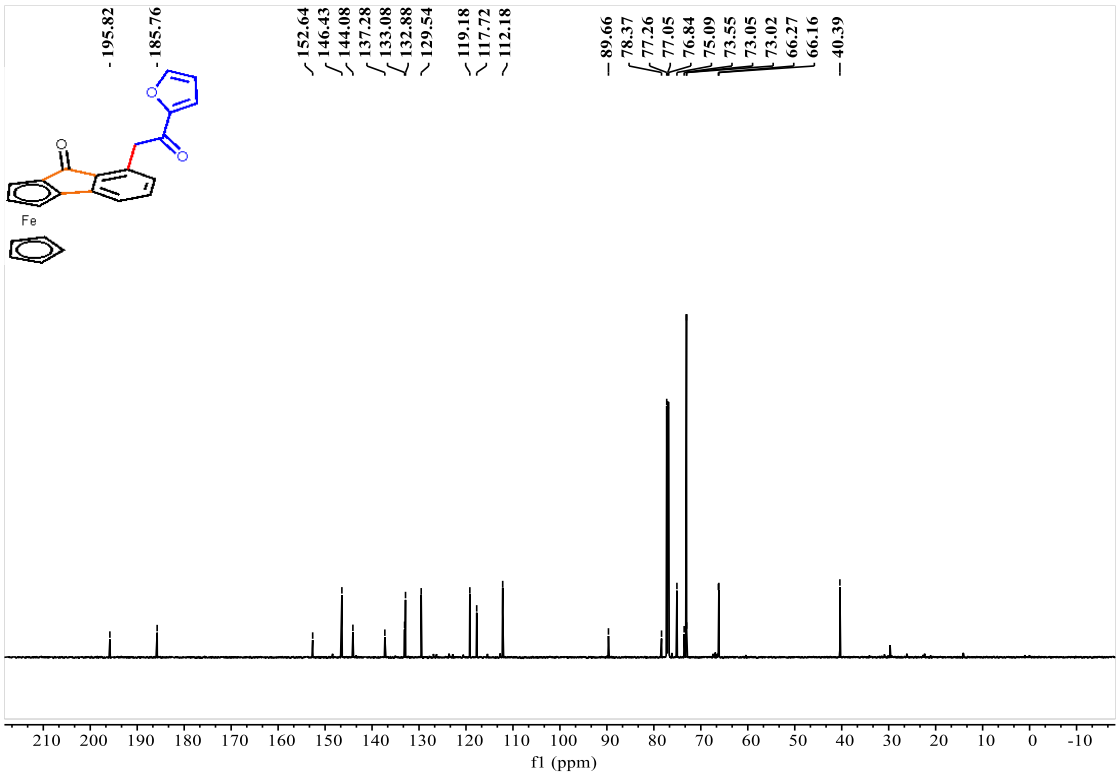


Figure S8.48 ^{13}C NMR of **3au** (151 MHz, $CDCl_3$)

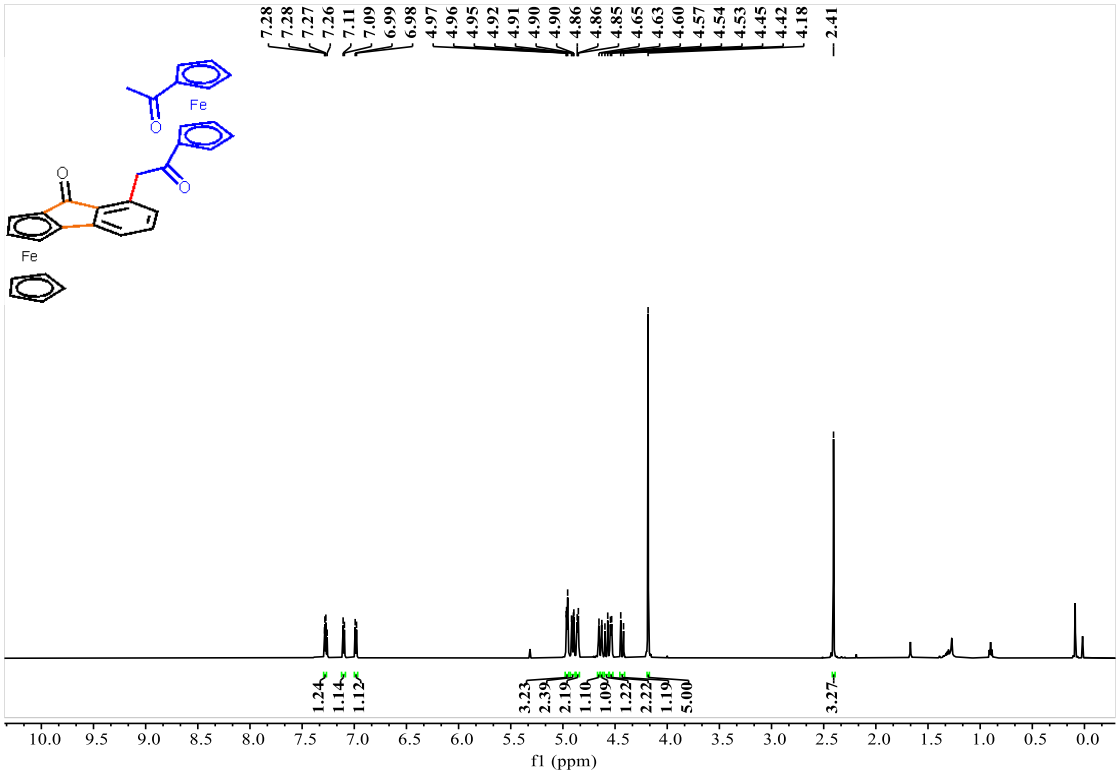


Figure S8.49 ^{1}H NMR of **3av** (600 MHz, $CDCl_3$)

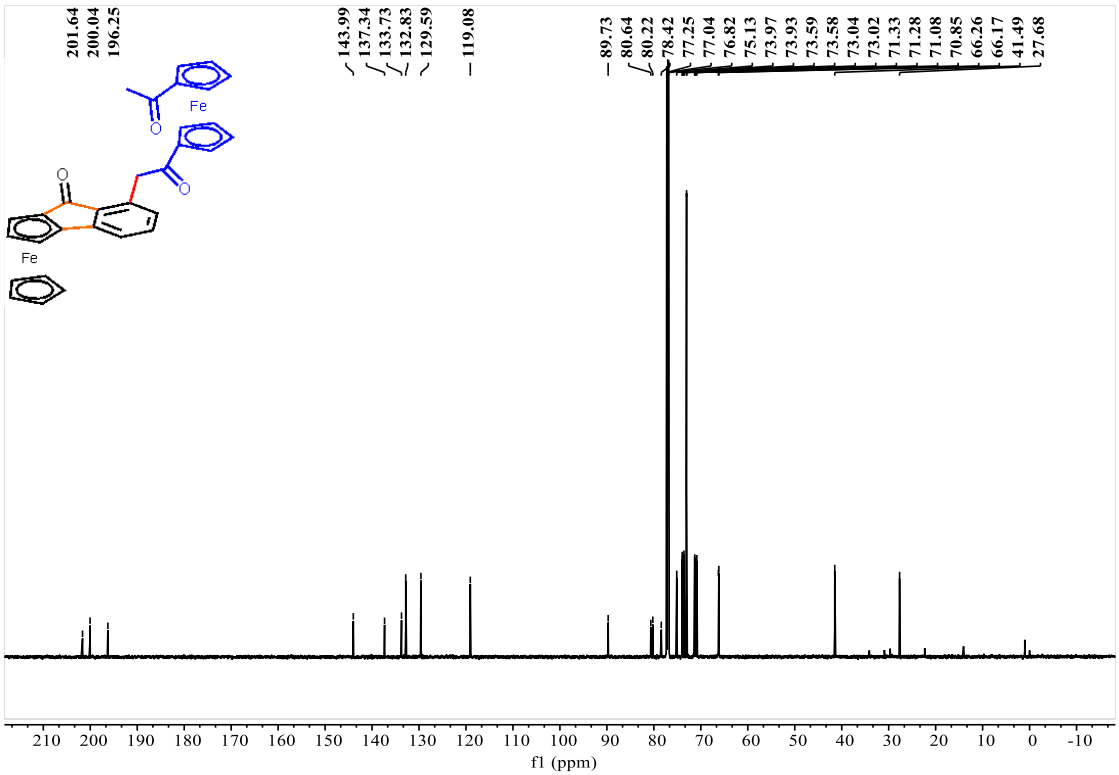


Figure S8.50 ^{13}C NMR of **3av** (151 MHz, $CDCl_3$)

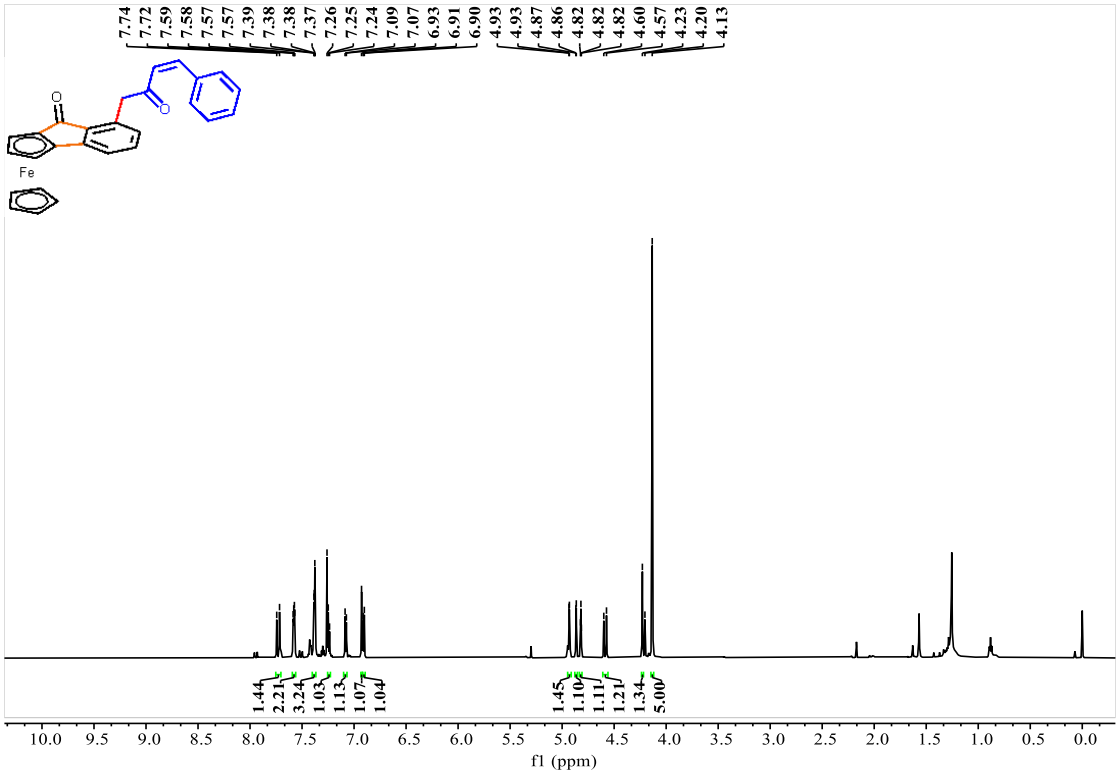


Figure S8.51 ^{1}H NMR of **3aw** (600 MHz, $CDCl_3$)

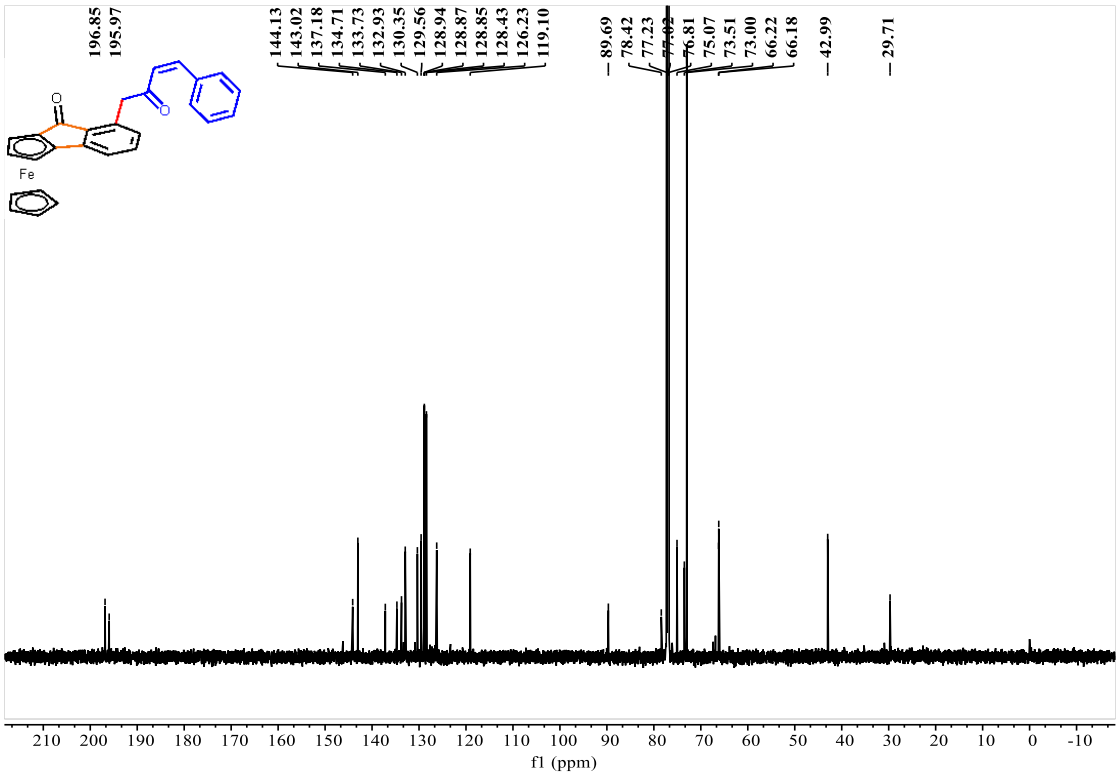


Figure S8.52 ^{13}C NMR of **3aw** (151 MHz, $CDCl_3$)

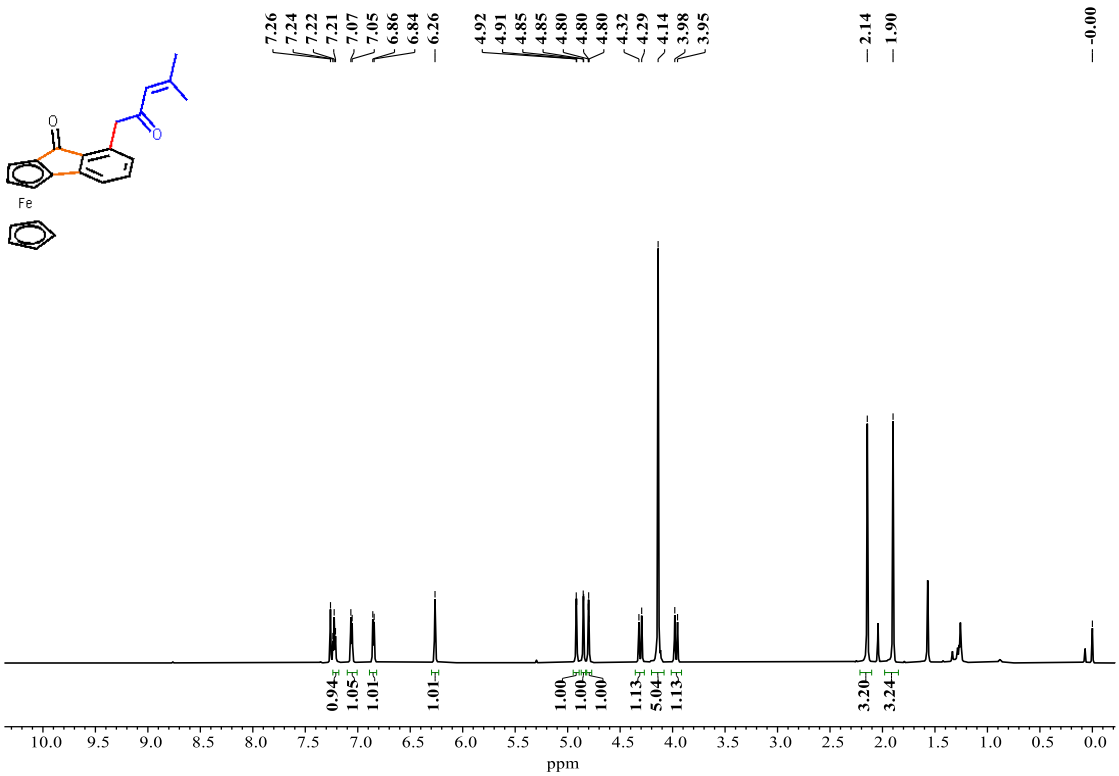


Figure S8.53 ^{1}H NMR of **3ax** (600 MHz, $CDCl_3$)

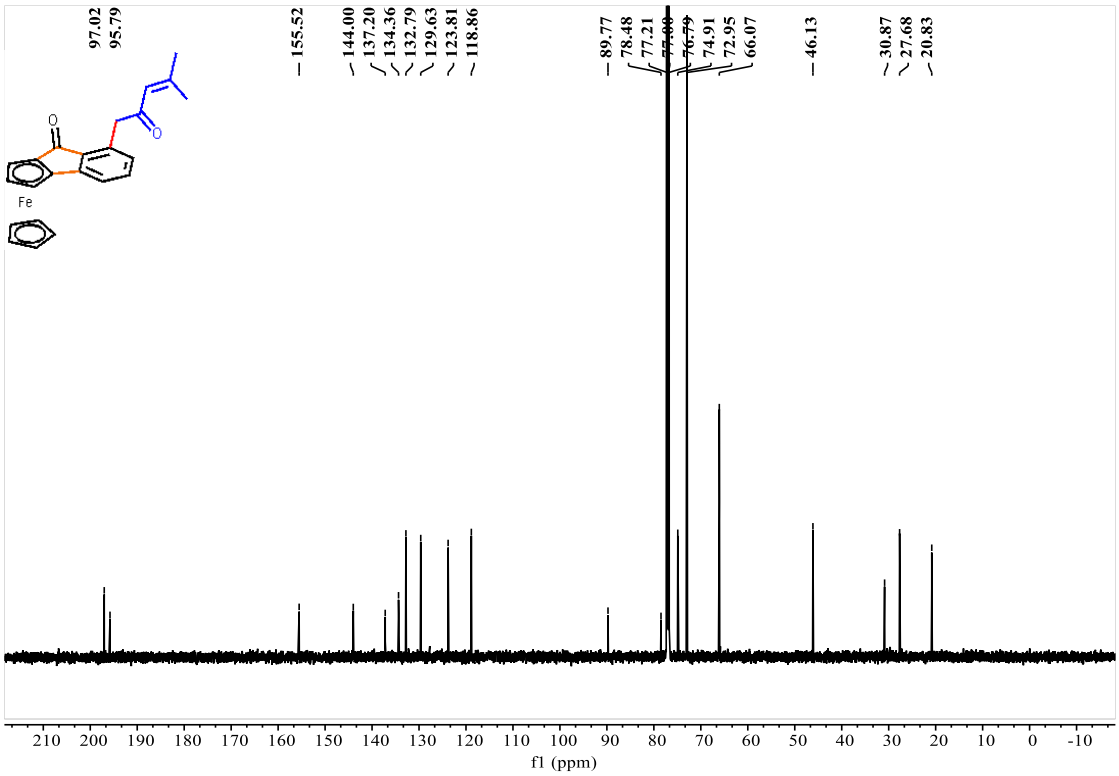


Figure S8.54 ^{13}C NMR of **3ax** (151 MHz, $CDCl_3$)

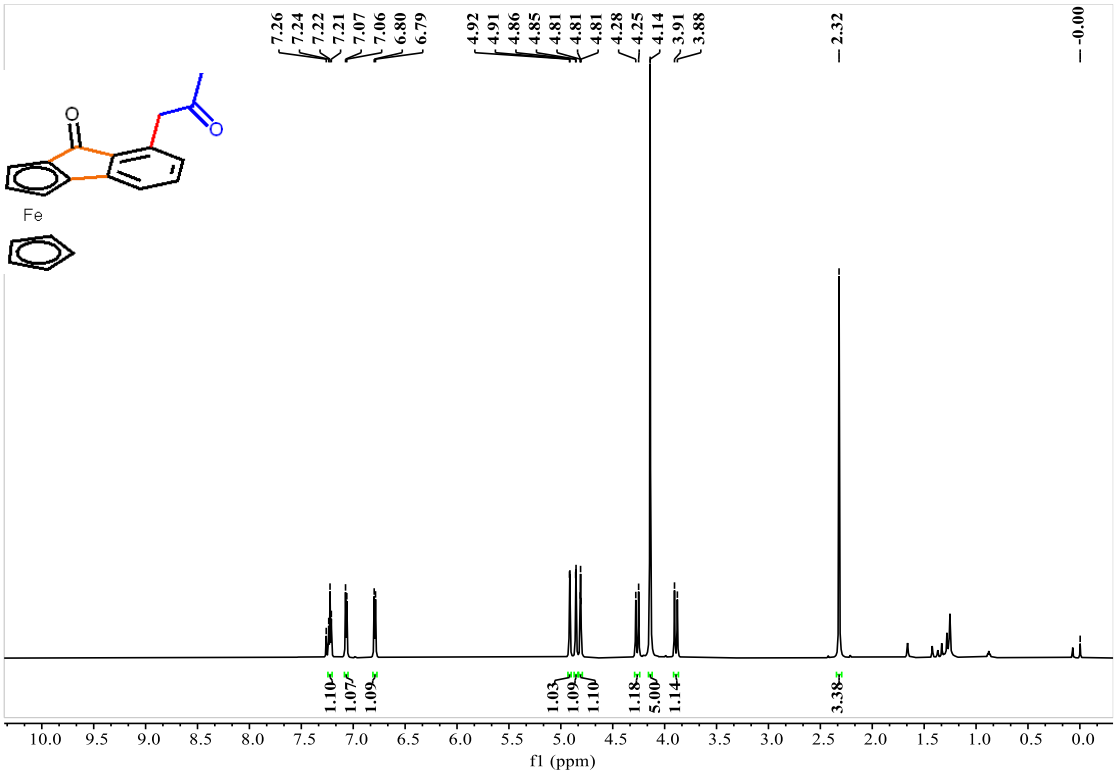


Figure S8.55 ^{1}H NMR of **3ay** (600 MHz, $CDCl_3$)

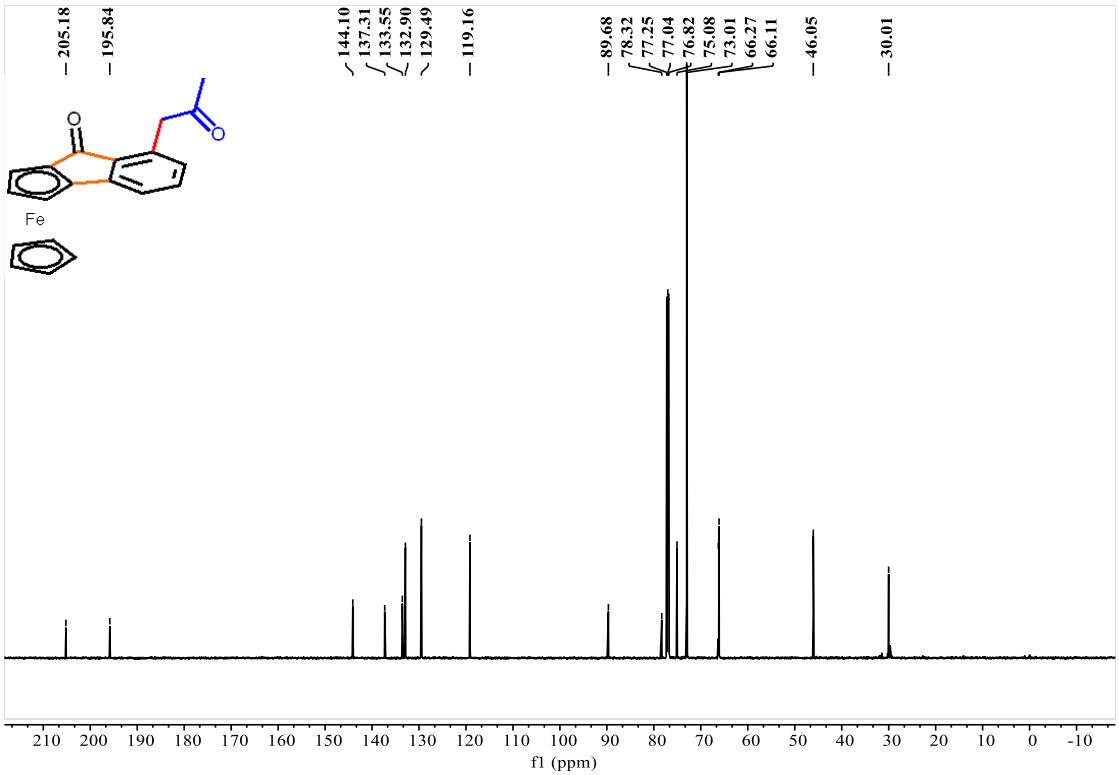


Figure S8.56 ^{13}C NMR of **3ay** (151 MHz, $CDCl_3$)

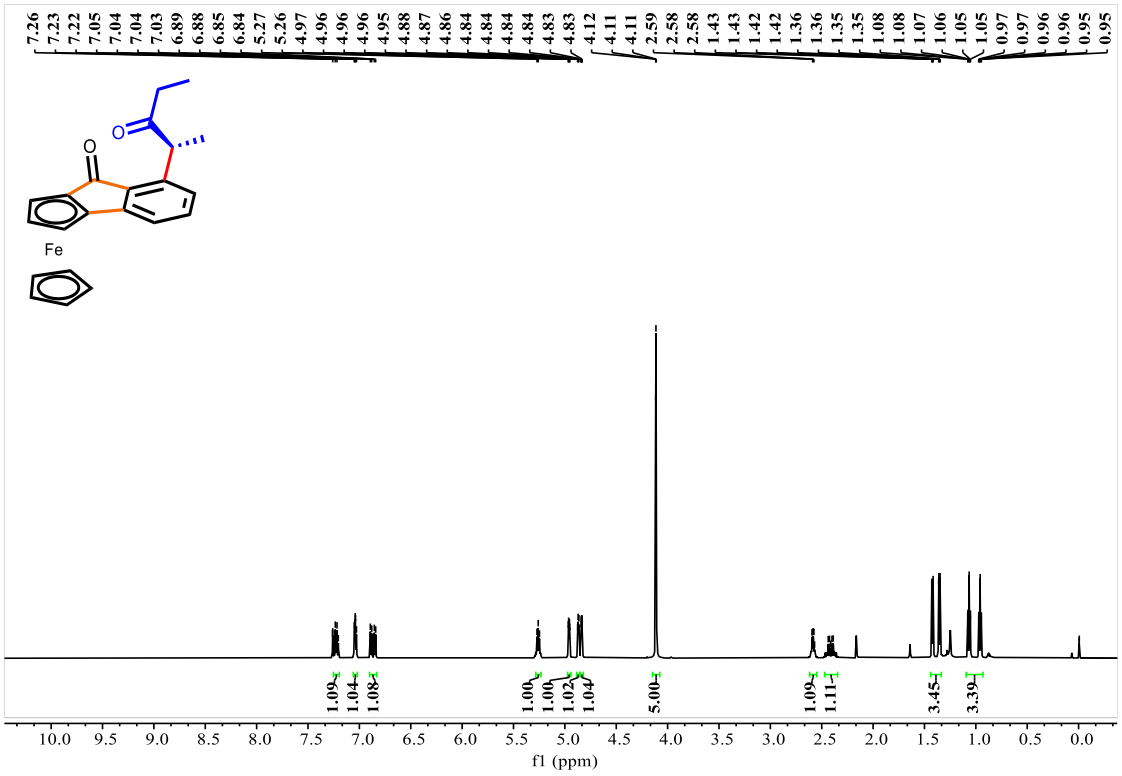


Figure S8.57 ^{1}H NMR of **(R_p, *R*)-3az** (600 MHz, $CDCl_3$)

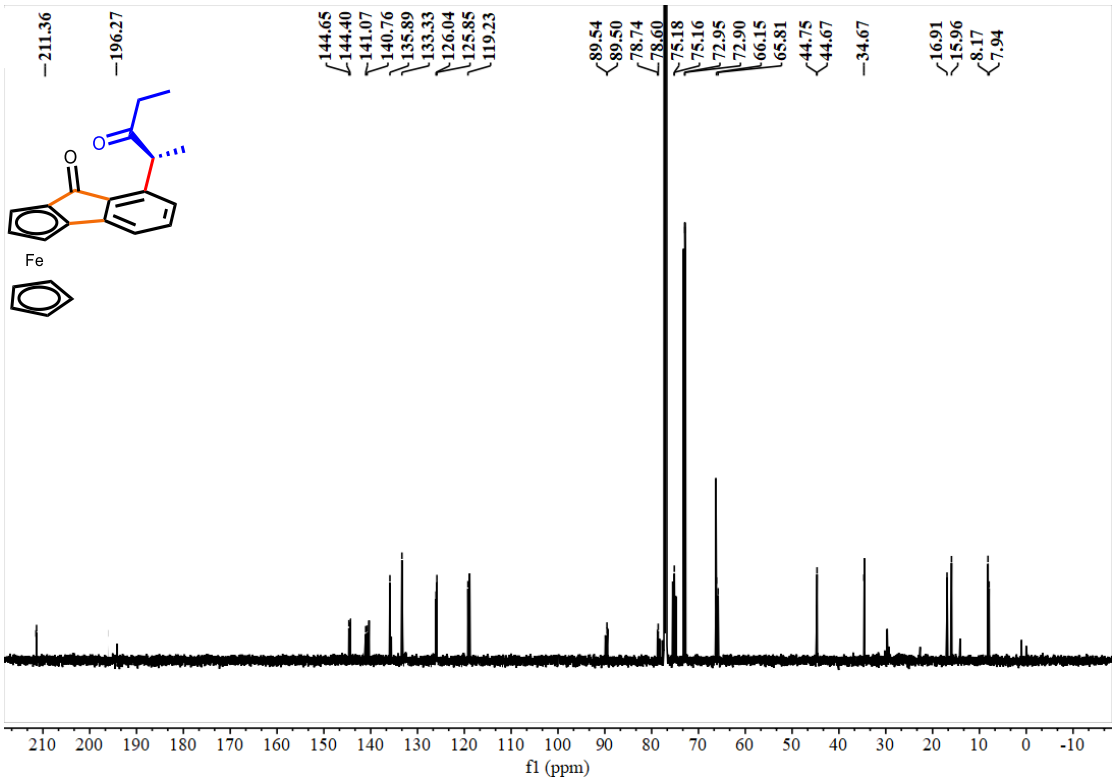


Figure S8.58 ^{13}C NMR of **(R_p, *R*)-3az** (151 MHz, $CDCl_3$)

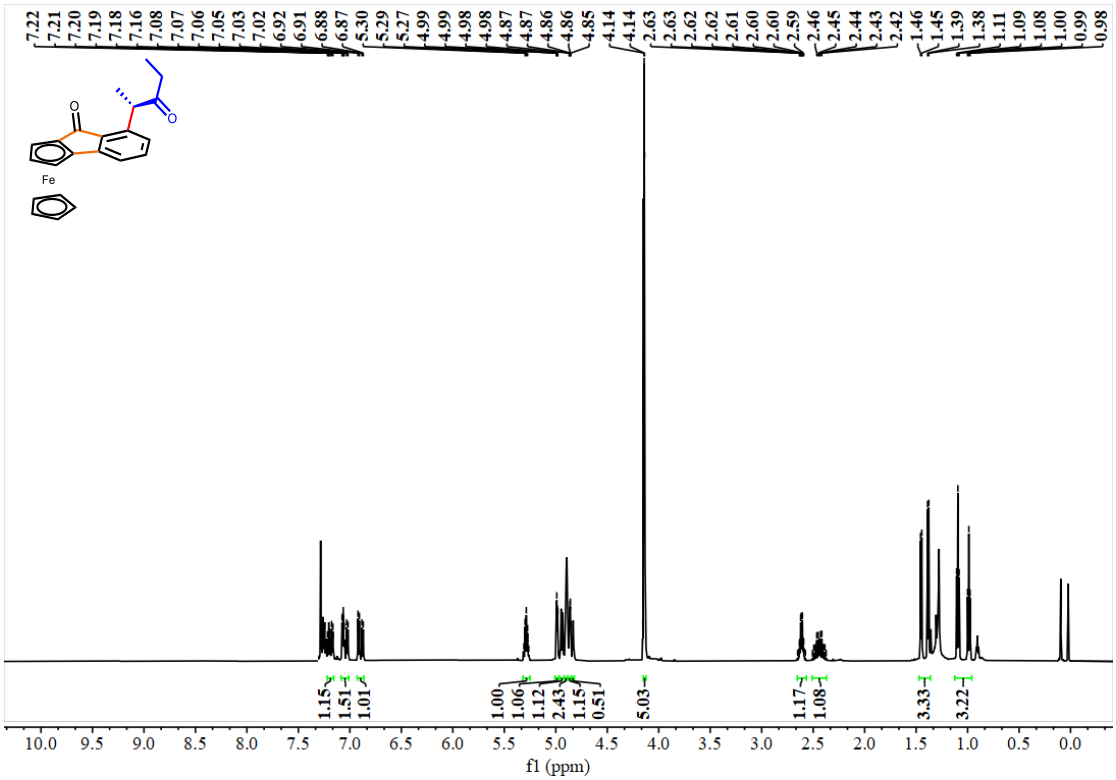


Figure S8.59 ^{1}H NMR of **(R_p, *S*)-3az** (600 MHz, $CDCl_3$)

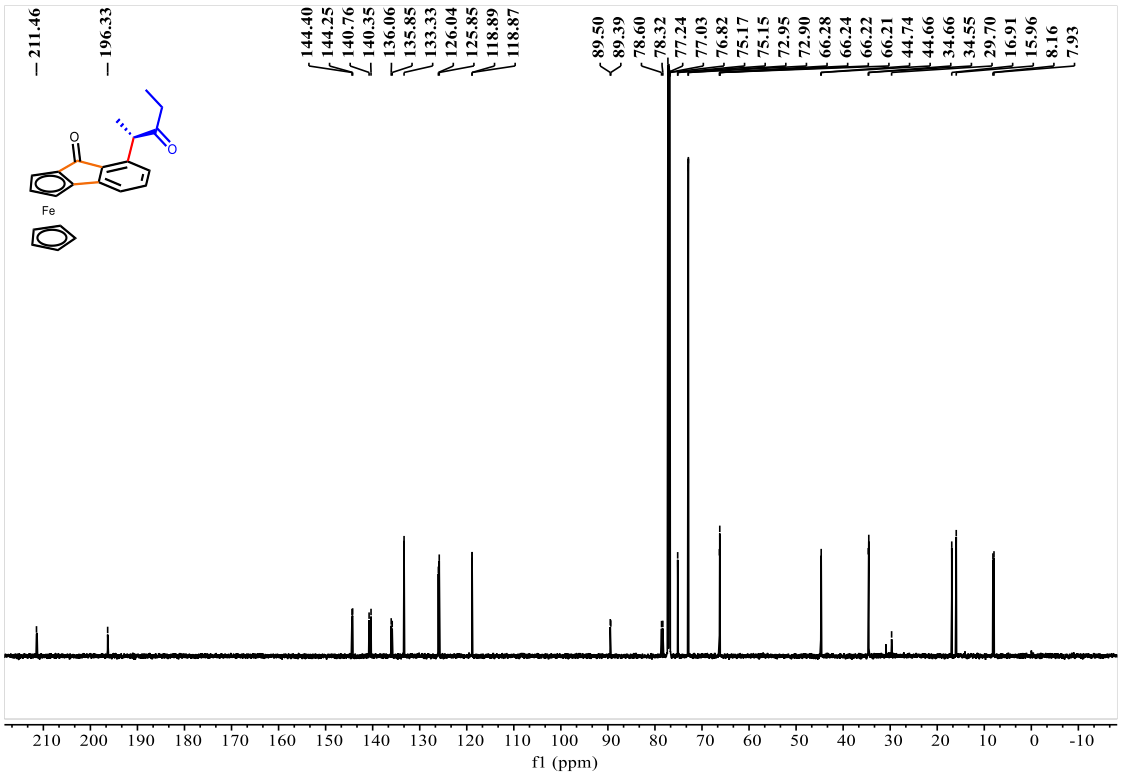


Figure S8.60 ^{13}C NMR of **(R_p, *S*)-3az** (151 MHz, $CDCl_3$)

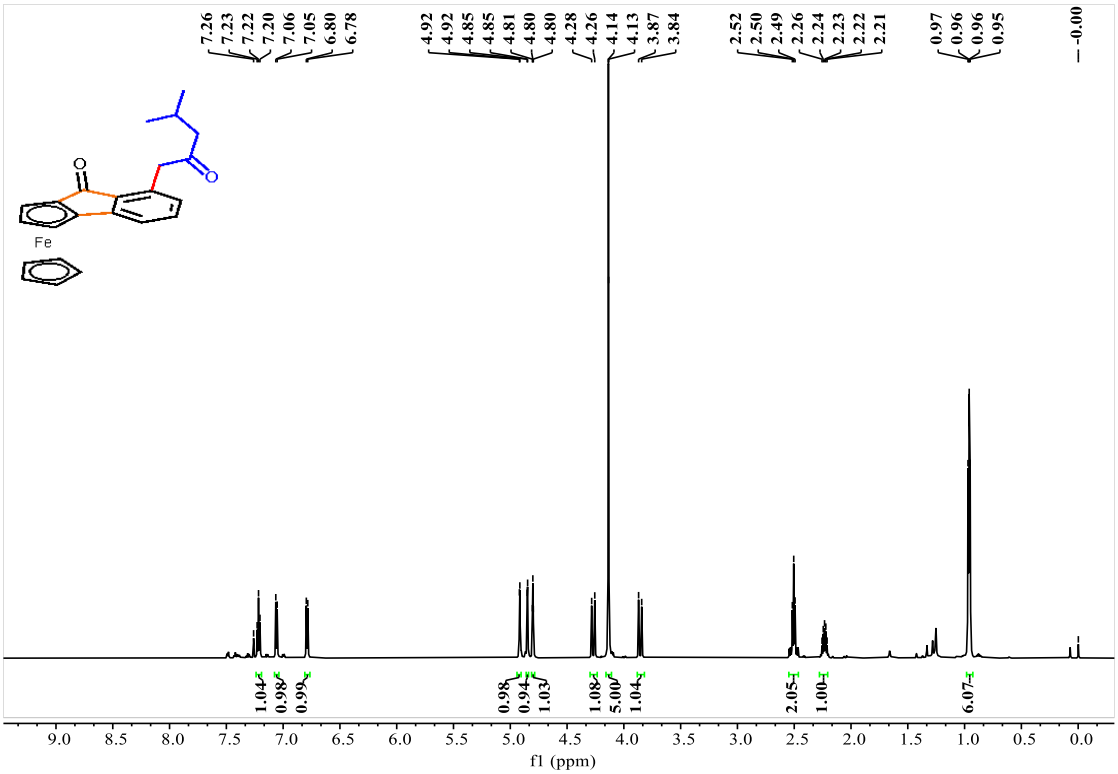


Figure S8.61 ^{1}H NMR of **3ba** (600 MHz, $CDCl_3$)

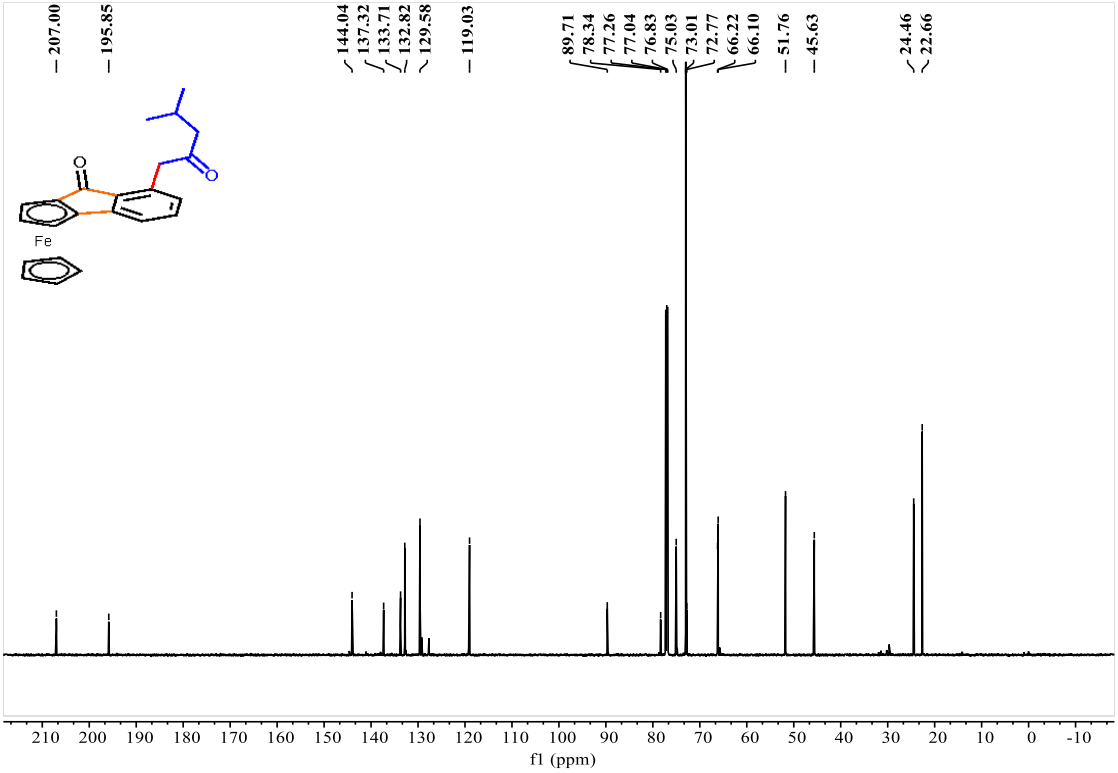


Figure S8.62 ^{13}C NMR of **3ba** (151 MHz, $CDCl_3$)

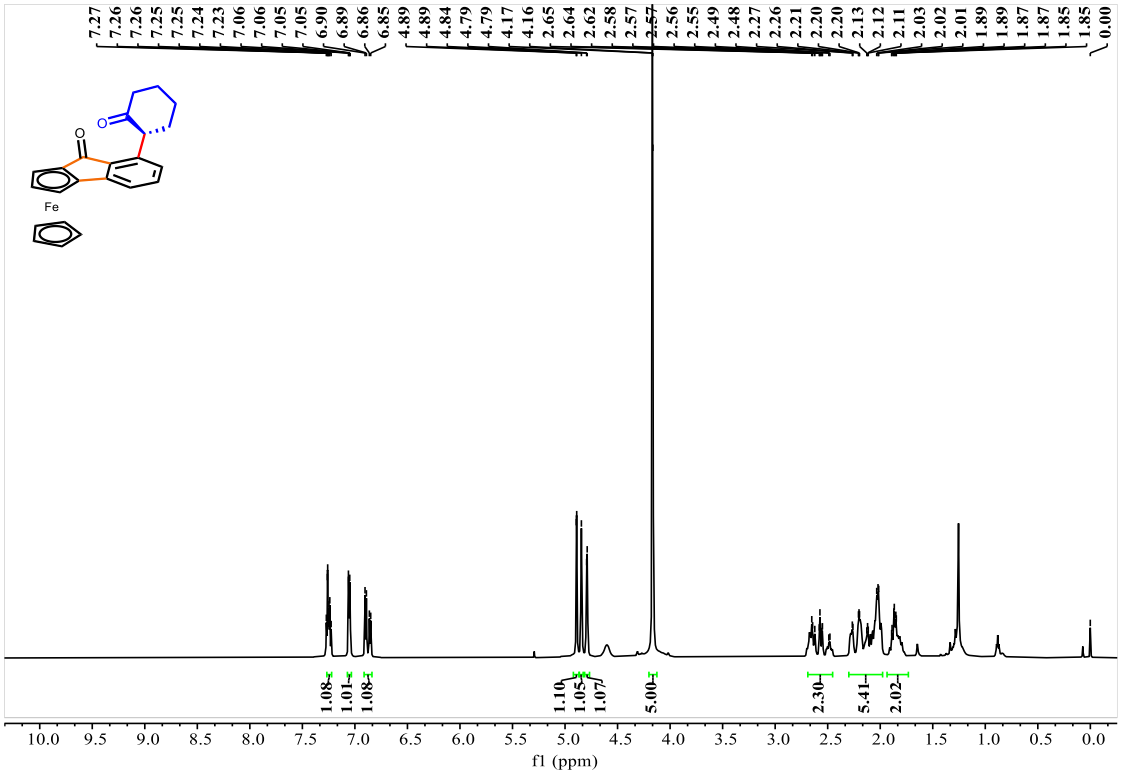


Figure S8.63 ^{1}H NMR of **(R_p, *R*)-3bb** (600 MHz, $CDCl_3$)

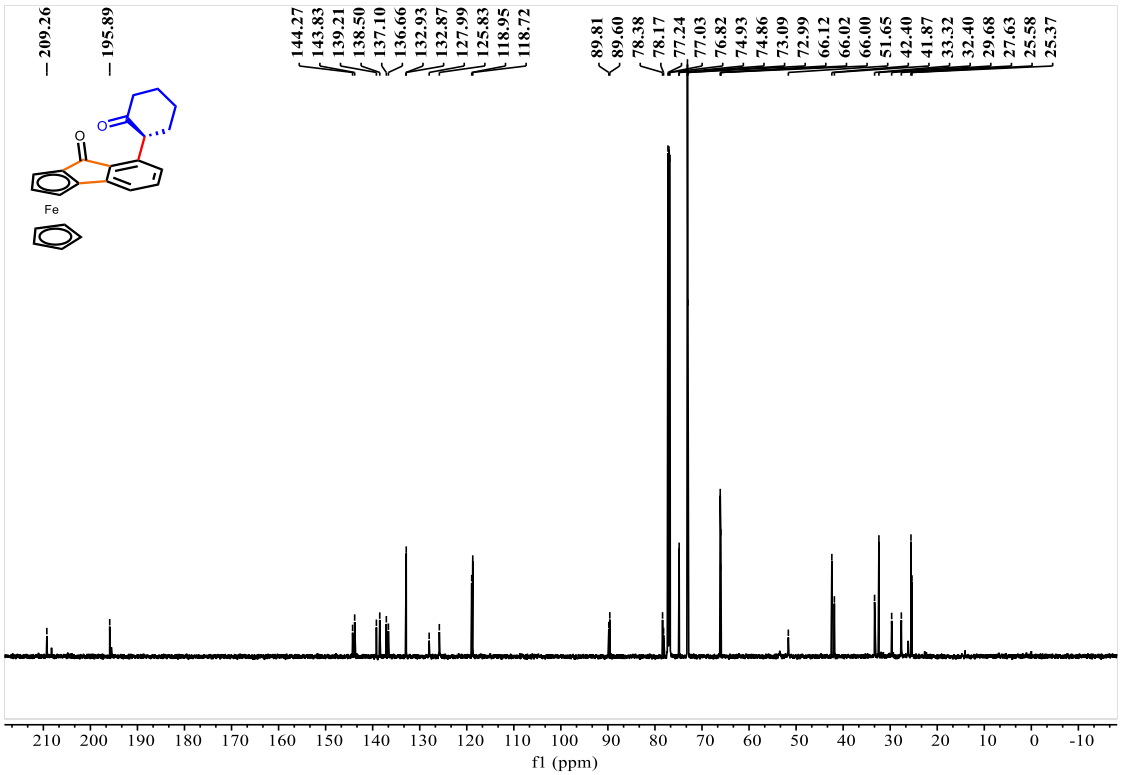


Figure S8.64 ^{13}C NMR of **(R_p, *R*)-3bb** (151 MHz, $CDCl_3$)

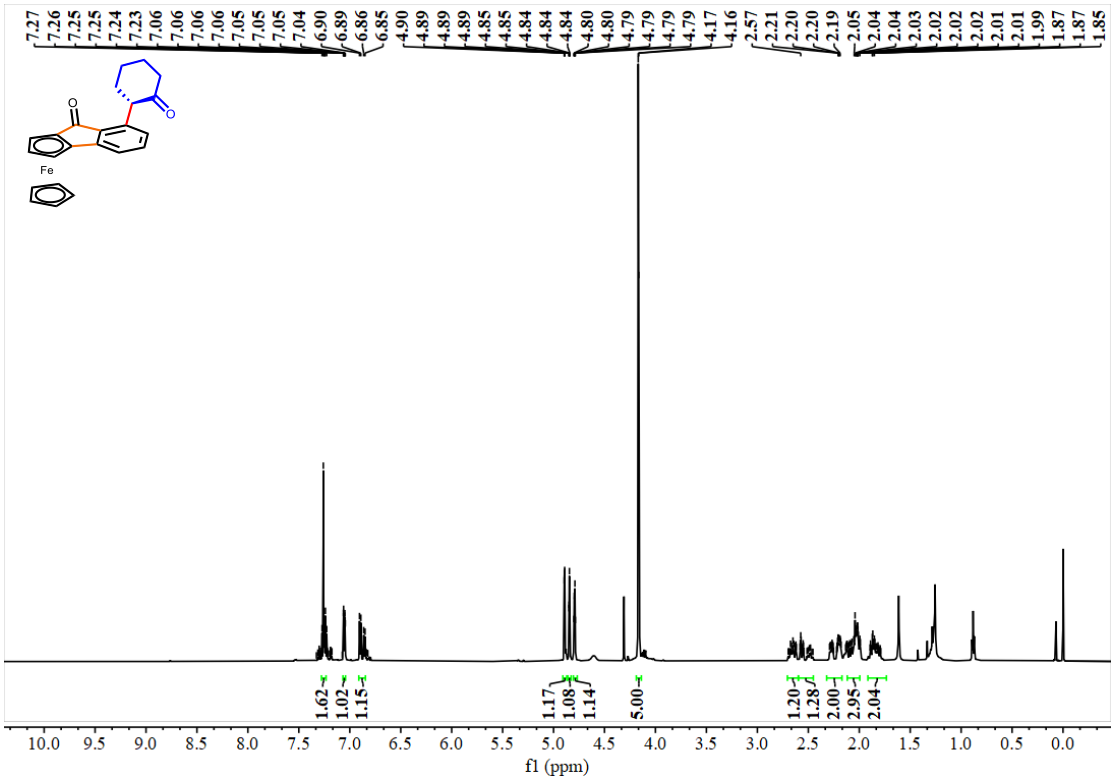


Figure S8.65 ^{1}H NMR of (***R*$_p$, *S*)-3bb** (600 MHz, $CDCl_3$)

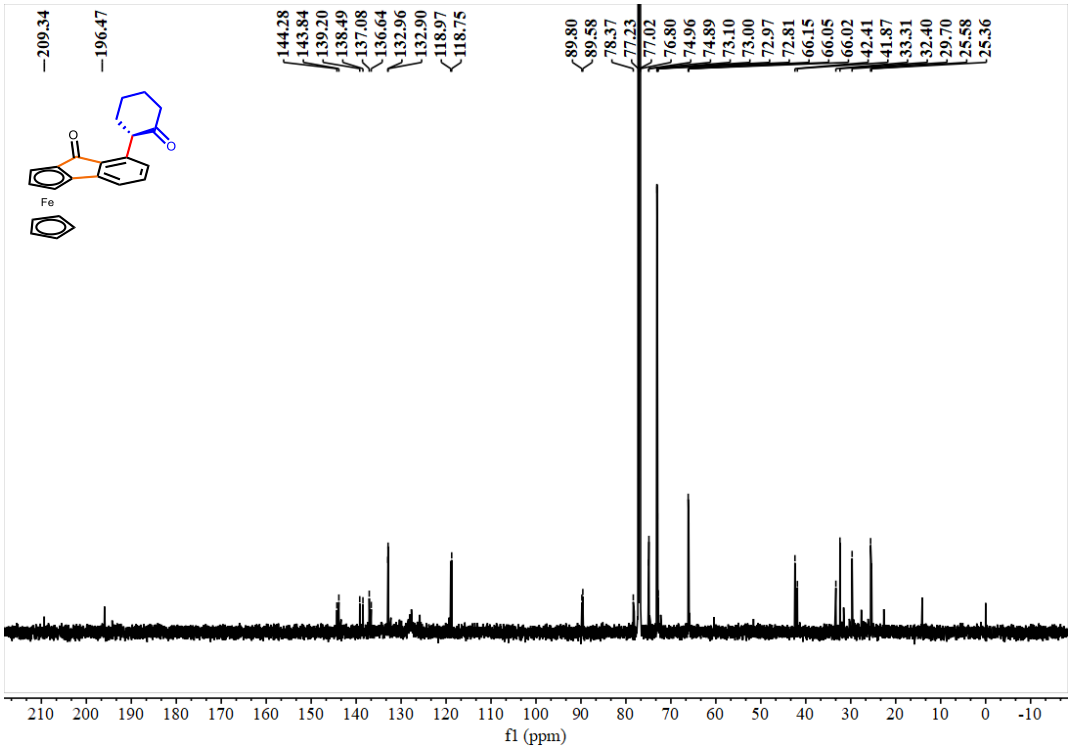


Figure S8.66 ^{13}C NMR of (***R*$_p$, *S*)-3bb** (151 MHz, $CDCl_3$)

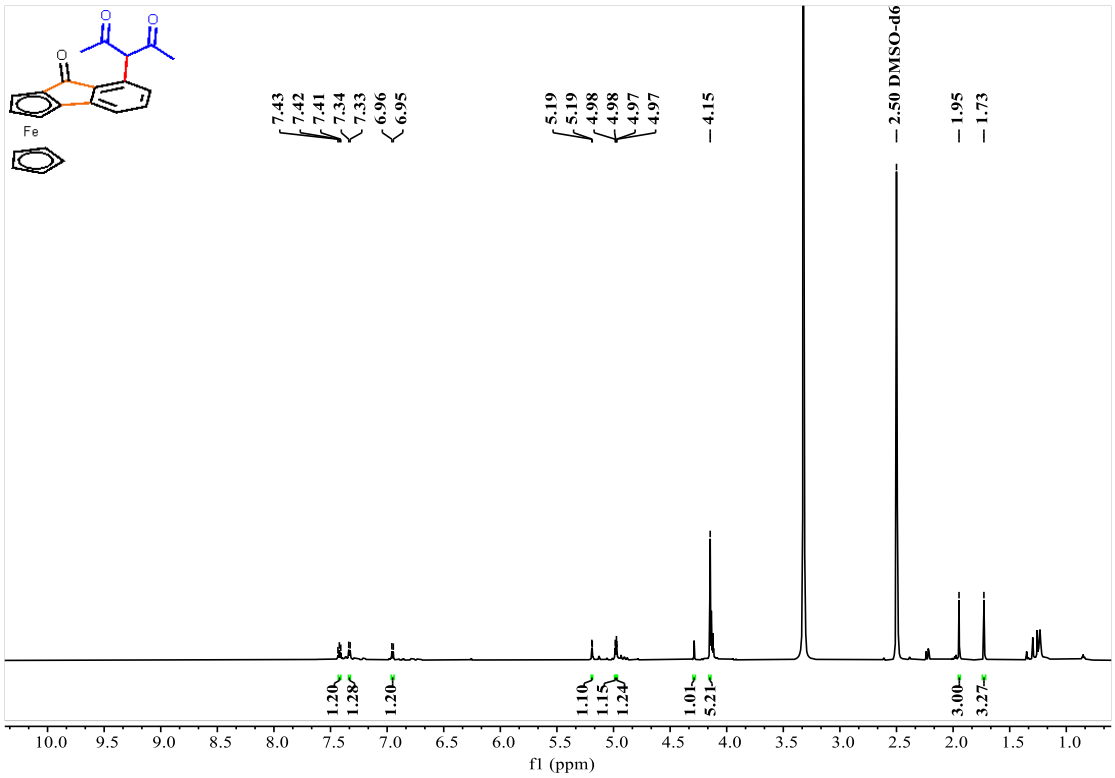


Figure S8.67 ^{1}H NMR of **3bc** (600 MHz, DMSO-d6)

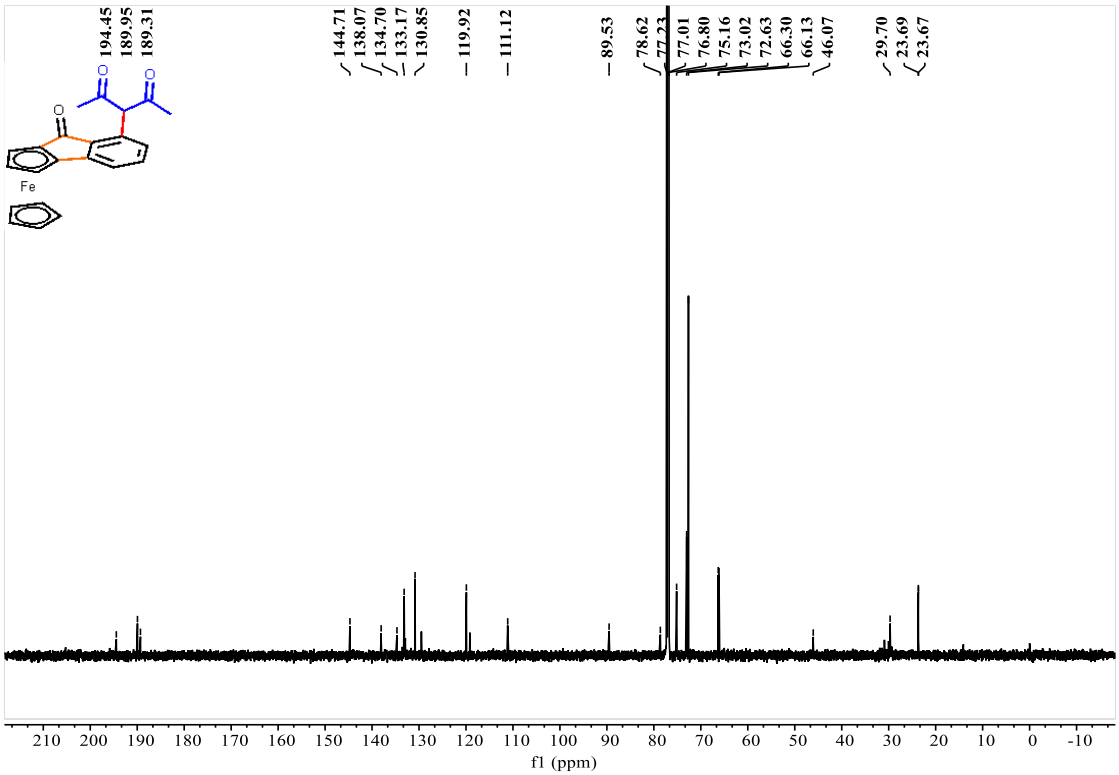


Figure S8.68 ^{13}C NMR of **3bc** (151 MHz, $CDCl_3$)

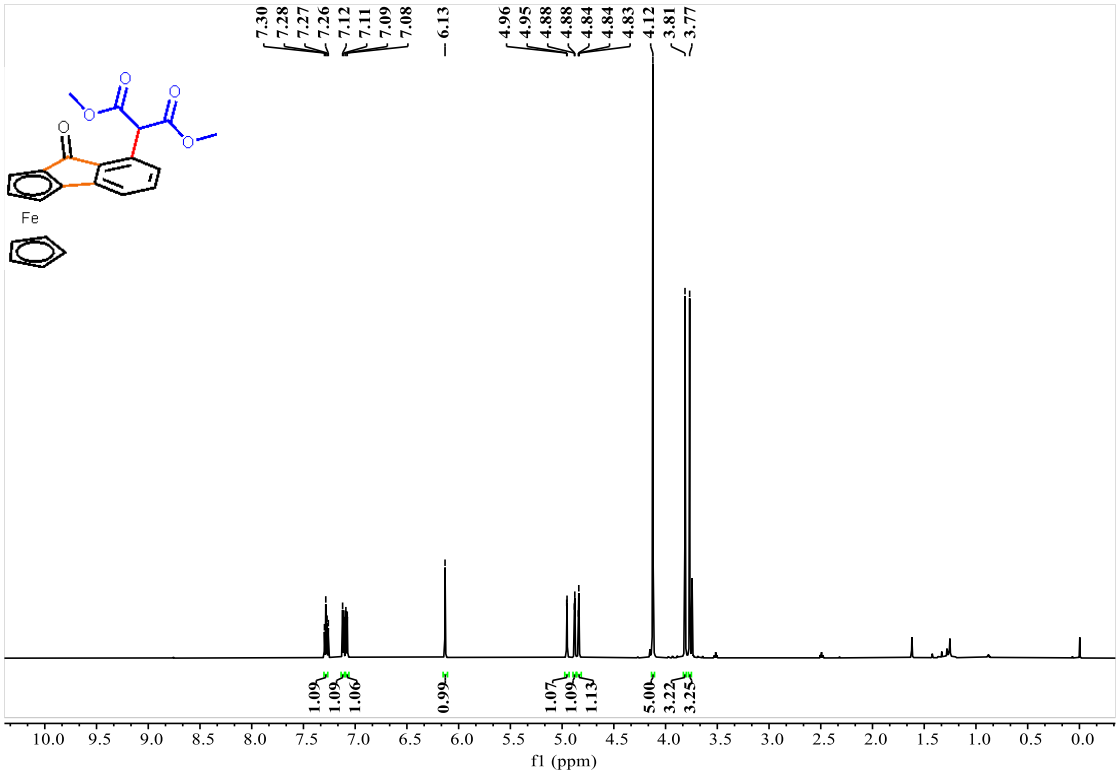


Figure S8.69 ^{1}H NMR of **3bd** (600 MHz, $CDCl_3$)

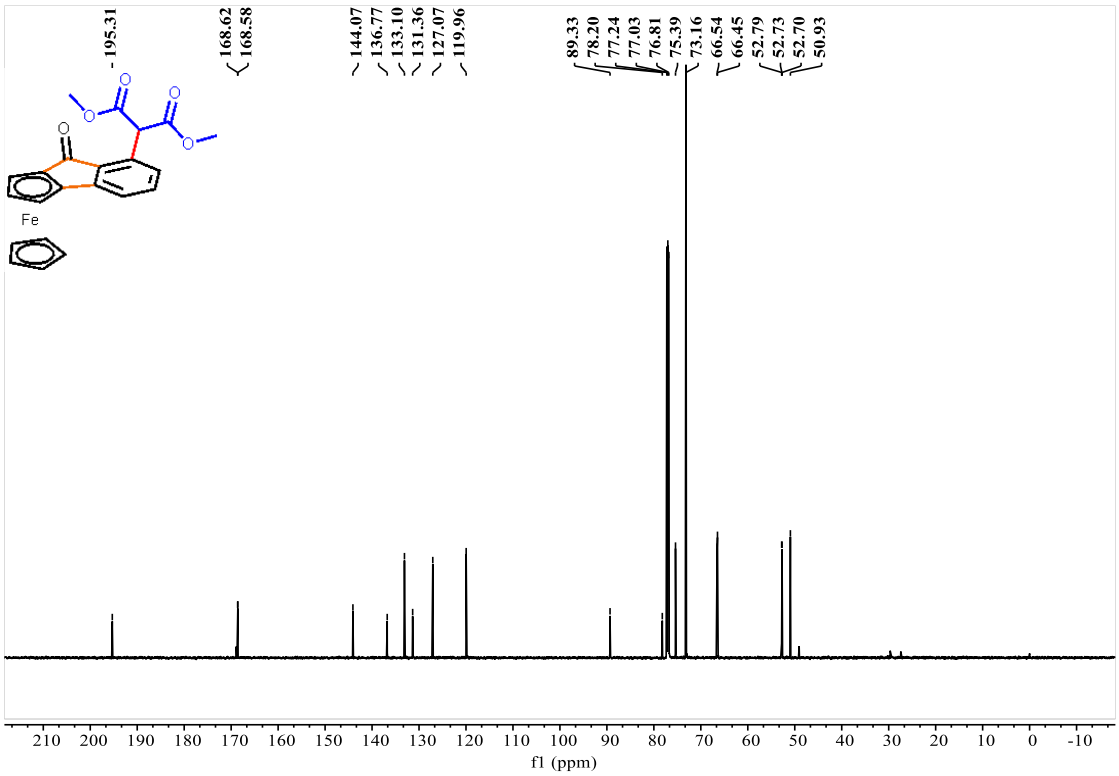


Figure S8.70 ^{13}C NMR of **3bd** (151 MHz, $CDCl_3$)

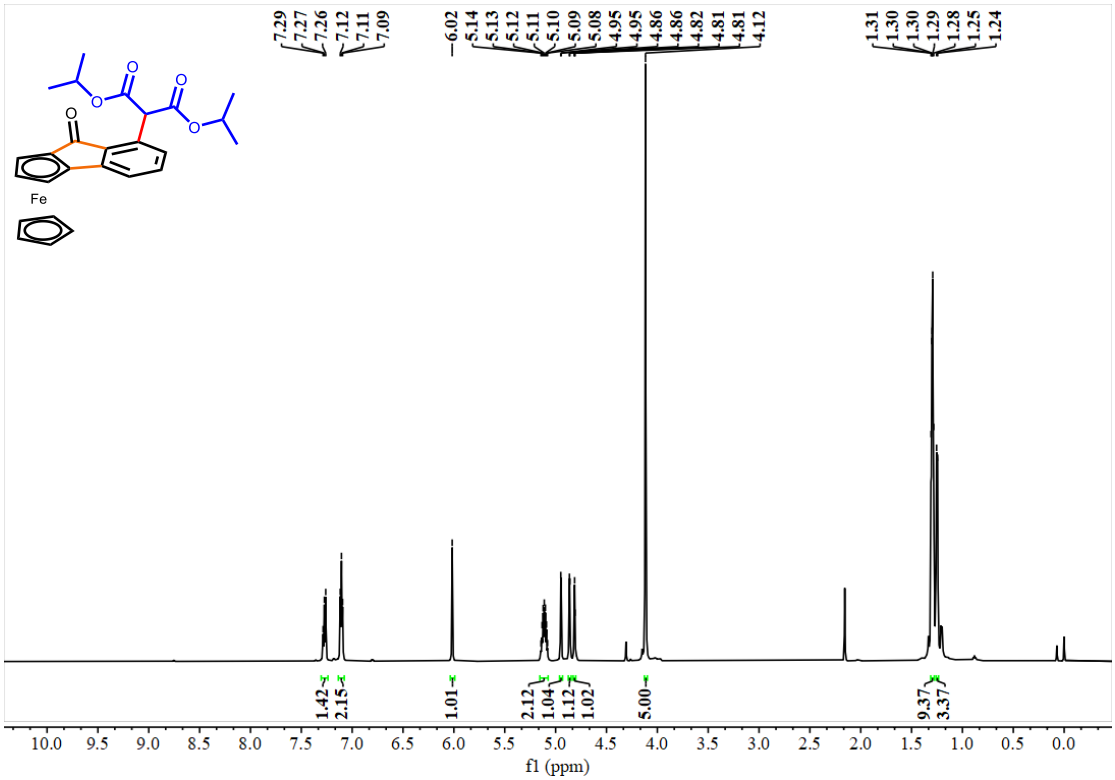


Figure S8.71 ^{1}H NMR of **3be** (600 MHz, $CDCl_3$)

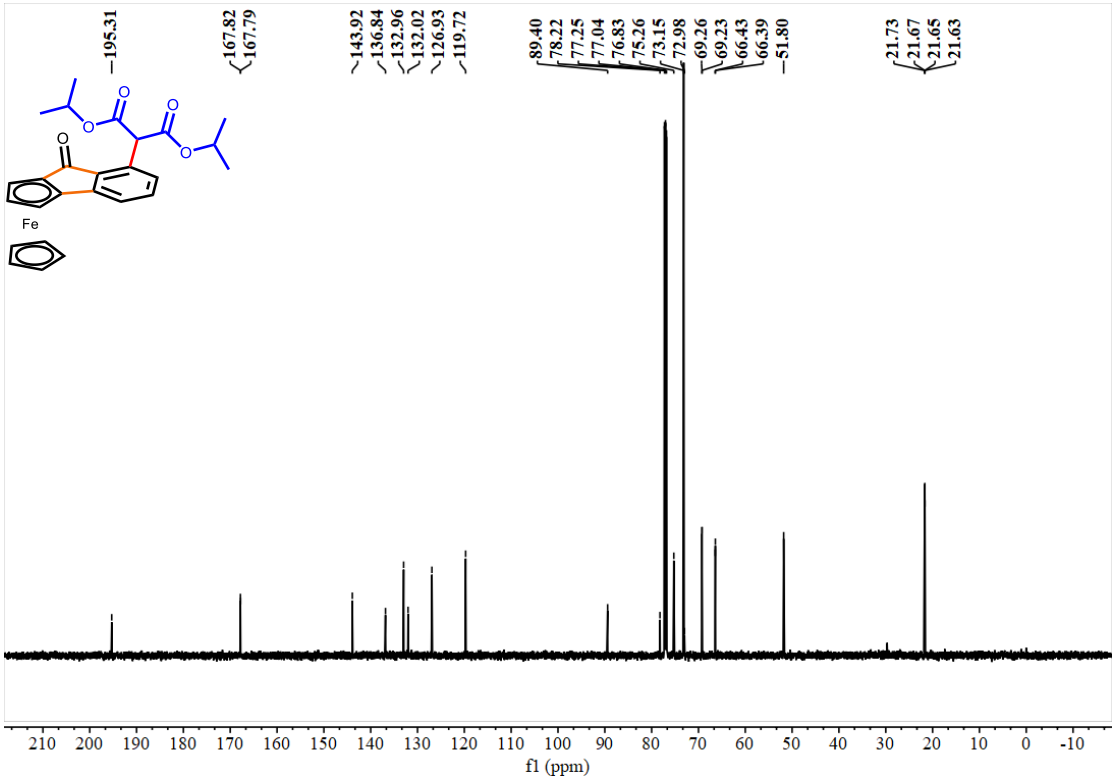


Figure S8.72 ^{13}C NMR of **3be** (151 MHz, $CDCl_3$)

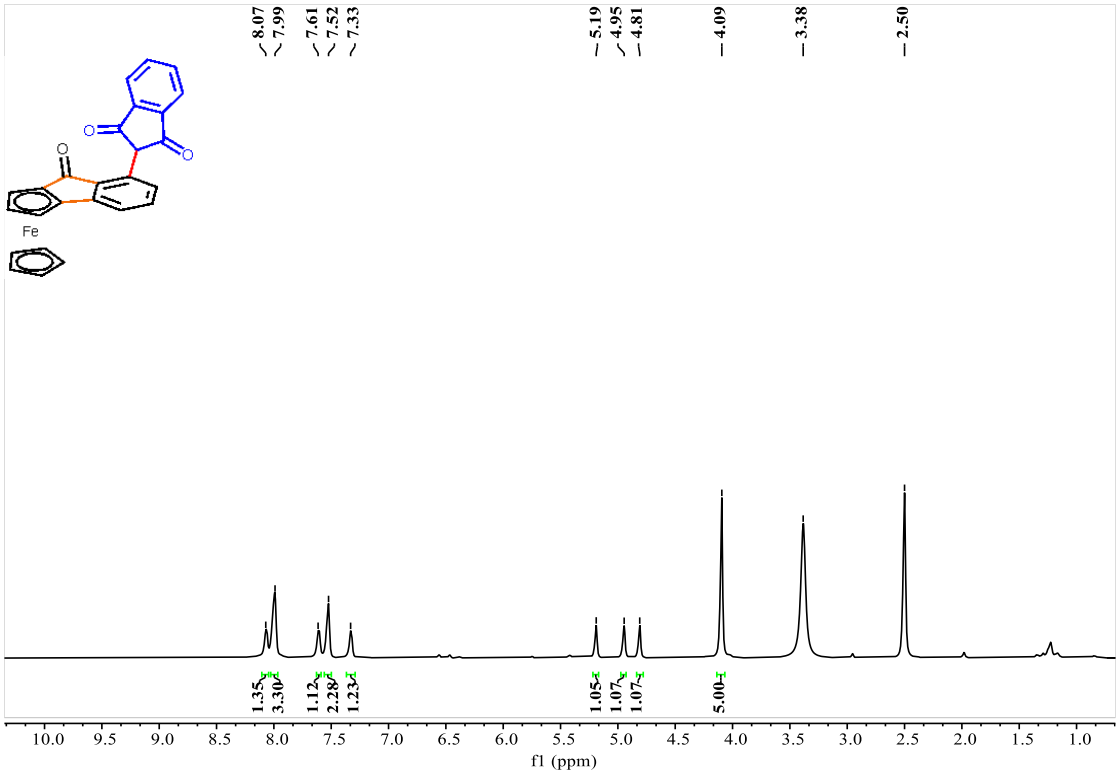


Figure S8.73 ^{1}H NMR of **3bf** (600 MHz, DMSO-d_6)

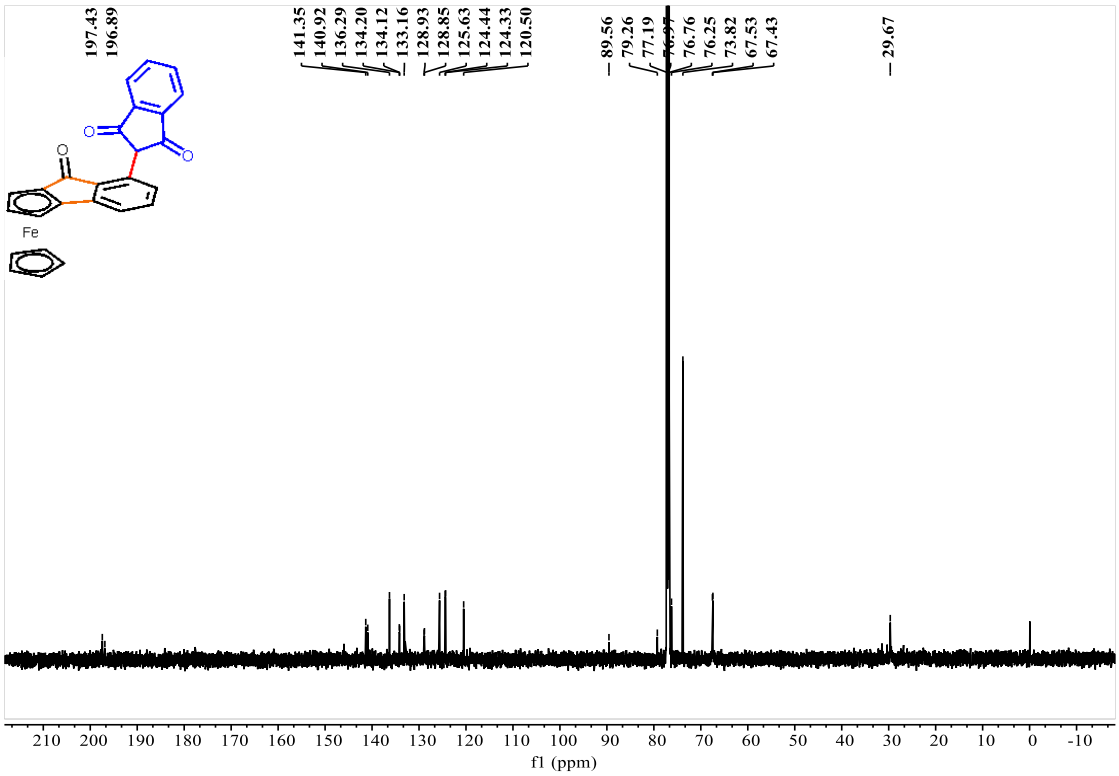


Figure S8.74 ^{13}C NMR of **3bf** (151 MHz, $CDCl_3$)

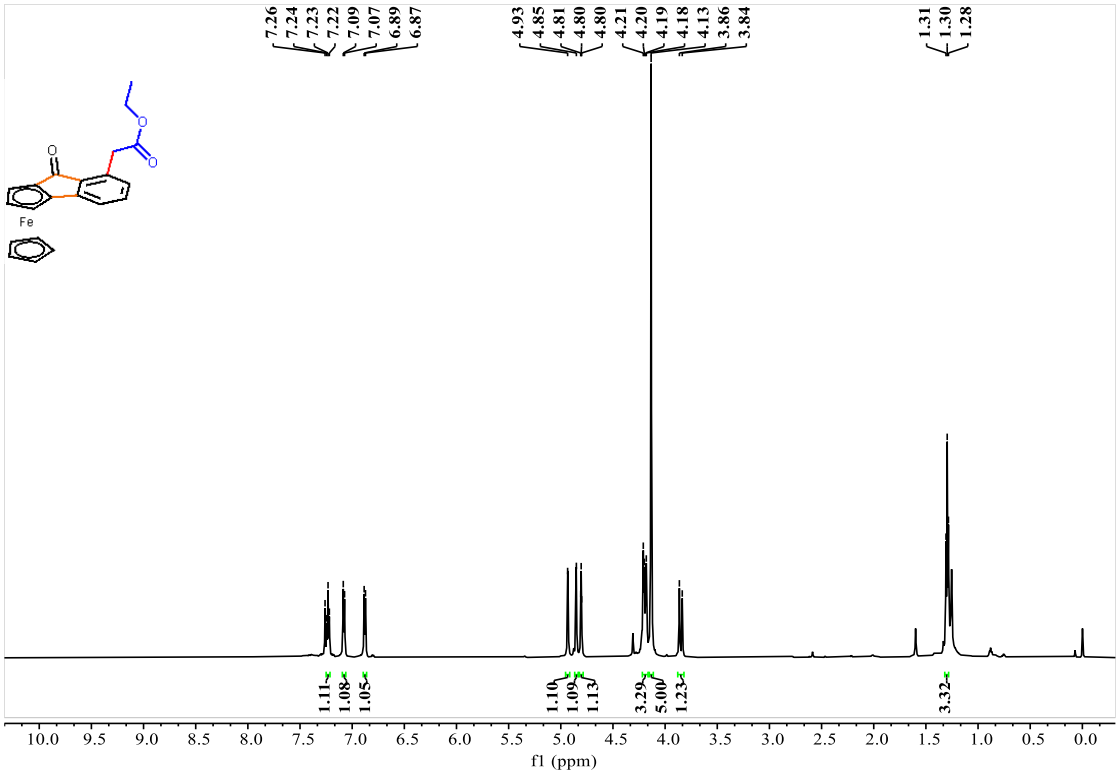


Figure S8.75 ^{1}H NMR of **3bg** (600 MHz, $CDCl_3$)

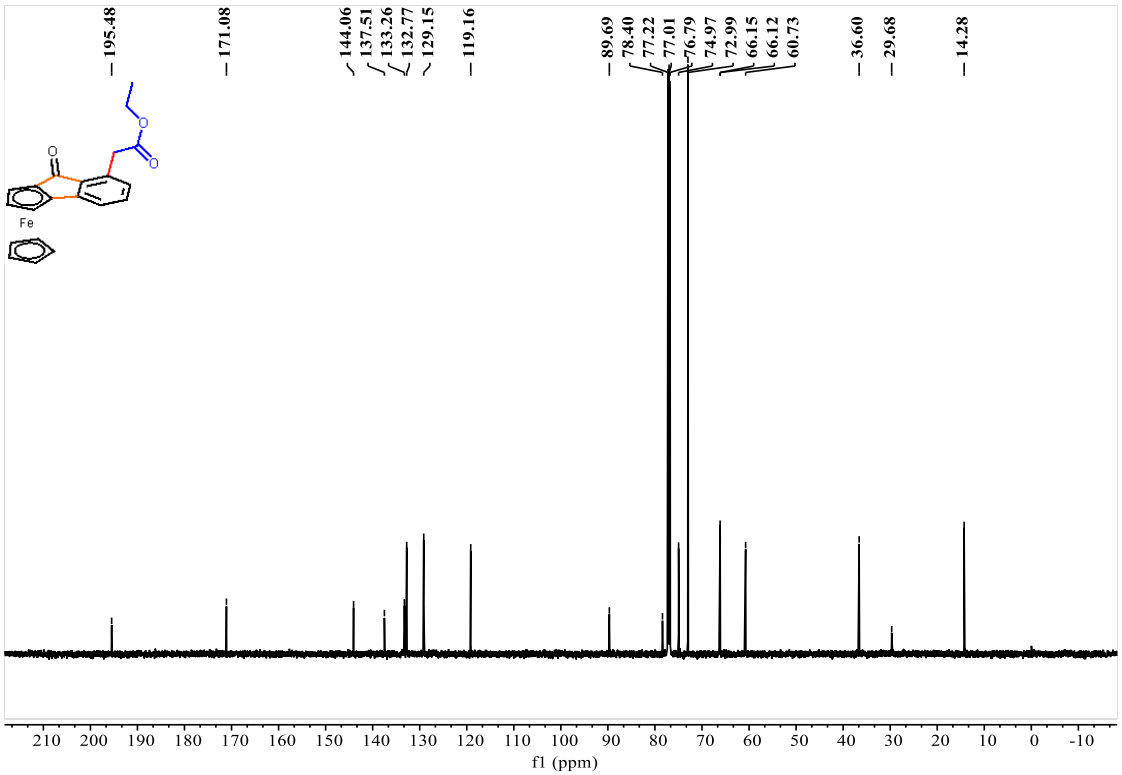


Figure S8.76 ^{13}C NMR of **3bg** (151 MHz, $CDCl_3$)

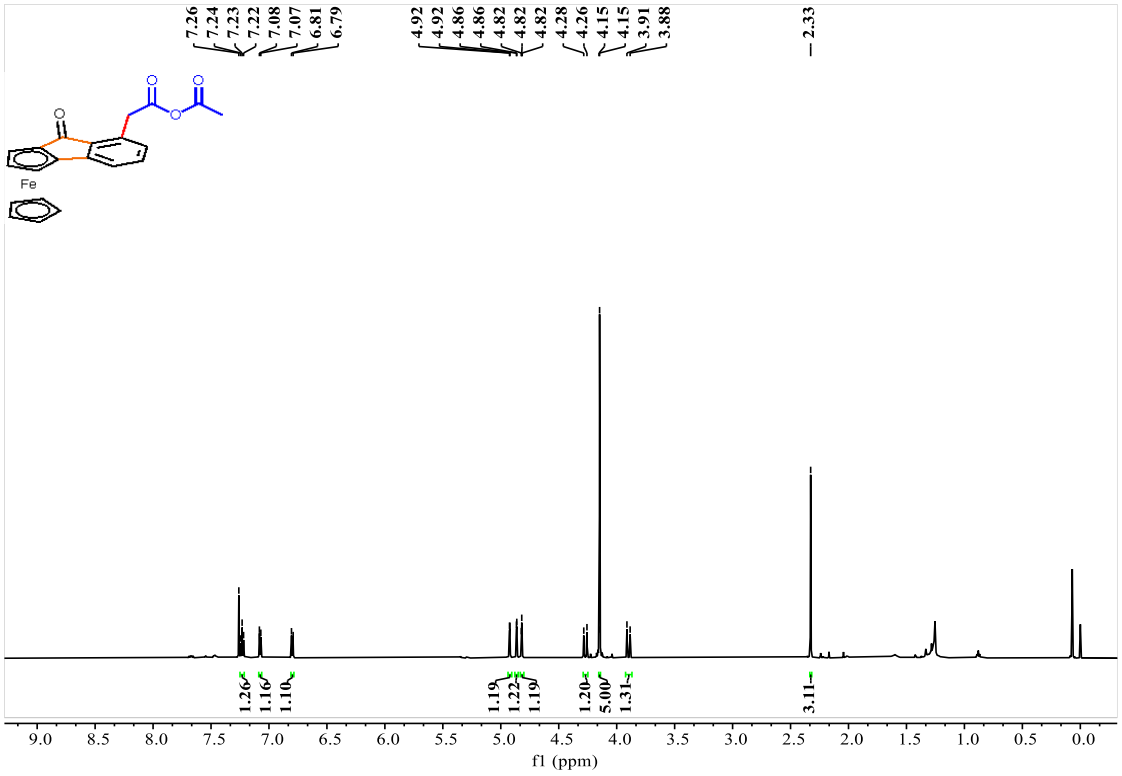


Figure S8.77 ^{1}H NMR of **3bh** (600 MHz, $CDCl_3$)

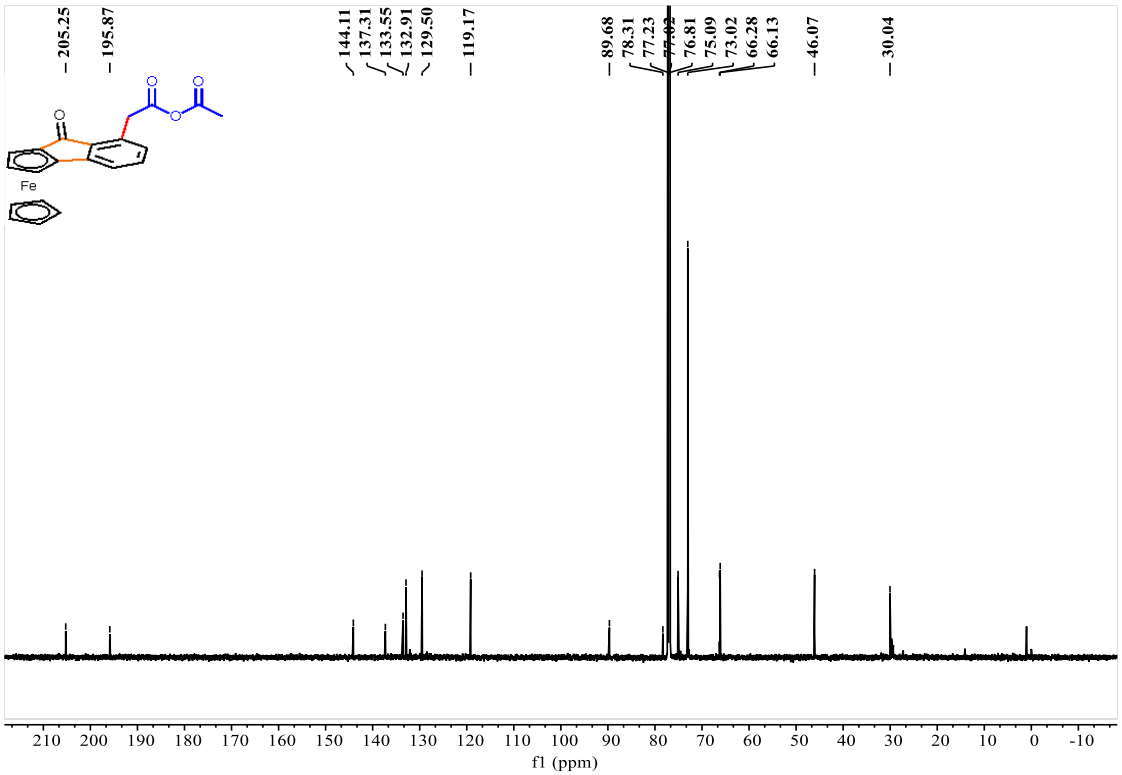


Figure S8.78 ^{13}C NMR of **3bh** (151 MHz, $CDCl_3$)

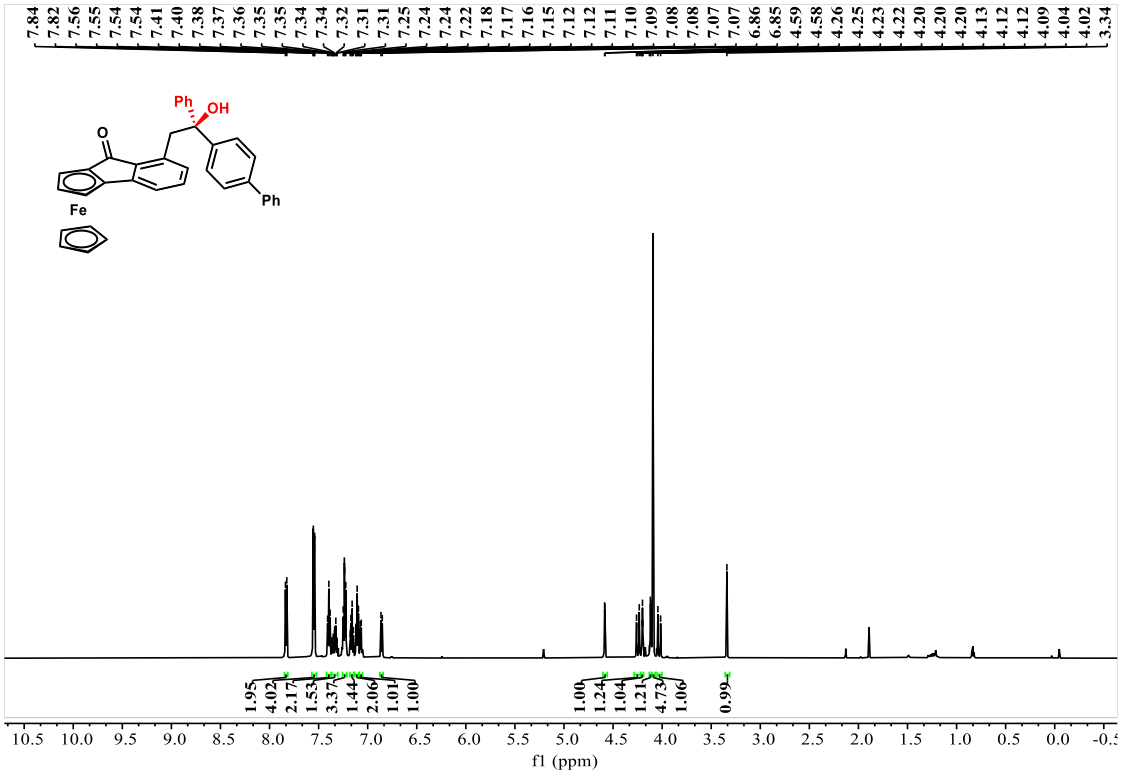


Figure S8.79 ^{1}H NMR of **(R_p, *S*)-4aa** (600 MHz, $CDCl_3$)

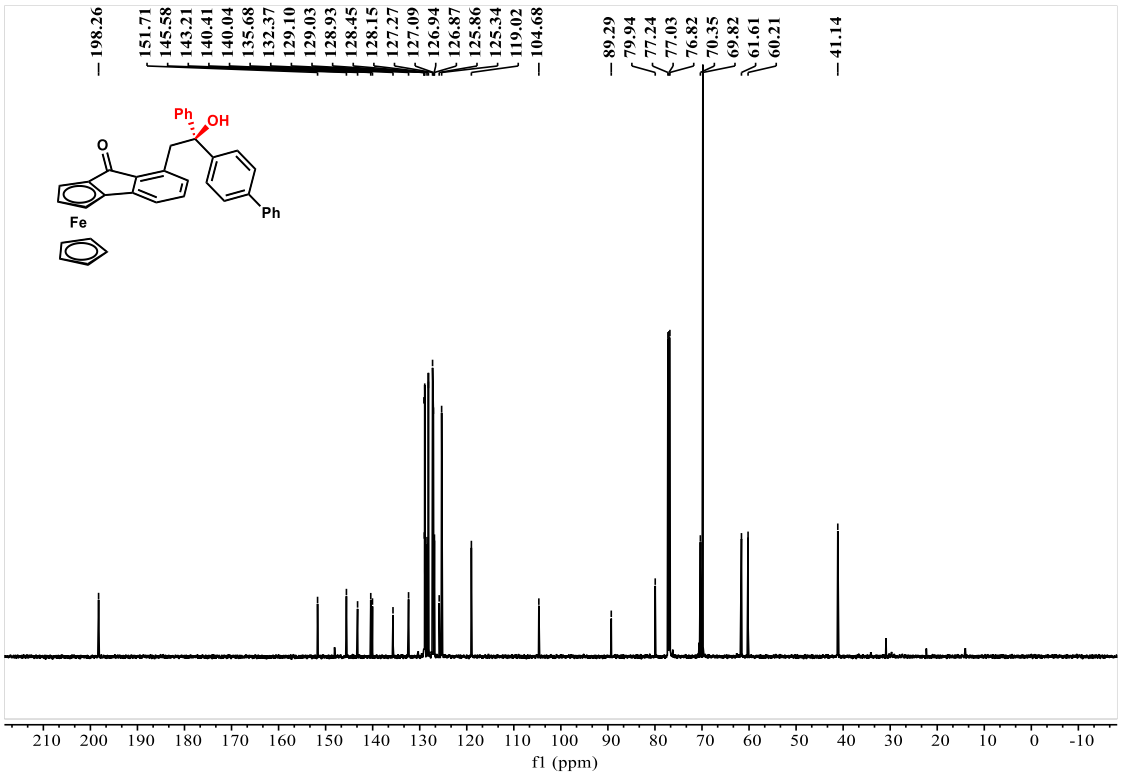


Figure S8.80 ^{13}C NMR of **(R_p, *S*)-4aa** (151 MHz, $CDCl_3$)

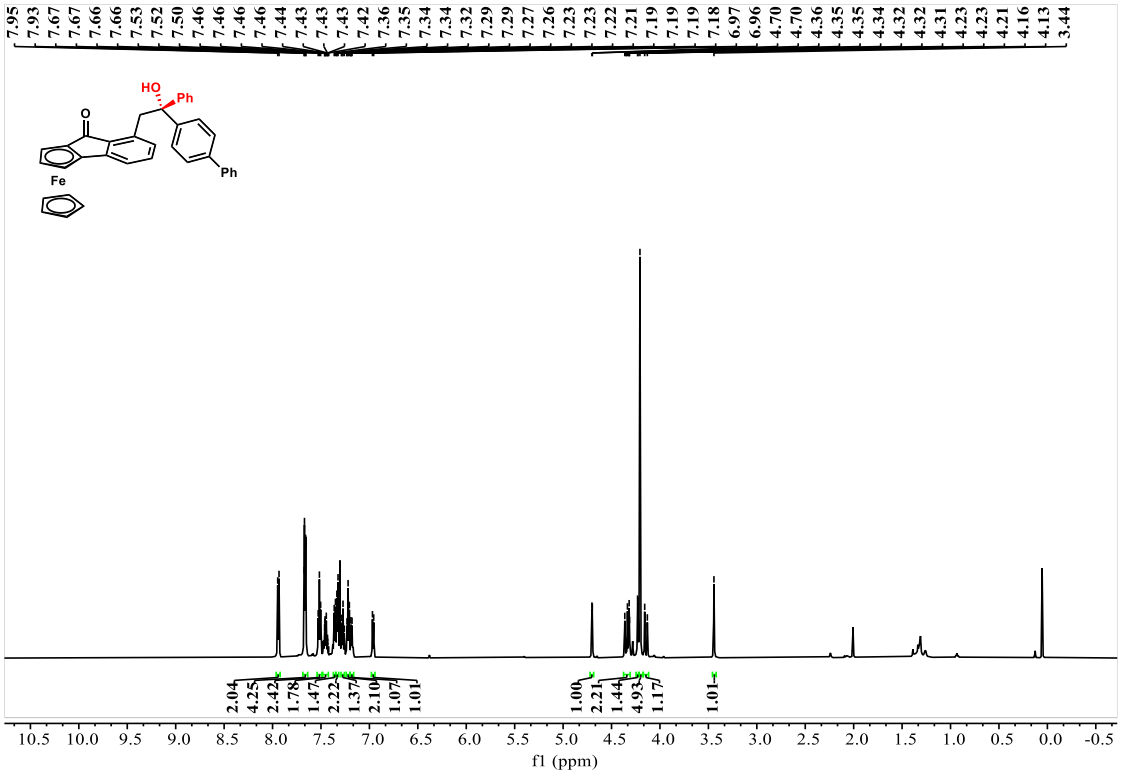


Figure S8.81 ^{1}H NMR of **(R_p, *R*)-4aa** (600 MHz, $CDCl_3$)

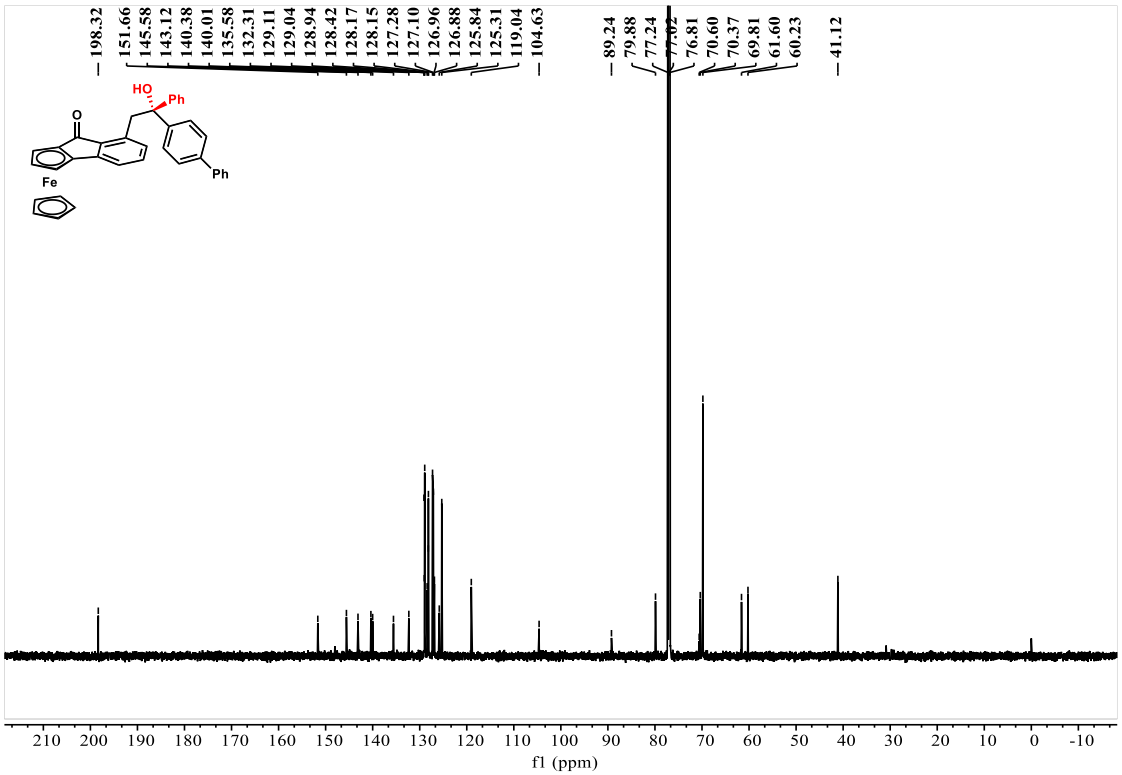


Figure S8.82 ^{13}C NMR of **(R_p, *R*)-4aa** (151 MHz, $CDCl_3$)

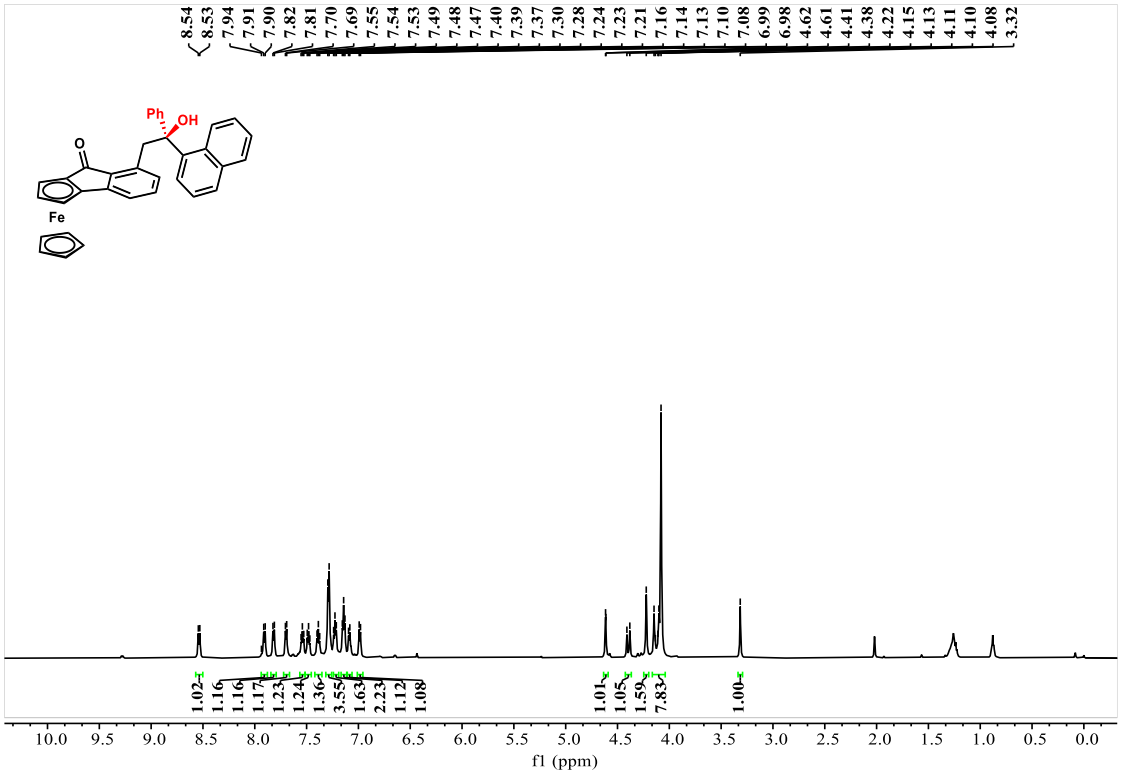


Figure S8.83 ^{1}H NMR of **(R_p, S)-4ab** (600 MHz, $CDCl_3$)

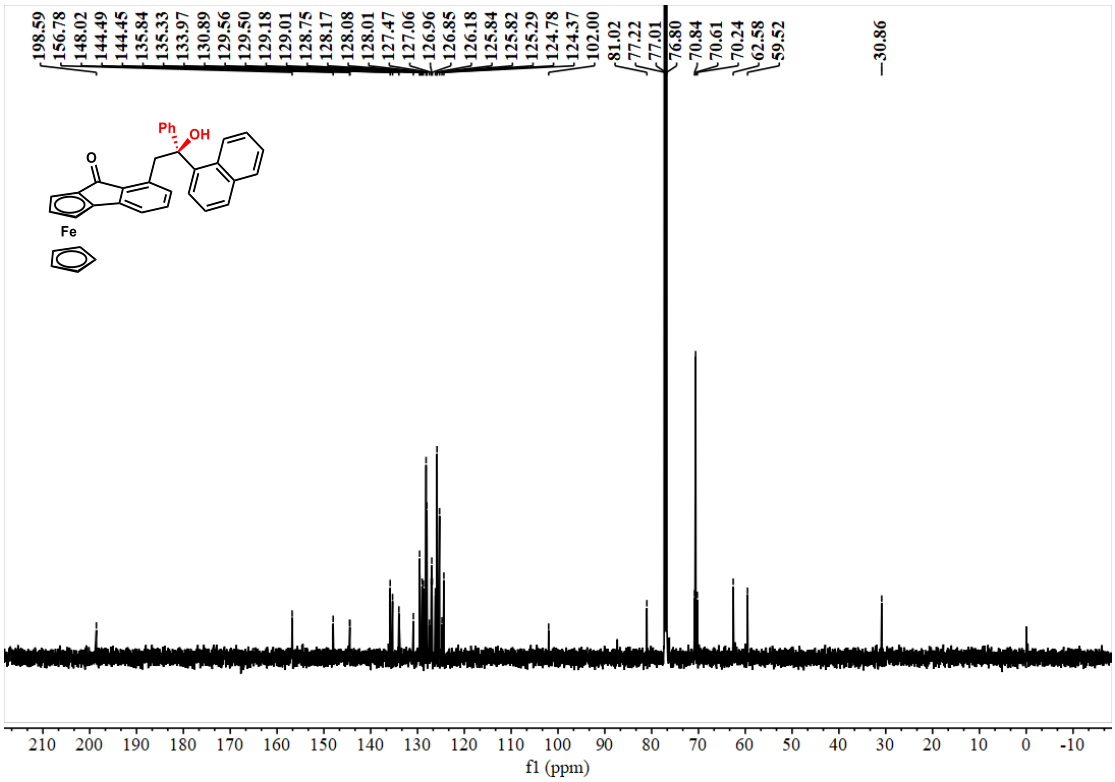


Figure S8.84 ^{13}C NMR of **(R_p, S)-4ab** (151 MHz, $CDCl_3$)

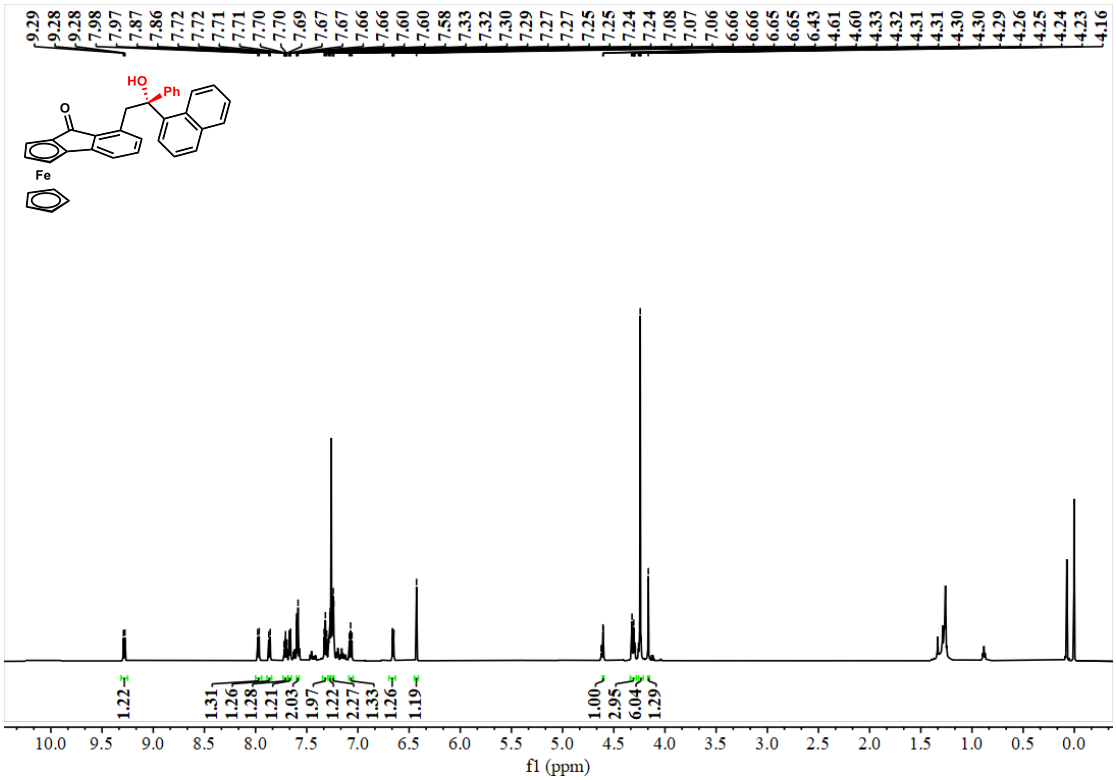


Figure S8.85 ^{1}H NMR of **(R_p, R)-4ab**(600 MHz, $CDCl_3$)

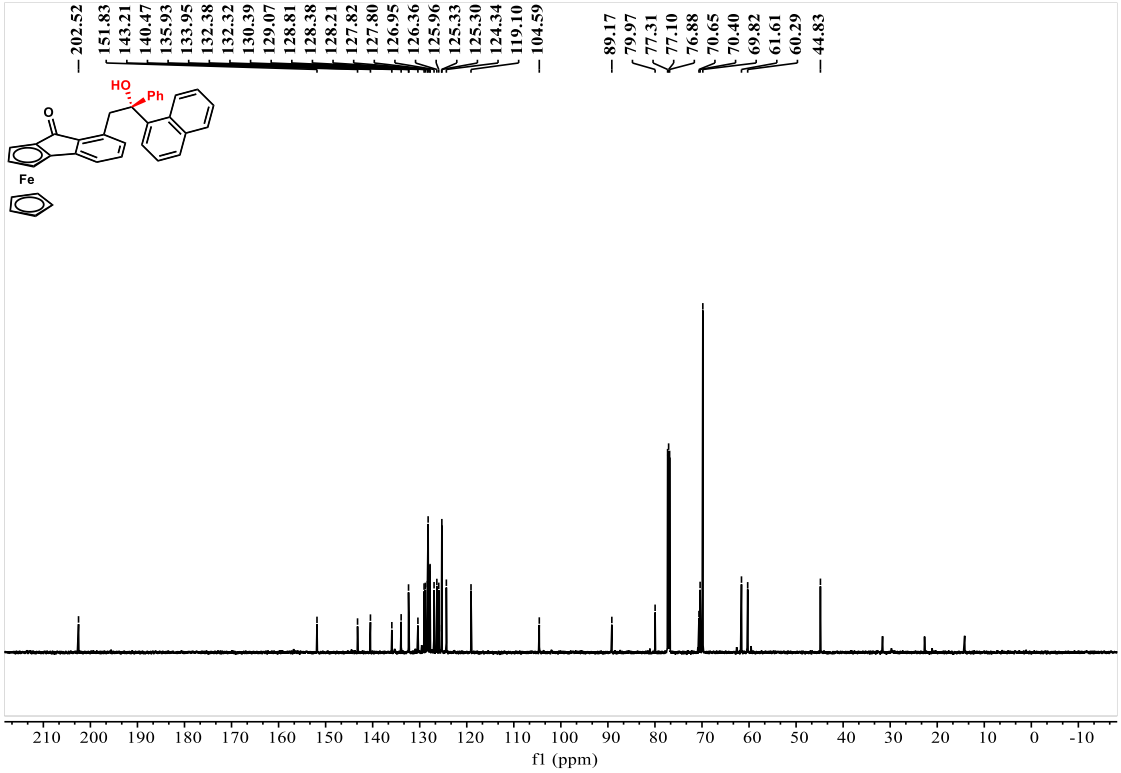


Figure S8.86 ^{13}C NMR of **(R_p, R)-4ab** (151 MHz, $CDCl_3$)

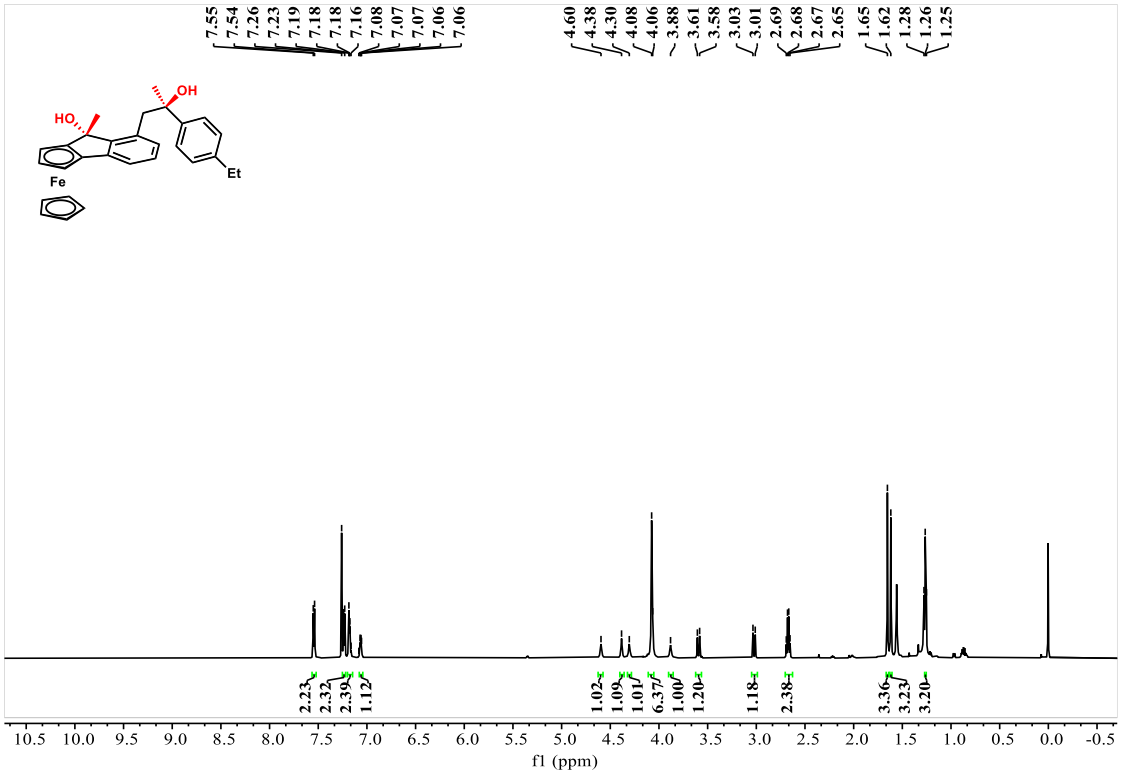


Figure S8.87 ^{1}H NMR of (***R*$_p$, *S*, *R*)-4ac**(600 MHz, $CDCl_3$)

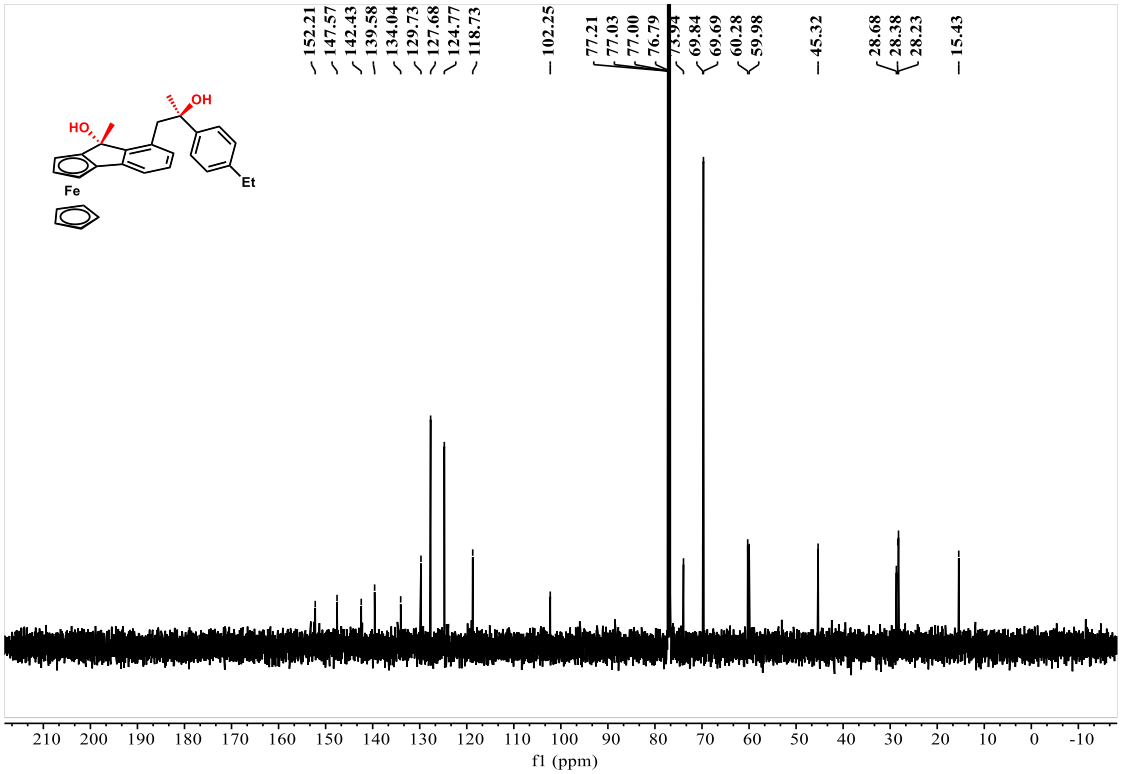


Figure S8.88 ^{13}C NMR of (***R*$_p$, *S*, *R*)-4ac** (151 MHz, $CDCl_3$)

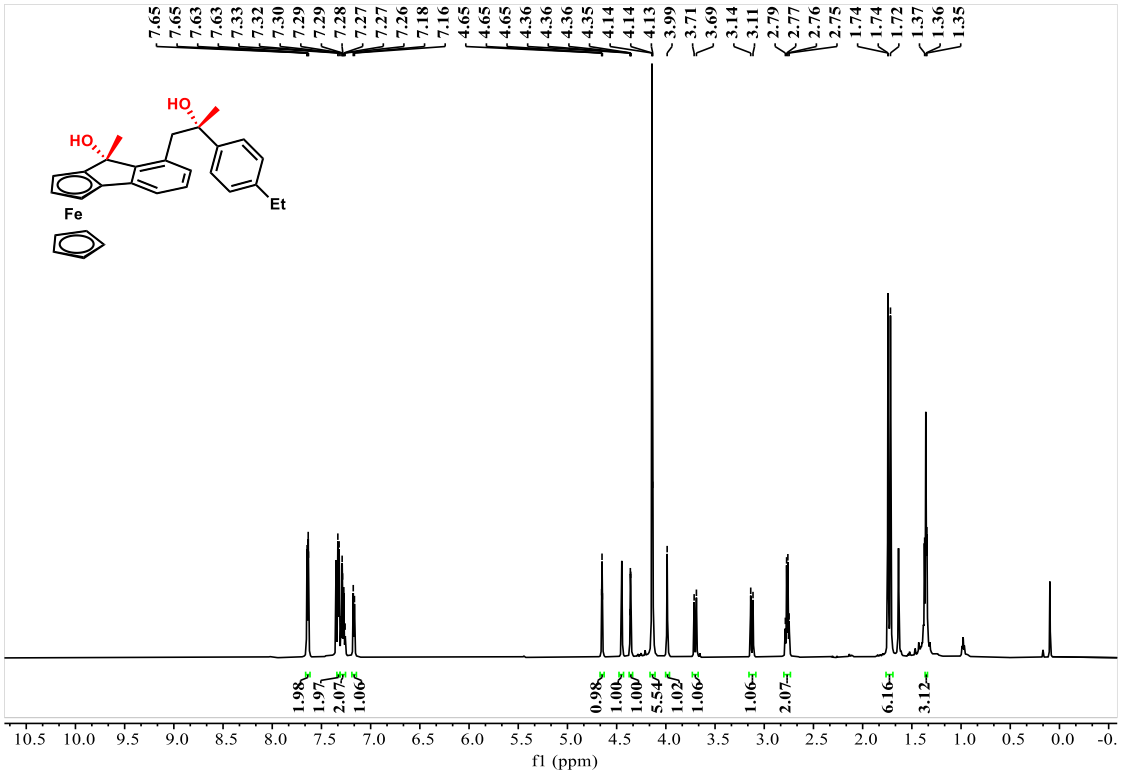


Figure S8.89 ^{1}H NMR of **(R_p, *S*, *S*)-4ac** (600 MHz, $CDCl_3$)

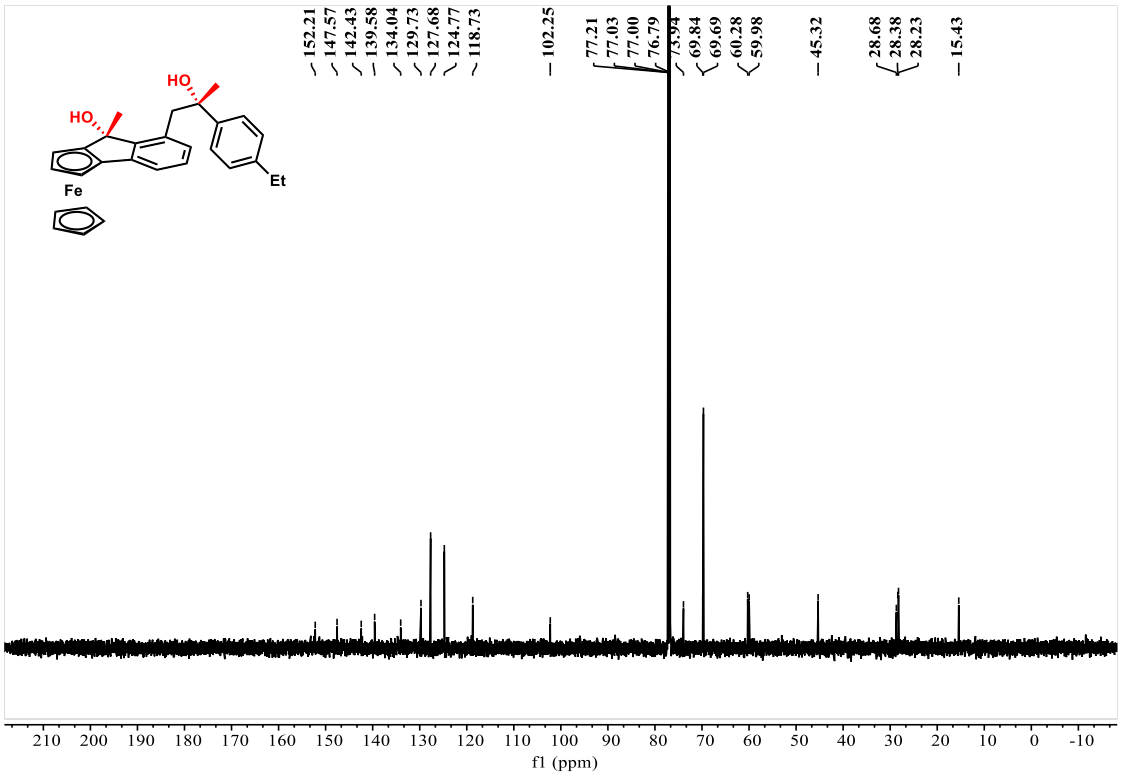


Figure S8.90 ^{13}C NMR of **(R_p, *S*, *S*)-4ac** (151 MHz, $CDCl_3$)

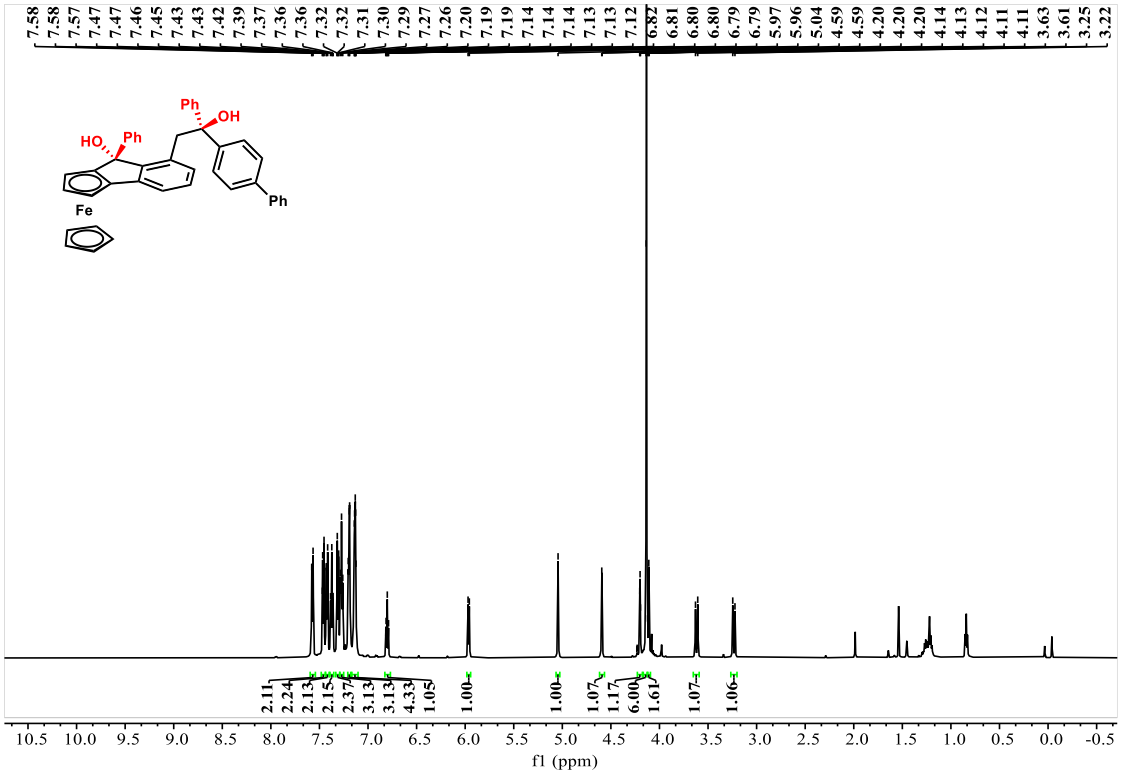


Figure S8.91 ^{1}H NMR of (***R*$_p$, *S*, *S*)-4ad** 600 MHz, $CDCl_3$)

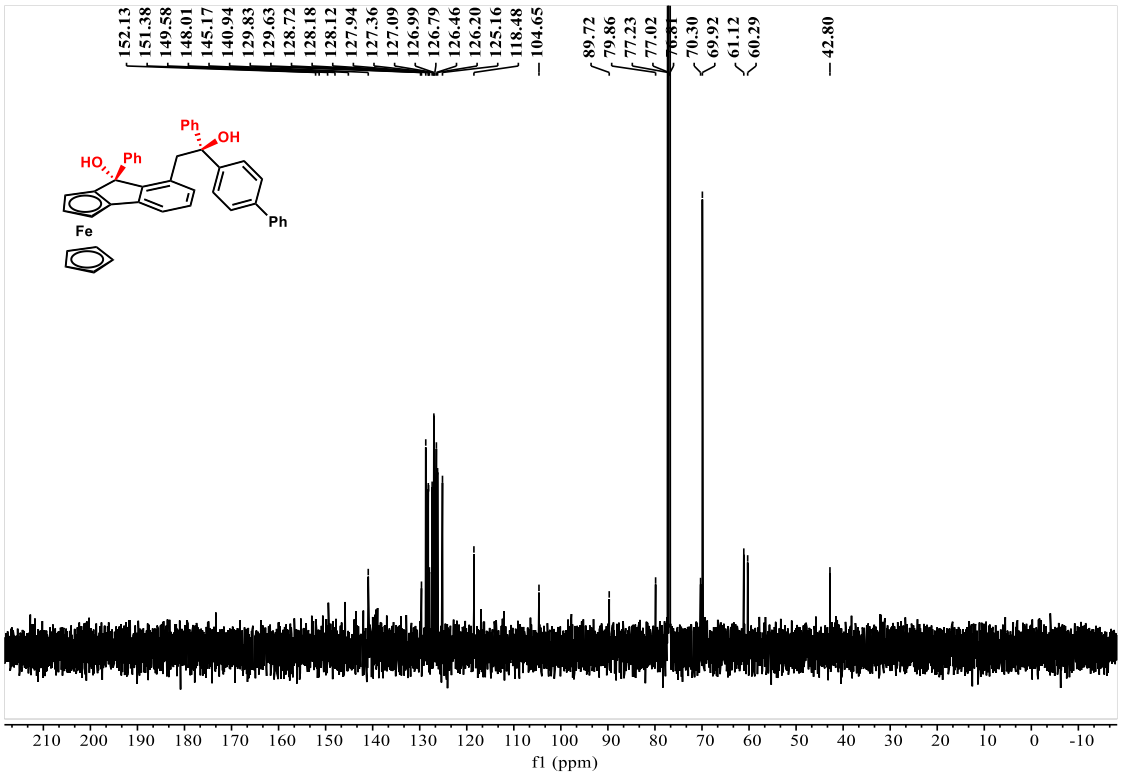


Figure S8.92 ^{13}C NMR of (***R*$_p$, *S*, *S*)-4ad** (151 MHz, $CDCl_3$)

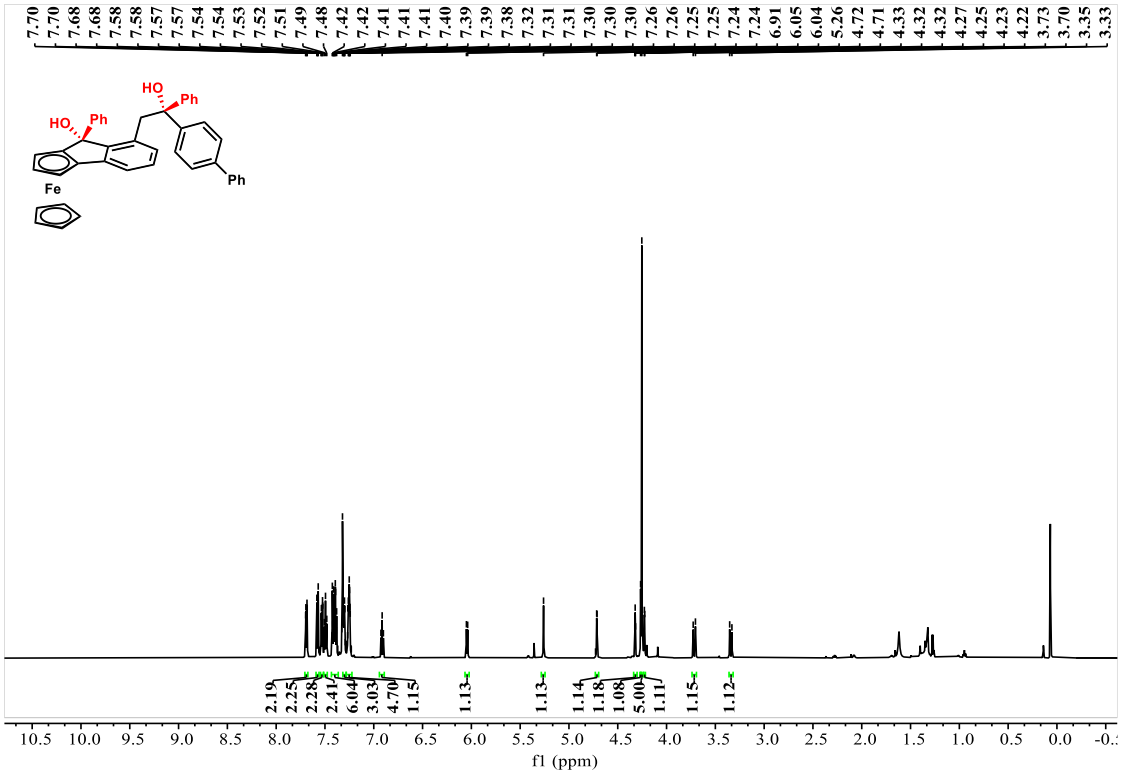


Figure S8.93 ^{1}H NMR of **(R_p, *S*, *R*)-4ad**(600 MHz, $CDCl_3$)

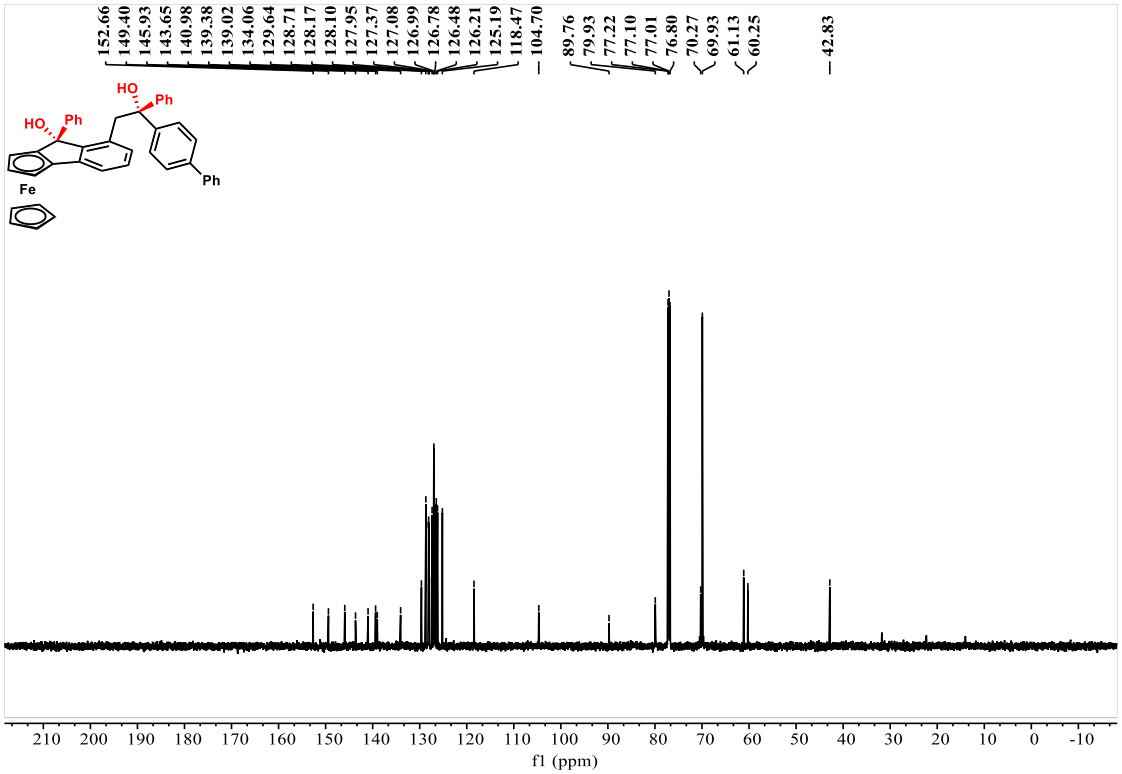


Figure S8.94 ^{13}C NMR of **(R_p, *S*, *R*)-4ad** (151 MHz, $CDCl_3$)

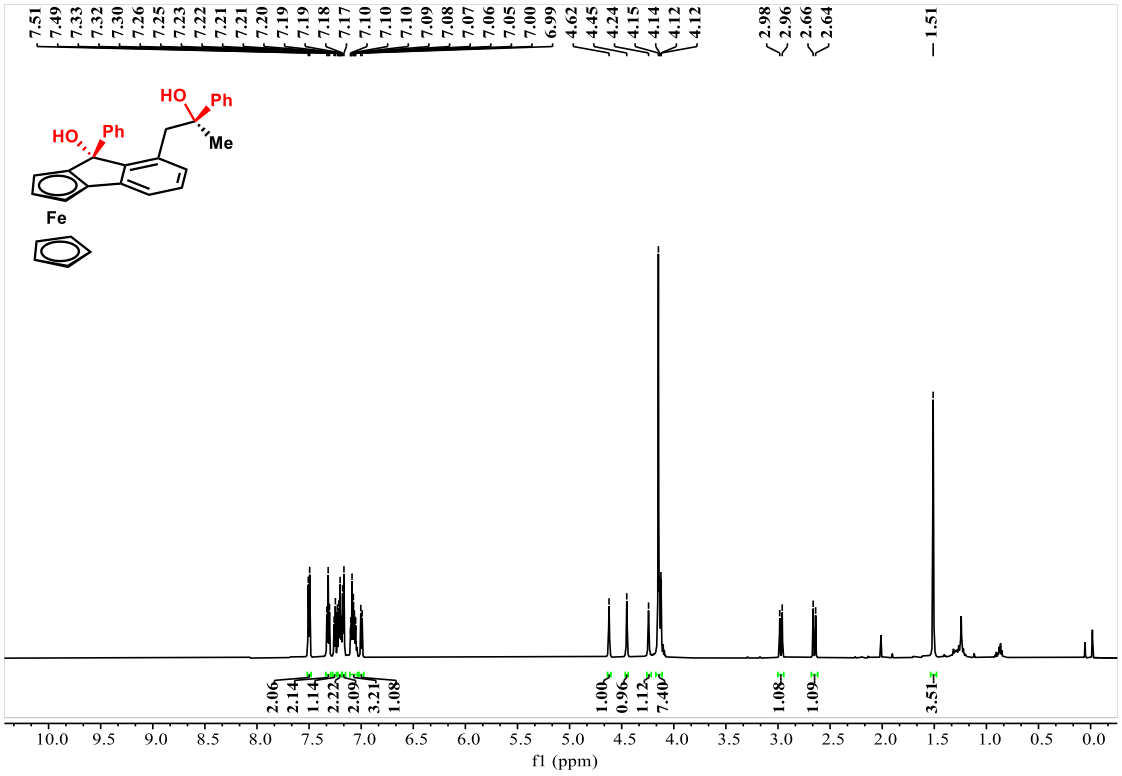


Figure S8.95 ^{1}H NMR of (***R*$_p$, *S*, *R*)-4ae**(600 MHz, $CDCl_3$)

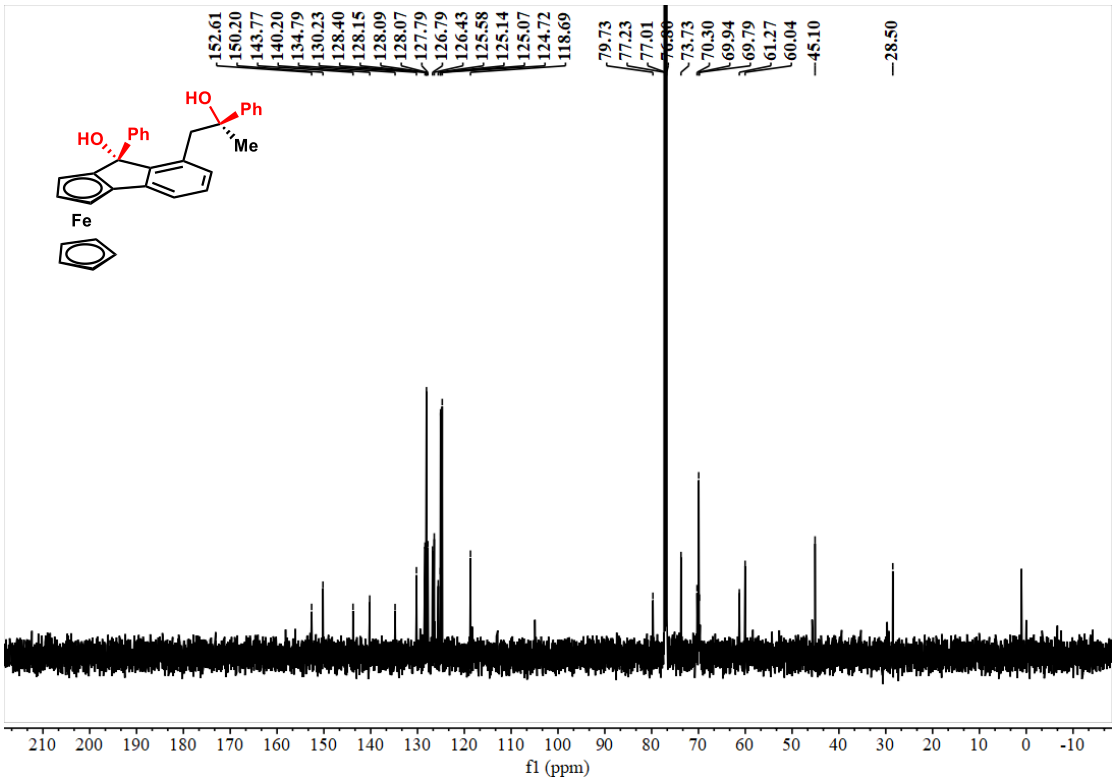


Figure S8.96 ^{13}C NMR of (***R*$_p$, *S*, *R*)-4ae** (151 MHz, $CDCl_3$)

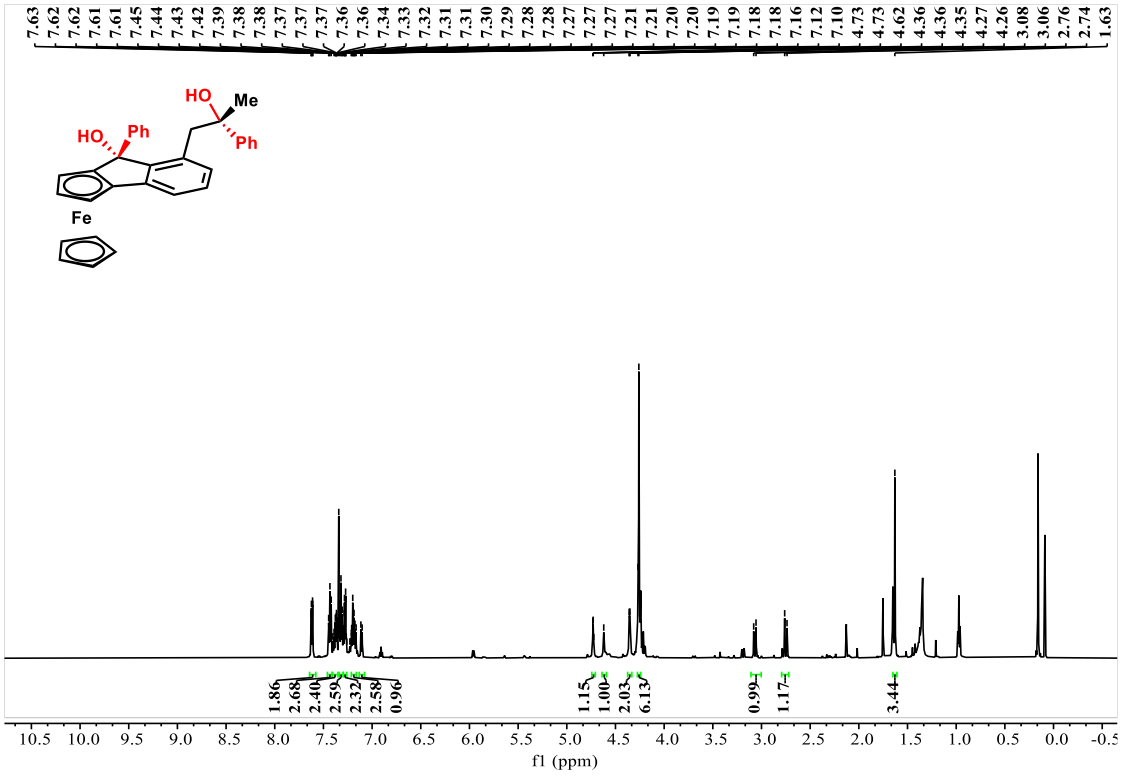


Figure S8.95 ^{1}H NMR of **(R_p, *S*, *S*)-4ae**(600 MHz, $CDCl_3$)

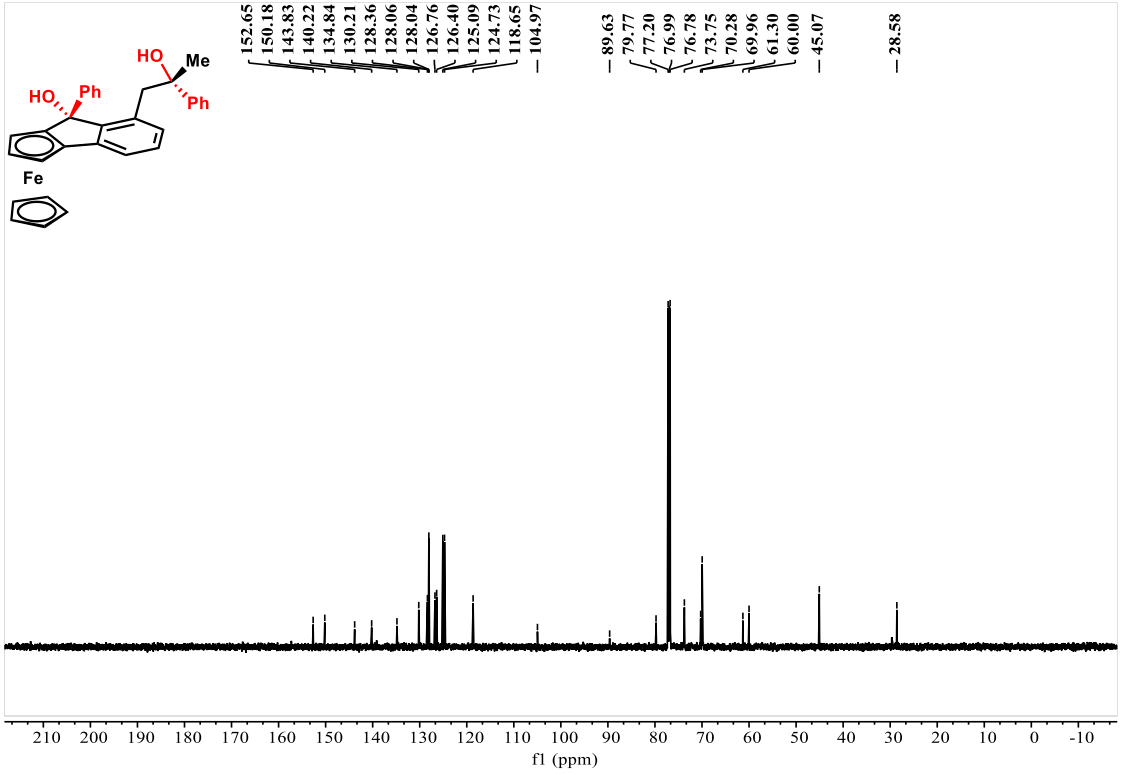
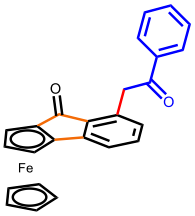
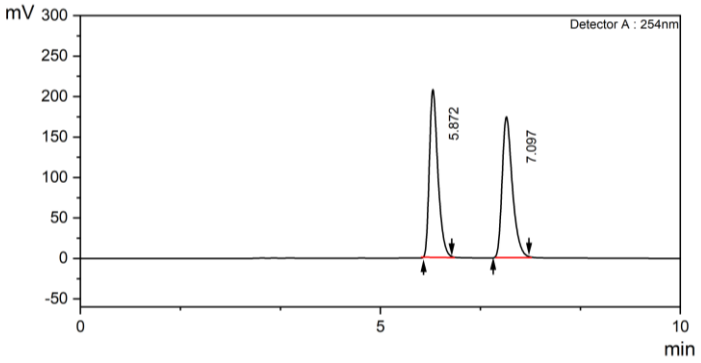


Figure S8.96 ^{13}C NMR of **(R_p, *S*, *S*)-4ae** (151 MHz, $CDCl_3$)

HPLC chromatographs

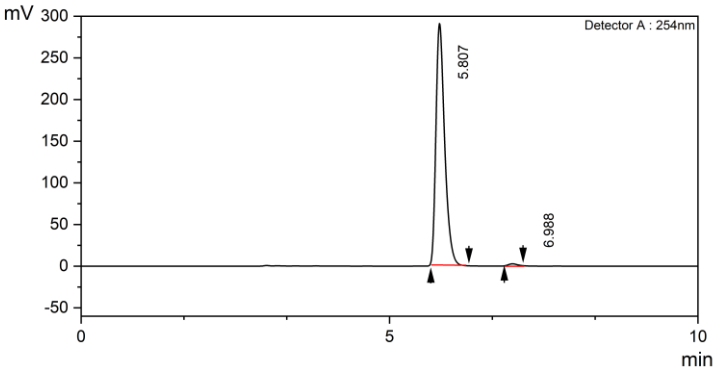
HPLC analysis 3aa:





Peak Results

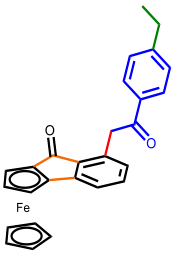
Peak#	Ret. Time	Area	Area%
1	5.872	3086611	49.9712
2	7.097	3090174	50.0288

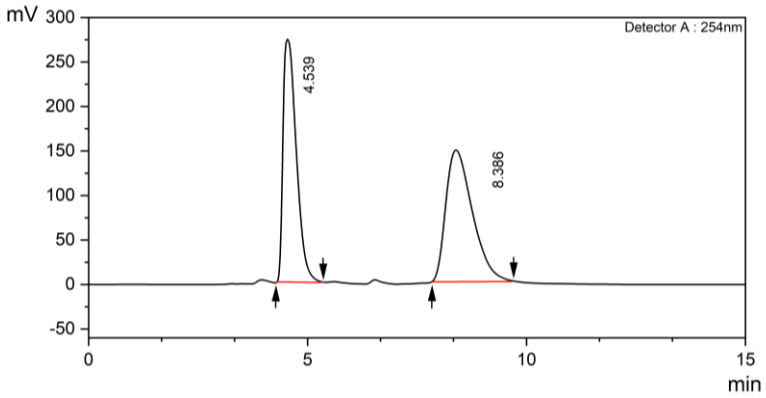


Peak Results

Peak#	Ret. Time	Area	Area%
1	5.807	5718277	99.2419
2	6.988	43683	0.7581

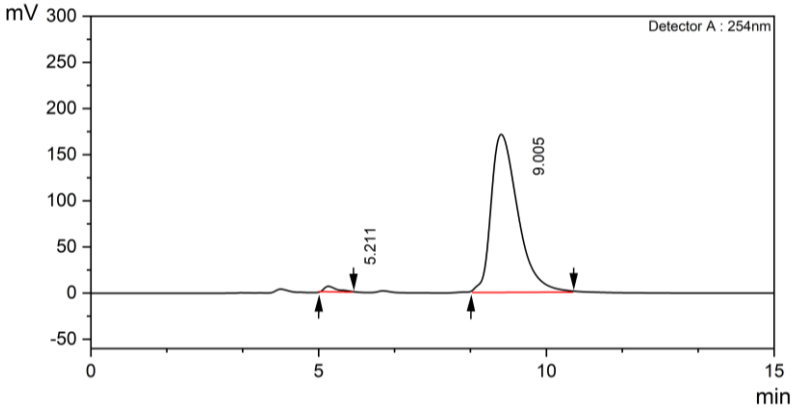
HPLC analysis 3ab:





Peak Results

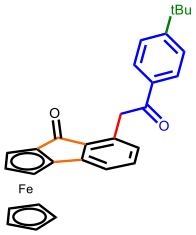
Peak#	Ret. Time	Area	Area%
1	4.539	62822468	48.3736
2	8.386	67046771	51.6264

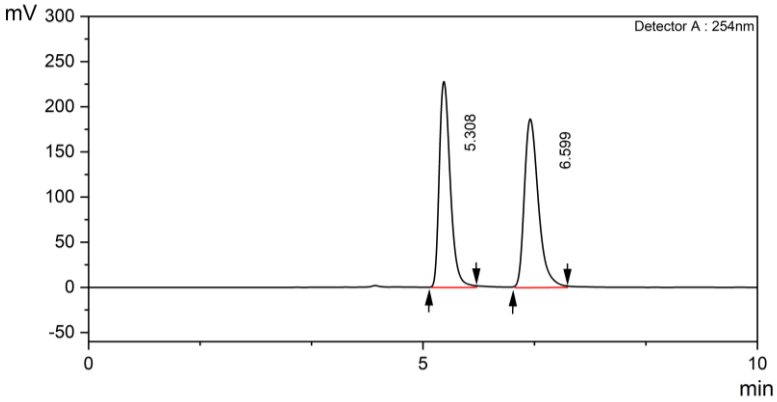


Peak Results

Peak#	Ret. Time	Area	Area%
1	5.211	1603461	1.5952
2	9.005	98911816	98.4048

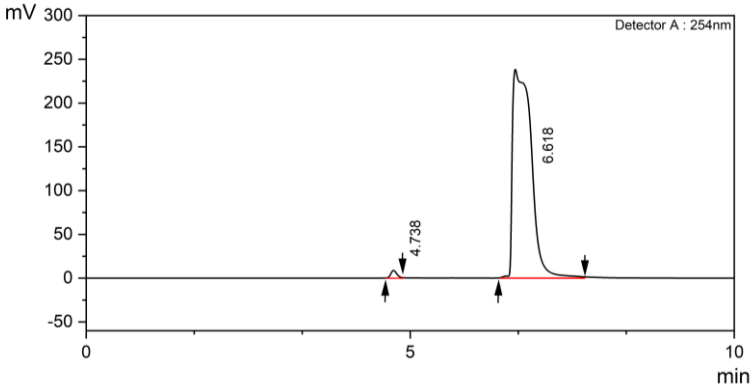
HPLC analysis 3ac:





Peak Results

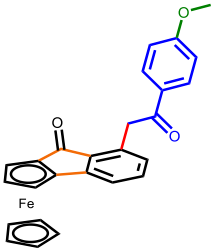
Peak#	Ret. Time	Area	Area%
1	5.308	30274251	49.0744
2	6.599	31416329	50.9256

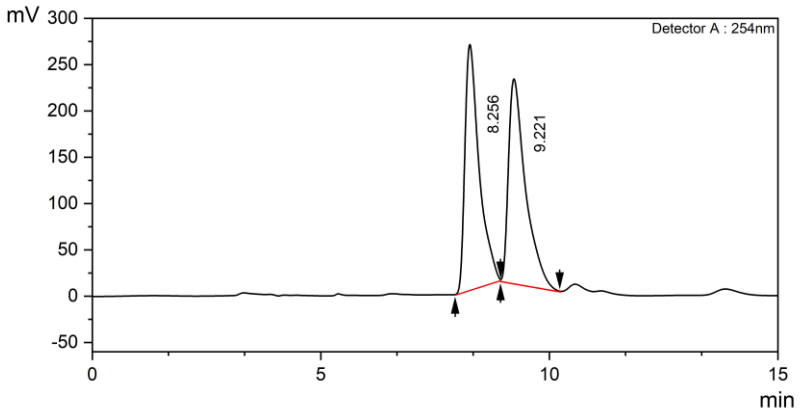


Peak Results

Peak#	Ret. Time	Area	Area%
1	4.738	449897	0.7497
2	6.618	59562282	99.2503

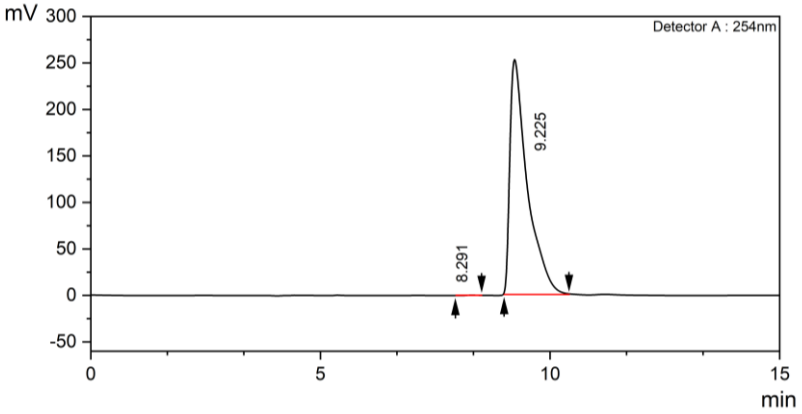
HPLC analysis 3ad:





Peak Results

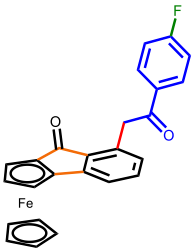
Peak#	Ret. Time	Area	Area%
1	8.256	6272223	50.4994
2	9.221	6148179	49.5006

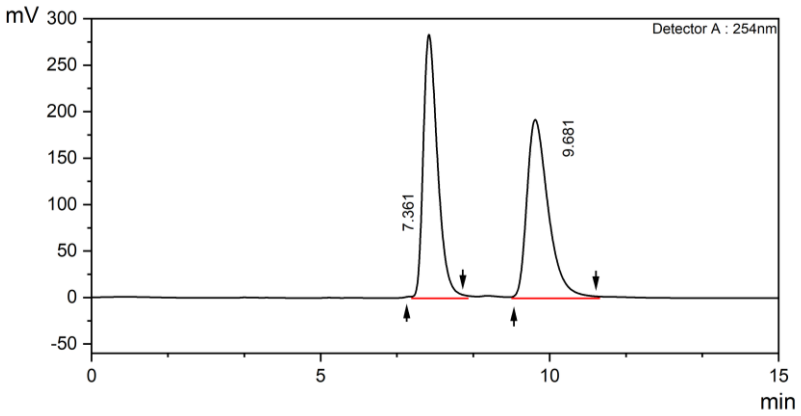


Peak Results

Peak#	Ret. Time	Area	Area%
1	8.291	32188	0.0992
2	9.225	32414365	99.9008

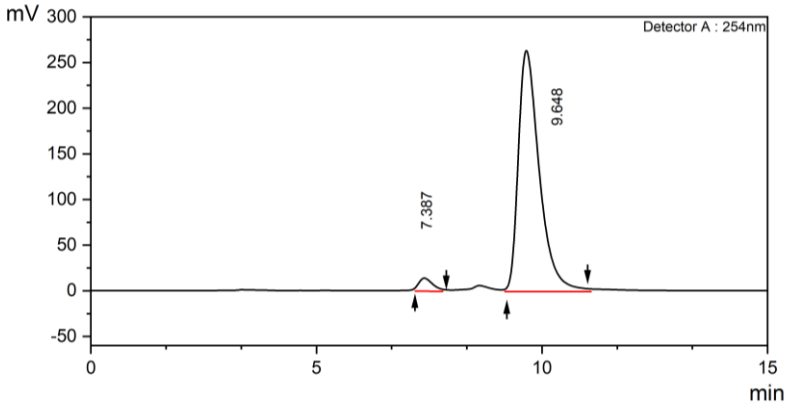
HPLC analysis 3ae:





Peak Results

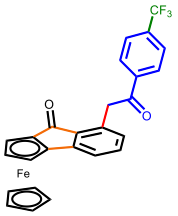
Peak#	Ret. Time	Area	Area%
1	7.361	18041562	49.975
2	9.681	18059581	50.025

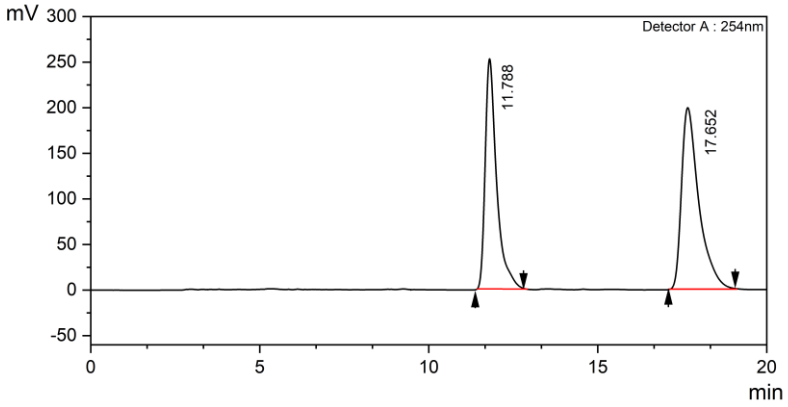


Peak Results

Peak#	Ret. Time	Area	Area%
1	7.387	842245	3.2327
2	9.648	25211514	96.7673

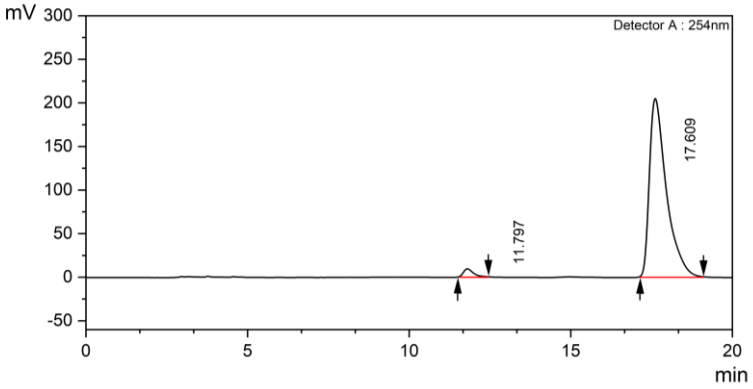
HPLC analysis 3af:





Peak Results

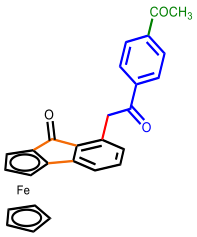
Peak#	Ret. Time	Area	Area%
1	11.788	2998830	50.255
2	17.652	3366368	49.745

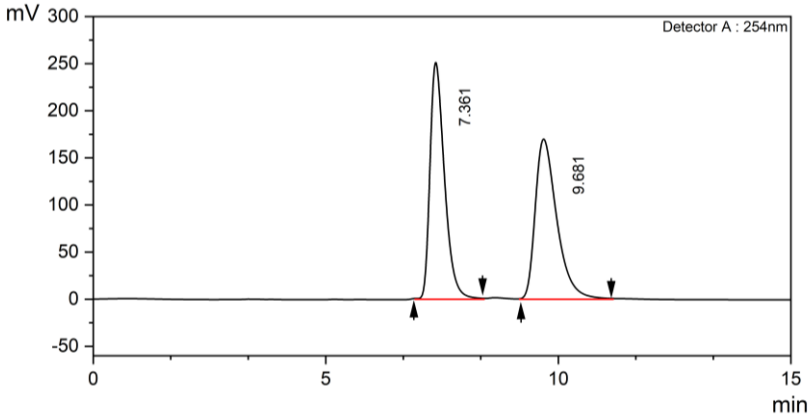


Peak Results

Peak#	Ret. Time	Area	Area%
1	11.797	132695	1.7516
2	17.609	7442958	98.2484

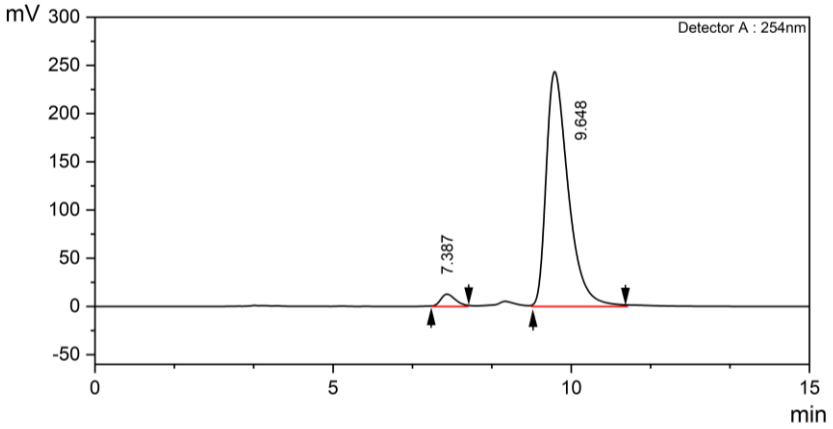
HPLC analysis 3ag:





Peak Results

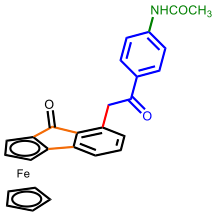
Peak#	Ret. Time	Area	Area%
1	7.361	18041562	49.975
2	9.681	18059581	50.025

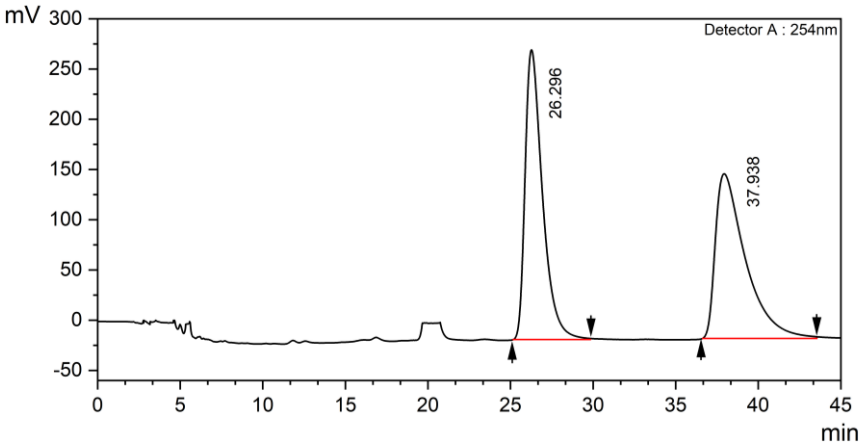


Peak Results

Peak#	Ret. Time	Area	Area%
1	7.387	842245	3.2327
2	9.648	25211514	96.7673

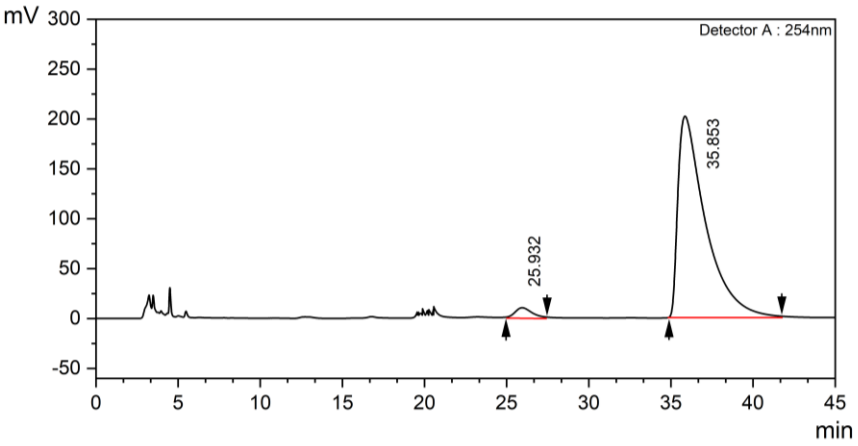
HPLC analysis 3ah:





Peak Results

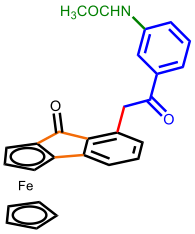
Peak#	Ret. Time	Area	Area%
1	26.296	1476676	50.0078
2	37.938	1476214	49.9922

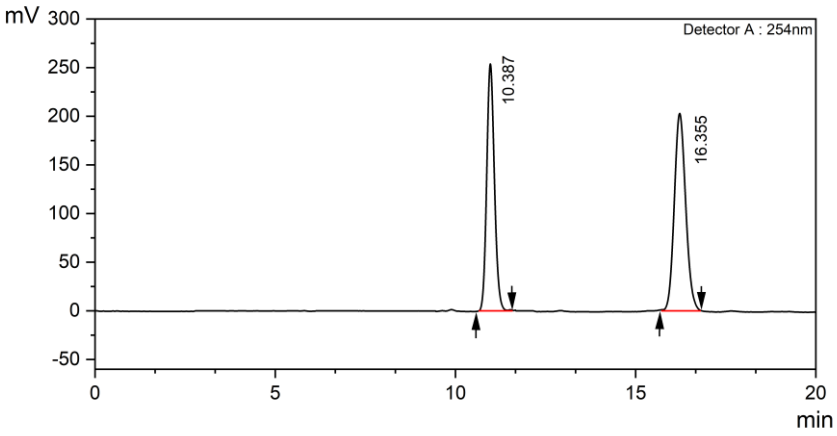


Peak Results

Peak#	Ret. Time	Area	Area%
1	25.932	184011	2.5545
2	35.853	7019456	97.4455

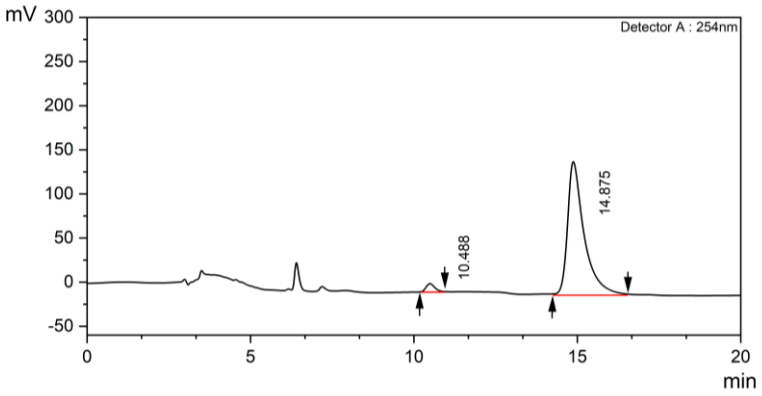
HPLC analysis 3ai:





Peak R esults

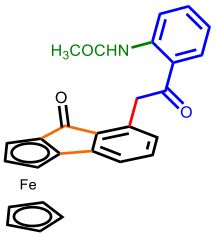
Peak#	Ret. Time	Area	Area%
1	10.387	617840	50.0703
2	16.355	616103	49.9297

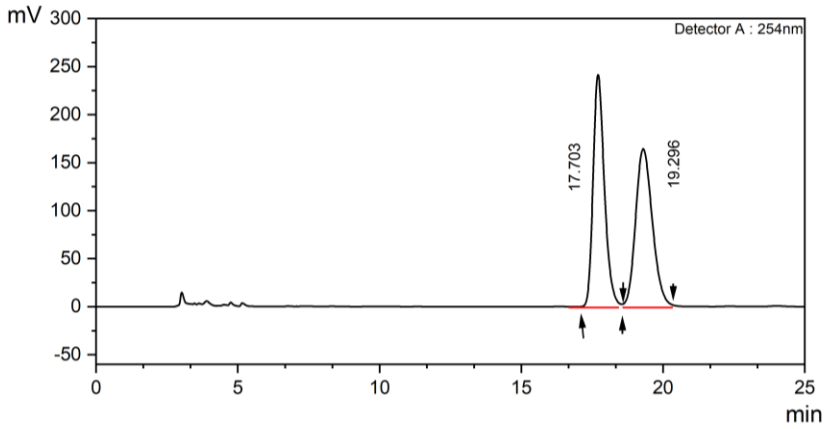


Peak Results

Peak#	Ret. Time	Area	Area%
1	10.488	27554	2.6664
2	14.875	1005847	97.3336

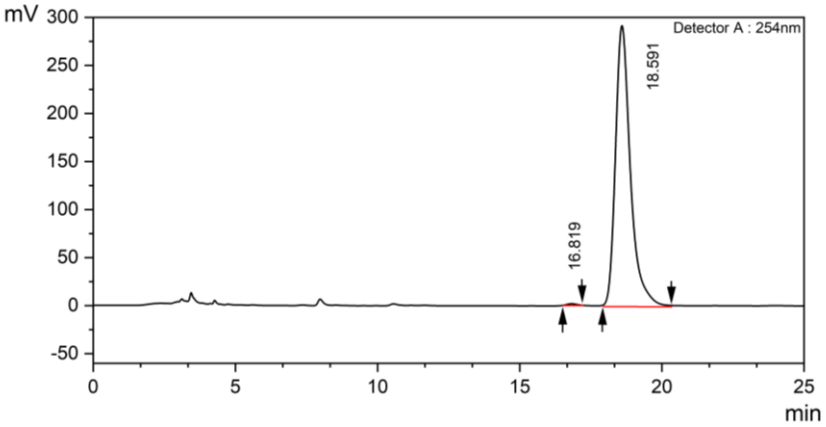
HPLC analysis 3aj:





Peak Results

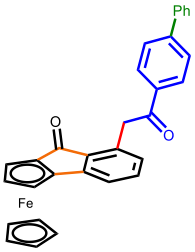
Peak#	Ret. Time	Area	Area%
1	17.703	6522491	49.8466
2	19.296	6562642	50.1534

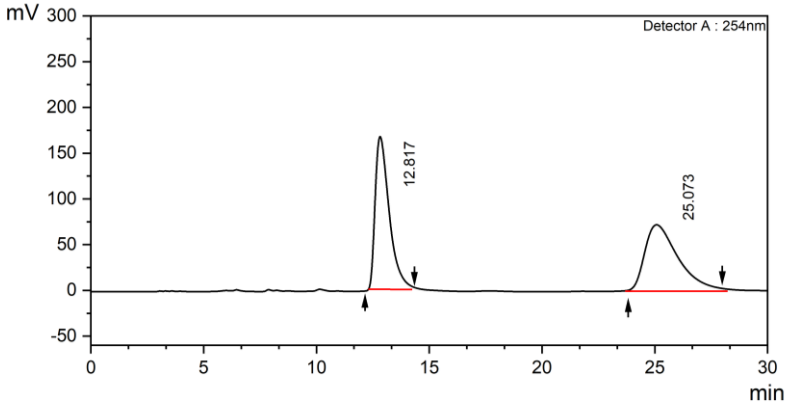


Peak Results

Peak#	Ret. Time	Area	Area%
1	16.819	12337	0.3886
2	18.591	3162266	99.6114

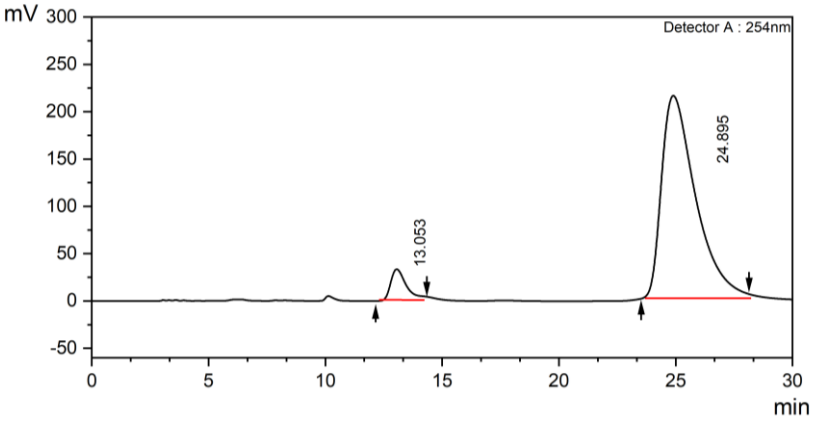
HPLC analysis 3ak:





Peak Results

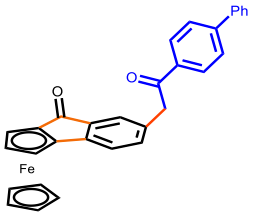
Peak#	Ret. Time	Area	Area%
1	12.817	74106544	50.86
2	25.073	71600381	49.14

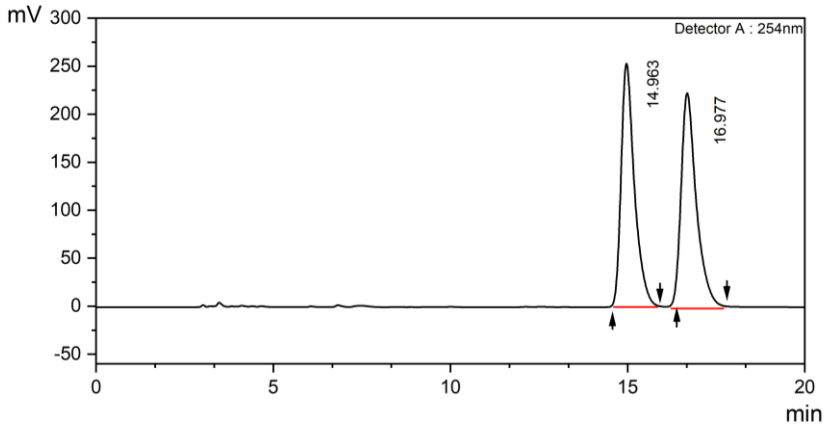


Peak Results

Peak#	Ret. Time	Area	Area%
1	13.053	6891214	5.9352
2	24.895	109215527	94.0648

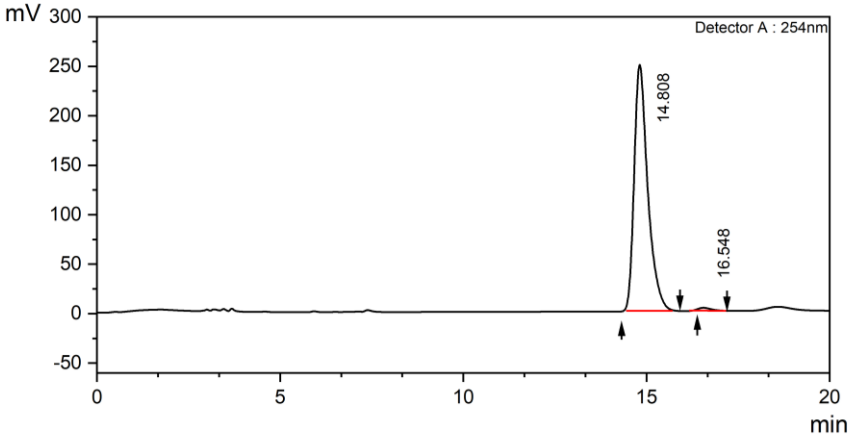
HPLC analysis 3al:





Peak Results

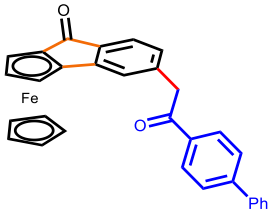
Peak#	Ret. Time	Area	Area%
1	14.963	1949198	49.8584
2	16.677	1960265	50.1416

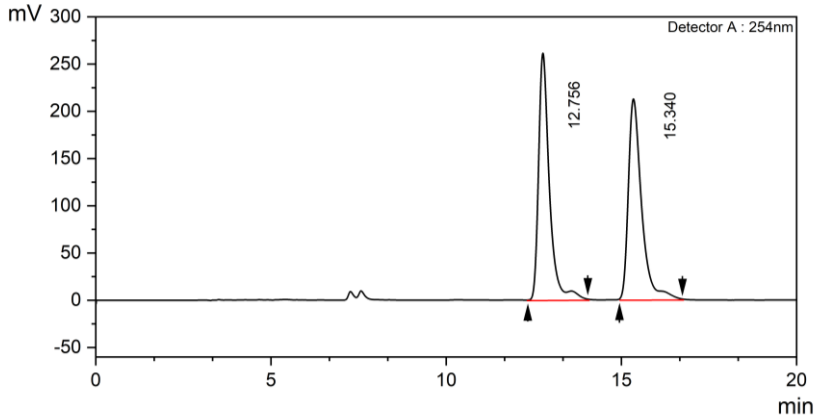


Peak Results

Peak#	Ret. Time	Area	Area%
1	14.809	2778261	98.9602
2	16.548	29192	1.0398

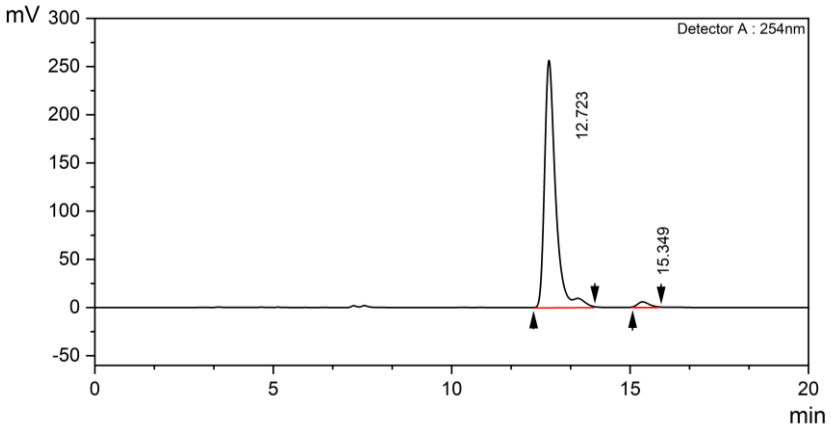
HPLC analysis 3am:





Peak Results

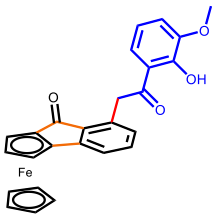
Peak#	Ret. Time	Area	Area%
1	12.756	6171589	50.3605
2	15.340	6083225	49.6395

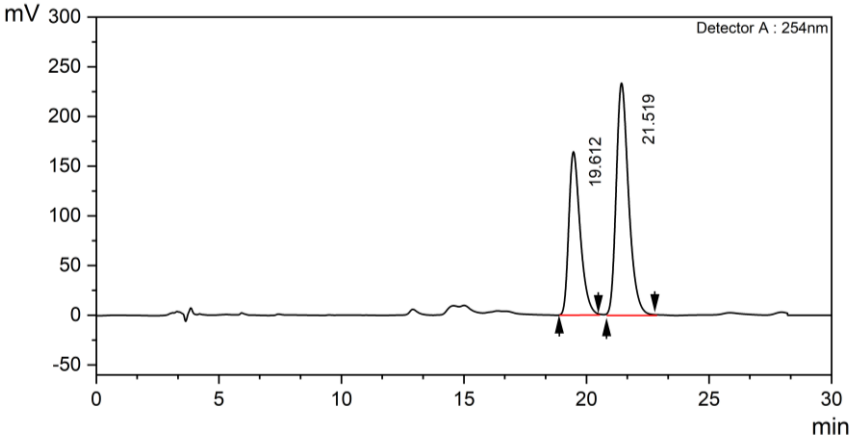


Peak Results

Peak#	Ret. Time	Area	Area%
1	12.723	18145299	97.5599
2	15.349	453842	2.4401

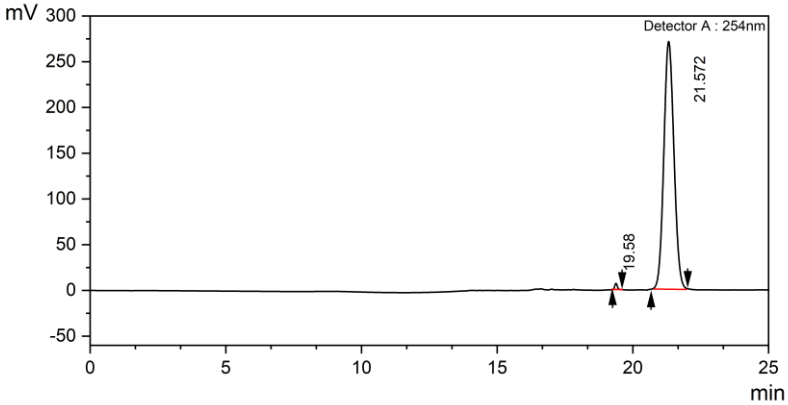
HPLC analysis 3an:





Peak Results

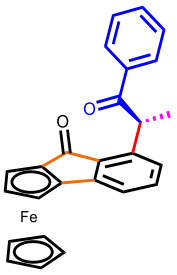
Peak#	Ret. Time	Area	Area%
1	19.612	2264583	49.1560
2	21.519	2342349	50.8448

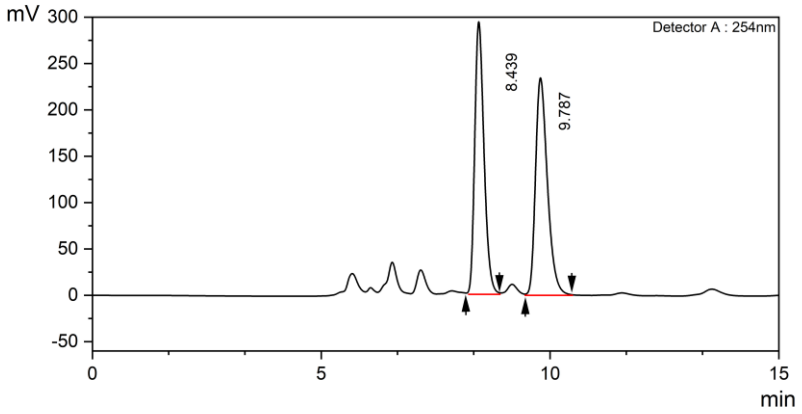


Peak Results

Peak#	Ret. Time	Area	Area%
1	19.580	124480	0.8167
2	21.572	15062077	99.1833

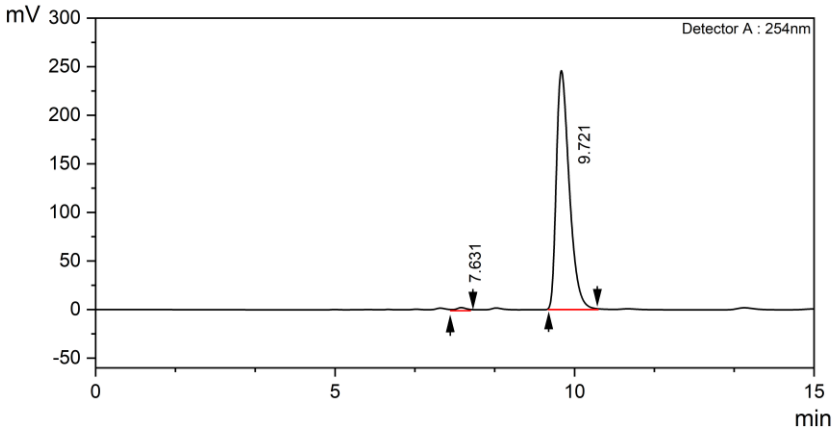
HPLC analysis (R_p, R)-3ao:





Peak Results

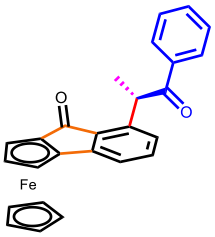
Peak#	Ret. Time	Area	Area%
1	8.439	7905657	48.9925
2	9.787	8230794	51.0075

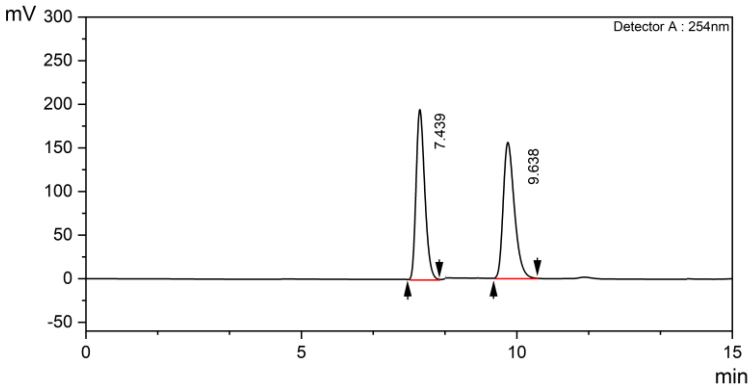


Peak Results

Peak#	Ret. Time	Area	Area%
1	7.631	99261	0.3572
2	9.721	27686629	99.6428

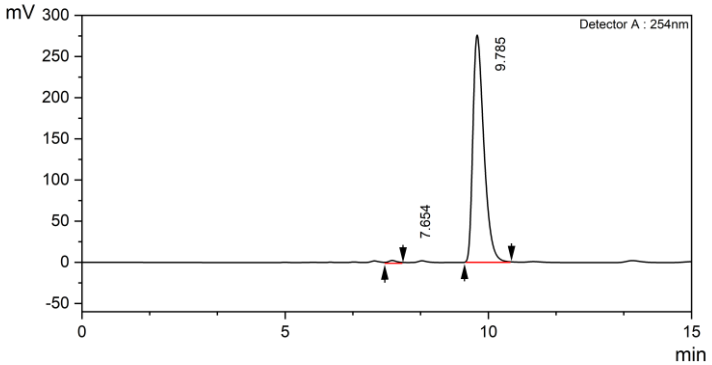
HPLC analysis (R_p, S)-3ao:





Peak Results

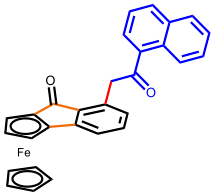
Peak#	Ret. Time	Area	Area%
1	7.439	4356568	49.7506
2	9.683	4400254	50.2494

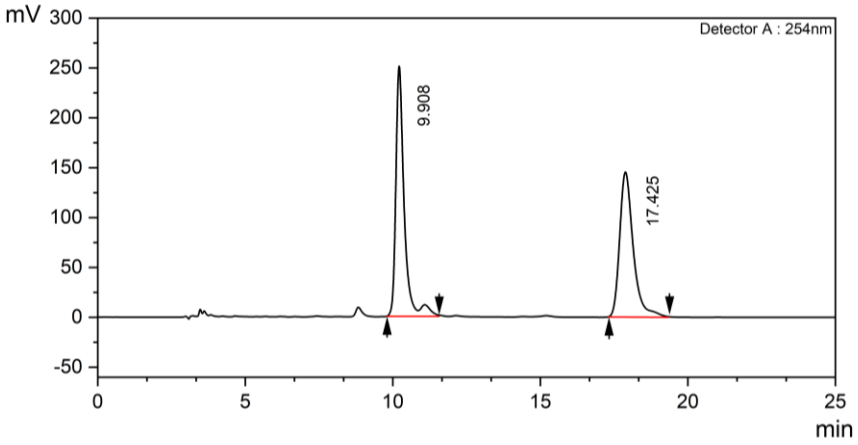


Peak Results

Peak#	Ret. Time	Area	Area%
1	7.654	45130	0.3137
2	9.785	14343320	99.6863

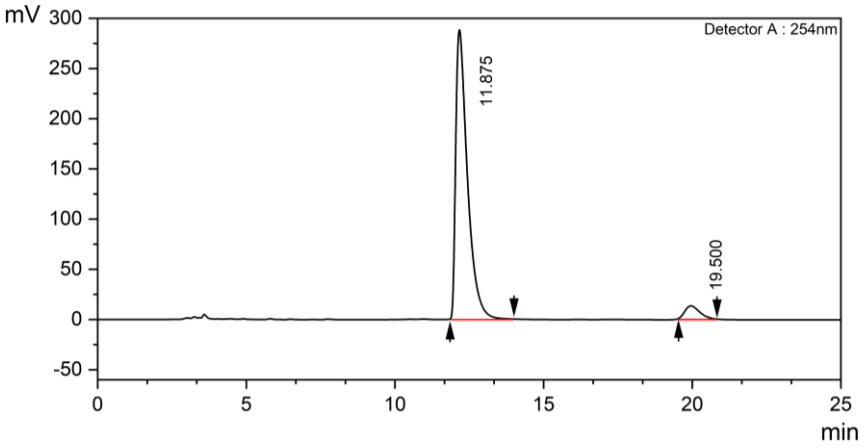
HPLC analysis 3ap:





Peak Results

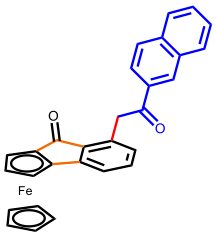
Peak#	Ret. Time	Area	Area%
1	9.908	866911	50.5287
2	17.425	848768	49.4713

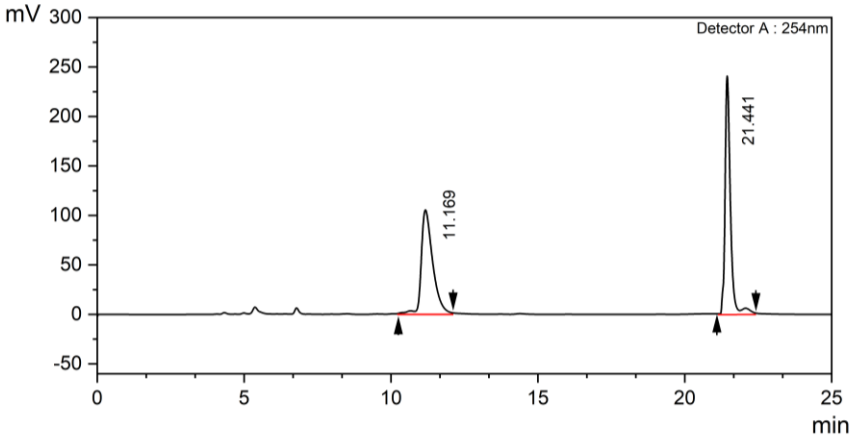


Peak Results

Peak#	Ret. Time	Area	Area%
1	11.875	6758284	95.7636
2	19.500	364334	4.2364

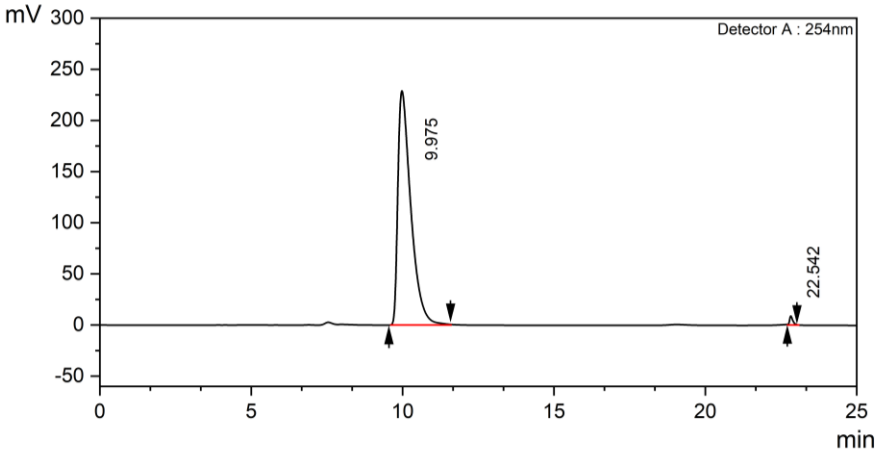
HPLC analysis 3aq:





Peak Results

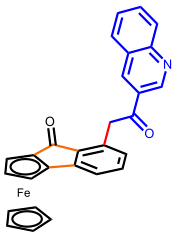
Peak#	Ret. Time	Area	Area%
1	11.169	5283284	47.9013
2	21.441	5746242	52.0987

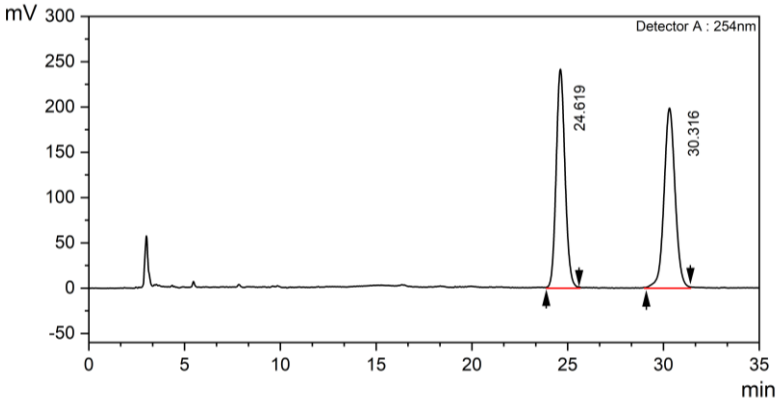


Peak Results

Peak#	Ret. Time	Area	Area%
1	9.975	13302115	99.7589
2	22.542	8394	0.0024

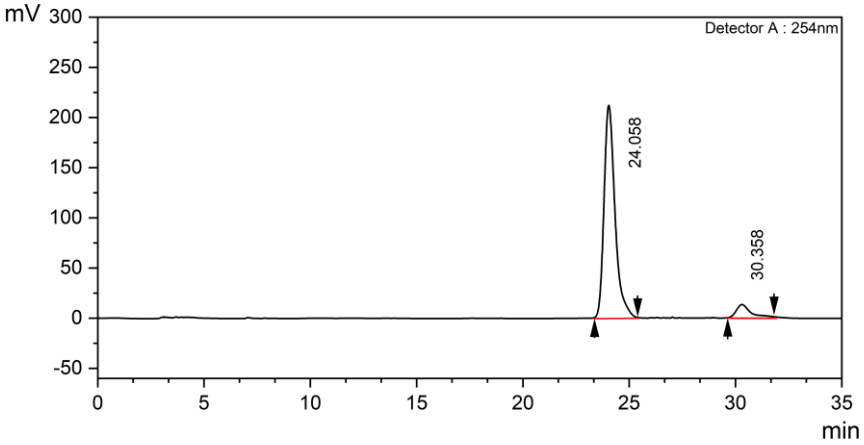
HPLC analysis 3ar:





Peak Results

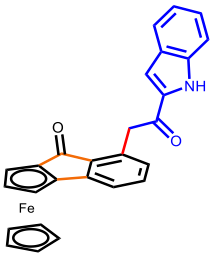
Peak#	Ret. Time	Area	Area%
1	24.619	514143	49.46
2	30.316	525361	50.54

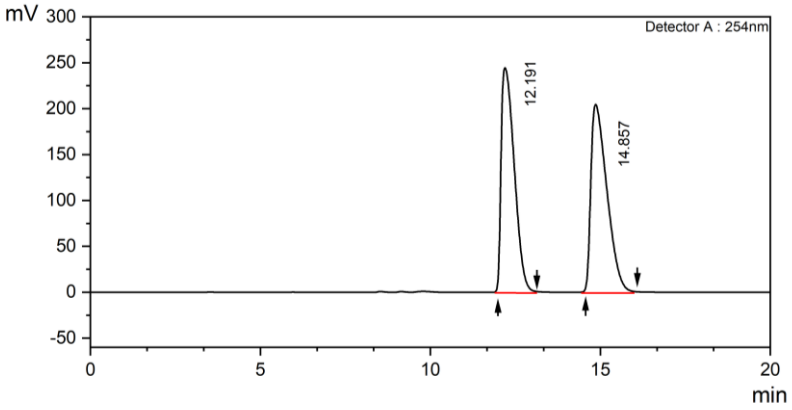


Peak Results

Peak#	Ret. Time	Area	Area%
1	24.058	5433874	98.6659
2	30.358	73472	1.3341

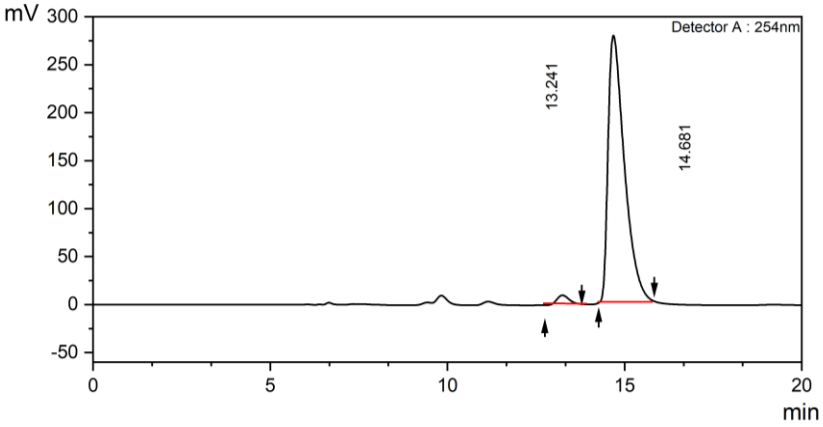
HPLC analysis 3as:





Peak Results

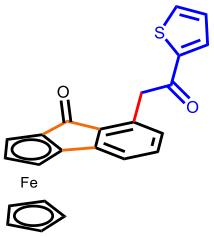
Peak#	Ret. Time	Area	Area%
1	12.191	65074319	49.8715
2	14.857	65396212	50.1182

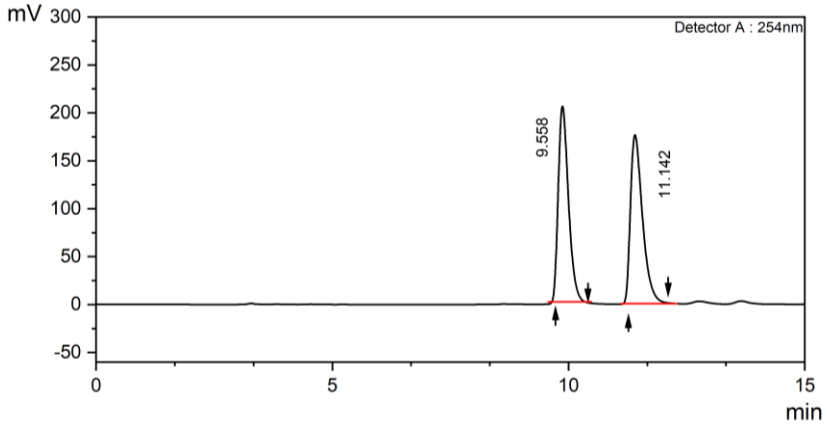


Peak Results

Peak#	Ret. Time	Area	Area%
1	13.241	446334	2.3875
2	14.681	18247975	97.6125

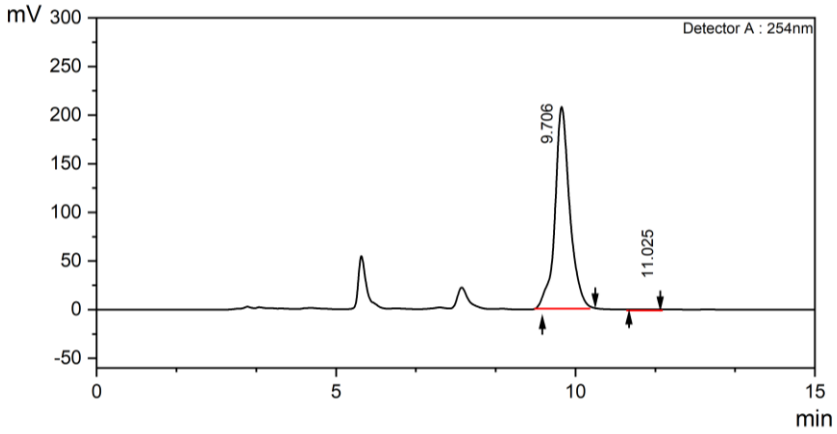
HPLC analysis 3at:





Peak Results

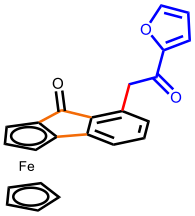
Peak#	Ret. Time	Area	Area%
1	9.558	6171589	50.3605
2	11.142	6083225	49.6395

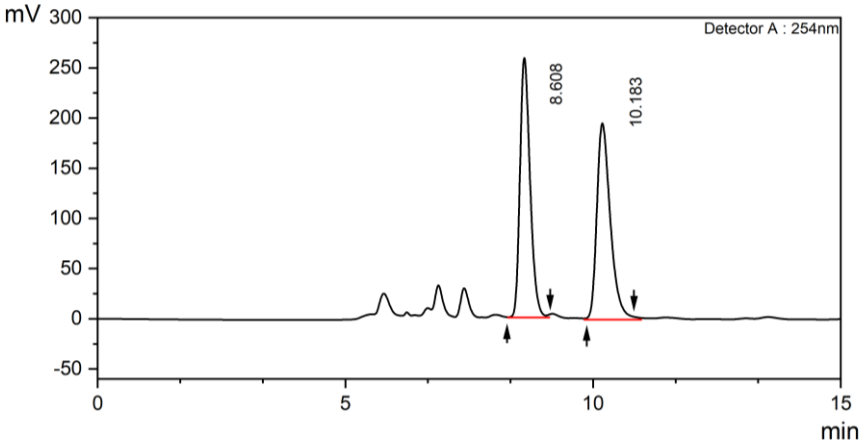


Peak Results

Peak#	Ret. Time	Area	Area%
1	9.706	18145299	99.7599
2	11.025	45384	0.2401

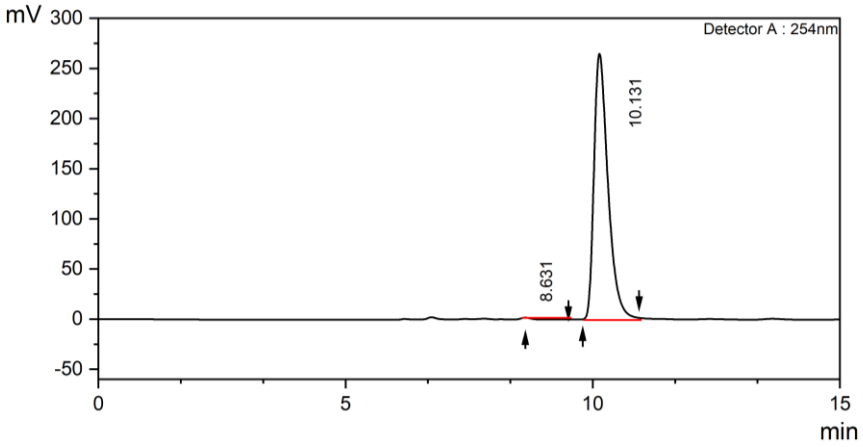
HPLC analysis 3au:





Peak Results

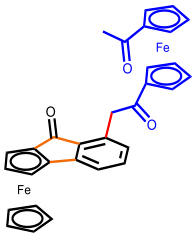
Peak#	Ret. Time	Area	Area%
1	8.608	5346206	49.5266
2	10.183	5448402	50.4734

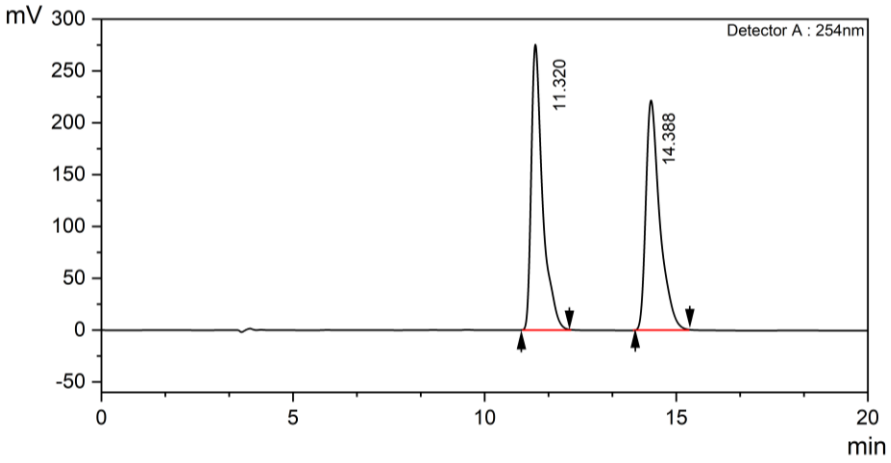


Peak Results

Peak#	Ret. Time	Area	Area%
1	8.631	28912	0.2479
2	10.131	11635114	99.7521

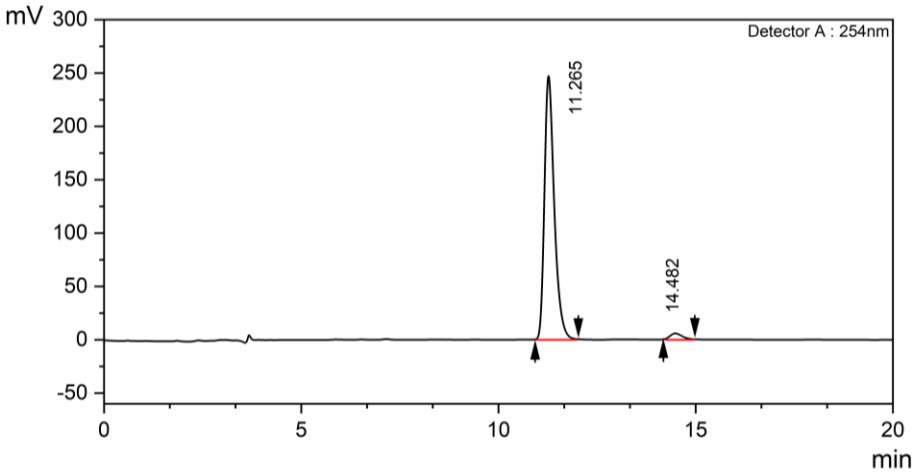
HPLC analysis 3av:





Peak Results

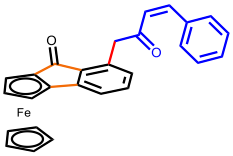
Peak#	Ret. Time	Area	Area%
1	11.32	8861112	50.1016
2	14.338	8825170	49.8984

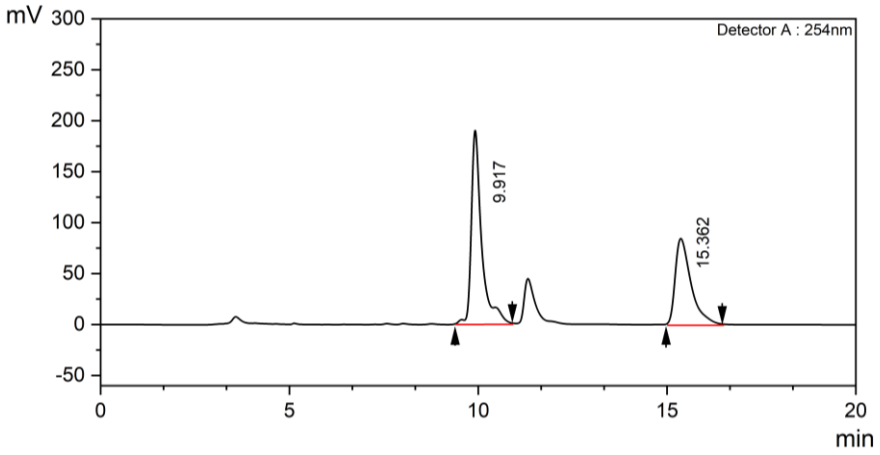


Peak Results

Peak#	Ret. Time	Area	Area%
1	11.265	6125898	97.3772
2	14.482	164997	2.6228

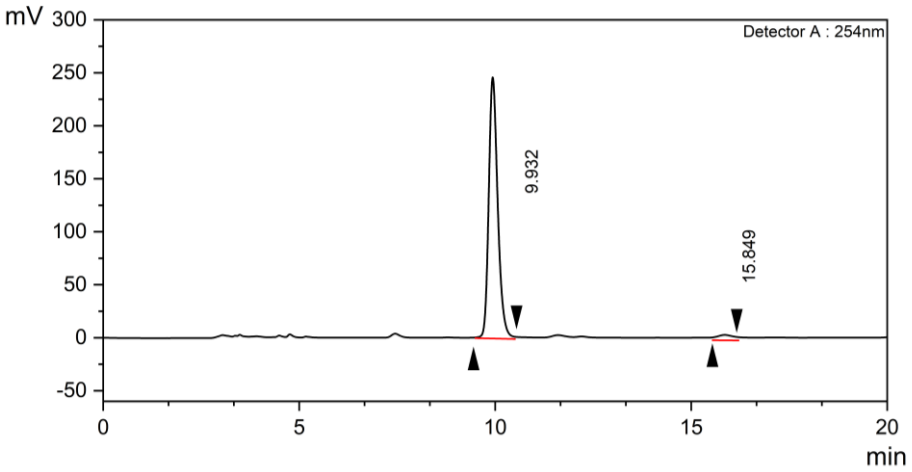
HPLC analysis 3aw:





Peak Results

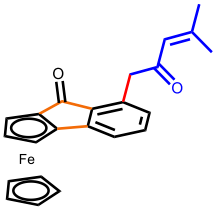
Peak#	Ret. Time	Area	Area%
1	9.917	7198528	49.5064
2	15.362	7342061	50.4936

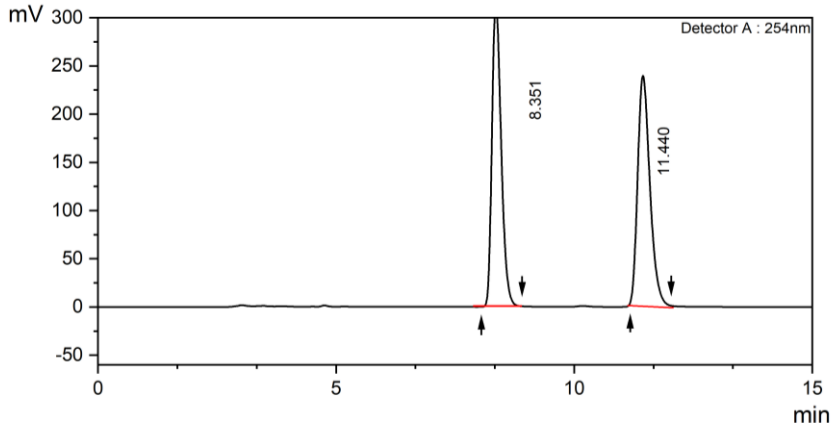


Peak Results

Peak#	Ret. Time	Area	Area%
1	9.932	3116526	98.3592
2	15.849	51990	1.6408

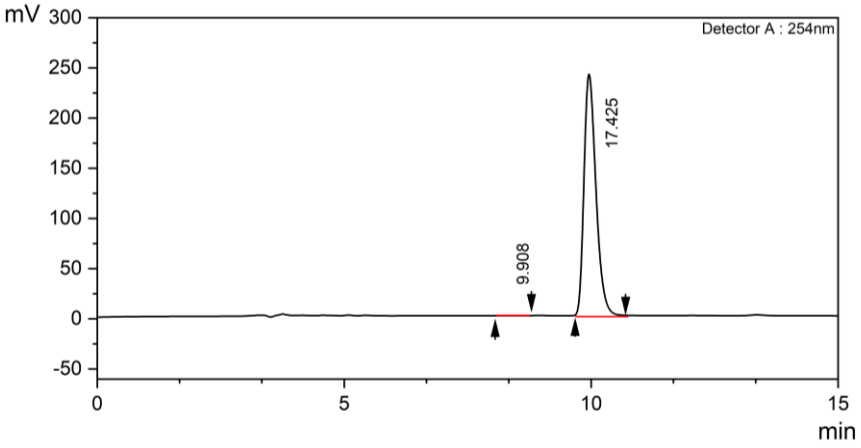
HPLC analysis 3ax:





Peak Results

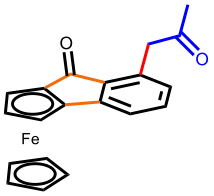
Peak#	Ret. Time	Area	Area%
1	8.351	10706134	49.7013
2	11.440	10834831	50.2987

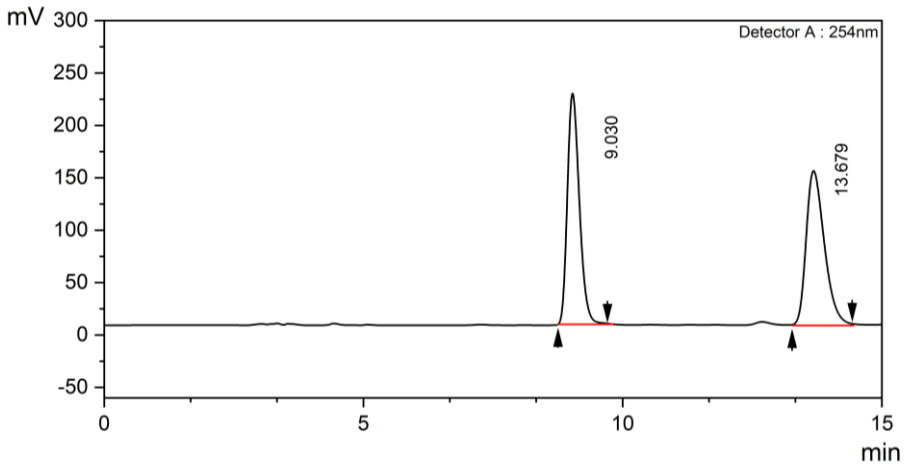


Peak Results

Peak#	Ret. Time	Area	Area%
1	8.254	22222	0.3613
2	9.954	609213	99.6369

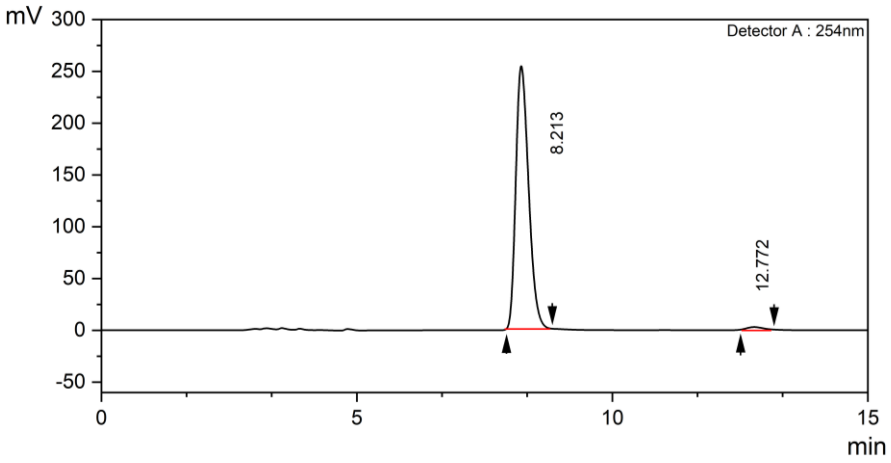
HPLC analysis 3ay:





Peak Results

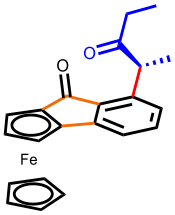
Peak#	Ret. Time	Area	Area%
1	9.030	4097053	49.3907
2	13.679	4198134	50.6093

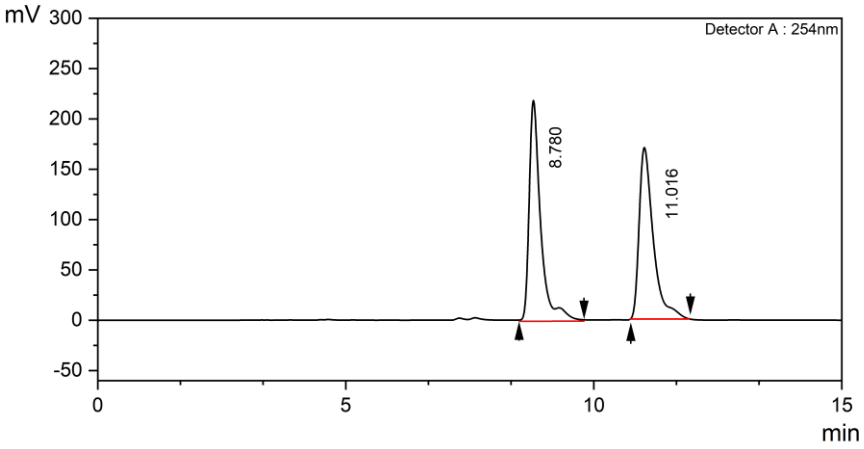


Peak Results

Peak#	Ret. Time	Area	Area%
1	8.213	7216428	98.8446
2	12.772	122543	1.1543

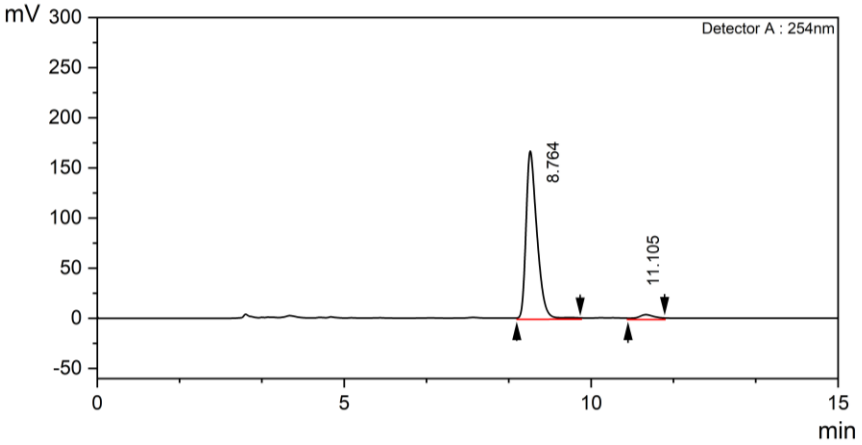
HPLC analysis (R_p, R)-3az:





Peak Results

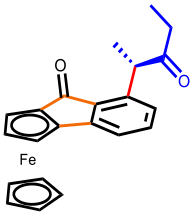
Peak#	Ret. Time	Area	Area%
1	8.870	13838800	50.1171
2	11.016	13774142	49.8829

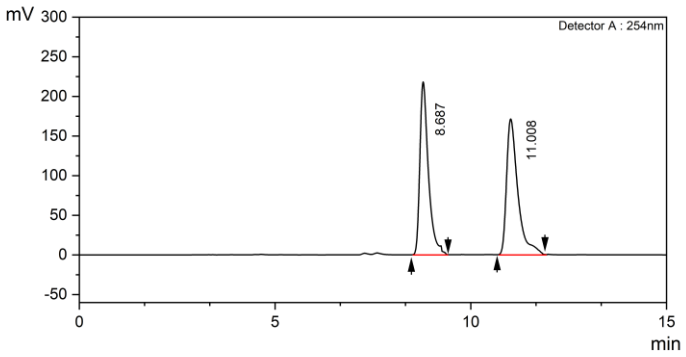


Peak Results

Peak#	Ret. Time	Area	Area%
1	8.764	5003559	97.4785
2	11.105	129427	2.5215

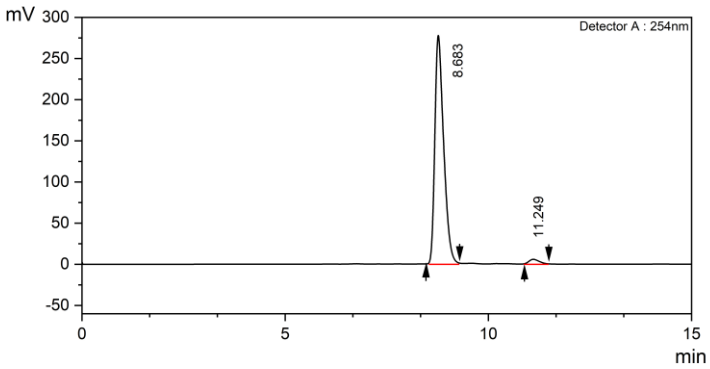
HPLC analysis (R_p, S)-3az:





Peak Results

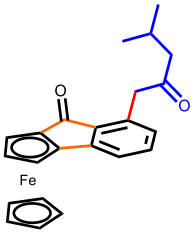
Peak#	Ret. Time	Area	Area%
1	8.687	5687258	50.3925
2	11.008	5598655	49.6075

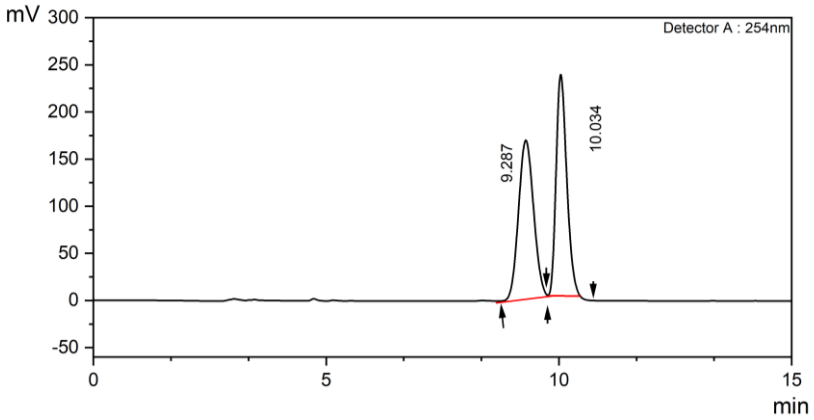


Peak Results

Peak#	Ret. Time	Area	Area%
1	8.683	3252313	97.668
2	11.249	77656	2.332

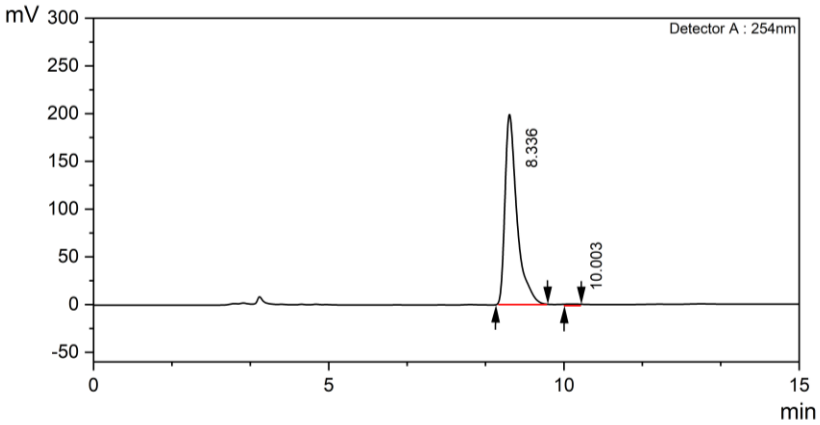
HPLC analysis 3ba:





Peak Results

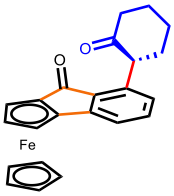
Peak#	Ret. Time	Area	Area%
1	9.283	3919113	49.6501
2	10.034	3974349	50.3499

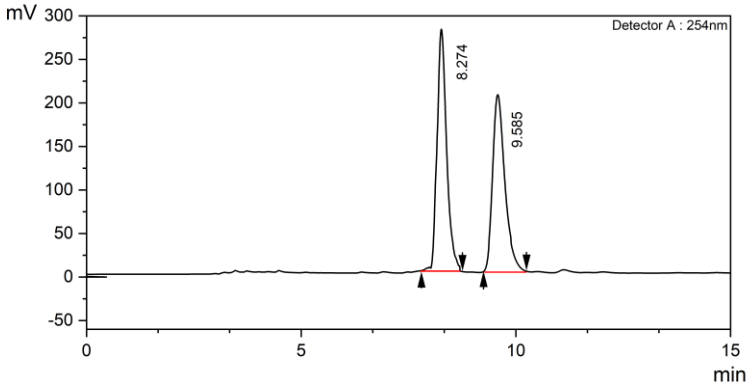


Peak Results

Peak#	Ret. Time	Area	Area%
1	8.336	3541759	99.8089
2	10.003	6783	0.1911

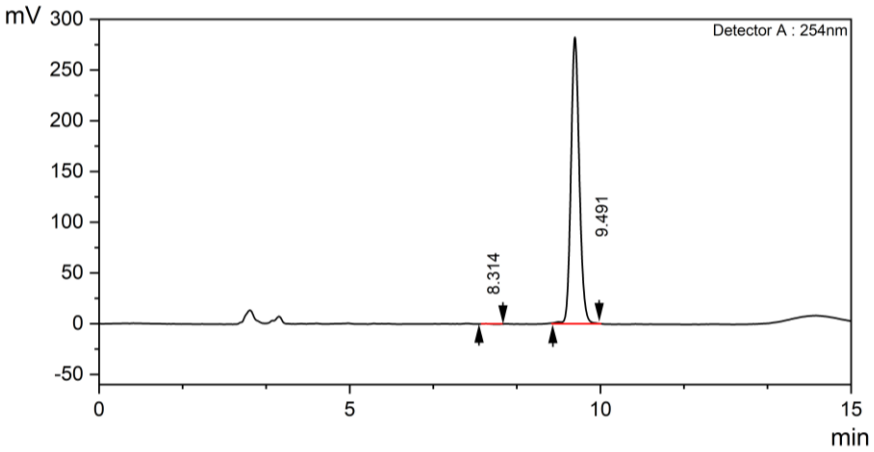
HPLC analysis (R_p, R)-3bb:





Peak Results

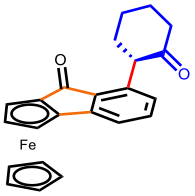
Peak#	Ret. Time	Area	Area%
1	8.274	2247533	50.0761
2	9.585	2240718	49.9239

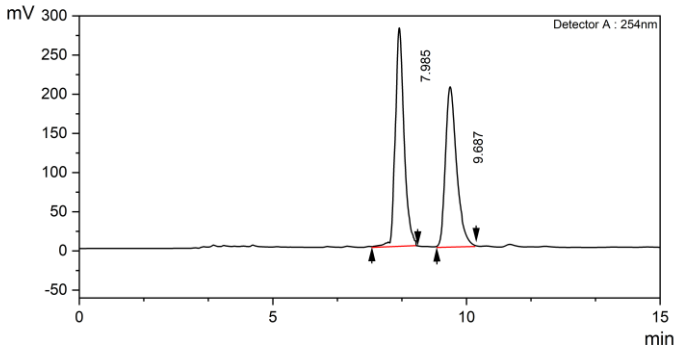


Peak Results

Peak#	Ret. Time	Area	Area%
1	8.314	1869	0.1963
2	9.491	950074	99.8037

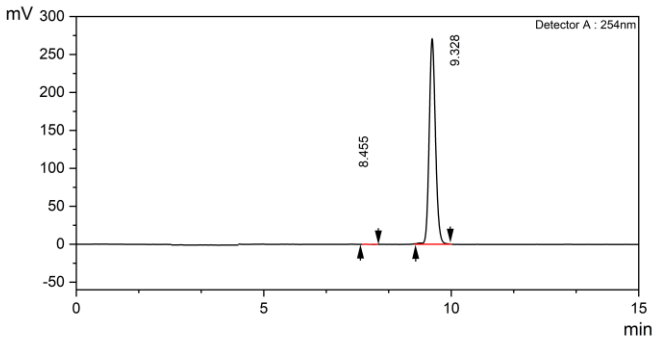
HPLC analysis (R_p, S)-3bb:





Peak Results

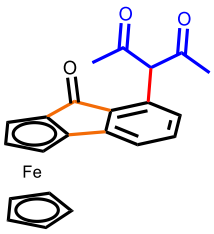
Peak#	Ret. Time	Area	Area%
1	7.985	2589764	50.4173
2	9.687	2546895	49.5827

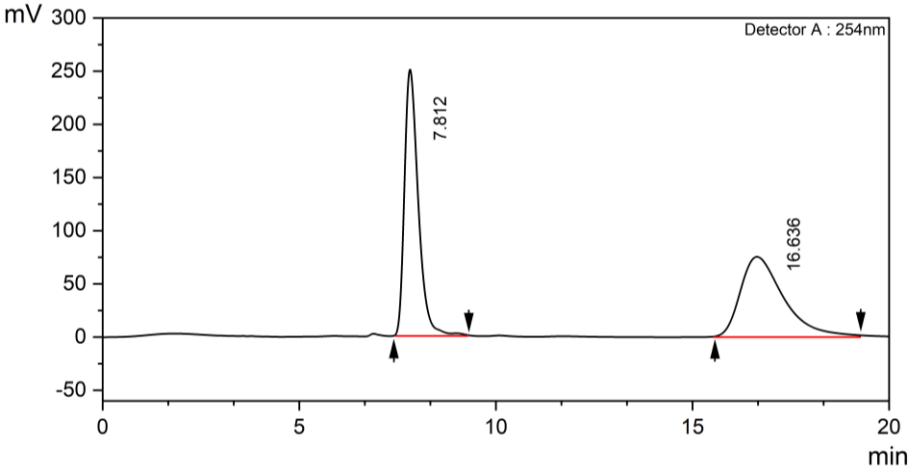


Peak Results

Peak#	Ret. Time	Area	Area%
1	8.455	2356	0.1262
2	9.328	1865242	99.8738

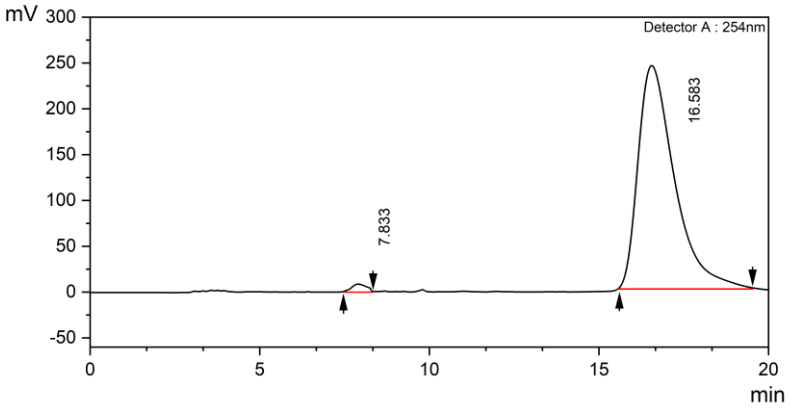
HPLC analysis 3bc:





Peak Results

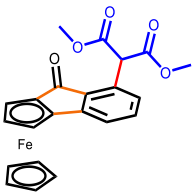
Peak#	Ret. Time	Area	Area%
1	7.812	23286673	53.0534
2	16.636	20606192	46.9466

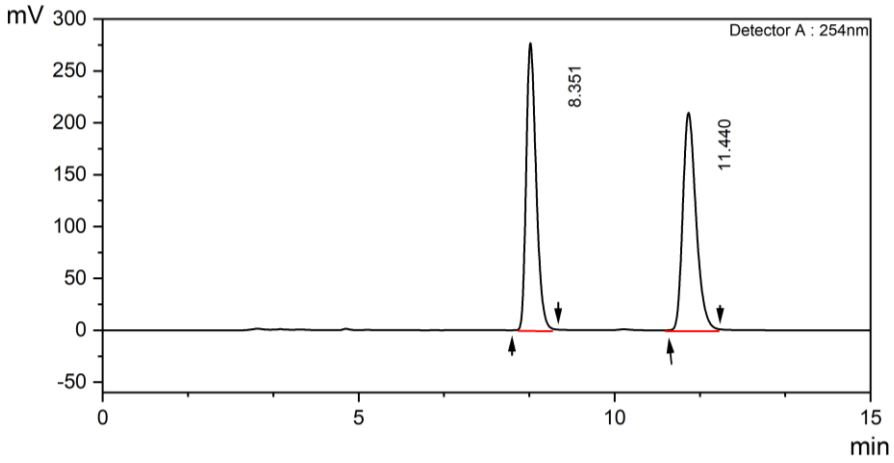


Peak Results

Peak#	Ret. Time	Area	Area%
1	7.833	229976	0.7221
2	16.582	31621512	99.2779

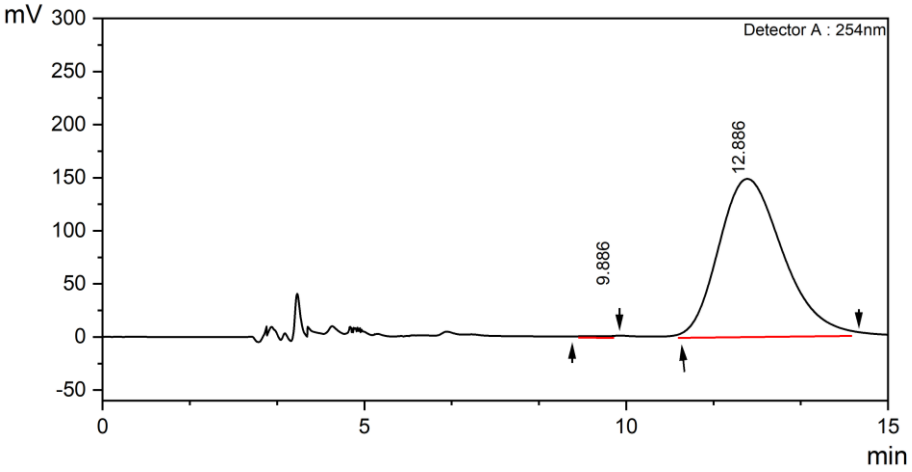
HPLC analysis 3bd:





Peak Results

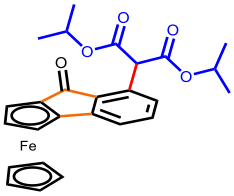
Peak#	Ret. Time	Area	Area%
1	8.351	10706134	49.7013
2	11.440	10834831	50.2987

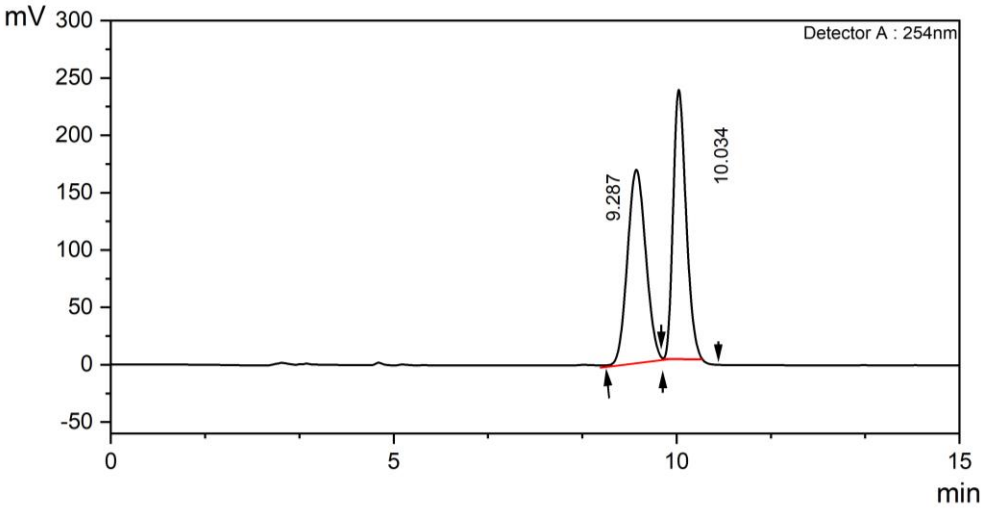


Peak Results

Peak#	Ret. Time	Area	Area%
1	9.886	33432	1.4749
2	12.886	2203144	98.5052

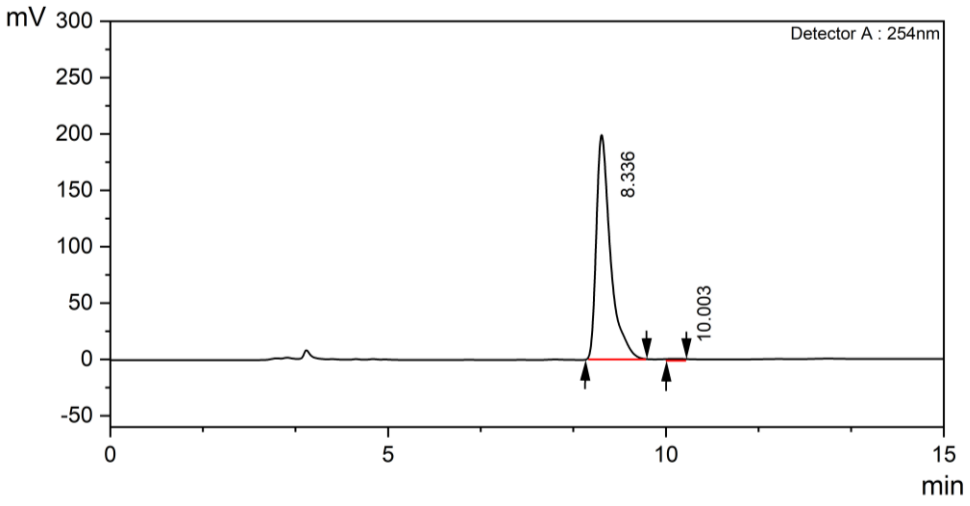
HPLC analysis 3be:





Peak Results

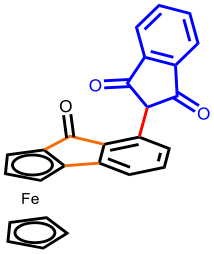
Peak#	Ret. Time	Area	Area%
1	8.006	2489687	49.9241
2	9.594	2497659	50.0759

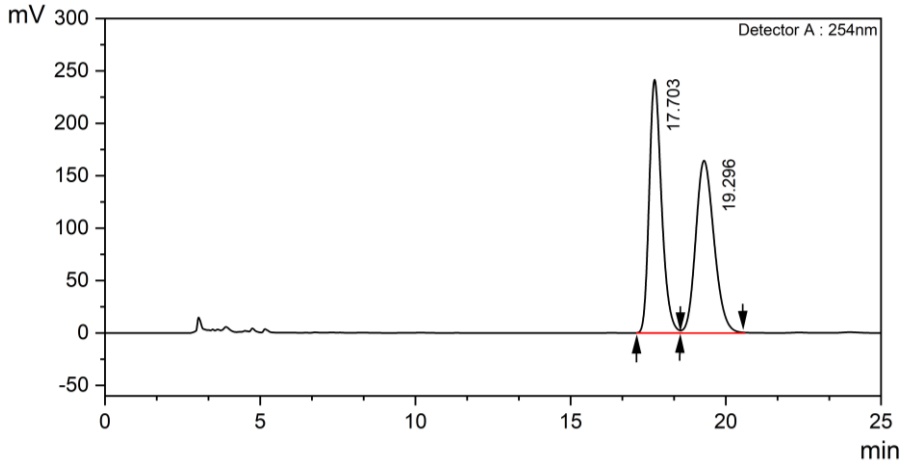


Peak Results

Peak#	Ret. Time	Area	Area%
1	7.618	407434	5.7518
2	9.706	6676159	94.2482

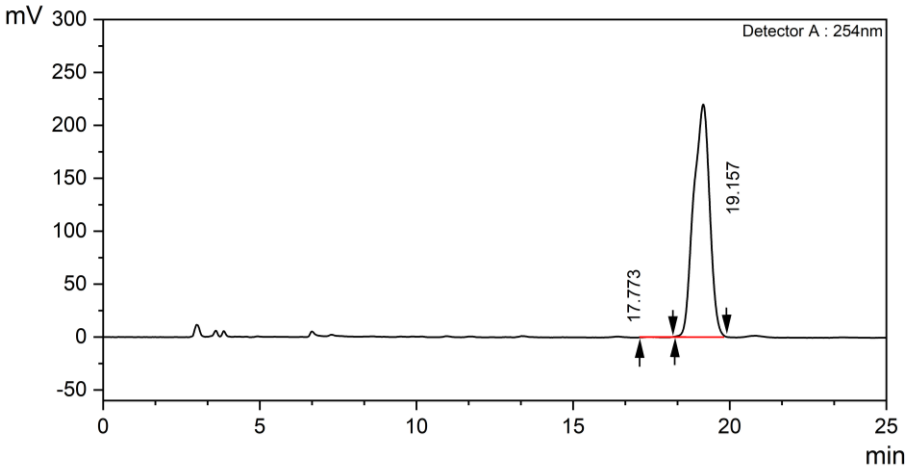
HPLC analysis 3bf:





Peak Results

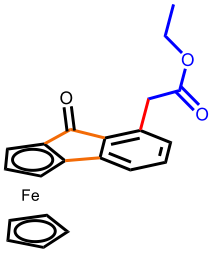
Peak#	Ret. Time	Area	Area%
1	17.703	6684604	49.6877
2	19.296	6768629	50.3123

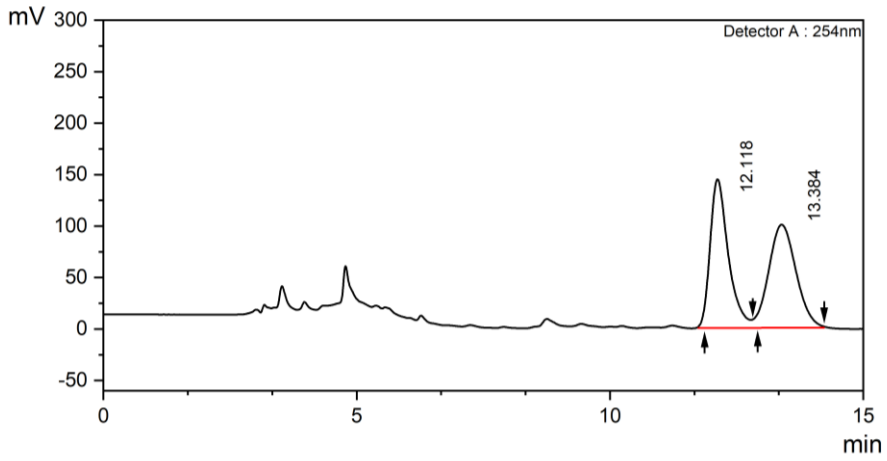


Peak Results

Peak#	Ret. Time	Area	Area%
1	17.773	4720	0.307
2	19.157	1531595	99.693

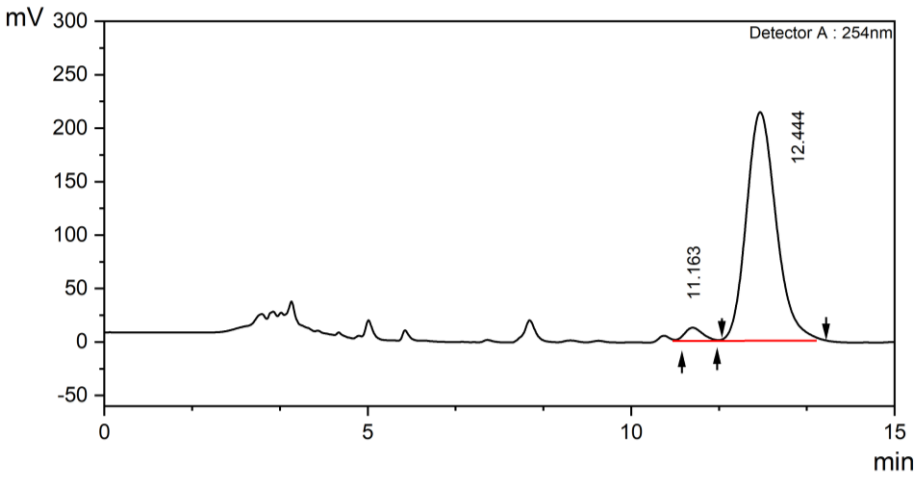
HPLC analysis 3bf:





Peak Results

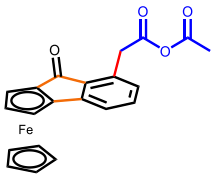
Peak#	Ret. Time	Area	Area%
1	12.118	365295	48.5251
2	13.384	387501	51.4749

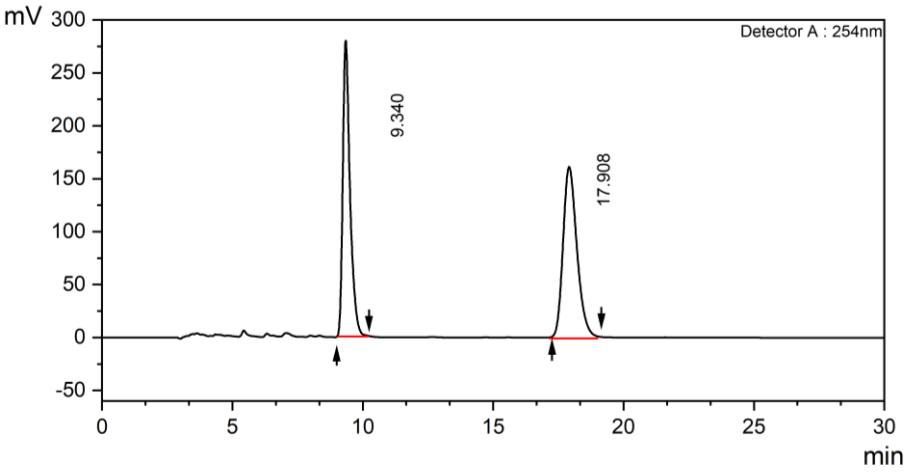


Peak Results

Peak#	Ret. Time	Area	Area%
1	11.163	31889	2.4996
2	12.444	1269884	97.5504

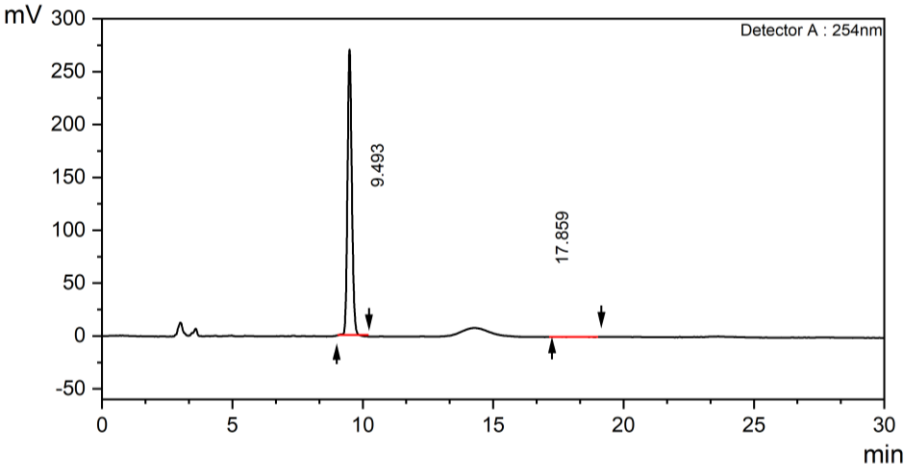
HPLC analysis 3bh:





Peak Results

Peak#	Ret. Time	Area	Area%
1	9.340	1651001	47.8090
2	17.908	1802330	52.1910



Peak Results

Peak#	Ret. Time	Area	Area%
1	9.493	950074	99.8900
2	17.859	1047	0.1100

9. Single Crystal Structure

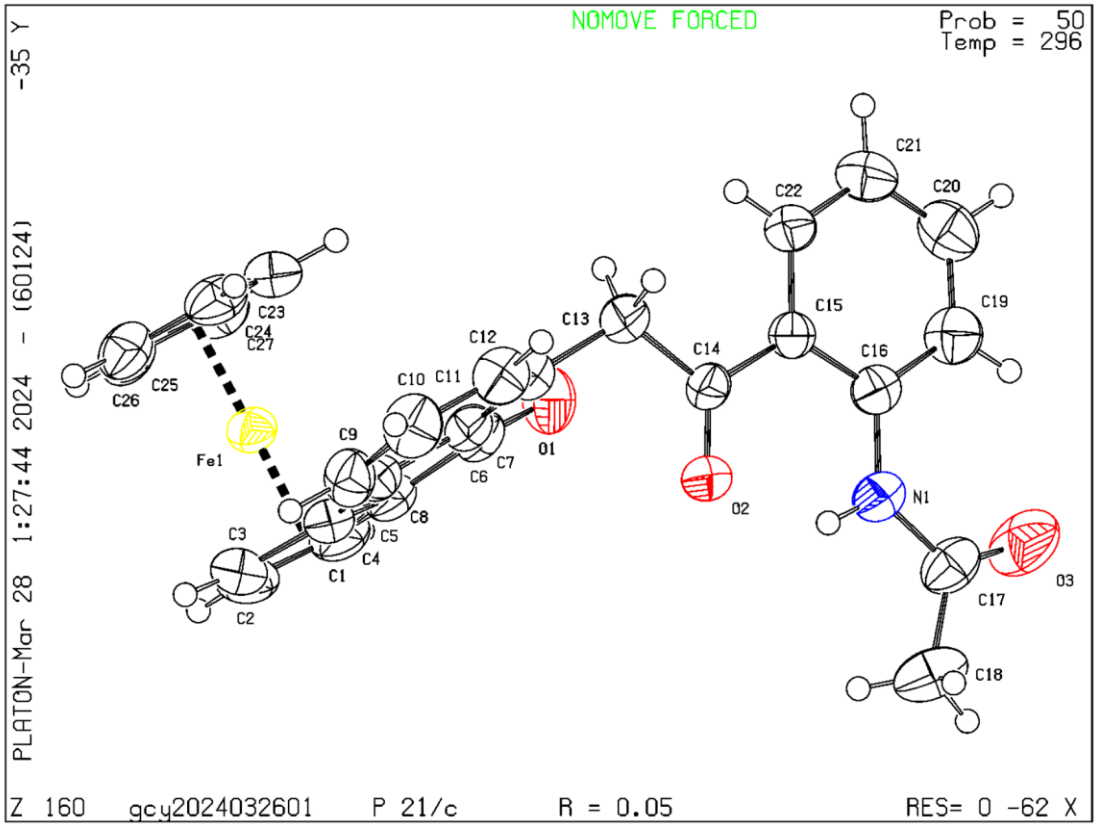


Figure S9.1 The single crystal dataspectra of the reduced product of (*rac*)-**3aj**.

Table S9.1 The crystal data and structure refinement of the reduced product of (*rac*)-**3aj**.

Identification code	**(*rac*)-3aj**	
Chemical formula	$C_{27}H_{21}FeNO_3$	
Formula weight	463.30 g/mol	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	P 1 21/n 1	
Unit cell dimensions	a = 14.2329(10) Å	α = 90°
	b = 13.9649(12) Å	β = 104.664(5)°
	c = 11.1832(8) Å	γ = 90°
Volume	2150.4(3) $Å^3$	

Z	4
Density (calculated)	1.431 g/cm^3
Absorption coefficient	0.731 mm^{-1}
F(000)	960.0
Index ranges	-18<=h<=19, -17<=k<=18, -15<=l<=14
Reflections collected	20661
Independent reflections	5419 [R(int) = 0.0599]
Largest diff. peak and hole	0.562 and -0.328 eÅ^{-3}

Table S9.2 The bond lengths (**Å**) of the reduced product of (*rac*)-**3aj**.

Fe1-C5	2.021(2)	Fe1-C2	2.025(3)
Fe1-C24	2.029(3)	Fe1-C4	2.030(3)
Fe1-C25	2.035(3)	Fe1-C1	2.035(3)
Fe1-C23	2.041(3)	Fe1-C27	2.045(3)
Fe1-C26	2.045(3)	Fe1-C3	2.046(3)
O1-C6	1.217(3)	O2-C14	1.214(3)
O3-C17	1.214(4)	N1-C17	1.364(3)
N1-C16	1.398(3)	N1-H8	0.86
C1-C2	1.408(5)	C1-C5	1.420(4)
C1-H16	0.93	C2-C3	1.433(5)
C2-H15	0.93	C3-C4	1.410(4)
C3-H1	0.93	C4-C5	1.427(4)
C4-C8	1.479(4)	C5-C6	1.474(4)
C6-C7	1.505(4)	C7-C12	1.387(4)
C7-C8	1.409(4)	C8-C9	1.378(4)
C9-C10	1.389(4)	C9-H14	0.93
C10-C11	1.380(4)	C10-H2	0.93
C11-C12	1.397(4)	C11-H3	0.93
C12-C13	1.501(4)	C13-C14	1.522(3)
C13-H13	0.97	C13-H4	0.97
C14-C15	1.490(4)	C15-C22	1.396(4)
C15-C16	1.414(4)	C16-C19	1.396(4)
C17-C18	1.503(5)	C18-H5	0.96
C18-H7	0.96	C18-H6	0.96
C19-C20	1.369(4)	C19-H12	0.93

C20-C21	1.366(4)	C20-H9	0.93
C21-C22	1.374(4)	C21-H10	0.93
C22-H11	0.93	C23-C24	1.406(4)
C23-C27	1.418(4)	C23-H21	0.93
C24-C25	1.412(4)	C24-H20	0.93
C25-C26	1.412(4)	C25-H19	0.93
C26-C27	1.395(4)	C26-H17	0.93
C27-H18	0.93		

Table S9.3 The bond angles (°) of the reduced product of (*rac*)-**3aj**.

C5-Fe1-C2	68.25(12)	C5-Fe1-C24	121.87(12)
C2-Fe1-C24	158.38(15)	C5-Fe1-C4	41.25(11)
C2-Fe1-C4	68.11(12)	C24-Fe1-C4	105.94(12)
C5-Fe1-C25	157.09(12)	C2-Fe1-C25	122.91(14)
C24-Fe1-C25	40.65(13)	C4-Fe1-C25	120.28(12)
C5-Fe1-C1	40.98(11)	C2-Fe1-C1	40.57(13)
C24-Fe1-C1	158.83(13)	C4-Fe1-C1	69.09(12)
C25-Fe1-C1	159.75(13)	C5-Fe1-C23	108.35(12)
C2-Fe1-C23	160.07(15)	C24-Fe1-C23	40.41(12)
C4-Fe1-C23	123.20(12)	C25-Fe1-C23	68.08(13)
C1-Fe1-C23	123.97(14)	C5-Fe1-C27	125.09(13)
C2-Fe1-C27	124.08(14)	C24-Fe1-C27	68.11(13)
C4-Fe1-C27	160.79(12)	C25-Fe1-C27	67.92(13)
C1-Fe1-C27	109.46(13)	C23-Fe1-C27	40.61(13)
C5-Fe1-C26	161.07(12)	C2-Fe1-C26	108.79(13)
C24-Fe1-C26	67.98(12)	C4-Fe1-C26	156.71(13)
C25-Fe1-C26	40.51(12)	C1-Fe1-C26	124.60(12)
C23-Fe1-C26	67.66(13)	C27-Fe1-C26	39.87(13)
C5-Fe1-C3	69.21(12)	C2-Fe1-C3	41.21(13)
C24-Fe1-C3	120.82(13)	C4-Fe1-C3	40.48(11)
C25-Fe1-C3	105.14(14)	C1-Fe1-C3	69.57(13)
C23-Fe1-C3	157.80(13)	C27-Fe1-C3	158.39(13)
C26-Fe1-C3	121.77(13)	C17-N1-C16	129.3(3)
C17-N1-H8	115.3	C16-N1-H8	115.3
C2-C1-C5	106.8(3)	C2-C1-Fe1	69.36(16)

C5-C1-Fe1	68.98(14)	C2-C1-H16	126.6
C5-C1-H16	126.6	Fe1-C1-H16	126.6
C1-C2-C3	110.1(3)	C1-C2-Fe1	70.07(16)
C3-C2-Fe1	70.16(16)	C1-C2-H15	125.0
C3-C2-H15	125.0	Fe1-C2-H15	126.4
C4-C3-C2	106.0(3)	C4-C3-Fe1	69.14(17)
C2-C3-Fe1	68.63(18)	C4-C3-H1	127.0
C2-C3-H1	127.0	Fe1-C3-H1	126.8
C3-C4-C5	109.0(3)	C3-C4-C8	141.7(3)
C5-C4-C8	109.2(2)	C3-C4-Fe1	70.38(17)
C5-C4-Fe1	69.04(15)	C8-C4-Fe1	121.46(17)
C1-C5-C4	108.1(3)	C1-C5-C6	142.5(3)
C4-C5-C6	109.1(2)	C1-C5-Fe1	70.04(15)
C4-C5-Fe1	69.71(15)	C6-C5-Fe1	119.72(17)
O1-C6-C5	128.8(3)	O1-C6-C7	126.8(3)
C5-C6-C7	104.5(2)	C12-C7-C8	121.4(2)
C12-C7-C6	128.2(3)	C8-C7-C6	110.4(2)
C9-C8-C7	121.0(2)	C9-C8-C4	132.1(3)
C7-C8-C4	106.8(2)	C8-C9-C10	117.4(3)
C8-C9-H14	121.3	C10-C9-H14	121.3
C11-C10-C9	122.0(3)	C11-C10-H2	119.0
C9-C10-H2	119.0	C10-C11-C12	121.2(3)
C10-C11-H3	119.4	C12-C11-H3	119.4
C7-C12-C11	117.0(3)	C7-C12-C13	121.1(3)
C11-C12-C13	121.9(2)	C12-C13-C14	114.4(2)
C12-C13-H13	108.7	C14-C13-H13	108.7
C12-C13-H4	108.7	C14-C13-H4	108.7
H13-C13-H4	107.6	O2-C14-C15	122.9(2)
O2-C14-C13	119.4(3)	C15-C14-C13	117.6(2)
C22-C15-C16	117.6(3)	C22-C15-C14	119.6(2)
C16-C15-C14	122.7(2)	C19-C16-N1	122.4(2)
C19-C16-C15	119.2(3)	N1-C16-C15	118.4(2)
O3-C17-N1	124.1(3)	O3-C17-C18	122.0(3)
N1-C17-C18	113.9(3)	C17-C18-H5	109.5
C17-C18-H7	109.5	H5-C18-H7	109.5
C17-C18-H6	109.5	H5-C18-H6	109.5
H7-C18-H6	109.5	C20-C19-C16	120.5(3)

C20-C19-H12	119.7	C16-C19-H12	119.7
C21-C20-C19	121.3(3)	C21-C20-H9	119.3
C19-C20-H9	119.3	C20-C21-C22	118.9(3)
C20-C21-H10	120.5	C22-C21-H10	120.5
C21-C22-C15	122.3(3)	C21-C22-H11	118.8
C15-C22-H11	118.8	C24-C23-C27	107.8(3)
C24-C23-Fe1	69.35(17)	C27-C23-Fe1	69.84(18)
C24-C23-H21	126.1	C27-C23-H21	126.1
Fe1-C23-H21	126.3	C23-C24-C25	108.1(3)
C23-C24-Fe1	70.24(16)	C25-C24-Fe1	69.87(16)
C23-C24-H20	125.9	C25-C24-H20	125.9
Fe1-C24-H20	125.5	C26-C25-C24	107.5(3)
C26-C25-Fe1	70.14(16)	C24-C25-Fe1	69.48(16)
C26-C25-H19	126.2	C24-C25-H19	126.2
Fe1-C25-H19	125.7	C27-C26-C25	108.6(3)
C27-C26-Fe1	70.05(17)	C25-C26-Fe1	69.35(16)
C27-C26-H17	125.7	C25-C26-H17	125.7
Fe1-C26-H17	126.5	C26-C27-C23	108.0(3)
C26-C27-Fe1	70.07(18)	C23-C27-Fe1	69.56(18)
C26-C27-H18	126.0	C23-C27-H18	126.0
Fe1-C27-H18	125.9		