Supplementary Information

Metal-Free Stereoretentive Click Coupling of Chiral Metallocenes in Water

Peng Chen,[1] Chao Yang,[1] Minnan Huang,[4] Lei Wang,[1] Xuefei Zhao,[4]* Zhenhua Jia,[1,3]* and Teck-Peng Loh[1,2]*

[1]*Henan Linker Technology Key Laboratory, College of Advanced Interdisciplinary Science and Technology (CAIST), Henan University of Technology, Zhengzhou, 450001, China*

[2]*Division of Chemistry and Biological Chemistry, School of Chemistry Chemical Engineering, and Biotechnology, Nanyang Technological University, Singapore, 637371, Singapore*

[3]*Department of Chemistry, Fudan University, Shanghai, 200433, China*

[4] *School of Chemistry and Molecular Engineering, Nanjing Tech University, Nanjing 211816, China*

*E-mail: xfzhao@njtech.edu.cn; zhenhua_jia@fudan.edu.cn; teckpeng@ntu.edu.sg

This PDF file includes:

Table of contents

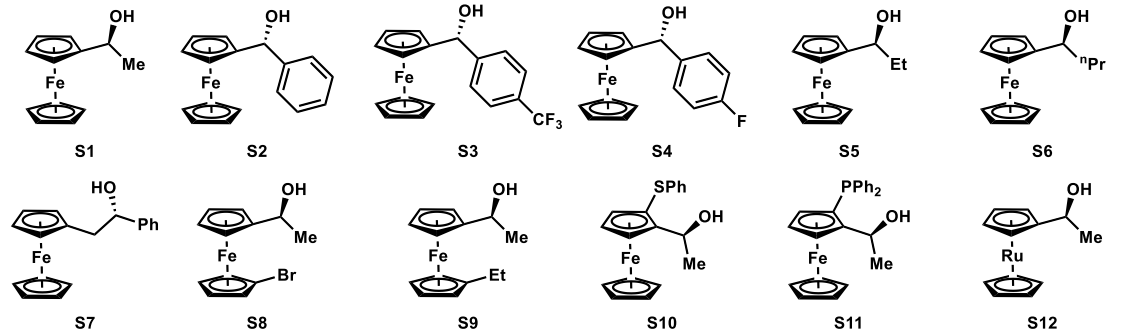
1. General Information

Materials and instruments: All reactions were carried out without exclusion of air or moisture. Chemicals were purchased from commercial suppliers and used without further purification. Metallocenes, alcohols, sulfonamides, indoles, heterocyclics and natural complexes were purchased from commercial suppliers and used directly as received. Flash column chromatographic purification of products was accomplished using forced-flow chromatography on Silica Gel (200–300 mesh). Preparative thin-layer chromatography (PTLC) was performed on glass plates (20 x 20 cm) impregnated with silica gel 60 F254 (0.3–0.4 mm thickness).

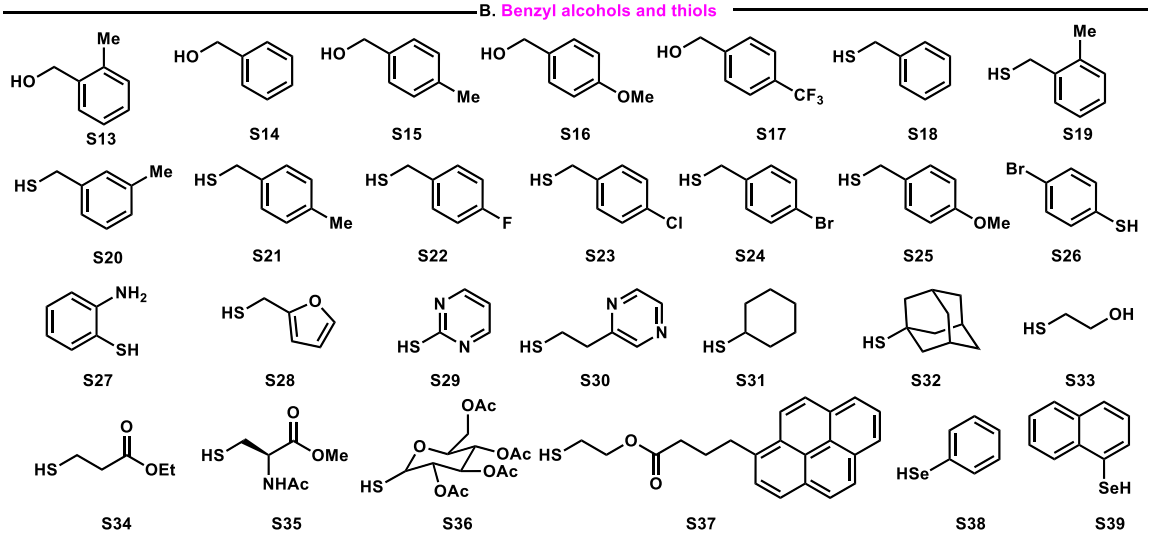
NMR spectra were recorded on a JEOL/JNM-ECZL400S NMR spectrometer (400 MHz for ^{1}H, 101 MHz for ^{13}C, 376 MHz for ^{19}F, 160 MHz for ^{31}P). Chemical shifts of ^{1}H NMR and ^{13}C NMR spectra were reported as parts per million in δ scale using residual solvent signal as internal standard (note: $CDCl_3$ referenced at δ 7.26 in ^{1}H and δ 77.0 for central line of the triplet in ^{13}C). Data are represented as follows: chemical shift, integration, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad) and coupling constant (*J*, Hz). High resolution mass spectra (HRMS) were obtained on a 3000-mass spectrometer, using Waters Q-Tof MS/MS system with the ESI technique. X-ray diffraction analysis of single crystals was performed on Bruker APEX II X-ray single crystal diffraction meter. Enantiomeric excesses were determined by HPLC analysis using chiral column described below in detail.

2. Starting materials

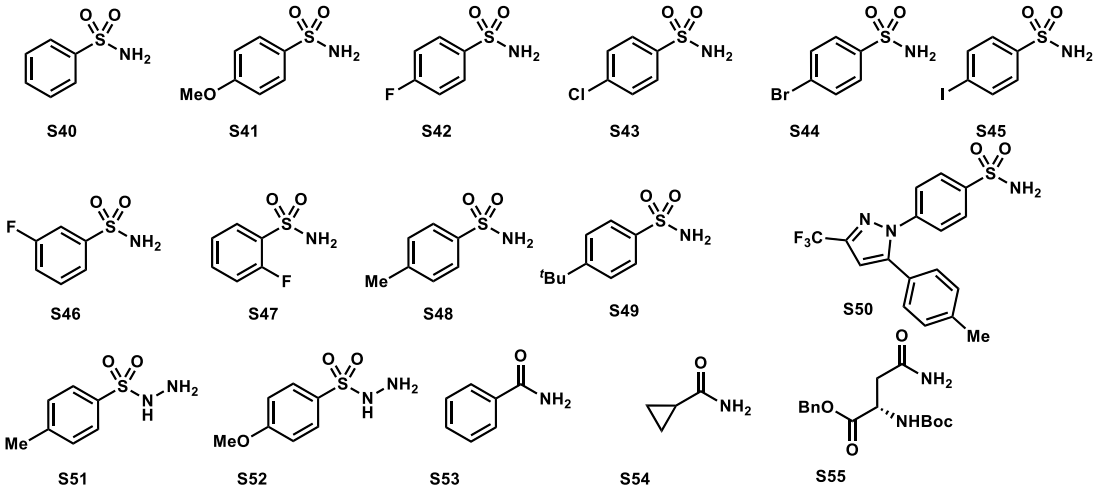
A. (*S*)-Metallocene alcohols



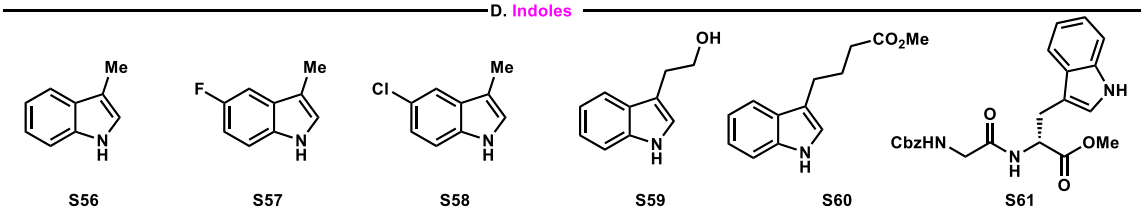
B. Benzyl alcohols and thiols



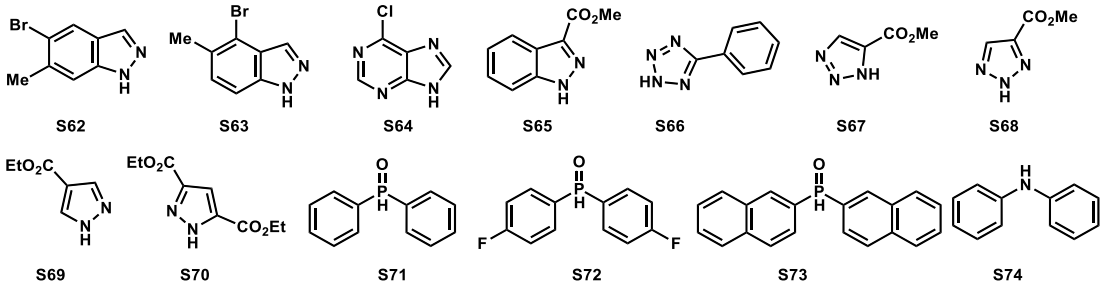
C. Sulfamides and amides



D. Indoles

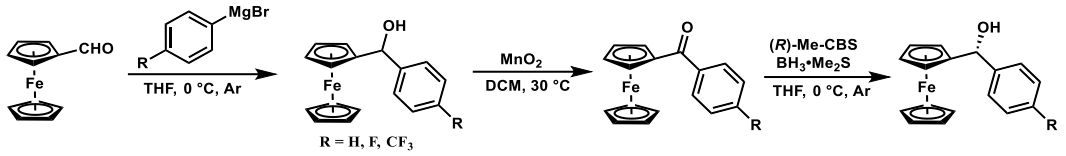


E. Other nucleophiles



Compounds **S1**, **S13**–**S36**, **S38**, **S40**–**S60** and **S62**–**S74** were commercially available. Compound **S10**[1], **S11**[1], **S37**[2], **S39**[3], and **S61**[4] were prepared in accordance with those previously reported in the literature. The spectral data are in full accordance with the literature report respectively.

2.1 Syntheses of compounds S2–S4



To an oven-dried 50 mL round bottom flask equipped with a stir was charged with ferrocene formaldehyde (10.0 mmol, 2.14 g) under argon atmosphere. Then, anhydrous THF (20.0 mL) was added *via* syringe. The reaction mixture was stirred at 0 °C, a solution of aryl magnesium bromide (15 mmol, 1.0 M in THF, 1.5 equiv.) was added slowly *via* syringe, and the mixture was stirred for 2 h at 0 °C. Upon completion, the reaction was quenched with saturated aqueous NH_4Cl solution, extracted with EtOAc (3 × 50 mL), dried over Na_2SO_4, filtered, concentrated under reduced pressure. The residue was purified by flash column chromatography (petroleum ether/ethyl acetate) to afford the corresponding ferrocene alcohol products.

To an oven-dried 50 mL round bottom flask equipped with a stir was charged with ferrocene alcohol (5 mmol, 1.0 equiv.) in anhydrous DCM (20.0 mL), activated MnO_2 (50 mmol, 4.35 g) was added and the reaction was allowed to stirred at room temperature for overnight. Upon completion, the mixture was filtered through a Büchner funnel to remove manganese dioxide, followed by concentration of the filtrate under reduced pressure. The residue was purified by silica gel flash chromatography (petroleum ether/Ethyl acetate = 10:1) to afford the corresponding ferrocene ketones.

To an oven-dried 50 mL round bottom flask equipped with a stir was charged with ferrocene ketone (5.0 mmol, 1.0 equiv.) in anhydrous THF (20.0 mL), (*R*)-Me-CBS (2.0 mmol, 0.4 equiv.) and BH_3•Me_2S (3.0 equiv.) were added slowly *via* syringe at 0 °C. Then, the reaction mixture was stirred at 0 °C for 30 min and was allowed to stirred at room temperature for overnight. Upon completion, MeOH was added slowly to quench the reaction, and extracted three times with EtOAc, dry with anhydrous $NaSO_4$, and concentrated under reduced pressure. The residue was purified by flash column chromatography to obtain products **S2**–**S4**. The products **S2** and **S3** exhibited improved enantioselectivity following recrystallization.

For example, the synthesis of compound **S2**. To an oven-dried 50 mL round bottom flask equipped with a stir was charged with ferrocene formaldehyde (10.0 mmol, 2.14 g) under argon atmosphere. Then, anhydrous THF (20.0 mL) was added *via* syringe. The reaction mixture was stirred at 0 °C, a solution of phenyl magnesium bromide (15 mmol, 1.0 M in THF, 1.5 equiv.) was added slowly *via* syringe, and the mixture was stirred for 2 h at 0 °C. Upon completion, the reaction was quenched with saturated aqueous NH_4Cl solution, extracted with EtOAc (3 × 50 mL), dried over Na_2SO_4, filtered, concentrated under reduced pressure. The residue was purified by flash column chromatography (petroleum ether/Ethyl acetate = 10/1) to afford ferrocenyl-(phenyl)methanol (2.4 g, 81% yield).

To an oven-dried 50 mL round bottom flask equipped with a stir was charged with ferrocenyl-(phenyl)methanol (5 mmol, 1.46 g) in anhydrous DCM (20.0 mL), activated MnO_2 (50 mmol, 4.35 g) was added and the reaction was allowed to stirred at room temperature for overnight. Upon completion, the mixture was filtered through a Büchner funnel to remove manganese dioxide, followed by concentration of the filtrate under reduced pressure. The residue was purified by silica gel flash chromatography (petroleum ether/Ethyl acetate = 10:1) to afford the ferrocenyl-(phenyl)methanone (1.4 g, 95% yield).

To an oven-dried 50 mL round bottom flask equipped with a stir was charged with ferrocenyl-(phenyl)methanone (4.0 mmol, 1.2 g, 1.0 equiv.) in anhydrous THF (20.0 mL), (*R*)-Me-CBS (1.6 mmol, 443 mg, 0.4 equiv.) and BH_3•Me_2S (12 mmol, 6 mL, 2 M in THF, 3.0 equiv.) were added slowly *via* syringe at 0 °C. Then, the reaction mixture was stirred at 0 °C for 30 min and was allowed to stirred at room temperature for overnight. Upon completion, MeOH was added slowly to quench the reaction, and extracted three times with EtOAc, dry with anhydrous Na_2SO_4, and concentrated under reduced pressure. The residue was purified by flash column chromatography to obtain product (*S*)-**S2** (1.05 g, 90% yield). The product **S2** exhibited improved enantioselectivity following recrystallization. The ee value was determined by HPLC.

TLC: R_f = 0.35 (petroleum ether/Ethyl acetate = 8/1); 1.05 g, yield: 90%; yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 – 7.37 (m, 2H), 7.34 – 7.30 (m, 2H), 7.27 – 7.22 (m, 1H), 5.46 (d, *J* = 3.2 Hz, 1H), 4.23 – 4.16 (m, 9H), 2.46 (d, *J* = 3.2 Hz, 1H).

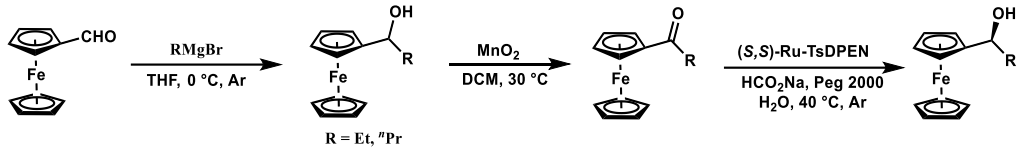
^{13}C NMR (101 MHz, $CDCl_3$) δ 143.2, 128.2, 127.4, 126.2, 94.3, 72.0, 68.5, 68.2, 68.1, 67.4, 65.9.

HRMS (ESI-TOF) m/z: $[M+K]^+$ Calcd for $C_{17}H_{16}FeOK$ 331.0177; Found: 331.0189.

Chiral HPLC: The ee value was 93%, t_R (minor) = 12.2 min, t_S (major) = 16.7 min (Chiralpak IA, λ = 254 nm, 10% isopropanol/hexanes, flow rate = 1.0 mL/min).

Data was in accordance with that reported in the literature.[5]

2.2 Syntheses of compounds S5–S6



To an oven-dried 50 mL round bottom flask equipped with a stir was charged with ferrocene formaldehyde (10.0 mmol, 2.14 g) under argon atmosphere. Then, anhydrous THF (20.0 mL) was added *via* syringe. The reaction mixture was stirred at 0 °C, a solution of alkyl magnesium bromide (15 mmol, 1.5 equiv.) was added slowly *via* syringe, and the mixture was stirred for 2 h at 0 °C. Upon completion, the reaction was quenched with saturated aqueous NH_4Cl solution, extracted with EtOAc (3 × 50 mL), dried over Na_2SO_4, filtered, concentrated under reduced pressure. The residue was purified by flash column chromatography (petroleum ether/ethyl acetate) to afford the corresponding ferrocene alcohol products.

To an oven-dried 50 mL round bottom flask equipped with a stir was charged with ferrocene alcohols (5 mmol, 1.0 equiv.) in anhydrous DCM (20.0 mL), activated MnO_2 (50 mmol, 4.35 g) was added and the reaction was allowed to stirred at room temperature for overnight. Upon completion, the mixture was filtered through a Büchner funnel to remove manganese dioxide, followed by concentration of the filtrate under reduced pressure. The residue was purified by silica gel flash chromatography (petroleum ether/Ethyl acetate = 10:1) to afford the corresponding ferrocene ketones.

To an oven-dried 5.0 mL vial equipped with a stir was charged with [(*S*,*S*)-N-(2-Amino-1,2-diphenylethyl)-*p*-toluenesulfonamide]chloro(mesitylene)ruthenium(II) (0.01

equiv.) in H_2O (1.0 mL), acetyl ferrocene ketones (1.0 mmol), sodium formate (5.0 mmol, 0.34 g) and PEG2000 (1.0 g) were added under argon atmosphere. Then, the reaction mixture was allowed to stirred at 40 °C for 24 h. Upon completion, Et_2O (10.0 mL) was added slowly to quench the reaction, and extracted three times with EtOAc, dry with anhydrous Na_2SO_4, and concentrated under reduced pressure. The residue was purified by flash column on silica (petroleum ether/Ethyl acetate = 10:1) to afford the product and the ee value was determined by HPLC analysis.

For example, the synthesis of compound (*S*)-**S5**. To an oven-dried 50 mL round bottom flask equipped with a stir was charged with ferrocene formaldehyde (10.0 mmol, 2.14 g) under argon atmosphere. Then, anhydrous THF (20.0 mL) was added *via* syringe. The reaction mixture was stirred at 0 °C, a solution of ethyl magnesium bromide (15 mmol, 15 mL, 1.0 M in THF) was added slowly, and the mixture was stirred for 2 h at 0 °C. Upon completion, the reaction was quenched with saturated aqueous NH_4Cl solution, extracted with EtOAc (3 × 50 mL), dried over Na_2SO_4, filtered, concentrated under reduced pressure. The residue was purified by flash column chromatography (petroleum ether/Ethyl acetate = 10/1) to afford 1-ferrocenylpropan-1-ol (2.07 g, 85% yield).

To an oven-dried 50 mL round bottom flask equipped with a stir was charged with 1-ferrocenylpropan-1-ol (5 mmol, 1.22 g) in anhydrous DCM (20.0 mL), activated MnO_2 (50 mmol, 4.35 g) was added and the reaction was allowed to stirred at room temperature for overnight. Upon completion, the mixture was filtered through a Büchner funnel to remove manganese dioxide, followed by concentration of the filtrate under reduced pressure. The residue was purified by silica gel flash chromatography (petroleum ether/Ethyl acetate = 10/1) to afford the ferrocenylpropenone (1.1 g, 91% yield).

To an oven-dried 5.0 mL vial equipped with a stir was charged with [(*S*,*S*)-N-(2-Amino-1,2-diphenylethyl)-*p*-toluenesulfonamide]chloro(mesitylene)ruthenium(II) (0.01 mmol, 6 mg) in H_2O (1.0 mL), ferrocenylpropenone (1.0 mmol, 242 mg), sodium formate (5.0 mmol, 0.34 g) and PEG2000 (1.0 g) were added under argon atmosphere. Then, the reaction mixture was allowed to stirred at 40 °C for 24 h. Upon completion, Et_2O (10.0

mL) was added slowly to quench the reaction, and extracted three times with EtOAc, dry with anhydrous Na_2SO_4, and concentrated under reduced pressure. The residue was purified by flash column on silica (petroleum ether/Ethyl acetate = 10:1) to afford the product **S5** (75 mg, 30% yield) and the ee value was determined by HPLC analysis.

TLC: R_f = 0.47 (petroleum ether/Ethyl acetate = 8:1); 75 mg, yield: 30%; yellow oil.

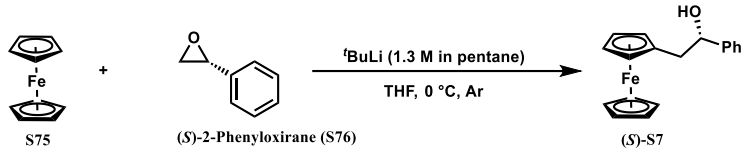
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.25 – 4.23 (m, 1H), 4.20 (s, 5H), 4.19 – 4.17 (m, 1H), 4.16 – 4.15 (m, 2H), 1.94 (d, *J* = 3.4 Hz, 1H), 1.73 – 1.64 (m, 2H), 0.95 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 94.3, 71.1, 68.2, 67.8, 67.7, 67.3, 65.1, 31.0, 10.3.

HRMS (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{13}H_{16}FeONa$ 267.0437; Found: 267.0443.

Chiral HPLC: The ee value was 98%, t_R (minor) = 9.2 min, t_S (major) = 14.1 min (Chiralpak IA, λ = 254 nm, 10% isopropanol/hexanes, flow rate = 1.0 mL/min).

2.3 Synthesis of compound S7



To a solution of *t*-butyllithium (9.2 mmol, 7.0 mL, 1.3 M in pentane) was added dropwise a solution of ferrocene **S75** (10.7 mmol, 2.0 g) in anhydrous THF (20 mL) under argon atmosphere at 0 °C. The reaction was stirred for 0.5 h, then 0.85 mL of (*S*)-styrene oxide **S76** (7.1 mmol) was added rapidly. The mixture was allowed to warm to room temperature and then stirred for 1 h. Upon completion, he reaction was quenched with saturated aqueous NH_4Cl solution, extracted with EtOAc (3 × 50 mL), dried over Na_2SO_4, filtered, concentrated under reduced pressure. The residue was purified by flash column chromatography (petroleum ether/Ethyl acetate = 4/1) to afford the product (*S*)-**S7** (400 mg, 12% yield), yellow solid. The ee value was determined by HPLC.

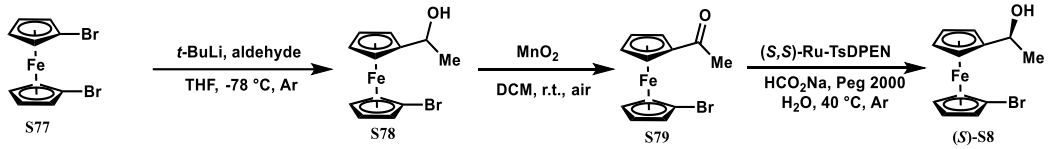
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 – 7.33 (m, 4H), 7.32 – 7.27 (m, 1H), 4.68 (dd, *J* = 8.2, 4.9 Hz, 1H), 4.17 – 4.07 (m, 8H), 4.07 (s, 1H), 2.82 – 2.71 (m, 2H), 2.36 (s, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.0, 128.2, 127.4, 125.7, 84.2, 75.0, 69.3, 68.8, 68.6, 67.9, 67.8, 40.2.

HRMS (ESI-TOF) m/z: $[M]^+$ Calcd for $C_{18}H_{18}FeO$ 306.0701; Found: 306.0703.

Chiral HPLC: The ee value was 97%, t_S (major) = 9.8 min, t_R (minor) = 10.6 min (Chiralpak IF, λ = 254 nm, 10% isopropanol/hexanes, flow rate = 1.0 mL/min).

2.4 Synthesis of compound S8



To a solution of *t*-butyllithium (3.3 mmol, 2.5 mL, 1.3 M in pentane) was added dropwise a solution of 1-1'-dibromoferrocene **S77** (3 mmol, 1.03 g) in anhydrous THF (20 mL) under argon atmosphere at -78 °C. The reaction was stirred for 0.5 h, then a solution of acetaldehyde (4.5 mmol, 0.25 mL) was added dropwise. The mixture was stirred at -78 °C for 4 h. Upon completion, the reaction was quenched with saturated aqueous NH_4Cl solution, extracted with EtOAc (3 × 50 mL), dried over Na_2SO_4, filtered, concentrated under reduced pressure. The residue was purified by flash column chromatography (petroleum ether/Ethyl acetate = 10/1) to afford the product **S78** (497 mg, 54% yield).

To an oven-dried 50 mL round bottom flask equipped with a stir was charged with **S78** (1.6 mmol, 497 mg) in anhydrous DCM (10.0 mL), activated MnO_2 (16mmol, 1.39 g) was added and the reaction was allowed to stirred at room temperature for overnight. Upon completion, the mixture was filtered through a Büchner funnel to remove manganese dioxide, followed by concentration of the filtrate under reduced pressure. The residue was purified by silica gel flash chromatography (petroleum ether/Ethyl acetate = 10/1) to afford **S79** (463 mg, 96% yield).

To an oven-dried 5.0 mL vial equipped with a stir was charged with [(*S*,*S*)-N-(2-Amino-1,2-diphenylethyl)-*p*-toluenesulfonamide]chloro(mesitylene)ruthenium(II) (0.01 mmol, 6 mg) in H_2O (1.0 mL), **S79** (1.0 mmol, 307 mg), sodium formate (5.0 mmol, 0.34 g) and PEG2000 (1.0 g) were added under argon atmosphere. Then, the reaction mixture was allowed to stirred at 40 °C for 24 h. Upon completion, Et_2O (10.0 mL) was added slowly to quench the reaction, and extracted three times with EtOAc, dry with anhydrous Na_2SO_4, and concentrated under reduced pressure. The residue was purified

by flash column on silica (petroleum ether/Ethyl acetate = 10:1) to afford the product (*S*)-**S8** (113 mg, 37% yield) and the ee value was determined by HPLC analysis.

TLC: R_f = 0.41 (petroleum ether/Ethyl acetate = 8/1); 113 mg, yield: 37%; yellow oil.

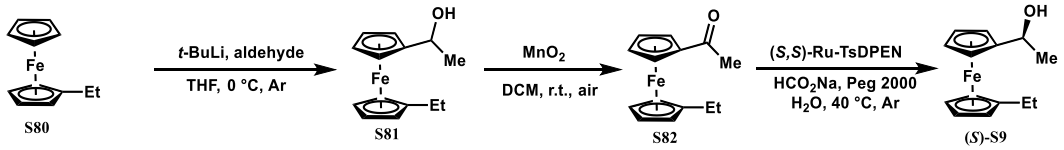
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.68 – 4.63 (m, 1H), 4.43 – 4.40 (m, 2H), 4.26 – 4.24 (m, 1H), 4.23 – 4.19 (m, 3H), 4.13 – 4.12 (m, 2H), 1.94 (d, *J* = 4.3 Hz, 1H), 1.46 – 1.44 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 96.2, 77.8, 70.5, 70.5, 70.4, 70.4, 68.5, 68.4, 67.4, 65.3, 24.1.

HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{12}H_{14}BrFeO$ 308.9566; Found: 308.9550.

Chiral HPLC: The ee value was 96%, t_S (major) = 6.5 min, t_R (minor) = 7.1 min (Chiralpak IC, λ = 254 nm, 10% isopropanol/hexanes, flow rate = 1.0 mL/min).

2.5 Synthesis of compound S9



To a solution of *t*-butyllithium (3.3 mmol, 2.5 mL, 1.3 M in pentane) was added dropwise a solution of ethylferrocene **S80** (3 mmol, 642 mg) in anhydrous THF (10 mL) under argon atmosphere at 0 °C. The reaction was stirred for 0.5 h, then a solution of acetaldehyde (4.5 mmol, 0.25 mL) was added dropwise and stirred at 0 °C for 4 h. Upon completion, the reaction was quenched with saturated aqueous NH_4Cl solution, extracted with EtOAc (3 × 50 mL), dried over Na_2SO_4, filtered, concentrated under reduced pressure. The residue was purified by flash column chromatography (petroleum ether/Ethyl acetate = 10/1) to afford the product **S81** (317 mg, 41% yield).

To an oven-dried 50 mL round bottom flask equipped with a stir was charged with **S81** (1.2 mmol, 317 mg) in anhydrous DCM (10.0 mL), activated MnO_2 (12 mmol, 1.04 g) was added and the reaction was allowed to stirred at room temperature for overnight. Upon completion, the mixture was filtered through a Büchner funnel to remove manganese dioxide, followed by concentration of the filtrate under reduced pressure. The residue was purified by silica gel flash chromatography (petroleum ether/Ethyl acetate = 10/1) to afford **S82** (291 mg, 95% yield).

To an oven-dried 5.0 mL vial equipped with a stir was charged with [(*S*,*S*)-N-(2-Amino-1,2-diphenylethyl)-*p*-toluenesulfonamide]chloro(mesitylene)ruthenium(II) (0.01 mmol, 6 mg) in H_2O (1.0 mL), **S82** (1.0 mmol, 258 mg), sodium formate (5.0 mmol, 0.34 g) and PEG2000 (1.0 g) were added under argon atmosphere. Then, the reaction mixture was allowed to stirred at 40 °C for 24 h. Upon completion, Et_2O (10.0 mL) was added slowly to quench the reaction, and extracted three times with EtOAc, dry with anhydrous Na_2SO_4, and concentrated under reduced pressure. The residue was purified by flash column on silica (petroleum ether/Ethyl acetate = 10:1) to afford the product (*S*)-**S8** (*S*)-**S9** (175 mg, 67% yield) and the ee value was determined by HPLC analysis.

TLC: R_f = 0.45 (petroleum ether/Ethyl acetate=8/1); 175 mg, yield: 67%; yellow oil.

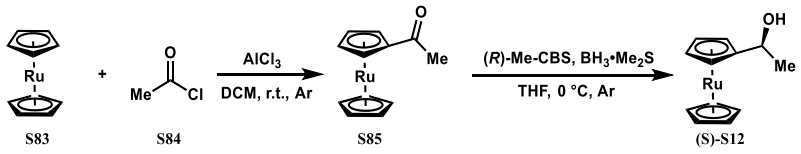
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.57 – 4.48 (m, 1H), 4.17 – 4.08 (m, 8H), 2.36 – 2.29 (m, 2H), 1.43 (dd, *J* = 6.5, 4.8 Hz, 3H), 1.16 (t, *J* = 7.5 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 95.0, 92.0, 69.1, 68.9, 68.9, 68.1, 68.1, 67.5, 66.8, 66.8, 65.4, 29.3 23.5, 22.0, 14.7.

HRMS (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{14}H_{18}FeONa$ 281.0593; Found: 281.0601.

Chiral HPLC: The ee value was 98%, t_S (major) = 13.8 min, t_R (minor) = 16.7 min (Chiralpak IC, λ = 254 nm, 3% isopropanol/hexanes, flow rate = 0.8 mL/min).

2.6 Synthesis of compound S12



In an argon-filled glovebox, to a 25 mL pressure-resistant sealed tube equipped with a stir was charged with aluminum trichloride (3.0 mmol, 402 mg) and ruthenocene **S83** (3.0 mmol, 693 mg) in DCM (10 mL), acetyl chloride **S84** (6.0 mmol, 471 mg) was added. The resulting solution was sealed, removed from the nitrogen filled dry box and the reaction mixture was allowed to stirred at 40 °C for 6 h. Upon completion, Et_2O (10.0 mL) was added slowly to quench the reaction and concentrated under reduced pressure. The residue was purified by flash column on silica (petroleum ether/Ethyl acetate = 10:1) to afford the product acetyl ruthenocene **S85** (274 mg, 33%).

To an oven-dried 50 mL round bottom flask equipped with a stir was charged with acetyl ruthenocene **S85** (1.3 mmol, 274 mg) in anhydrous THF (10.0 mL), (*R*)-Me-CBS (0.52 mmol, 144 mg) and BH_3•Me_2S (3.9 mmol, 1.45 mL, 2 M in THF) were added slowly *via* syringe at 0 °C. Then, the reaction mixture was stirred at 0 °C for 30 min and was allowed to stirred at room temperature for overnight. Upon completion, MeOH was added slowly to quench the reaction, and extracted three times with EtOAc, dry with anhydrous Na_2SO_4, and concentrated under reduced pressure. The residue was purified by flash column chromatography to obtain product (*S*)-**S12** (242 mg, 88%). The product **S12** exhibited improved enantioselectivity following recrystallization. The ee value was determined by HPLC.

TLC: R_f = 0.39 (petroleum ether/Ethyl acetate = 8/1); 242 mg, yield: 88%; white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 4.68 – 4.67 (m, 1H), 4.66 – 4.64 (m, 1H), 4.61 (s, 5H), 4.53 – 4.51 (m, 2H), 4.28 – 4.26 (m, 1H), 1.34 (d, *J* = 6.3 Hz, 3H).

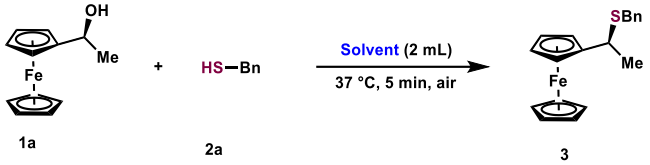
^{13}C NMR (101 MHz, $CDCl_3$) δ 100.7, 70.4, 70.2, 70.2, 69.8, 68.8, 63.7, 23.5.

HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{12}H_{15}ORu$ 277.0161; Found: 277.0158.

Chiral HPLC: The ee value was 93%, t_S (major) = 7.0 min, t_R (minor) = 7.6 min (Chiralpak IC, λ = 254 nm, 10% isopropanol/hexanes, flow rate = 1.0 mL/min).

3. Optimization of Reaction Conditions

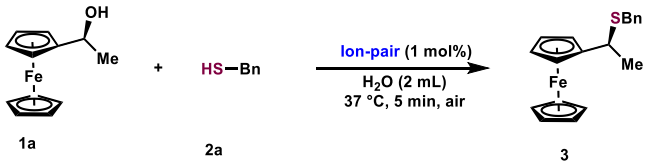
3.1 Table S1: Screening buffer as the reaction solvent



[a]Entry	**1a** (mmol)	**2a** (mmol)	Solvent	Yield (%)[b]
1	0.2	0.4	PB buffer pH = 6	n.r.
2	0.2	0.4	PB buffer pH = 7	n.r.
3	0.2	0.4	PB buffer pH = 8	n.r.
4	0.2	0.4	PB buffer pH = 9	n.r.
5	0.2	0.4	Tris-HCl buffer pH = 6	n.r.
6	0.2	0.4	Tris-HCl buffer pH = 7	n.r.
7	0.2	0.4	Tris-HCl buffer pH = 8	n.r.
8	0.2	0.4	Tris-HCl buffer pH = 9	n.r.

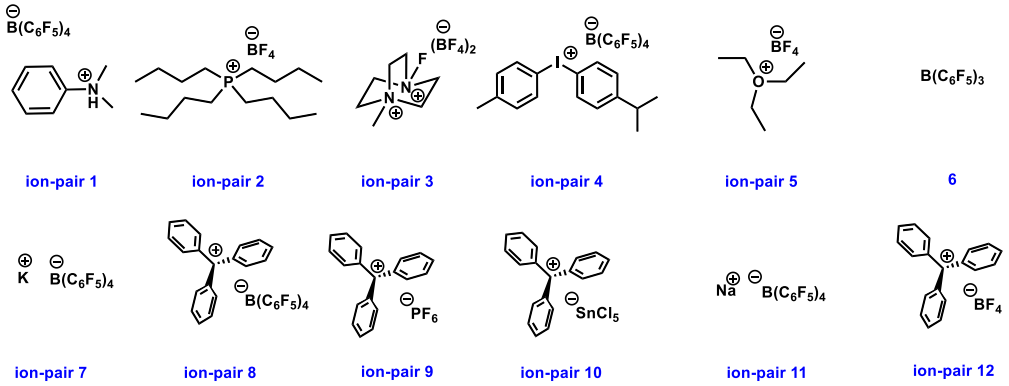
[a]Reaction conditions unless otherwise noted: **1a** (0.2 mmol) and **2a** (0.4 mmol) in buffer (2.0 mL) as solvent at 37 °C for 5 min under air. [b]n.r. = no reaction.

3.2 Table S2: Screening ion-pairs for the reaction

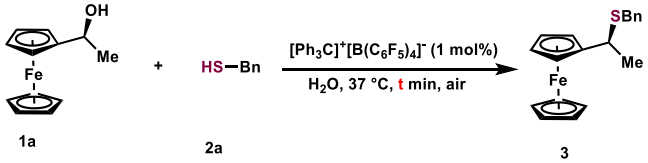


[a]Entry	**1a** (mmol)	**2a** (mmol)	Ion-pair (1 mol%)	Yield (%)[b]	Ee (%)[c]
1	0.2	0.4	ion-pair-1	98	98
2	0.2	0.4	ion-pair-2	n.r.	-
3	0.2	0.4	3	n.r.	-
4	0.2	0.4	ion-pair-4	15	98
5	0.2	0.4	ion-pair-5	n.r.	-
6	0.2	0.4	6	92	98
7	0.2	0.4	ion-pair-7	90	97
8	0.2	0.4	ion-pair-8	99	99
9	0.2	0.4	ion-pair-9	90	96
10	0.2	0.4	ion-pair-10	21	95
11	0.2	0.4	ion-pair-11	92	97
12	0.2	0.4	ion-pair-12	44	99

[a]Reaction conditions unless otherwise noted: **1a** (0.2 mmol), **2a** (0.4 mmol) and ion-pair (1 mol%) in H_2O (2.0 mL) at 37 °C for the 5 min under air. [b]Yields were determined by ^1H NMR with CH_2Br_2 as an internal standard. [c]Enantiomeric excess (Ee) was determined by HPLC on chiral stationary phases.



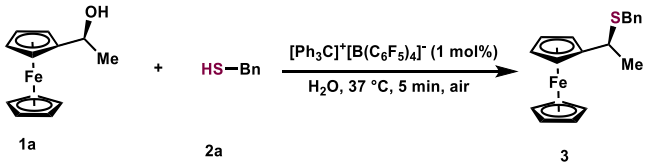
3.3 Table S3: Screening the reaction time



[a]Entry	**1a** (mmol)	**2a** (mmol)	Time (min)	Yield (%)[b]	Ee (%)[c]
1	0.2	0.4	1	88	98
2	0.2	0.4	3	95	98
3	0.2	0.4	5	97	99

[a]Reaction conditions unless otherwise noted: **1a** (0.2 mmol), **2a** (0.4 mmol) and $[Ph_3C]^+[B(C_6F_5)_4]^-$ (1 mol%) in H_2O (2.0 mL) at 37 °C for the indicated time under air. [b]Yields were determined by ^1H NMR with CH_2Br_2 as an internal standard.

3.4 Table S4: Screening the equivalent of 2a

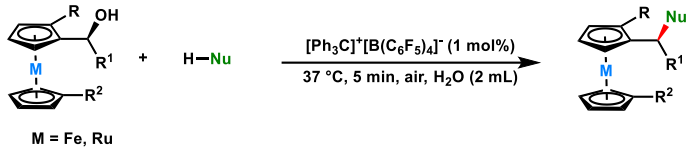


[a]Entry	**1a** (mmol)	**2a** (mmol)	t (min)	Yield (%)[b]	Ee (%)[c]
1	0.2	0.24	5	89	99
2	0.2	0.3	5	94	97
3	0.2	0.36	5	94	99
4	0.2	0.4	5	95	98

[a]Reaction conditions unless otherwise noted: **1a** (0.2 mmol), **2a** (x mmol) and $[Ph_3C]^+[B(C_6F_5)_4]^-$ (1 mol%) in H_2O (2.0 mL) at 37 °C for the 5 min under air. [b]Yield was determined by isolated yield.

4. Experimental Section

4.1 General Procedure Condition A



To a glass vials (10 mL) equipped with a magnetic stirrer, alcohols (0.2 mmol), $[Ph_3C]^+[B(C_6F_5)_4]^-$ (0.002 mmol, 1.8 mg) and nucleophiles (0.3 mmol) were added. Then, 2.0 mL H_2O were charged *via* syringe. Subsequently, the tube was sealed and the solution was stirred at 37 °C for 5 min. Upon completion of the reaction, the mixture was extracted with EtOAc (3 × 10 mL), dry with anhydrous Na_2SO_4, and concentrate under reduced pressure. The crude mixture was purified by flash column chromatography on silica gel to afford the products. For example, **1a** (0.2 mmol, 46 mg), $[Ph_3C]^+[B(C_6F_5)_4]^-$ (0.002 mmol, 1.8 mg) and **2a** (0.3 mmol, 37.3 mg) were added. Then, 2.0 mL H_2O were charged *via* syringe. Subsequently, the tube was sealed and the solution was stirred at 37 °C for 5 min. Upon completion of the reaction, the mixture was extracted with EtOAc (3 × 10 mL), dry with anhydrous Na_2SO_4, and concentrate under reduced pressure. The crude mixture was purified by flash column chromatography on silica gel (PE) to obtain product **3** as a yellow oil, 63 mg, 94% yield.

TLC: R_f = 0.68 (petroleum ether/Ethyl acetate = 20/1); 63 mg, yield: 94%; yellow oil. $[\alpha]_D^{23.8}$ = 8 (*c* = 1.0, $CHCl_3$).

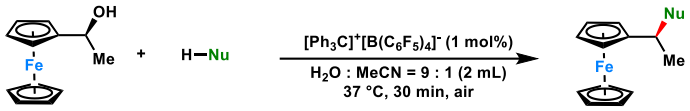
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 – 7.23 (m, 5H), 4.19 – 4.14 (m, 9H), 3.71 – 3.61 (m, 3H), 1.64 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 138.5, 128.8, 128.4, 126.8, 91.5, 68.6, 67.8, 67.7, 67.4, 65.9, 38.6, 35.5, 21.3.

HRMS (ESI-TOF) m/z: $[M+K]^+$ Calcd for $C_{19}H_{20}FeSK$ 375.0261; Found: 375.0274.

Chiral HPLC: The ee value was 99%, t_R (minor) = 6.3 min, t_S (major) = 7.3 min (Chiralpak IA, λ = 254 nm, 3% isopropanol/hexanes, flow rate = 0.8 mL/min).

4.2 General Procedure Condition B



To a glass vials (10 mL) equipped with a magnetic stirrer, *(S)*-1-ferrocenylethanol (0.2 mmol), $[Ph_3C]^+[B(C_6F_5)_4]^-$ (0.002 mmol, 1.8 mg) and nucleophiles (sulfonamides or indoles) (0.3 mmol) were added. Then, 0.2 mL MeCN and 1.8 mL H_2O were charged *via* syringe. Subsequently, the tube was sealed and the solution was stirred at 37 °C for 0.5 h. When the reaction was complete, the mixture was extracted with EtOAc (3 × 10 mL), dry with anhydrous Na_2SO_4, and concentrate under reduced pressure. The crude mixture was purified by flash column chromatography on silica gel to afford the products. For example, **1a** (0.2 mmol, 46 mg), $[Ph_3C]^+[B(C_6F_5)_4]^-$ (0.002 mmol, 1.8 mg) and **S56** (0.3 mmol, 43.2 mg) were added. Then, 0.2 mL MeCN and 1.8 mL H_2O were charged *via* syringe. Subsequently, the tube was sealed and the solution was stirred at 37 °C for 30 min. When the reaction was complete, the mixture was extracted with EtOAc (3 × 10 mL), dry with anhydrous Na_2SO_4, and concentrate under reduced pressure. The crude mixture was purified by flash column chromatography on silica gel (petroleum ether/Ethyl acetate=15/1) to obtain product **64** as a yellow solid, 41 mg, 60% yield.

TLC: R_f = 0.72 (petroleum ether/Ethyl acetate = 10:1); 41 mg, yield: 60%; yellow solid.

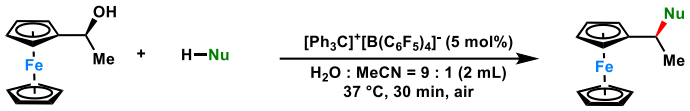
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 7.8 Hz, 1H), 7.44 (d, *J* = 8.2 Hz, 1H), 7.26 – 7.22 (m, 1H), 7.15 – 7.11(m, 1H), 6.81 (s, 1H), 5.53 (q, *J* = 6.9 Hz, 1H), 4.34 – 4.33 (m, 1H), 4.22 – 4.15 (m, 8H), 2.31 (d, *J* = 1.1 Hz, 3H), 1.83 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 135.7, 128.6, 122.4, 121.1, 119.0, 118.4, 110.1, 109.1, 89.6, 68.8, 68.4, 68.1, 67.5, 66.4, 50.4, 20.6, 9.7.

HRMS (ESI-TOF) m/z: $[M]^+$ Calcd for $C_{21}H_{21}FeN$ 343.1018; Found: 343.1021.

Chiral HPLC: The ee value was 95%, t_R (minor) = 19.0 min, t_S (major) = 21.1 min (Chiralpak IA, λ = 254 nm, 1% isopropanol/hexanes, flow rate = 0.2 mL/min).

4.3 General Procedure Condition C



To a glass vials (10 mL) equipped with a magnetic stirrer, *(S)*-1-ferrocenylethanol (0.2 mmol), $[Ph_3C]^+[B(C_6F_5)_4]^-$ (0.01 mmol, 9.2 mg) and heterocyclics or other nucleophiles (0.4 mmol) were added. Then, 0.2 mL MeCN and 1.8 mL H_2O were charged *via* syringe. Subsequently, the tube was sealed and the solution was stirred at 37 °C for 0.5 h. When the reaction was complete, the mixture was extracted with EtOAc (3 × 10 mL), dry with anhydrous Na_2SO_4, and concentrate under reduced pressure. The crude mixture was purified by flash column chromatography on silica gel to afford the heterocyclics. For example, **1a** (0.2 mmol, 46 mg), $[Ph_3C]^+[B(C_6F_5)_4]^-$ (0.01 mmol, 9.2 mg) and **S62** (0.3 mmol, 63 mg) were added. Then, 0.2 mL MeCN and 1.8 mL H_2O were charged *via* syringe. Subsequently, the tube was sealed and the solution was stirred at 37 °C for 30 min. When the reaction was complete, the mixture was extracted with EtOAc (3 × 10 mL), dry with anhydrous Na_2SO_4, and concentrate under reduced pressure. The crude mixture was purified by flash column chromatography on silica gel (petroleum ether/Ethyl acetate=15/1) to obtain product **55** as a yellow solid, 65 mg, 77% yield.

TLC: R_f = 0.46 (petroleum ether/Ethyl acetate = 8/1); 65 mg, yield: 77%; yellow solid.

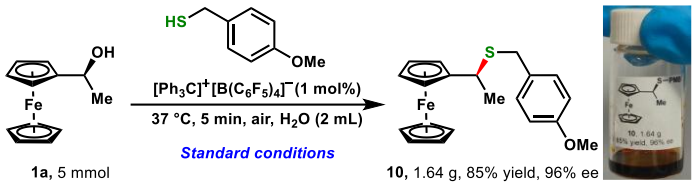
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (s, 1H), 7.87 (s, 1H), 7.28 (s, 1H), 5.67 (q, *J* = 7.0 Hz, 1H), 4.29 (d, *J* = 1.9 Hz, 1H), 4.16 (t, *J* = 2.1 Hz, 2H), 4.13 (s, 6H), 2.51 (s, 3H), 1.92 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 138.0, 135.2, 131.5, 124.0, 117.1, 110.4, 89.1, 68.8, 68.4, 67.8, 67.6, 66.5, 54.6, 24.2, 20.0.

HRMS (ESI-TOF) m/z: $[M+K]^+$ Calcd for $C_{20}H_{19}BrFeN_2K$ 460.9707; Found: 460.9708.

Chiral HPLC: The ee value was 99%, t_S (major) = 6.7 min, t_R (minor) = 12.8 min (Chiralcel OD-H, λ = 254 nm, 15% isopropanol/hexanes, flow rate = 1.0 mL/min).

4.4 Gram Scale Reaction



To a well-dried Schlenk tube (250 mL) equipped with a magnetic stir bar, *(S)*-1-ferrocenylethanol (5 mmol, 1.15 g), $[Ph_3C]^+[B(C_6F_5)_4]^-$ (0.05 mmol, 45 mg) and *p*-methoxybenzyl mercaptan (7.5 mmol, 1.16 g) were added. Then, 50 mL H_2O were charged *via* syringe. Subsequently, the tube was sealed and the solution was stirred at 37 °C for 5 min. When the reaction was complete, the mixture was extracted with EtOAc (3 × 150 mL), dry with anhydrous Na_2SO_4, and concentrate under reduced pressure. The crude mixture was purified by flash column chromatography on silica gel (petroleum ether/Ethyl acetate 20:1) to obtain product **10** as a yellow oil, 1.64 g, 85% yield, 96% ee.

5. Mechanistic Study

5.1 Competition experiments of 1a with 2a and 2c

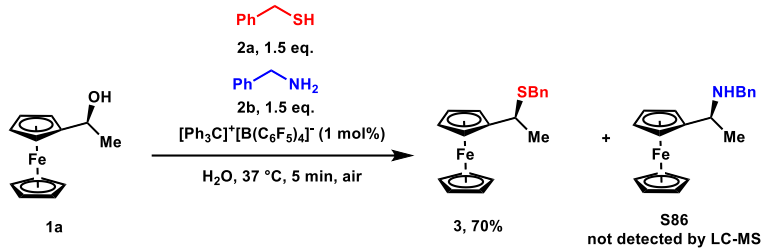


Figure S1. Competition experiments of **1a** with **2a** and **2b**.

General procedure of the reaction shown in Figure **S1**: To a glass vial (10 mL) equipped with a magnetic stirrer, 2.0 mL H_2O was added to the mixture of **1a** (0.2 mmol), $[Ph_3C]^+[B(C_6F_5)_4]^-$ (0.002 mmol, 1.8 mg), **2a** (0.3 mmol) and **2b** (0.3 mmol). Subsequently, the tube was sealed and the solution was stirred at 37 °C for 5 minutes. Upon completion of the reaction, the mixture was extracted with EtOAc (3 × 10 mL), dry with anhydrous Na_2SO_4, and concentrate under reduced pressure. The residue was purified by silica flash column chromatography to obtain the pure product **3** (47 mg, 70% yield). However, **S86** was not detected by LC-MS.

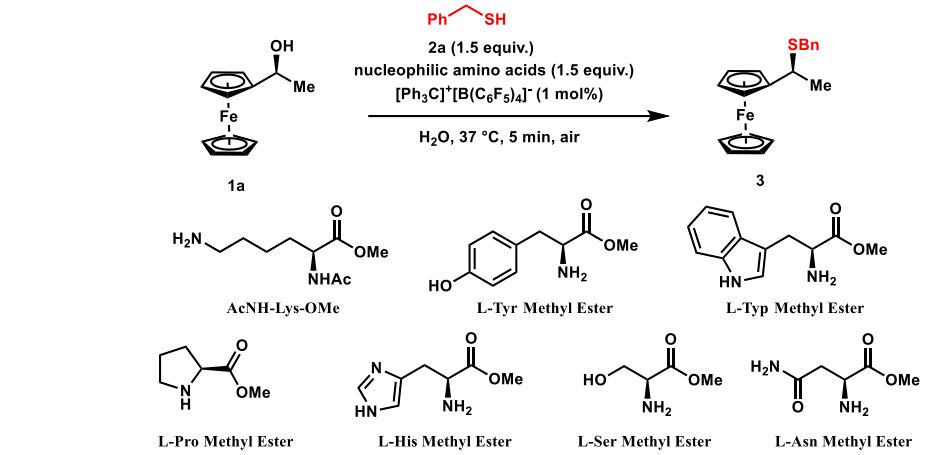
***(S)*-1-(benzylthio)ethylferrocene (3)**

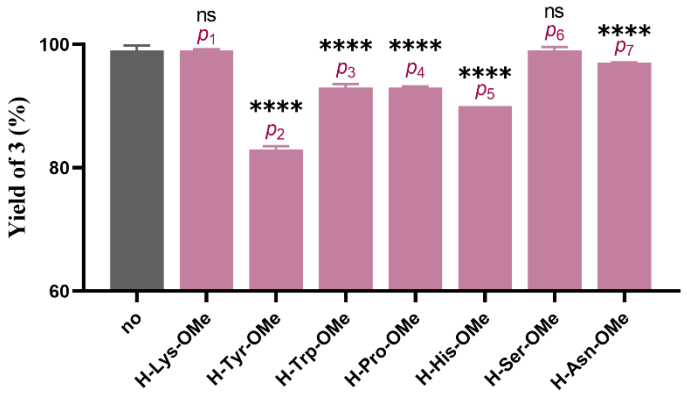
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 – 7.23 (m, 5H), 4.19 – 4.14 (m, 9H), 3.71 – 3.61 (m, 3H), 1.64 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 138.5, 128.8, 128.4, 126.8, 91.5, 68.6, 67.8, 67.7, 67.4, 65.9, 38.6, 35.5, 21.3.

HRMS (ESI-TOF) m/z: $[M+K]^+$ Calcd for $C_{19}H_{20}FeSK$ 375.0261; Found: 375.0274.

5.2 Chemo-selectivity of 1a conjugating with 2a in the presence of nucleophilic amino acids



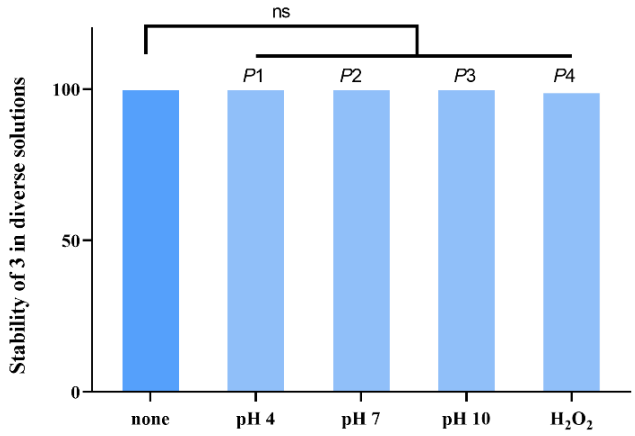


P	value
P_1	>0.9999
P_2	<0.0001
P_3	<0.0001
P_4	<0.0001
P_5	<0.0001
P_6	>0.9999
P_7	0.0004

Figure S2. Chemo-selectivity of **1a** towards various nucleophiles. Statistical significance between the two groups was calculated *via* a Tukey post-hoc test: ns, $p > 0.05$. The mean values and SD are presented (n = 3 independent times).

General procedure of the reaction shown in Figure **S2**: To a glass vial (10 mL) equipped with a magnetic stir bar, 2 mL of H_2O was added to the mixture of **1a** (23 mg, 0.1 mmol), **2a** (18.6 mg, 0.15 mmol, 1.5 equiv.) and $[Ph_3C]^+[B(C_6F_5)_4]^-$ (0.002 mmol, 1.8 mg), respectively. Afterwards, the corresponding nucleophilic amino acid (0.15 mmol, 1.5 equiv.) was added. After stirring for 5 min at 37 °C, the reaction was quenched and extracted with EtOAc. Then, the organic phases were collected and concentrated under reduced pressure. The crude ^{1}H-NMR was analyzed to determine the yields of **3** using CH_2Br_2 as the internal standard.

5.3 Studies on stability of 3 under various conditions



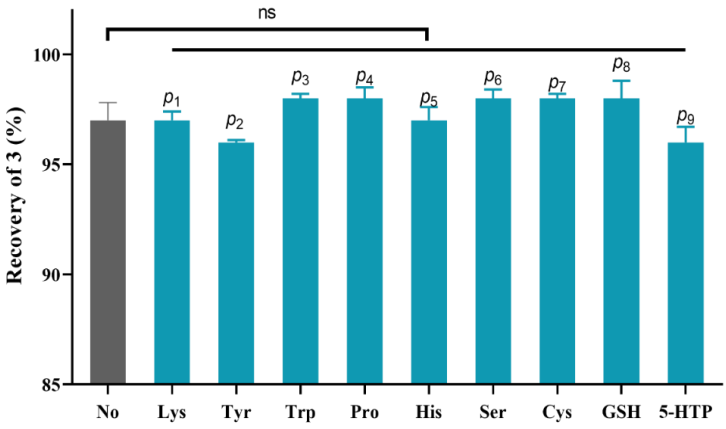
P	value
P_1	0.9457
P_2	0.8564
P_3	0.9913
P_4	0.9643

Figure S3. Stability of **3** under various conditions.

Stability of 3 under various conditions. Statistical significance between the two groups was calculated via a Tukey post-hoc test, ns means no significance, $p > 0.05$. The mean values and SD are presented (n = 3 independent times).

General procedure of the reaction shown in Figure **S3**: To a glass vials (10 mL) equipped with a magnetic stir bar, 2 mL of the depicted solution was added and mixed with **3** (0.05 mmol, 16.8 mg, 1.0 equiv. After stirring for 24 hours at 37 ℃. Subsequently, the mixture was extracted with EtOAc (3 × 5 mL). The organic layer was washed with brine and dried over anhydrous sodium sulfate and concentrated under the reduced pressure to obtain the crude samples. The yield was determined by ^{1}H NMR analysis with CH_2Br_2 as an internal standard.

General procedure of the reaction shown in Figure S4: To 10 mL reaction tube, 2 mL of H_2O was added to the mixture of **3** (16.8 mg, 0.05 mmol, 1.0 equiv.) and different endogenous molecules (0.05 mmol, 1.0 equiv.). After stirring for 24 hours at 37 °C, the reaction was quenched and extracted with EtOAc. Then, the organic phases were collected and concentrated under reduced pressure. The crude ^{1}H-NMR was analyzed to determine the yields of **3** using CH_2Br_2 as the internal standard.

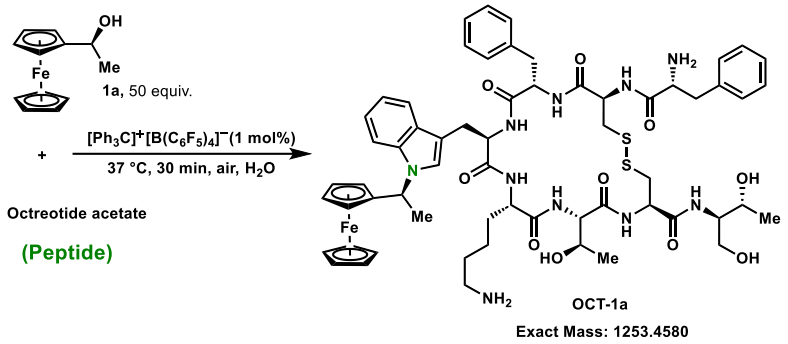


P	value
P_1	>0.9999
P_2	0.6369
P_3	>0.9999
P_4	>0.9999
P_5	>0.9999
P_6	>0.9999
P_7	>0.9999
P_8	0.8776
P_9	>0.9999
P_{10}	>0.9999

Figure S4. Stability of **3** in the presence of endogenous molecules. Statistical significance between the two groups was calculated *via* a Tukey post-hoc test: ns, > 0.05. The mean values and SD are presented (n = 3 independent times).

5.4 Modification of peptides Octreotide acetate

*General procedure for reactions of peptides Octreotide acetate with **1a***: To a 10 mL reaction tube, **1a** (57.5 mg, 250 μmol, 50 equiv.), Octreotide acetate (6.0 mg, 5 μmol), $[Ph_3C]^+[B(C_6F_5)_4]^-$ (0.5 mg, 0.05 μmol, 0.1 equiv.) and H_2O (2.0 mL) were added. After slow stirring at 37 °C for 30 minutes, a 20 μL aliquot of the reaction mixture was evaluated by performing ESI-MS, obtain the product OCT-**1a**.



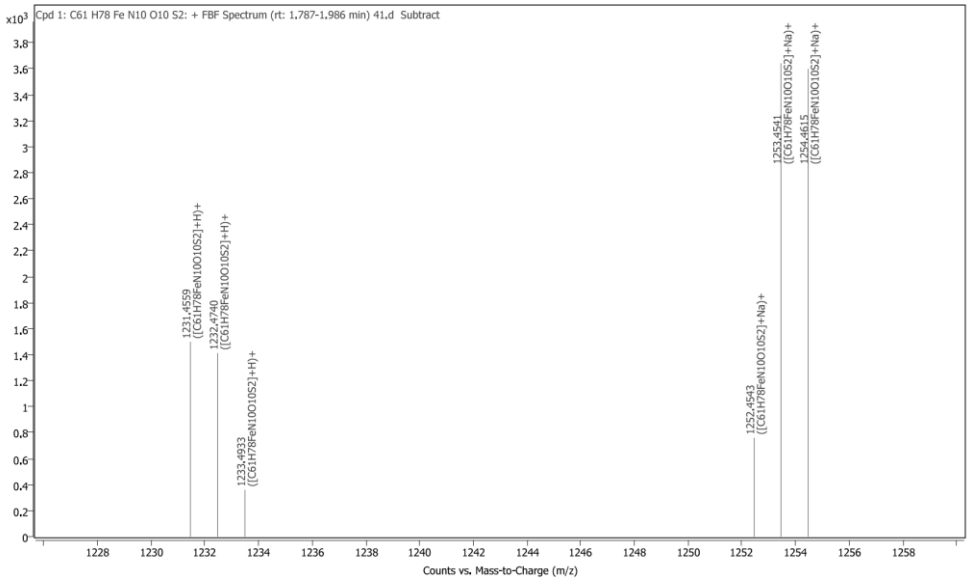


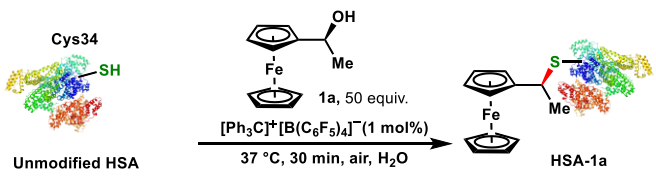
Figure S5. Showing HRMS of the peptide Octreotide acetate modified with **1a**.

5.5 Modification of Human Serum Albumin protein

ESI-MS was performed on a linear quadrupole ion trap detector mass spectrometer (LC/Q-TOF from Agilent). Data were processed using Agilent BioConfirm 12.1. Data were processed using Thermo BioPharma Finder 3.1. Albumin from human serum was purchased from Sigma-Aldrich (catalog No.: A3782). Protein was used without further purification. Sequence of albumin from human serum (HSA): HSA is composed of 585 amino acids and contains one free cysteine (Cys34) and 60 lysines.

DAHKSEVAHRFKDLGEENFKALVLIAFAQYLQQCPFEDHVKLVNEVTEFAKTCVAD
ESAENCDKSLHTLFGDKLCTVATLRETYGEMADCCAKQEPERNECFLQHKDDNPNL
PRLVRPEVDVMCTAFHDNEETFLKKYLYEIARRHPYFYAPELLFFAKRYKAAFTECC
QAADKAACLLPKLDELRDEGKASSAKQRLKCASLQKFGERAFKAWAVARLSQRFPK
AEFAEVSKLVTDLTKVHTECCHGDLLECADDRADLAKYICENQDSISSKLKECCEKP
LLEKSHCIAEVENDEMRADLPSLAADFVESKDVCKNYAEAKDVFLGMFLYEYARRH
PDYSVVLLLRLAKTYETTLEKCCAAADPHECYAKVFDEFKPLVEEPQNLIKQNCELF
EQLGEYKFQNALLVRYTKKVPQVSTPTLVEVSRNLGKVGSKCCKHPEAKRMPCAED
YLSVVLNQLCVLHEKTPVSDRVTKCCTESLVNRRPCFSALEVDETYVPKEFNAETFTF
HADICTLSEKERQIKKQTALVELVKHKPKATKEQLKAVMDDFAAFVEKCCKADDKE
TCFAEEGKKLVAASQAALGL

*General procedure for reactions of HSA with **1a*****:** To a 10 mL reaction tube, **1a** (3.4 mg, 15 μmol, 50 equiv.), albumin from human serum (HSA) (19.9 mg, 0.3 μmol), $[Ph_3C]^+[B(C_6F_5)_4]^-$ (0.13 mg, 0.003 μmol, 0.01 equiv.) and H_2O (4.0 mL) were added. After slow stirring at 37 °C for 30 minutes, a 20 μL aliquot of the reaction mixture was evaluated by performing ESI-MS, obtain the product HSA-**1a**.



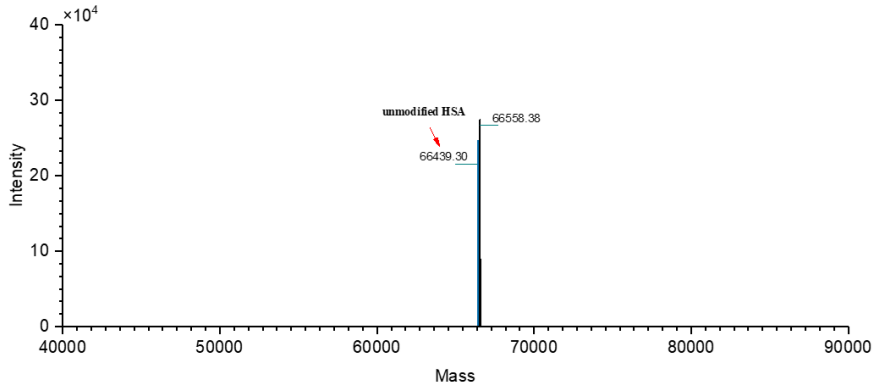


Figure S6. Deconvoluted mass spectrum of unmodified HSA.

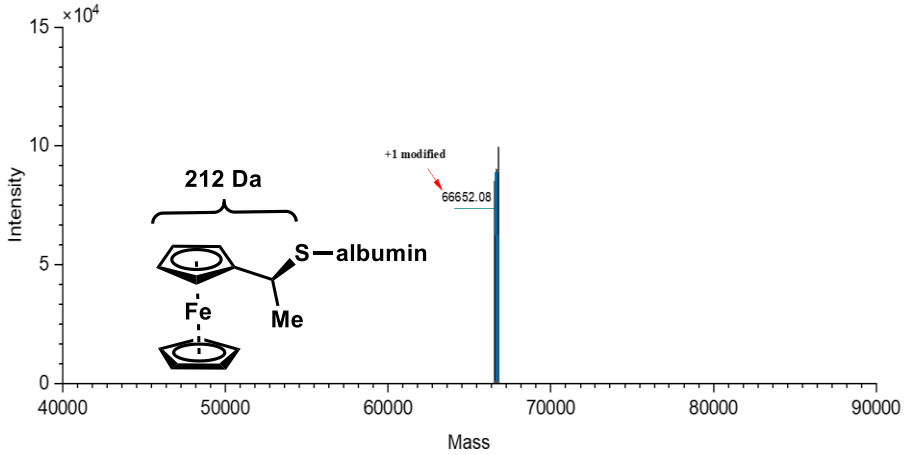


Figure S7. Modification results of HSA with **1a** in H_2O: +1 modified = singly modified protein.

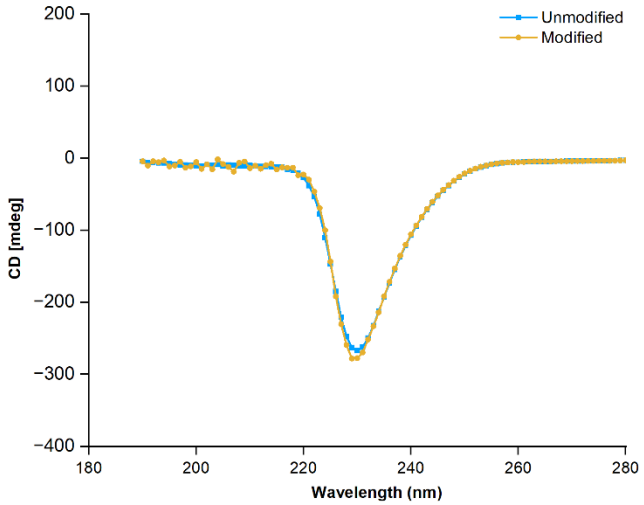


Figure S8. The CD spectra of native HSA and modified HSA with **1a**. The HSA concentrations were 0.5 mg/mL. All spectra were measured at 20 °C with 1 cm path length.

5.6 Proton scavenging experiment

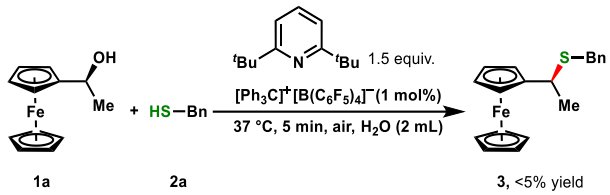


Figure S9. Proton scavenging experiment with 2,6-di-*tert*-butylpyridine.

To an over-dried reaction tube (10 mL) equipped with a magnetic stir bar, **1a** (0.2 mmol, 46 mg), 2,6-di-*tert*-butylpyridine (57.3 mg, 0.3 mmol), **2a** (0.3 mmol, 37.3 mg) and $[Ph_3C]^+[B(C_6F_5)_4]^-$ (0.002 mmol, 1.8 mg) were added. Then, 2.0 mL H_2O were charged *via* syringe. Subsequently, the tube was sealed and the solution was stirred at 37 °C for 5 min. Then, the mixture was extracted with EtOAc (3 × 10 mL), dry with anhydrous Na_2SO_4, and concentrate under reduced pressure. The filtrate was concentrated under reduced pressure and the residue was analyzed by ^1H NMR. The result showed that the yield of **3** was down to less than 5%, which indicated the possible involvement of Brønsted acid achieving this sustainable process.

5.7 The linear effect of substrate (*S*)-1a

To an over-dried reaction tube (10 mL) equipped with a magnetic stir bar, varying optical purity **1a** (0.2 mmol, 46 mg), **2a** (0.3 mmol, 37.3 mg) and $[Ph_3C]^+[B(C_6F_5)_4]^-$ (0.002 mmol, 1.8 mg) were added. Then, 2.0 mL H_2O were charged *via* syringe. Subsequently, the tube was sealed and the solution was stirred at 37 °C for 5 min. Upon completion of the reaction, the mixture was extracted with EtOAc (3 × 10 mL), dry with anhydrous Na_2SO_4, and concentrate under reduced pressure. The filtrate was concentrated under reduced pressure and the residue was analyzed by HPLC. The studies of nonlinear effect using standard condition with varying optical purity **1a** resulted in a linear correlation between the the ee values of **1a** and **3**. This observation suggests that the chirality of the product is exclusively determined by the substrate and remains stereochemically stable throughout the reaction process, with no observed racemization.

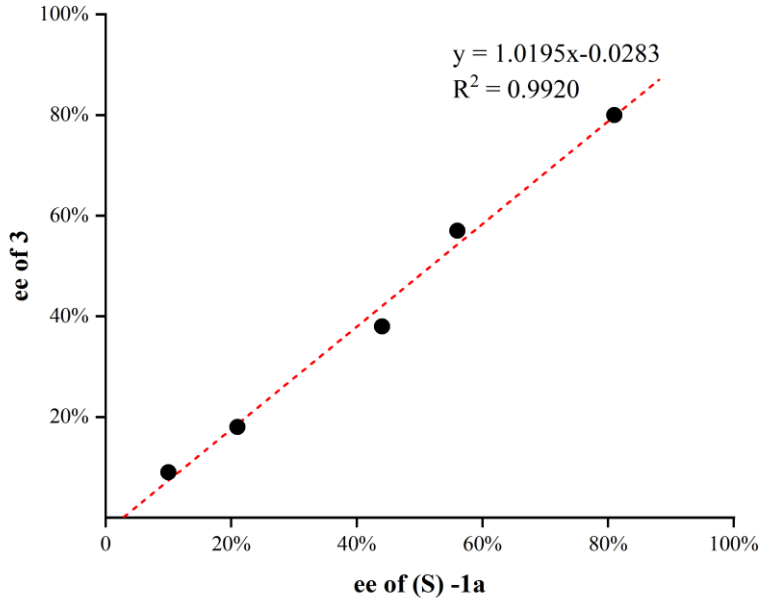


Figure S10. The linear effect of substrate (*S*)-**1a**.

5.8 The stability of 3 at varying time intervals

To an over-dried reaction tube (10 mL) equipped with a magnetic stir bar, **1a** (0.2 mmol, 46 mg), **2a** (0.3 mmol, 37.3 mg) and $[Ph_3C]^+[B(C_6F_5)_4]^-$ (0.002 mmol, 1.8 mg) were added. Then, 2.0 mL H_2O were charged *via* syringe. After stirring for 5–25 minutes at 37 °C, the mixture was extracted with EtOAc (3 × 10 mL), dry with anhydrous Na_2SO_4, and concentrate under reduced pressure. The filtrate was concentrated under reduced pressure and enantiomeric excess (ee) was determined by HPLC.

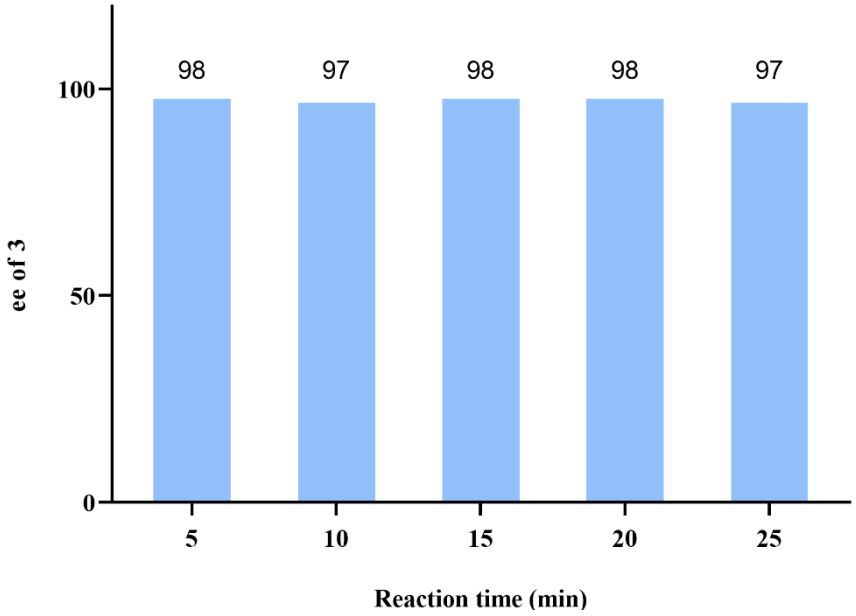


Figure S11. The stability of **3** at the reaction duration.

To an over-dried reaction tube (10 mL) equipped with a magnetic stir bar, **1a** (0.2 mmol, 46 mg) and $[Ph_3C]^+[B(C_6F_5)_4]^-$ (0.002 mmol, 1.8 mg) were added. Then, 2.0 mL H_2O were charged *via* syringe. After stirring for 0.5–72 hours at 37 °C, **2a** (0.3 mmol, 37.3 mg) was added. After stirring 5 min at 37 °C, the mixture was extracted with EtOAc (3 × 10 mL), dry with anhydrous Na_2SO_4, and concentrate under reduced pressure. The filtrate was concentrated under reduced pressure by ^1H NMR and enantiomeric excess (ee) was determined by HPLC.

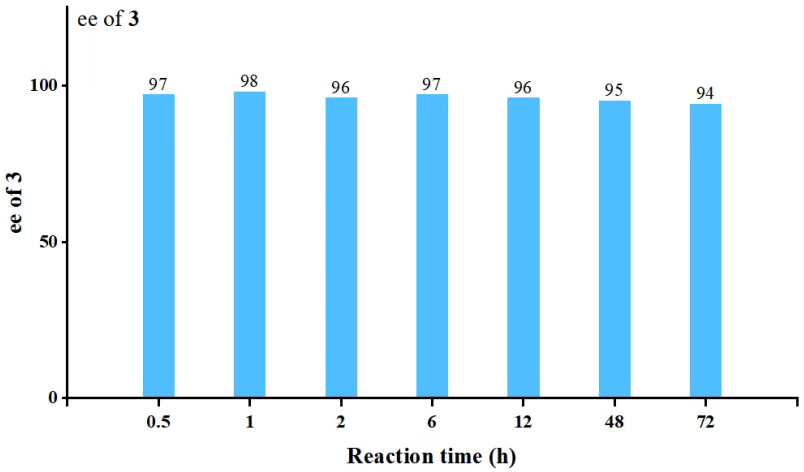


Figure S12. The stability of product **3** under the sequential addition protocol involving **2a**.

The results indicate that neither the reaction duration nor the sequential addition protocol, specifically, the addition of (*S*)-1-ferrocenylethanol (**1a**) followed by catalyst introduction and subsequent addition of substrate **2a** at varying time intervals, affects the enantiomeric excess (ee) of product **3**. This observation confirms the configurational stability of product **3** under the reaction conditions and its resistance to racemization.

5.9 DFT Calculations

Computational details

All density functional theory (DFT) calculations were carried out with the Gaussian 16 program package,[6] and the structures were illustrated by CYLview20[7] (Figure S13). The geometry optimizations were carried out for all molecules using the B3PW91 functional.[8,9] 6-31G**[10] basis set was used for C, H, O, F, B and S atoms, while the effective core potential (ECPs) of Dolg with a corresponding basis set was used for Fe atom.[11,12] To take long range interactions into account, the Grimme's D3 dispersion corrections and Becke-Johnson damping (DFT-D3BJ) were employed.[13] The effects of solvation in water were accounted for implicitly using the SMD polarizable continuum model.[14] Intrinsic reaction coordinate (IRC)[15] calculations were conducted to verify the critical reaction steps involved in our proposed mechanisms. The energetic results were further improved by the single-point calculations at the M06-2X+D3[16] /6-311++G** [17] /SMD.

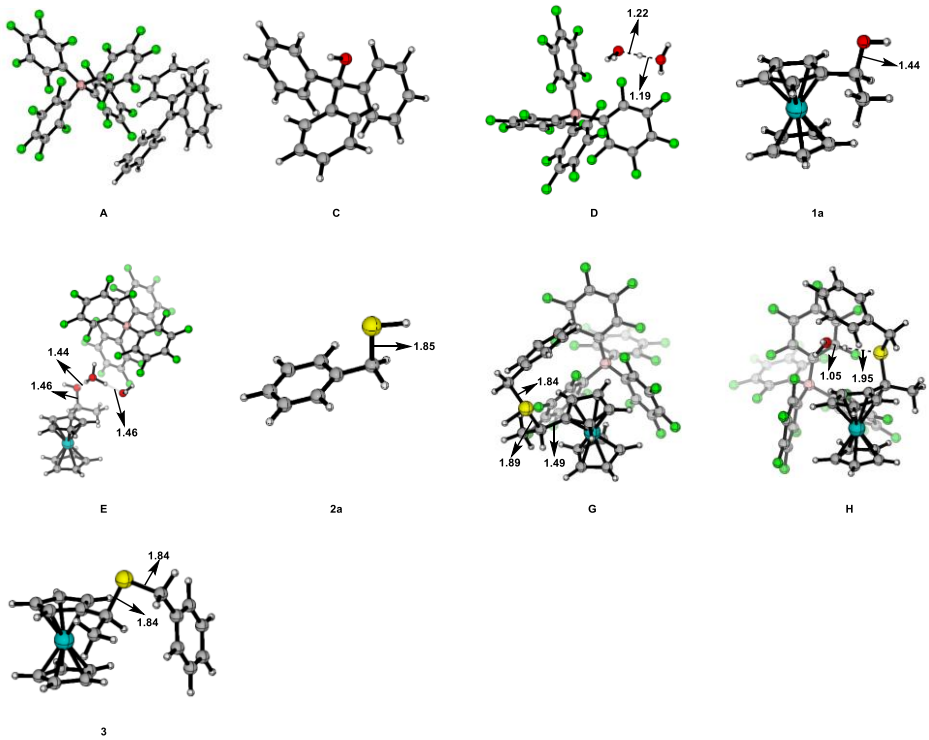


Figure S13. Computed structures of **A**, **C**, **D**, **1a**, **E**, **2a**, **G**, **H**, **3** selected bond distance is given in Å (color code, C: grey, Fe: blue, O: red, H: white, F: green, S: yellow, B: pink).

To begin with, the addition of H_2O to triphenyl carbenium ion-pair **A** affording the triphenylmethanol and tetrakis-(pentafluorophenyl)-boric acid was investigated (Figure S14).

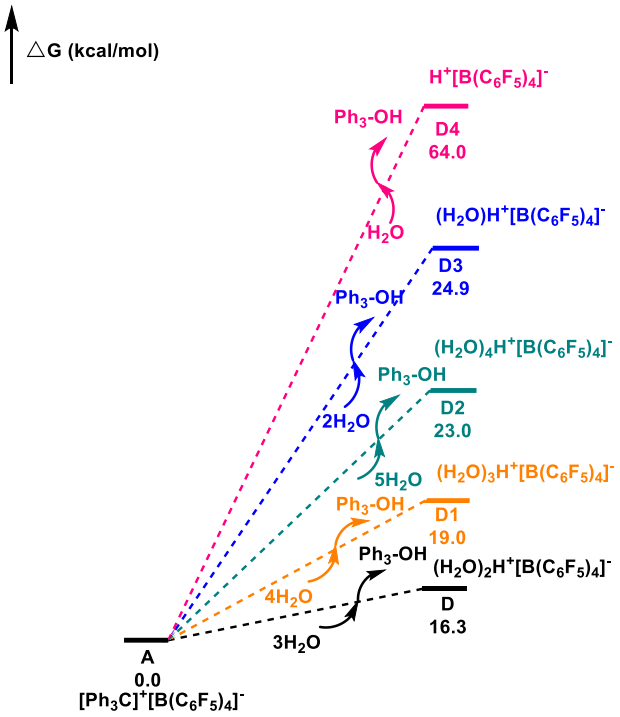


Figure S14. Computed energy profiles (DFT, M06-2X+D3/6-311++G**/SMD//B3PW91 +D3BJ/6-31G**/SMD and ECP basis set was used for Fe atom) for the addition of H_2O to $[Ph_3C]^+[B(C_6F_5)_4]^-$ (**A**).

Our investigation of water-mediated proton transfer from intermediate **G** revealed that the process employing one molecule of water exhibits the lowest energy barrier (Figure S15).

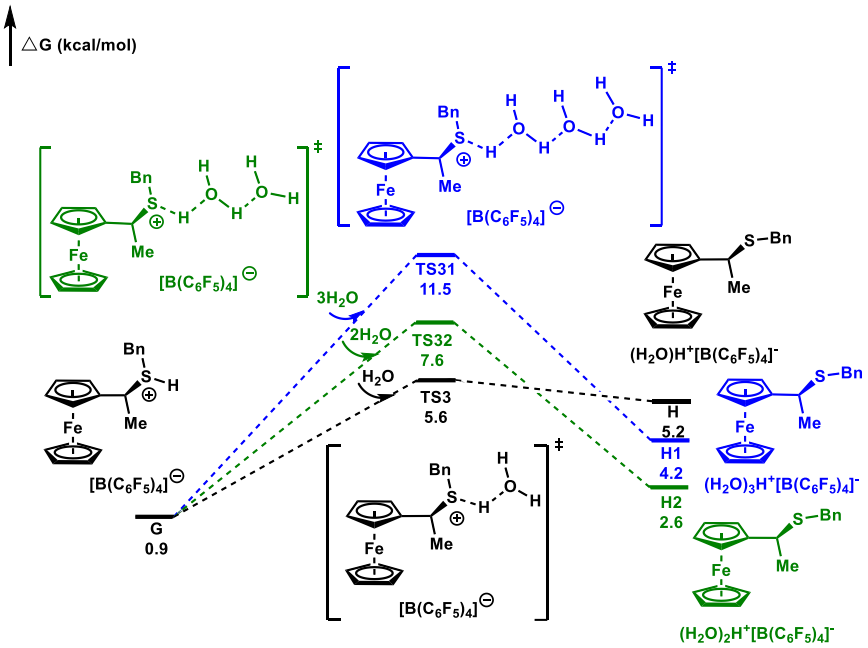


Figure S15. Computed energy profiles (DFT, M06-2X+D3/6-311++G**/SMD//B3PW91 +D3BJ/6-31G**/SMD and ECP basis set was used for Fe atom) for the addition of H_2O to intermediate **G**.

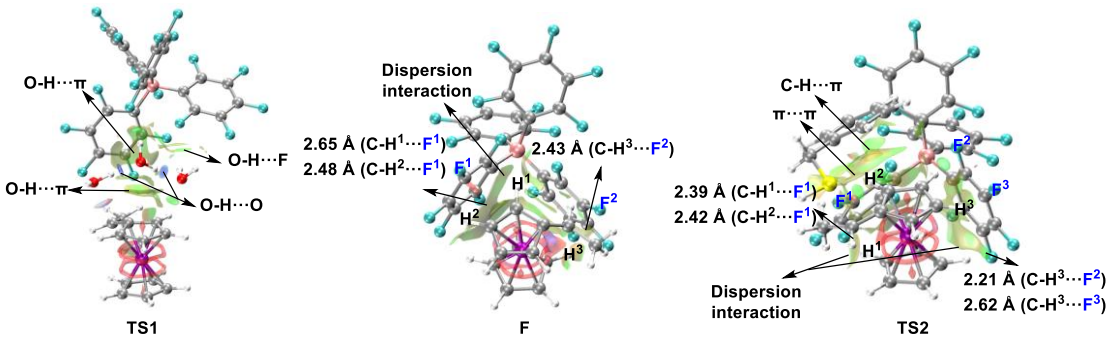


Figure S16. IGMH analysis of the non-covalent interactions. A green isosurface represents the dispersion interactions; a blue isosurface represents the hydrogen-bond interactions.

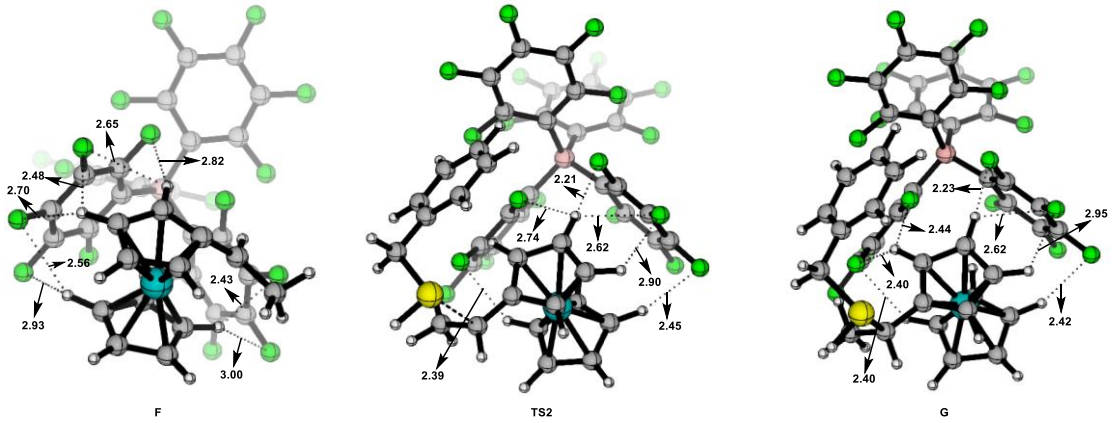


Figure S17. Computed structures of **F, TS2, G**, The distances for the C–H···F dispersion interactions are given in Å (color code, C: grey, Fe: blue, H: white, F: green, S: yellow, B: pink).

Coordinates and energies (hartree) of the calculated structures at the M06-2X+D3/6-311++G**/SMD//B3PW91+D3BJ/6-31G**/SMD and ECP basis set was used for Fe atom level.

A

Free energy: -3668.547485

C	4.356228000	-0.140583000	-0.314896000
C	3.749774000	-1.240862000	-1.028630000
C	3.358388000	-1.099234000	-2.377529000
C	3.521463000	-2.467549000	-0.364857000
C	2.781737000	-2.166213000	-3.047265000
H	3.553243000	-0.166824000	-2.894963000
C	2.900567000	-3.510682000	-1.031977000
H	3.776841000	-2.561656000	0.683748000
C	2.541680000	-3.365475000	-2.374210000
H	2.503633000	-2.061949000	-4.089732000
H	2.691152000	-4.437673000	-0.508591000
H	2.067635000	-4.190574000	-2.896845000
C	3.869746000	1.196450000	-0.518005000
C	2.519992000	1.391738000	-0.894867000
C	4.690195000	2.328300000	-0.296799000
C	2.000175000	2.668692000	-1.013145000
H	1.882410000	0.527707000	-1.015046000
C	4.163362000	3.601855000	-0.427004000
H	5.741908000	2.193374000	-0.070500000
C	2.818806000	3.773955000	-0.771758000
H	0.953576000	2.804796000	-1.261323000
H	4.798097000	4.467234000	-0.268834000
H	2.409251000	4.775768000	-0.855710000
C	5.418936000	-0.415260000	0.617470000
C	5.594388000	0.370064000	1.780074000
C	6.296692000	-1.499867000	0.381069000
C	6.612216000	0.075595000	2.671456000
H	4.890360000	1.160752000	2.002075000
C	7.324983000	-1.770865000	1.268133000
H	6.189895000	-2.084036000	-0.525941000
C	7.481112000	-0.988091000	2.414927000
H	6.724394000	0.664813000	3.575426000
H	8.010472000	-2.587494000	1.068050000
H	8.281456000	-1.210446000	3.113959000
C	-3.073082000	0.588016000	0.757725000
C	-4.247318000	0.522147000	0.007601000
C	-3.264240000	0.963552000	2.083957000
C	-5.506227000	0.835257000	0.497650000
C	-4.508439000	1.286089000	2.620429000
C	-5.639859000	1.224994000	1.823548000
C	-0.336597000	0.453394000	0.965420000
C	-0.126443000	1.786686000	1.315777000
C	0.695469000	-0.402544000	1.341434000
C	0.971764000	2.245673000	2.026467000
C	1.806424000	0.008960000	2.075026000
C	1.943996000	1.341782000	2.426292000
C	-1.951587000	-1.550877000	-0.015213000
C	-2.287306000	-2.265695000	-1.161517000
C	-2.032802000	-2.293530000	1.162983000
C	-2.628304000	-3.615892000	-1.154908000
C	-2.365402000	-3.638652000	1.218328000
C	-2.667457000	-4.311560000	0.042304000
C	-1.338684000	0.776268000	-1.363569000
C	-1.857614000	1.983592000	-1.823230000
C	-0.343076000	0.236821000	-2.175883000
C	-1.439211000	2.601568000	-2.999496000
C	0.105527000	0.813743000	-3.354648000
C	-0.451384000	2.014575000	-3.773428000
F	0.681005000	-1.708283000	1.015064000
F	2.752217000	-0.873798000	2.428822000
F	3.007628000	1.763317000	3.121313000
F	1.112332000	3.546367000	2.311438000
F	-1.027409000	2.722231000	0.960124000
F	-1.777560000	-1.701998000	2.346751000
F	-2.406978000	-4.289179000	2.389195000
F	-2.994614000	-5.607489000	0.066537000
F	-2.929250000	-4.244831000	-2.299686000
F	-2.309106000	-1.683514000	-2.375211000
F	-4.195954000	0.134487000	-1.282066000
F	-6.588971000	0.760011000	-0.288287000
F	-6.841566000	1.530742000	2.323045000
F	-4.619526000	1.648521000	3.906027000
F	-2.237579000	1.034732000	2.952350000
F	0.266936000	-0.906624000	-1.799907000
F	1.072739000	0.243936000	-4.086214000
F	-0.037221000	2.595164000	-4.903487000
F	-1.988570000	3.759439000	-3.389918000
F	-2.814520000	2.643479000	-1.145964000
B	-1.668432000	0.065563000	0.080691000

B

Free energy: -76.431055

O	0.000000000	0.000000000	0.120241000
H	0.000000000	0.754776000	-0.480965000
H	0.000000000	-0.754776000	-0.480965000

C

Free energy: -808.510313

C	0.035120000	-0.016758000	0.720538000
C	-0.306403000	1.390175000	0.231134000
C	0.269755000	1.930429000	-0.920448000
C	-1.276826000	2.128980000	0.915872000
C	-0.111167000	3.192407000	-1.376474000
H	1.021338000	1.366491000	-1.463272000
C	-1.650388000	3.392333000	0.466102000
H	-1.740118000	1.710227000	1.802991000
C	-1.068610000	3.929291000	-0.683085000
H	0.347246000	3.599304000	-2.273114000
H	-2.400371000	3.957470000	1.012079000
H	-1.361529000	4.914140000	-1.034843000
C	1.428908000	-0.454662000	0.266844000
C	1.667218000	-1.594742000	-0.500303000
C	2.521225000	0.314071000	0.692954000
C	2.971076000	-1.954583000	-0.848215000
H	0.838368000	-2.210270000	-0.831691000
C	3.819274000	-0.041622000	0.345770000
H	2.344135000	1.198016000	1.297998000
C	4.049055000	-1.180006000	-0.430313000
H	3.138658000	-2.845576000	-1.446322000
H	4.653663000	0.568191000	0.679963000
H	5.062418000	-1.459236000	-0.703512000
C	-1.065792000	-0.964737000	0.234010000
C	-1.741312000	-1.797597000	1.125768000
C	-1.411340000	-1.006111000	-1.122442000
C	-2.738870000	-2.662245000	0.672586000
H	-1.497936000	-1.766561000	2.182102000
C	-2.402126000	-1.871006000	-1.576517000
H	-0.901431000	-0.356221000	-1.827292000
C	-3.071701000	-2.704125000	-0.678714000
H	-3.256542000	-3.301452000	1.382103000
H	-2.655393000	-1.890961000	-2.632543000
H	-3.848722000	-3.375934000	-1.031295000
O	0.043440000	0.061087000	2.149722000
H	0.406127000	-0.773290000	2.478471000

D

Free energy: -3089.304318

C	0.748154000	-0.607823000	-1.209754000
C	1.838065000	0.118919000	-1.670931000
C	0.687755000	-1.910409000	-1.707132000
C	2.792157000	-0.385046000	-2.547812000
C	1.607848000	-2.453538000	-2.591878000
C	2.683413000	-1.682960000	-3.016297000
C	-0.230321000	1.439809000	0.347630000
C	-0.424101000	2.372769000	-0.671437000
C	-0.129638000	1.995806000	1.620095000
C	-0.461009000	3.745034000	-0.476893000
C	-0.162763000	3.367577000	1.863684000
C	-0.325359000	4.251151000	0.809086000
C	0.209195000	-1.134490000	1.207491000
C	-0.444580000	-2.266485000	1.684739000
C	1.478132000	-0.937924000	1.750457000
C	0.091683000	-3.113388000	2.651670000
C	2.052560000	-1.750434000	2.715629000
C	1.347959000	-2.854900000	3.175428000
C	-1.875384000	-0.346377000	-0.409466000
C	-2.839403000	-0.178452000	0.584158000
C	-2.394722000	-0.505996000	-1.690003000
C	-4.206885000	-0.199667000	0.356092000
C	-3.759323000	-0.533290000	-1.967296000
C	-4.674804000	-0.380821000	-0.938746000
F	-4.193352000	-0.698300000	-3.224500000
F	-1.592632000	-0.637333000	-2.763207000
F	-5.987871000	-0.404204000	-1.187908000
F	-5.075519000	-0.043226000	1.364283000
F	-2.454455000	0.018655000	1.860432000
F	-1.657282000	-2.625571000	1.225077000
F	-0.596554000	-4.182910000	3.073475000
F	1.876503000	-3.657949000	4.103805000
F	3.273622000	-1.486831000	3.199732000
F	2.230947000	0.102063000	1.333512000
F	-0.310718000	-2.725272000	-1.318511000
F	1.478198000	-3.711864000	-3.030371000
F	3.589208000	-2.184640000	-3.858939000
F	3.832690000	0.382074000	-2.926678000
F	2.057775000	1.393905000	-1.282028000
F	0.007979000	1.228011000	2.716477000
F	-0.046523000	3.837298000	3.112809000
F	-0.358830000	5.569261000	1.025645000
F	-0.629363000	4.582059000	-1.509106000
F	-0.572402000	1.950193000	-1.941900000

B	-0.293773000	-0.161041000	-0.017784000
H	4.142943000	2.599444000	0.070056000
O	3.310704000	2.924106000	0.903030000
H	3.518848000	2.492411000	1.747193000
H	2.447712000	2.569731000	0.632473000
O	4.953798000	2.293528000	-0.739784000
H	5.199814000	3.081084000	-1.251770000
H	4.548950000	1.678298000	-1.374967000

1a

Free energy: -664.517786

C	1.477124000	-1.524878000	-0.816952000
C	2.661135000	-0.094535000	0.557232000
C	1.047819000	-1.746808000	0.526470000
H	2.974598000	-0.086306000	-1.662177000
H	1.658362000	-0.765667000	2.446651000
Fe	0.721810000	0.192435000	-0.014839000
C	2.474637000	-0.503509000	-0.797740000
C	1.779298000	-0.863039000	1.375615000
H	1.086569000	-2.016588000	-1.698293000
H	3.326750000	0.687249000	0.899595000
H	0.274547000	-2.435179000	0.841465000
C	0.197218000	1.853330000	-1.082137000
C	-0.631560000	1.317830000	1.002790000
C	-0.773478000	0.822012000	-1.246630000
C	0.283894000	2.161839000	0.309115000
C	-1.284752000	0.477790000	0.045042000
H	0.793687000	2.295199000	-1.869812000
H	-0.782707000	1.280647000	2.074177000
H	-1.040336000	0.347486000	-2.181456000
H	0.958194000	2.877984000	0.760681000
C	-2.339030000	-0.537061000	0.369939000
H	-2.077208000	-1.001162000	1.332242000
O	-3.568701000	0.191243000	0.521364000
H	-4.247045000	-0.456062000	0.756089000
C	-2.485256000	-1.623380000	-0.683201000
H	-2.767732000	-1.189897000	-1.647467000
H	-1.551591000	-2.177885000	-0.809611000
H	-3.265844000	-2.330615000	-0.384441000

E

Free energy: -3753.825361

C	-2.593644000	-1.111462000	-1.247431000
C	-1.583979000	-1.437554000	-2.143557000
C	-3.722243000	-1.926935000	-1.340562000
C	-1.676921000	-2.462724000	-3.080077000
C	-3.865380000	-2.957972000	-2.256728000
C	-2.828574000	-3.230648000	-3.140134000
C	-1.238659000	1.005632000	-0.100985000
C	-1.051149000	1.762229000	-1.259344000
C	-0.398970000	1.364222000	0.947628000
C	-0.089745000	2.752656000	-1.396955000
C	0.567443000	2.361559000	0.865290000
C	0.728353000	3.062014000	-0.317972000
C	-2.428799000	-1.031604000	1.286124000
C	-3.410831000	-1.250772000	2.247072000
C	-1.307060000	-1.845688000	1.423279000
C	-3.265571000	-2.153512000	3.298237000
C	-1.108977000	-2.744372000	2.458798000
C	-2.103570000	-2.900689000	3.414757000
C	-3.768598000	1.023592000	0.023221000
C	-3.915553000	1.866757000	1.124772000
C	-4.641901000	1.294191000	-1.026041000
C	-4.867842000	2.870672000	1.216969000
C	-5.612335000	2.292112000	-0.978967000
C	-5.729939000	3.086657000	0.149931000
F	-6.428167000	2.495034000	-2.022335000
F	-4.595968000	0.599266000	-2.177625000
F	-6.655411000	4.048811000	0.210392000
F	-4.960027000	3.633367000	2.314476000
F	-3.098012000	1.727987000	2.186635000
F	-4.583961000	-0.594078000	2.216490000
F	-4.244535000	-2.306997000	4.199400000
F	-1.946504000	-3.761530000	4.423879000
F	0.027822000	-3.451635000	2.546488000
F	-0.314571000	-1.774166000	0.509940000
F	-4.758516000	-1.726856000	-0.504199000
F	-4.984070000	-3.692534000	-2.296066000
F	-2.939788000	-4.219876000	-4.031052000
F	-0.662009000	-2.715098000	-3.915906000
F	-0.408125000	-0.763245000	-2.165583000
F	-0.467672000	0.749131000	2.153059000
F	1.337950000	2.642924000	1.923594000
F	1.650669000	4.022391000	-0.422543000
F	0.046858000	3.422502000	-2.547609000
F	-1.839163000	1.548340000	-2.329145000
B	-2.512781000	-0.031861000	-0.013909000
O	1.972920000	-0.548687000	-0.540016000
H	2.503161000	0.292445000	-0.880109000
H	1.974366000	-0.605011000	0.506086000

O	2.013803000	-0.749732000	1.953330000
H	1.273383000	-0.238300000	2.313930000
H	1.056201000	-0.495251000	-0.858585000
C	7.806867000	0.597100000	1.648888000
C	9.157015000	-0.412879000	0.069967000
C	7.952950000	1.498026000	0.550962000
H	8.614388000	-1.469231000	1.970869000
H	9.059077000	1.288115000	-1.386575000
Fe	7.125254000	-0.259058000	-0.071768000
C	8.551672000	-0.584134000	1.351303000
C	8.786950000	0.873901000	-0.424513000
H	7.205278000	0.764433000	2.532681000
H	9.758744000	-1.145669000	-0.451855000
H	7.481430000	2.467360000	0.456154000
C	5.985276000	-1.953201000	-0.181254000
C	6.064092000	-0.315680000	-1.804797000
C	5.208561000	-0.849285000	0.274856000
C	6.513369000	-1.624822000	-1.466316000
C	5.260707000	0.174569000	-0.724911000
H	6.176918000	-2.864609000	0.370073000
H	6.315224000	0.237800000	-2.700796000
H	4.701508000	-0.781035000	1.227134000
H	7.175592000	-2.243305000	-2.058116000
C	4.568693000	1.500638000	-0.702352000
H	5.163788000	2.226525000	-1.265561000
O	3.284234000	1.390910000	-1.393979000
H	3.463186000	1.180601000	-2.323084000
C	4.266403000	2.032875000	0.680480000
H	3.636178000	1.337430000	1.239239000
H	5.195653000	2.178017000	1.235018000
H	3.746173000	2.989097000	0.607311000
H	1.799556000	-1.671046000	2.158573000

TS1

Free energy: -3753.801723

C	-2.650984000	-1.067892000	-1.252507000
C	-1.697749000	-1.381521000	-2.213332000
C	-3.798837000	-1.859857000	-1.309576000
C	-1.862265000	-2.376945000	-3.172627000
C	-4.010782000	-2.860337000	-2.245829000
C	-3.028772000	-3.123868000	-3.192130000
C	-1.203516000	0.995936000	-0.105656000
C	-1.057241000	1.788397000	-1.245850000
C	-0.321106000	1.315274000	0.921214000
C	-0.095316000	2.777518000	-1.389984000
C	0.645215000	2.312323000	0.832404000
C	0.759982000	3.052963000	-0.331193000
C	-2.359347000	-1.070488000	1.267648000
C	-3.318838000	-1.329293000	2.241314000
C	-1.235777000	-1.890542000	1.342010000
C	-3.155751000	-2.283156000	3.243452000
C	-1.023120000	-2.842619000	2.325891000
C	-1.997124000	-3.042490000	3.294784000
C	-3.723454000	1.044273000	0.135860000
C	-3.813243000	1.848535000	1.272048000
C	-4.632801000	1.366409000	-0.867368000
C	-4.741479000	2.865762000	1.436116000
C	-5.582360000	2.378068000	-0.746867000
C	-5.640354000	3.134618000	0.412349000
F	-6.435009000	2.631458000	-1.749070000
F	-4.645423000	0.712282000	-2.043558000
F	-6.544093000	4.110603000	0.542645000
F	-4.776367000	3.590739000	2.562245000
F	-2.959495000	1.656420000	2.296490000
F	-4.486894000	-0.663214000	2.271961000
F	-4.114537000	-2.474892000	4.159224000
F	-1.823365000	-3.954956000	4.254944000
F	0.110435000	-3.560429000	2.351693000
F	-0.257220000	-1.770606000	0.419134000
F	-4.786861000	-1.666146000	-0.414919000
F	-5.144318000	-3.573574000	-2.245722000
F	-3.206458000	-4.083893000	-4.104389000
F	-0.899968000	-2.620071000	-4.071769000
F	-0.517336000	-0.725885000	-2.281641000
F	-0.345068000	0.662841000	2.106612000
F	1.460161000	2.557158000	1.867442000
F	1.681663000	4.015093000	-0.438586000
F	0.001255000	3.483180000	-2.523000000
F	-1.890128000	1.614986000	-2.288860000
B	-2.486746000	-0.027164000	0.006536000
O	1.991205000	-0.422538000	-0.839908000
H	2.637751000	0.931170000	-1.575452000
H	2.088089000	-0.481420000	0.137009000
O	2.193464000	-0.838528000	1.886045000
H	1.482230000	-0.285971000	2.238126000
H	1.038163000	-0.417154000	-0.994216000
C	7.491558000	0.548913000	1.801222000
C	9.001573000	-0.445358000	0.364289000
C	7.815022000	1.485595000	0.771822000

H	8.181001000	-1.557170000	2.125667000	C	5.122321000	-1.178921000	1.270027000
H	9.140674000	1.310865000	-1.022356000	C	5.545358000	-2.094964000	0.316169000
Fe	7.012376000	-0.232234000	-0.024798000	C	0.471599000	-0.699037000	-1.017686000
C	8.234828000	-0.642015000	1.551230000	C	0.108087000	-2.040452000	-0.893117000
C	8.740177000	0.871454000	-0.118843000	C	-0.249149000	0.002339000	-1.978623000
H	6.784764000	0.704606000	2.605014000	C	-0.855174000	-2.662546000	-1.673897000
H	9.629480000	-1.185155000	-0.114017000	C	-1.207799000	-0.585387000	-2.798321000
H	7.386130000	2.472373000	0.656828000	C	-1.522431000	-1.924003000	-2.641316000
C	6.009979000	-2.025606000	-0.319499000	F	-1.851394000	0.146661000	-3.720267000
C	6.244140000	-0.354953000	-1.894948000	F	-0.064877000	1.321116000	-2.177210000
C	5.129357000	-0.993471000	0.063705000	F	-2.484195000	-2.489427000	-3.381345000
C	6.689075000	-1.637851000	-1.517956000	F	-1.170374000	-3.950516000	-1.486249000
C	5.251867000	0.068622000	-0.919115000	F	0.705999000	-2.812465000	0.033040000
H	6.191265000	-2.937192000	0.233951000	F	2.700298000	-2.187652000	-1.871078000
H	6.585976000	0.235684000	-2.734039000	F	5.088670000	-3.290187000	-1.663725000
H	4.498292000	-0.975863000	0.940536000	F	6.755971000	-2.654974000	0.403671000
H	7.462212000	-2.210482000	-2.012244000	F	5.933321000	-0.849368000	2.284488000
C	4.963735000	1.416815000	-0.675253000	F	3.527080000	0.284276000	2.101365000
H	5.421476000	2.142110000	-1.340595000	F	2.617137000	0.547506000	-2.573480000
O	3.102586000	1.681283000	-2.034343000	F	3.784638000	2.800085000	-3.391007000
H	3.467507000	1.274677000	-2.831109000	F	4.015632000	4.930783000	-1.693954000
C	4.280675000	1.925990000	0.533413000	F	3.033798000	4.732960000	0.846635000
H	3.661547000	1.169969000	1.014125000	F	1.867024000	2.520485000	1.683813000
H	5.039698000	2.262116000	1.250174000	F	1.741527000	-1.919253000	2.453585000
H	3.679080000	2.798109000	0.279418000	F	0.151999000	-1.858664000	4.560296000
H	1.807985000	-1.724179000	1.869586000	F	-1.803823000	0.043392000	4.785252000
F				F	-2.112667000	1.887009000	2.812711000
Free energy: -3524.548125				F	-0.608144000	1.776482000	0.605895000
C	2.132774000	1.413783000	-0.418672000	B	1.557672000	-0.058517000	0.032194000
C	2.298151000	2.521099000	0.408502000	C	-5.299668000	-1.076077000	1.421434000
C	2.676782000	1.566652000	-1.694245000	C	-3.999732000	-2.011942000	-0.239167000
C	2.916614000	3.700448000	0.000351000	C	-3.949778000	-0.648895000	1.607257000
C	3.297944000	2.721883000	-2.145070000	H	-6.204308000	-2.379898000	-0.154529000
C	3.419611000	3.805997000	-1.286154000	H	-2.090287000	-1.039229000	0.424802000
C	0.693189000	-0.034810000	1.427063000	Fe	-4.652366000	-0.078386000	-0.248749000
C	-0.345637000	0.882923000	1.581675000	C	-5.324538000	-1.928882000	0.284010000
C	0.809208000	-0.949998000	2.469860000	C	-3.145872000	-1.215768000	0.577474000
C	-1.151603000	0.954336000	2.706432000	H	-6.149305000	-0.776012000	2.019011000
C	-0.009350000	-0.942456000	3.596883000	H	-3.718555000	-2.544157000	-1.135992000
C	-0.997346000	0.019814000	3.720310000	H	-3.610078000	0.016298000	2.385849000
C	2.957685000	-0.912708000	0.134270000	C	-5.948129000	0.238662000	-1.863567000
C	3.436042000	-1.821805000	-0.804684000	C	-3.887199000	1.241606000	-1.596807000
C	3.862029000	-0.612037000	1.152840000	C	-6.118141000	1.203243000	-0.856440000
C	4.693718000	-2.415312000	-0.728469000	C	-4.590898000	0.263531000	-2.317413000

C	-4.821488000	1.836380000	-0.644540000
H	-6.700746000	-0.462248000	-2.198575000
H	-2.836471000	1.484093000	-1.660561000
H	-7.016833000	1.384086000	-0.284468000
H	-4.173130000	-0.414075000	-3.046981000
C	-4.357937000	2.054995000	0.653792000
H	-3.285137000	2.185865000	0.768400000
C	-5.204847000	2.408390000	1.819377000
H	-6.252053000	2.133259000	1.690082000
H	-4.818733000	1.960480000	2.737501000
H	-5.146158000	3.497449000	1.952824000

2a

Free energy: -669.598165

C	0.651655000	-1.205363000	0.259365000
C	-0.023960000	0.000493000	0.475235000
C	0.652362000	1.205787000	0.258723000
C	1.981980000	1.206267000	-0.157926000
C	2.649270000	-0.000553000	-0.367936000
C	1.981241000	-1.206886000	-0.157235000
C	-1.463194000	0.000914000	0.899280000
S	-2.525479000	-0.000184000	-0.610862000
H	0.130328000	-2.144922000	0.423583000
H	0.131651000	2.145769000	0.422459000
H	2.497608000	2.148841000	-0.317470000
H	3.685976000	-0.000964000	-0.691542000
H	2.496323000	-2.149853000	-0.316217000
H	-1.697483000	-0.888722000	1.487322000
H	-1.697342000	0.891388000	1.486093000
H	-3.715519000	-0.002547000	0.022531000

TS2

Free energy: -4194.137880

C	-1.608246000	-1.190722000	-0.934743000
C	-0.692414000	-0.995867000	-1.962626000
C	-1.884467000	-2.532109000	-0.664120000
C	-0.108987000	-2.034051000	-2.683693000
C	-1.334685000	-3.599251000	-1.360016000
C	-0.437298000	-3.346000000	-2.388448000
C	-2.035261000	1.500135000	-0.495745000
C	-2.484899000	1.818398000	-1.776981000
C	-1.583913000	2.594684000	0.236427000
C	-2.440134000	3.091332000	-2.326656000
C	-1.516508000	3.888152000	-0.273221000
C	-1.943672000	4.142284000	-1.566477000
C	-1.381238000	-0.329045000	1.437763000
C	-1.846218000	-0.989211000	2.570575000
C	-0.025848000	-0.007851000	1.474018000
C	-1.042737000	-1.282853000	3.670677000
C	0.796663000	-0.235950000	2.563905000
C	0.290026000	-0.903897000	3.669890000
C	-3.850095000	-0.118694000	0.244317000
C	-4.459947000	0.645923000	1.238317000
C	-4.738506000	-0.769055000	-0.606438000
C	-5.832314000	0.743047000	1.414124000
C	-6.122530000	-0.700038000	-0.468896000
C	-6.676509000	0.059323000	0.549142000
F	-6.923381000	-1.357756000	-1.318551000
F	-4.304551000	-1.514435000	-1.639958000
F	-8.003050000	0.136866000	0.694491000
F	-6.349283000	1.489229000	2.399655000
F	-3.700597000	1.351841000	2.098796000
F	-3.125378000	-1.391946000	2.673396000
F	-1.549459000	-1.929986000	4.728524000
F	1.081775000	-1.178276000	4.710723000
F	2.082203000	0.150750000	2.558545000
F	0.544402000	0.580363000	0.404585000
F	-2.735181000	-2.851095000	0.329006000
F	-1.649505000	-4.861764000	-1.045041000
F	0.132764000	-4.353880000	-3.058776000
F	0.793762000	-1.775455000	-3.641170000
F	-0.286114000	0.240682000	-2.319492000
F	-1.161611000	2.470603000	1.510292000
F	-1.033392000	4.886609000	0.478645000
F	-1.884810000	5.377689000	-2.072666000
F	-2.871046000	3.316826000	-3.575001000
F	-2.990164000	0.850489000	-2.566374000
B	-2.223122000	-0.035557000	0.060471000
C	1.936754000	-2.879989000	0.181298000
C	3.925764000	-3.906270000	-0.395532000
C	2.857492000	-2.687340000	1.250937000
H	2.182756000	-3.901963000	-1.798526000
H	4.996988000	-3.315089000	1.476099000
Fe	3.590263000	-1.884242000	-0.477365000
C	2.598175000	-3.627535000	-0.839593000
C	4.085465000	-3.326126000	0.892791000
H	0.935502000	-2.474672000	0.126940000
H	4.690881000	-4.420240000	-0.961852000
H	2.679740000	-2.127993000	2.157239000
C	2.871846000	-0.302234000	-1.609433000

C	5.050023000	-1.058093000	-1.625880000
C	3.455313000	0.135619000	-0.406159000
C	3.843170000	-1.040026000	-2.355410000
C	4.832499000	-0.304582000	-0.402643000
H	1.849194000	-0.131860000	-1.902461000
H	5.970909000	-1.557224000	-1.896099000
H	2.969390000	0.696539000	0.373451000
H	3.660791000	-1.548426000	-3.292337000
C	5.682010000	-0.350431000	0.710996000
H	6.611551000	-0.901434000	0.586511000
C	5.284821000	0.003484000	2.090997000
H	4.512929000	0.771553000	2.126533000
H	4.878157000	-0.906019000	2.554191000
H	6.149700000	0.301552000	2.686112000
S	7.017616000	1.908097000	0.186154000
C	4.560632000	3.182698000	0.367408000
C	4.416028000	3.262009000	-1.022088000
C	3.148270000	3.311756000	-1.598328000
C	2.008376000	3.299095000	-0.794494000
C	2.142941000	3.244430000	0.592176000
C	3.411985000	3.177864000	1.167358000
C	5.915664000	3.125896000	1.020246000
H	7.997540000	1.935221000	1.112034000
H	5.295704000	3.275425000	-1.660341000
H	3.051325000	3.356018000	-2.679206000
H	1.021922000	3.316924000	-1.247390000
H	1.260592000	3.231594000	1.222455000
H	3.515065000	3.113299000	2.247268000
H	6.421607000	4.094733000	0.969050000
H	5.823272000	2.840955000	2.069876000

G

Free energy: -4194.151776

C	-1.564641000	-1.180467000	-0.954150000
C	-0.650783000	-0.944767000	-1.975508000
C	-1.816057000	-2.532459000	-0.714556000
C	-0.048370000	-1.955093000	-2.719974000
C	-1.248071000	-3.572705000	-1.435937000
C	-0.356241000	-3.279045000	-2.458207000
C	-2.057941000	1.490203000	-0.472130000
C	-2.516565000	1.814399000	-1.748762000
C	-1.635746000	2.586231000	0.274995000
C	-2.506533000	3.095600000	-2.280677000
C	-1.604746000	3.888102000	-0.216306000
C	-2.038766000	4.148927000	-1.505922000
C	-1.353139000	-0.354338000	1.432804000
C	-1.799362000	-1.056333000	2.548077000
C	-0.008171000	0.007573000	1.479993000
C	-0.988944000	-1.353673000	3.641911000
C	0.818661000	-0.222132000	2.566591000
C	0.331312000	-0.933825000	3.653716000
C	-3.828959000	-0.182737000	0.250059000
C	-4.451837000	0.548461000	1.261035000
C	-4.706336000	-0.838239000	-0.608221000
C	-5.825191000	0.609829000	1.445109000
C	-6.090899000	-0.804580000	-0.462849000
C	-6.657568000	-0.077642000	0.571731000
F	-6.880276000	-1.465538000	-1.320736000
F	-4.260663000	-1.554724000	-1.657067000
F	-7.984828000	-0.034357000	0.724845000
F	-6.354312000	1.324939000	2.447146000
F	-3.705326000	1.255619000	2.131702000
F	-3.066596000	-1.498052000	2.639631000
F	-1.477491000	-2.041981000	4.682286000
F	1.129843000	-1.210297000	4.688916000
F	2.091358000	0.204305000	2.575991000
F	0.545905000	0.638368000	0.426795000
F	-2.660449000	-2.890464000	0.270739000
F	-1.541421000	-4.847865000	-1.152047000
F	0.227171000	-4.260988000	-3.155411000
F	0.846791000	-1.658159000	-3.673075000
F	-0.270214000	0.306935000	-2.304933000
F	-1.208498000	2.455776000	1.546461000
F	-1.147300000	4.888685000	0.549080000
F	-2.012959000	5.392496000	-1.994677000
F	-2.943281000	3.326500000	-3.526034000
F	-2.995766000	0.844811000	-2.552190000
B	-2.204580000	-0.057933000	0.061936000
C	1.968031000	-2.845662000	0.166944000
C	3.973573000	-3.818351000	-0.442761000
C	2.904175000	-2.628236000	1.221446000
H	2.204349000	-3.881601000	-1.808722000
H	5.063488000	-3.195966000	1.412884000
Fe	3.589394000	-1.814416000	-0.521661000
C	2.629976000	-3.583071000	-0.861483000
C	4.143743000	-3.226352000	0.843177000
H	0.951622000	-2.476570000	0.135362000
H	4.740459000	-4.318319000	-1.019936000
H	2.725869000	-2.071785000	2.129676000

C	2.916269000	-0.207111000	-1.600915000
C	5.101845000	-0.940814000	-1.569165000
C	3.490371000	0.208109000	-0.371753000
C	3.905611000	-0.921362000	-2.339660000
C	4.846045000	-0.241288000	-0.344301000
H	1.898384000	-0.027486000	-1.905634000
H	6.032793000	-1.427257000	-1.830889000
H	2.985641000	0.743183000	0.413974000
H	3.758833000	-1.405151000	-3.296082000
C	5.844952000	0.002933000	0.730412000
H	6.671084000	-0.710679000	0.638833000
C	5.332250000	0.064593000	2.152537000
H	4.521503000	0.784637000	2.264517000
H	4.944673000	-0.924160000	2.407751000
H	6.133593000	0.310174000	2.854077000
S	6.738537000	1.598228000	0.256241000
C	4.461096000	3.184500000	0.351749000
C	4.336042000	3.344566000	-1.032210000
C	3.075504000	3.479701000	-1.607478000
C	1.933346000	3.475496000	-0.805360000
C	2.055126000	3.346605000	0.577215000
C	3.315508000	3.191359000	1.153019000
C	5.803479000	3.005992000	0.996267000
H	7.730372000	1.557459000	1.178965000
H	5.220871000	3.351401000	-1.663830000
H	2.984342000	3.586845000	-2.684116000
H	0.951541000	3.565989000	-1.259424000
H	1.169650000	3.343928000	1.202734000
H	3.412738000	3.061551000	2.227081000
H	6.473572000	3.853275000	0.816510000
H	5.729234000	2.831897000	2.070108000

TS3

Free energy: -4270.575325

C	1.606203000	1.384615000	0.024666000
C	1.073367000	2.036150000	1.134902000
C	1.794750000	2.211930000	-1.084536000
C	0.707946000	3.380153000	1.137387000
C	1.459150000	3.558307000	-1.121901000
C	0.902470000	4.150610000	0.003785000
C	1.812150000	-1.045571000	1.297719000
C	0.472396000	-1.231561000	1.629672000
C	2.697849000	-1.787056000	2.073594000
C	0.024410000	-2.042262000	2.659161000
C	2.295627000	-2.616725000	3.118034000
C	0.949603000	-2.747656000	3.416904000
C	3.780028000	0.070651000	-0.248421000
C	4.510757000	-0.194750000	-1.400806000
C	4.495659000	0.725102000	0.753561000
C	5.855843000	0.135632000	-1.547603000
C	5.833814000	1.073349000	0.652300000
C	6.524358000	0.773640000	-0.515091000
C	1.471633000	-1.085802000	-1.215071000
C	1.885279000	-2.415227000	-1.337011000
C	0.359044000	-0.778643000	-1.985997000
C	1.240910000	-3.368715000	-2.111311000
C	-0.326950000	-1.696353000	-2.775762000
C	0.112577000	-3.007251000	-2.836706000
F	-1.413727000	-1.324733000	-3.464827000
F	-0.162157000	0.475771000	-2.020921000
F	-0.537049000	-3.907995000	-3.579218000
F	1.690601000	-4.627783000	-2.164721000
F	2.968948000	-2.839504000	-0.660832000
F	3.944760000	-0.784668000	-2.469990000
F	6.505860000	-0.149319000	-2.684301000
F	7.814772000	1.098682000	-0.640103000
F	6.464065000	1.691580000	1.659992000
F	3.881800000	1.045740000	1.909615000
F	2.316579000	1.699004000	-2.215116000
F	1.648400000	4.282897000	-2.232033000
F	0.531707000	5.433927000	-0.017169000
F	0.132301000	3.923037000	2.219861000
F	0.853725000	1.392519000	2.296966000
F	4.022971000	-1.766844000	1.847580000
F	3.202820000	-3.299335000	3.828071000
F	0.545140000	-3.538851000	4.413501000
F	-1.283883000	-2.159501000	2.938382000
F	-0.476531000	-0.585353000	0.914677000
B	2.172074000	-0.160037000	-0.042551000
C	-4.661701000	-3.875867000	-1.124116000
C	-2.570858000	-3.282715000	-0.337628000
C	-4.744236000	-3.748657000	0.295389000
H	-2.941372000	-3.562210000	-2.528306000
H	-3.194878000	-3.175687000	1.808849000
Fe	-4.131863000	-1.989986000	-0.545000000
C	-3.318868000	-3.587676000	-1.515408000
C	-3.452349000	-3.383283000	0.780030000
H	-5.480909000	-4.112423000	-1.790694000
H	-1.532826000	-2.978477000	-0.303843000

H	-5.636763000	-3.870696000	0.895193000
C	-5.490385000	-0.651533000	-1.306611000
C	-3.276276000	-0.202042000	-0.854859000
C	-5.358405000	-0.479377000	0.102056000
C	-4.206515000	-0.467117000	-1.899544000
C	-3.985214000	-0.200130000	0.390658000
H	-6.401331000	-0.910632000	-1.830083000
H	-2.211372000	-0.093447000	-0.970193000
H	-6.149040000	-0.586605000	0.832000000
H	-3.968852000	-0.568729000	-2.949462000
C	-3.371560000	-0.026008000	1.740303000
H	-2.450283000	-0.602196000	1.793245000
C	-4.268125000	-0.402120000	2.906699000
H	-5.164131000	0.222162000	2.955650000
H	-4.587671000	-1.440824000	2.783957000
H	-3.727656000	-0.316313000	3.852164000
S	-2.707841000	1.692137000	1.990485000
C	-4.040685000	3.671603000	0.626399000
C	-3.183389000	4.774976000	0.708514000
C	-2.925334000	5.550805000	-0.419108000
C	-3.526448000	5.234647000	-1.637973000
C	-4.391313000	4.142110000	-1.724321000
C	-4.645464000	3.360148000	-0.596872000
C	-4.206324000	2.756772000	1.800135000
H	-2.051895000	2.022207000	0.482385000
H	-2.691956000	5.004450000	1.650566000
H	-2.244367000	6.393325000	-0.349287000
H	-3.320036000	5.835126000	-2.518858000
H	-4.863312000	3.892920000	-2.670076000
H	-5.299212000	2.494775000	-0.665232000
H	-4.313722000	3.299596000	2.740686000
H	-5.059808000	2.087539000	1.674167000
O	-1.601640000	2.447291000	-0.621091000
H	-1.005189000	1.775344000	-0.997125000
H	-2.349228000	2.542018000	-1.237976000

H

Free energy: -4270.575970

C	1.612237000	1.382349000	0.052490000
C	1.073085000	2.015425000	1.170690000
C	1.812062000	2.229350000	-1.039986000
C	0.711389000	3.360754000	1.194508000
C	1.478608000	3.576816000	-1.056650000
C	0.914161000	4.150186000	0.075124000
C	1.808214000	-1.067355000	1.287238000
C	0.468292000	-1.255726000	1.618119000
C	2.694070000	-1.816235000	2.055738000
C	0.021282000	-2.073506000	2.642604000
C	2.292540000	-2.653600000	3.094236000
C	0.946841000	-2.785210000	3.393950000
C	3.775704000	0.051097000	-0.256135000
C	4.498902000	-0.218165000	-1.412271000
C	4.502917000	0.691991000	0.746200000
C	5.847484000	0.095866000	-1.562566000
C	5.844953000	1.023948000	0.641580000
C	6.527514000	0.720914000	-0.529656000
C	1.449941000	-1.065762000	-1.226032000
C	1.836944000	-2.402685000	-1.356394000
C	0.347730000	-0.732022000	-2.000046000
C	1.174219000	-3.338416000	-2.136774000
C	-0.356317000	-1.630020000	-2.796501000
C	0.055498000	-2.949559000	-2.862770000
F	-1.430365000	-1.231431000	-3.489733000
F	-0.143075000	0.537387000	-2.037505000
F	-0.609629000	-3.831885000	-3.613480000
F	1.598406000	-4.605685000	-2.197140000
F	2.912365000	-2.852568000	-0.684037000
F	3.921586000	-0.795897000	-2.482138000
F	6.489667000	-0.191967000	-2.702964000
F	7.821434000	1.030343000	-0.657880000
F	6.486655000	1.629327000	1.649824000
F	3.897619000	1.012997000	1.906627000
F	2.339315000	1.735527000	-2.176642000
F	1.678236000	4.320526000	-2.152143000
F	0.550545000	5.435708000	0.075693000
F	0.140799000	3.889947000	2.285864000
F	0.852177000	1.354207000	2.321531000
F	4.018864000	-1.797625000	1.827023000
F	3.200103000	-3.343205000	3.797212000
F	0.542887000	-3.583429000	4.385236000
F	-1.286406000	-2.191194000	2.923668000
F	-0.480237000	-0.604306000	0.909224000
B	2.166935000	-0.165224000	-0.042611000
C	-4.687464000	-3.868066000	-1.111720000
C	-2.590773000	-3.297361000	-0.323555000
C	-4.770260000	-3.737232000	0.307447000
H	-2.961576000	-3.577312000	-2.514226000
H	-3.216907000	-3.179228000	1.822247000
Fe	-4.136333000	-1.987577000	-0.535033000

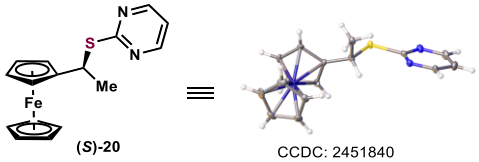
C	-3.340829000	-3.595956000	-1.501790000
C	-3.474812000	-3.385585000	0.793345000
H	-5.508372000	-4.097091000	-1.778873000
H	-1.549192000	-3.005024000	-0.289862000
H	-5.664782000	-3.848519000	0.906422000
C	-5.469507000	-0.634618000	-1.309980000
C	-3.256619000	-0.209667000	-0.832502000
C	-5.350038000	-0.460769000	0.100429000
C	-4.177061000	-0.465959000	-1.888954000
C	-3.978087000	-0.195396000	0.404727000
H	-6.377845000	-0.883678000	-1.842923000
H	-2.188341000	-0.113305000	-0.931676000
H	-6.150306000	-0.557423000	0.821437000
H	-3.928691000	-0.573005000	-2.935701000
C	-3.376193000	-0.003913000	1.760019000
H	-2.465953000	-0.596593000	1.827090000
C	-4.293232000	-0.369848000	2.914540000
H	-5.181445000	0.266864000	2.951385000
H	-4.626676000	-1.405343000	2.795336000
H	-3.763712000	-0.283823000	3.866176000
S	-2.685297000	1.701280000	1.977407000
C	-3.998555000	3.691694000	0.621997000
C	-3.134100000	4.789511000	0.711903000
C	-2.861454000	5.568452000	-0.410646000
C	-3.452339000	5.260569000	-1.636474000
C	-4.322420000	4.172392000	-1.733332000
C	-4.594031000	3.390020000	-0.609145000
C	-4.175822000	2.773456000	1.792406000
H	-1.943083000	2.109016000	0.220577000
H	-2.648213000	5.012760000	1.658308000
H	-2.175557000	6.406126000	-0.331376000
H	-3.234035000	5.861960000	-2.513782000
H	-4.787166000	3.928209000	-2.684019000
H	-5.253976000	2.530041000	-0.686959000
H	-4.293660000	3.321094000	2.729330000
H	-5.037473000	2.116295000	1.657211000
O	-1.592949000	2.473742000	-0.696644000
H	-0.988575000	1.813450000	-1.094458000
H	-2.352706000	2.603304000	-1.299741000
H	4.699599000	0.965208000	0.799077000
H	1.081657000	2.595452000	-1.027041000
Fe	2.177413000	0.173933000	-0.146961000
C	3.680573000	1.300579000	0.655918000
C	1.767946000	2.165192000	-0.309342000
H	2.673256000	0.682985000	2.561416000
H	3.715398000	2.146108000	-1.420070000
H	0.437283000	1.688673000	1.428189000
C	2.956853000	-1.637170000	-0.681572000
C	0.984721000	-0.761792000	-1.497417000
C	1.955481000	-1.798248000	0.321789000
C	2.355188000	-1.000070000	-1.808638000
C	0.731287000	-1.250099000	-0.175498000
H	3.997977000	-1.918226000	-0.589807000
H	0.258326000	-0.266048000	-2.128417000
H	2.107927000	-2.216167000	1.307688000
H	2.860616000	-0.711567000	-2.721185000
C	-0.575314000	-1.136545000	0.545344000
H	-0.996829000	-0.151273000	0.324396000
S	-1.750009000	-2.335925000	-0.218102000
C	-3.343769000	-1.635018000	0.370468000
H	-4.104904000	-2.216296000	-0.158549000
H	-3.455995000	-1.825818000	1.440788000
C	-0.470789000	-1.317986000	2.050631000
H	-1.447221000	-1.192754000	2.525438000
H	-0.093460000	-2.312806000	2.303795000
H	0.208573000	-0.570593000	2.473639000
C	-3.465427000	-0.169523000	0.072701000
C	-3.369297000	0.770135000	1.104217000
C	-3.608143000	0.285066000	-1.244348000
C	-3.412312000	2.137596000	0.828259000
H	-3.254368000	0.424969000	2.128376000
C	-3.655037000	1.648307000	-1.521897000
H	-3.672347000	-0.438168000	-2.053233000
C	-3.552918000	2.580200000	-0.485719000
H	-3.332434000	2.854586000	1.640475000
H	-3.770205000	1.986892000	-2.547753000
H	-3.584637000	3.643786000	-0.703806000

3

Free energy: -1257.707997

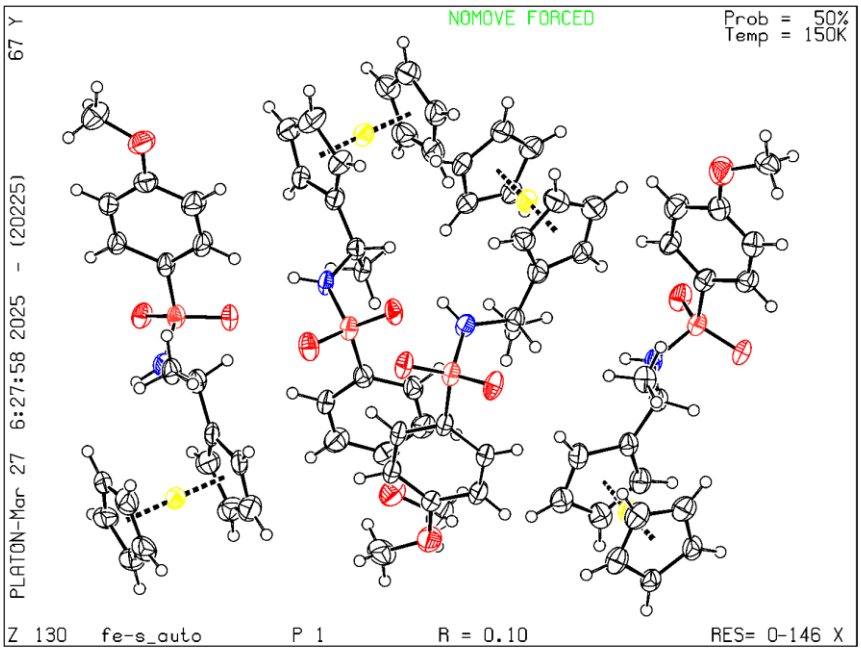
C	2.609587000	1.153159000	1.588782000
C	3.160124000	1.925354000	-0.517638000
C	1.427779000	1.688133000	0.991825000

6. X-ray Crystallographic Data



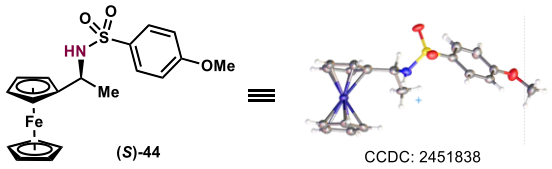
ORTEP drawing of compound (*S*)-**20** with 50% thermal ellipsoids.

Crystal sample preparation: compound (*S*)-**20** (10 mg) was added to a 10 mL glass vial and dissolved by the addition of methanol (2 mL). Stuff the bottle mouth with an absorbent cotton, place at room temperature for 3 days, a colorless crystal of (*S*)-**20** was obtained for X-ray analysis.



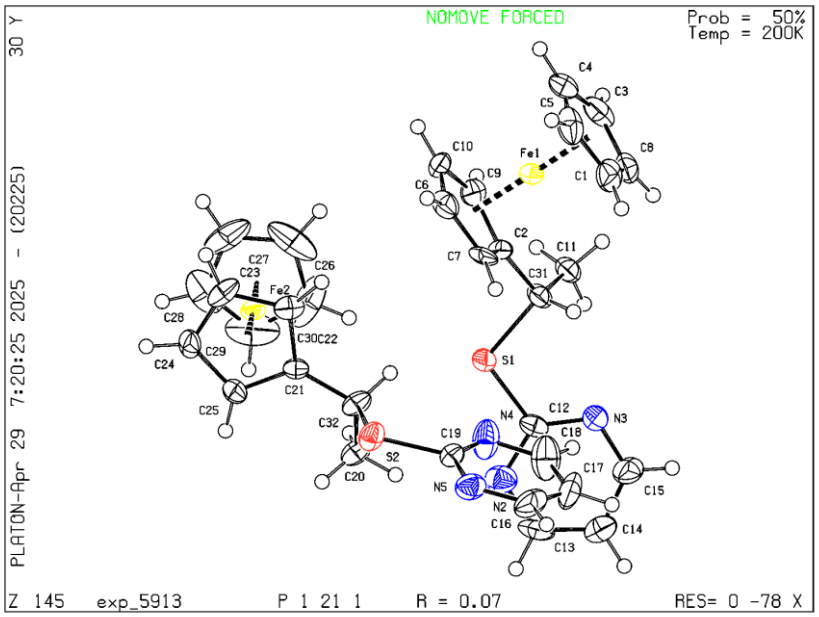
Identification code	CCDC: 2451840
Empirical formula	$C_{19}H_{21}FeNO_3S$
Formula weight	399.28
Temperature/K	150.00(10)
Crystal system	triclinic
Space group	P1
a/Å	7.5160(3)
b/Å	14.8861(8)

c/Å	17.0616(7)
α/°	68.584(4)
β/°	89.263(3)
γ/°	80.833(4)
Volume/Å^3	1752.29(14)
Z	4
ρ_{calc}g/cm^3	1.513
μ/mm^{-1}	8.167
F(000)	832.0
Crystal size/mm^3	0.15 × 0.12 × 0.1
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	9.976 to 146.088
Index ranges	-8 ≤ h ≤ 5, -18 ≤ k ≤ 18, -21 ≤ l ≤ 20
Reflections collected	37770
Independent reflections	10087 [R_{int} = 0.0729, R_{sigma} = 0.0740]
Data/restraints/parameters	10087/1068/918
Goodness-of-fit on F^2	1.093
Final R indexes [I>=2σ (I)]	R_1 = 0.0978, wR_2 = 0.2553
Final R indexes [all data]	R_1 = 0.1213, wR_2 = 0.2771
Largest diff. peak/hole / e Å^{-3}	2.18/-0.97
Flack parameter	-0.016(9)



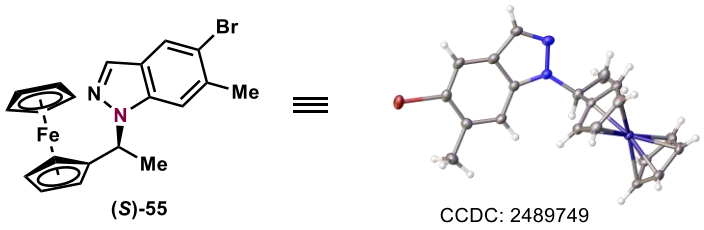
ORTEP drawing of compound (*S*)-**44** with 50% thermal ellipsoids.

Crystal sample preparation: compound (*S*)-**44** (10 mg) was added to a 10 mL glass vial and dissolved by the addition of methanol (2 mL). Stuff the bottle mouth with an absorbent cotton, place at room temperature for 3 days, a colorless crystal of (*S*)-**44** was obtained for X-ray analysis.



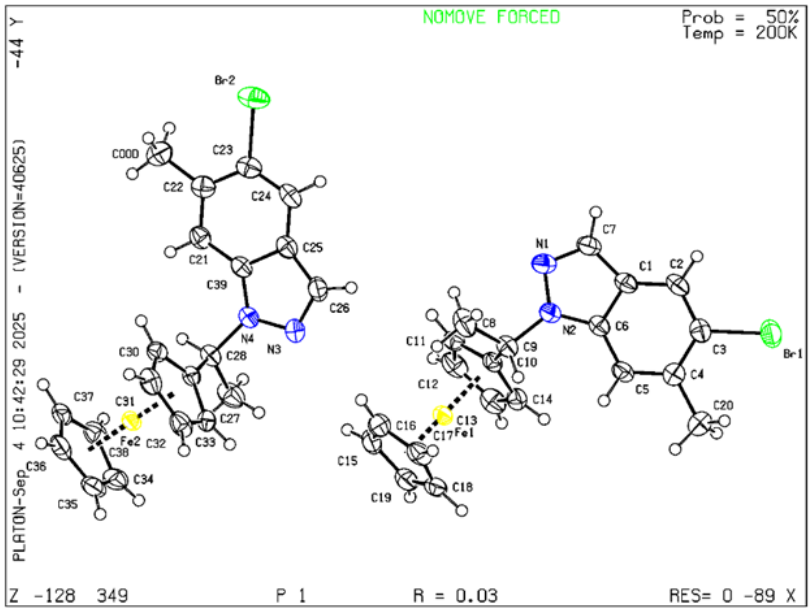
Identification code	CCDC: 2451838
Empirical formula	$C_{16}H_{16}FeN_2S$
Formula weight	324.22
Temperature/K	200.00(10)
Crystal system	monoclinic
Space group	$P2_1$
a/Å	10.7826(3)
b/Å	7.7550(3)
c/Å	17.6467(5)

α/°	90
β/°	100.124(3)
γ/°	90
Volume/Å^3	1452.62(8)
Z	4
ρ_{calc}g/cm^3	1.482
μ/mm^{-1}	9.573
F(000)	672.0
Crystal size/mm^3	0.15 × 0.13 × 0.11
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	5.086 to 147.79
Index ranges	-13 ≤ h ≤ 13, -9 ≤ k ≤ 9, -21 ≤ l ≤ 15
Reflections collected	8996
Independent reflections	5293 [R_{int} = 0.0756, R_{sigma} = 0.1045]
Data/restraints/parameters	5293/13/363
Goodness-of-fit on F^2	1.027
Final R indexes [I>=2σ (I)]	R_1 = 0.0692, wR_2 = 0.1747
Final R indexes [all data]	R_1 = 0.0884, wR_2 = 0.1898
Largest diff. peak/hole / e Å^{-3}	0.60/-0.99
Flack parameter	-0.006(9)



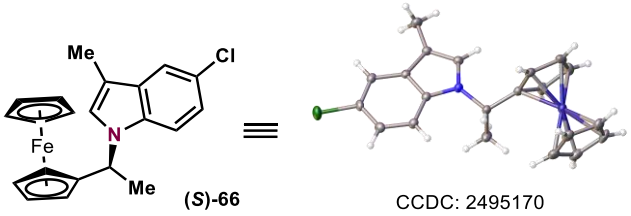
ORTEP drawing of compound (*S*)-**55** with 50% thermal ellipsoids.

Crystal sample preparation: compound (*S*)-**55** (10 mg) was added to a 10 mL glass vial and dissolved by the addition of methanol (2 mL). Stuff the bottle mouth with an absorbent cotton, place at room temperature for 3 days, a colorless crystal of (*S*)-**55** was obtained for X-ray analysis.



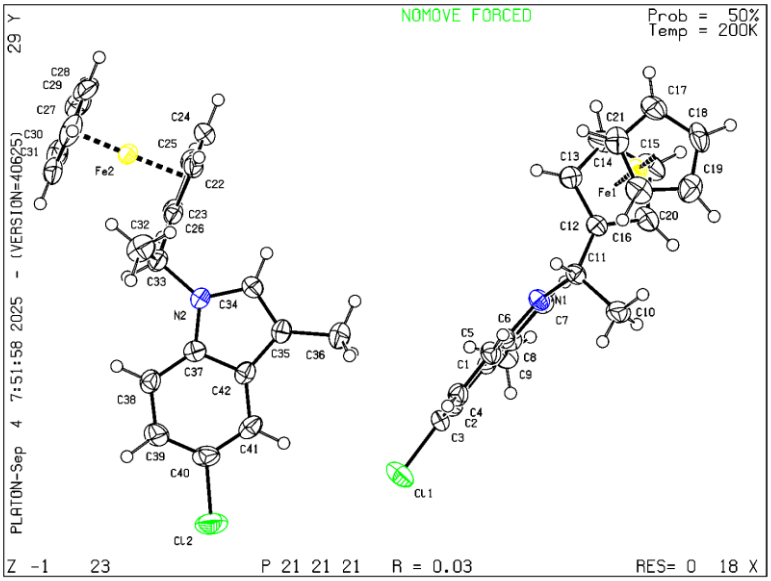
Identification code	CCDC: 2489749
Empirical formula	$C_{40}H_{38}Br_2Fe_2N_4$
Formula weight	846.26
Temperature/K	200.00(10)
Crystal system	triclinic
Space group	P1
a/Å	6.04841(16)

b/Å	12.0883(3)
c/Å	12.3620(4)
α/°	85.012(2)
β/°	89.508(2)
γ/°	77.839(2)
Volume/Å^3	880.17(4)
Z	1
ρ_{calc}g/cm^3	1.597
μ/mm^{-1}	9.534
F(000)	428.0
Crystal size/mm^3	0.13 × 0.12 × 0.11
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.178 to 146.844
Index ranges	-7 ≤ h ≤ 7, -14 ≤ k ≤ 14, -13 ≤ l ≤ 15
Reflections collected	19153
Independent reflections	5419 [R_{int} = 0.0280, R_{sigma} = 0.0184]
Data/restraints/parameters	5419/3/437
Goodness-of-fit on F^2	1.054
Final R indexes [I>=2σ (I)]	R_1 = 0.0263, wR_2 = 0.0718
Final R indexes [all data]	R_1 = 0.0268, wR_2 = 0.0720
Largest diff. peak/hole / e Å^{-3}	0.41/-0.32
Flack/Hooft parameter	0.001(3)/-0.004(11)



ORTEP drawing of compound (*S*)-**66** with 50% thermal ellipsoids.

Crystal sample preparation: compound (*S*)-**66** (10 mg) was added to a 10 mL glass vial and dissolved by the addition of methanol (2 mL) and dichloromethane (0.5 mL). Stuff the bottle mouth with an absorbent cotton, place at room temperature for 3 days, a colorless crystal of (*S*)-**66** was obtained for X-ray analysis.

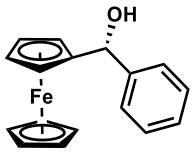


Identification code	CCDC: 2495170
Empirical formula	$C_{21}H_{20}ClFeN$
Formula weight	377.68
Temperature/K	200.00(10)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	7.60479(6)
b/Å	12.96157(9)

c/Å	36.3865(3)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	3586.61(5)
Z	8
ρ_{calc}g/cm^3	1.399
μ/mm^{-1}	8.100
F(000)	1568.0
Crystal size/mm^3	0.14 × 0.12 × 0.11
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.24 to 145.898
Index ranges	$-9 \leq h \leq 8$, $-15 \leq k \leq 16$, $-44 \leq l \leq 42$
Reflections collected	54553
Independent reflections	6976 [R_{int} = 0.0398, R_{sigma} = 0.0242]
Data/restraints/parameters	6976/0/437
Goodness-of-fit on F^2	1.066
Final R indexes [I>=2σ (I)]	R_1 = 0.0277, wR_2 = 0.0553
Final R indexes [all data]	R_1 = 0.0306, wR_2 = 0.0561
Largest diff. peak/hole / e Å^{-3}	0.20/-0.24
Flack/Hooft parameter	-0.0115(13)/-0.0108(11)

7. Characterization Data of Products

***(S)*-phenyl(ferrocene-2-yl)methanol (S2)**



TLC: R_f = 0.35 (petroleum ether/Ethyl acetate=8/1); 1.05 g, yield: 90%; yellow solid.

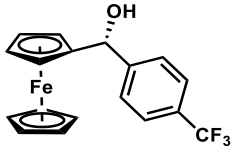
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 – 7.37 (m, 2H), 7.34 – 7.30 (m, 2H), 7.27 – 7.22 (m, 1H), 5.46 (d, *J* = 3.2 Hz, 1H), 4.23 – 4.16 (m, 9H), 2.46 (d, *J* = 3.2 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 143.2, 128.2, 127.4, 126.2, 94.3, 72.0, 68.5, 68.2, 68.1, 67.4, 65.9.

HRMS (ESI-TOF) m/z: $[M+K]^+$ Calcd for $C_{17}H_{16}FeOK$ 331.0177; Found: 331.0189.

Chiral HPLC: The ee value was 93%, t_R (minor) = 12.2 min, t_S (major) = 16.7 min (Chiralpak IA, λ = 254 nm, 10% isopropanol/hexanes, flow rate = 1.0 mL/min).

***(S)*-ferrocene-2-yl(4-(trifluoromethyl)phenyl)methanol (S3)**



TLC: R_f = 0.35 (petroleum ether/Ethyl acetate=8/1); 1.55 g, yield: 43%; yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 8.3 Hz, 2H), 7.51 (d, *J* = 8.1 Hz, 2H), 5.49 (d, *J* = 3.0 Hz, 1H), 4.26 – 4.17 (m, 9H), 2.63 (d, *J* = 3.0 Hz, 1H).

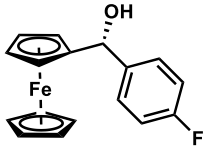
^{13}C NMR (101 MHz, $CDCl_3$) δ 147.1, 129.6, 129.3, 126.3, 125.2, 125.1, 125.1, 125.1, 93.8, 71.2, 68.5, 68.4, 68.3, 67.4, 65.6.

^{19}F NMR (376 MHz, $CDCl_3$) δ -115.16.

HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{18}H_{16}F_3FeO$ 361.0492; Found: 361.0522.

Chiral HPLC: The ee value was 96%, t_R (minor) = 11.7 min, t_S (major) = 13.3 min (Chiralpak IA, λ = 254 nm, 10% isopropanol/hexanes, flow rate = 1.0 mL/min).

***(S)*-(4-fluorophenyl)(ferrocene-2-yl)methanol (S4)**



TLC: R_f = 0.28 (petroleum ether/Ethyl acetate=8/1); 650 mg, yield: 19%; yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.33 (m, 2H), 7.04 – 6.98 (m, 2H), 5.45 (d, *J* = 3.0 Hz, 1H), 4.24 – 4.18 (m, 9H), 2.48 (d, *J* = 3.0 Hz, 1H).

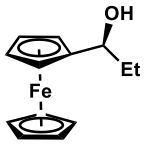
^{13}C NMR (101 MHz, $CDCl_3$) δ 163.3, 160.8, 139.0, 139.0, 127.9, 127.8, 115.1, 114.9, 94.2, 71.3, 68.5, 68.3, 68.2, 67.4, 65.7.

^{19}F NMR (376 MHz, $CDCl_3$) δ -115.16.

HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{17}H_{15}FFeO$ 311.0524; Found: 311.0520.

Chiral HPLC: The ee value was 83%, t_R (minor) = 12.6 min, t_S (major) = 14.6 min (Chiralpak IA, λ = 254 nm, 10% isopropanol/hexanes, flow rate = 1.0 mL/min).

***(S)*-1-(ferrocene-2-yl)propan-1-ol (S5)**



TLC: R_f = 0.47 (petroleum ether/Ethyl acetate = 8:1); 75 mg, yield: 30%; yellow oil.

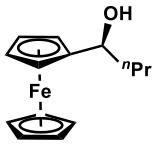
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.25 – 4.23 (m, 1H), 4.20 (s, 5H), 4.19 – 4.17 (m, 1H), 4.16 – 4.15 (m, 2H), 1.94 (d, *J* = 3.4 Hz, 1H), 1.73 – 1.64 (m, 2H), 0.95 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 94.3, 71.1, 68.2, 67.8, 67.7, 67.3, 65.1, 31.0, 10.3.

HRMS (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{13}H_{16}FeONa$ 267.0437; Found: 267.0443.

Chiral HPLC: The ee value was 98%, t_R (minor) = 9.2 min, t_S (major) = 14.1 min (Chiralpak IA, λ = 254 nm, 10% isopropanol/hexanes, flow rate = 1.0 mL/min).

***(S)*-1-(ferrocene-2-yl)butan-1-ol (S6)**



TLC: R_f = 0.41 (petroleum ether/Ethyl acetate = 8:1); 80 mg, yield: 31%; yellow oil.

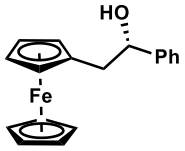
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.33 (ddd, *J* = 8.2, 4.9, 3.3 Hz, 1H), 4.25 – 4.23 (m, 1H), 4.21 – 4.19 (m, 5H), 4.19 – 4.15 (m, 3H), 1.92 (d, *J* = 3.4 Hz, 1H), 1.72 – 1.64 (m, 1H), 1.61 – 1.53 (m, 1H), 1.52 – 1.43 (m, 1H), 1.43 – 1.31 (m, 1H), 0.93 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 94.6, 69.4, 68.2, 67.8, 67.7, 67.2, 65.2, 40.3, 19.2, 14.0.

HRMS (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{14}H_{18}FeONa$ 281.0593; Found: 281.0602.

Chiral HPLC: The ee value was 98%, t_R (minor) = 8.8 min t_S (major) = 11.8 min (Chiralpak IA, λ = 254 nm, 10% isopropanol/hexanes, flow rate = 1.0 mL/min).

***(S)*-1-phenyl-2-(ferrocene-2-yl)ethan-1-ol (S7)**



TLC: R_f = 0.37 (petroleum ether/Ethyl acetate = 8/1); 400 mg, yield: 12%; yellow solid.

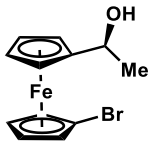
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 – 7.33 (m, 4H), 7.32 – 7.27 (m, 1H), 4.68 (dd, *J* = 8.2, 4.9 Hz, 1H), 4.17 – 4.07 (m, 8H), 4.07 (s, 1H), 2.82 – 2.71 (m, 2H), 2.36 (s, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.0, 128.2, 127.4, 125.7, 84.2, 75.0, 69.3, 68.8, 68.6, 67.9, 67.8, 40.2.

HRMS (ESI-TOF) m/z: $[M]^+$ Calcd for $C_{18}H_{18}FeO$ 306.0701; Found: 306.0703.

Chiral HPLC: The ee value was 97%, t_S (major) = 9.8 min, t_R (minor) = 10.6 min (Chiralpak IF, λ = 254 nm, 10% isopropanol/hexanes, flow rate = 1.0 mL/min).

***(S)*-1-(1-Hydroxyethyl)-1'-bromoferrocene (S8)**



TLC: R_f = 0.41 (petroleum ether/Ethyl acetate=8/1); 113 mg, yield: 37%; yellow oil.

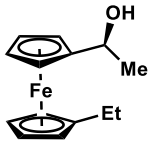
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.68 – 4.63 (m, 1H), 4.43 – 4.40 (m, 2H), 4.26 – 4.24 (m, 1H), 4.23 – 4.19 (m, 3H), 4.13 – 4.12 (m, 2H), 1.94 (d, *J* = 4.3 Hz, 1H), 1.46 – 1.44 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 96.2, 77.8, 70.5, 70.5, 70.4, 70.4, 68.5, 68.4, 67.4, 65.3, 24.1.

HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{12}H_{14}BrFeO$ 308.9566; Found: 308.9550.

Chiral HPLC: The ee value was 96%, t_S (major) = 6.5 min, t_R (minor) = 7.1 min (Chiralpak IC, λ = 254 nm, 10% isopropanol/hexanes, flow rate = 1.0 mL/min).

***(S)*-1-(1-Hydroxyethyl)-1'-ethylferrocene (S9)**



TLC: R_f = 0.45 (petroleum ether/Ethyl acetate=8/1); 175 mg, yield: 67%; yellow oil.

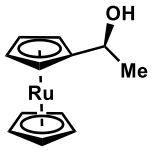
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.57 – 4.48 (m, 1H), 4.17 – 4.08 (m, 8H), 2.36 – 2.29 (m, 2H), 1.43 (dd, *J* = 6.5, 4.8 Hz, 3H), 1.16 (t, *J* = 7.5 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 95.0, 92.0, 69.1, 68.9, 68.9, 68.1, 68.1, 67.5, 66.8, 66.8, 65.4, 29.3 23.5, 22.0, 14.7.

HRMS (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{14}H_{18}FeONa$ 281.0593; Found: 281.0601.

Chiral HPLC: The ee value was 98%, t_S (major) = 13.8 min, t_R (minor) = 16.7 min (Chiralpak IC, λ = 254 nm, 3% isopropanol/hexanes, flow rate = 0.8 mL/min).

***(S)*-1-(ruthenocene-2-yl)ethan-1-ol (S12)**



TLC: R_f = 0.39 (petroleum ether/Ethyl acetate = 8/1); 242 mg, yield: 88%; white solid.

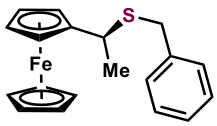
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.68 – 4.67 (m, 1H), 4.66 – 4.64 (m, 1H), 4.61 (s, 5H), 4.53 – 4.51 (m, 2H), 4.28 – 4.26 (m, 1H), 1.34 (d, *J* = 6.3 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 100.7, 70.4, 70.2, 70.2, 69.8, 68.8, 63.7, 23.5.

HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{12}H_{15}ORu$ 277.0161; Found: 277.0158.

Chiral HPLC: The ee value was 93%, t_S (major) = 7.0 min, t_R (minor) = 7.6 min (Chiralpak IC, λ = 254 nm, 10% isopropanol/hexanes, flow rate = 1.0 mL/min).

***(S)*-1-(benzylthio)ethylferrocene (3)**



TLC: R_f = 0.68 (petroleum ether/Ethyl acetate = 20/1); 63 mg, yield: 94%; yellow oil.

$[\alpha]_D^{23.8}$ = 8 (*c* = 1.0, $CHCl_3$).

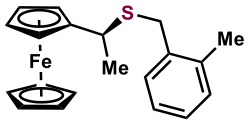
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 – 7.23 (m, 5H), 4.19 – 4.14 (m, 9H), 3.71 – 3.61 (m, 3H), 1.64 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 138.5, 128.8, 128.4, 126.8, 91.5, 68.6, 67.8, 67.7, 67.4, 65.9, 38.6, 35.5, 21.3.

HRMS (ESI-TOF) m/z: $[M+K]^+$ Calcd for $C_{19}H_{20}FeSK$ 375.0261; Found: 375.0274.

Chiral HPLC: The ee value was 99%, t_R (minor) = 6.3 min, t_S (major) = 7.3 min (Chiralpak IA, λ = 254 nm, 3% isopropanol/hexanes, flow rate = 0.8 mL/min).

***(S)*-1-((2-methylbenzyl)thio)ethylferrocene (4)**



TLC: R_f = 0.57 (petroleum ether/Ethyl acetate = 20/1); 65 mg, yield: 93%; yellow oil.

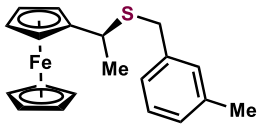
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 – 7.23 (m, 1H), 7.17 – 7.12 (m, 3H), 4.23 (s, 1H), 4.18 – 4.15 (m, 8H), 3.77 – 3.64 (m, 3H), 2.34 (s, 3H), 1.71 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 136.7, 136.0, 130.4, 129.4, 127.1, 125.8, 91.5, 68.6, 67.8, 67.6, 67.5, 66.0, 39.2, 33.3, 21.3, 19.1.

HRMS (ESI-TOF) m/z: $[M]^+$ Calcd for $C_{20}H_{22}FeS$ 350.0786; Found: 350.0789.

Chiral HPLC: The ee value was 97%, t_R (minor) = 5.8 min, t_S (major) = 6.4 min (Chiralpak IF, λ = 254 nm, 3% isopropanol/hexanes, flow rate = 0.8 mL/min).

***(S)*-1-((3-methylbenzyl)thio)ethylferrocene (5)**



TLC: R_f = 0.44 (petroleum ether/Ethyl acetate = 20/1); 65 mg, yield: 93%; yellow oil.

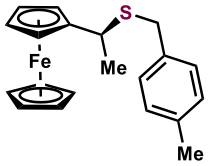
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22 (dd, *J* = 15.0, 7.5 Hz, 1H), 7.15 – 7.12 (m, 2H), 7.06 (d, *J* = 7.5 Hz, 1H), 4.22 (d, *J* = 1.8 Hz, 1H), 4.16 – 4.15 (m, 8H), 3.70 – 3.62 (m, 3H), 2.36 (s, 3H), 1.67 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 138.3, 138.0, 129.5, 128.2, 127.5, 125.8, 91.5, 68.6, 67.8, 67.6, 67.4, 65.8, 38.6, 35.4, 21.3, 21.2.

HRMS (ESI-TOF) m/z: $[M]^+$ Calcd for $C_{20}H_{22}FeS$ 350.0786; Found: 350.0789.

Chiral HPLC: The ee value was 99%, t_R (minor) = 5.9 min, t_S (major) = 7.1 min (Chiralpak IF, λ = 254 nm, 3% isopropanol/hexanes, flow rate = 0.8 mL/min)

***(S)*-1-((4-methylbenzyl)thio)ethylferrocene (6)**



TLC: R_f = 0.57 (petroleum ether/Ethyl acetate = 20/1); 66 mg, yield: 94%; yellow oil.

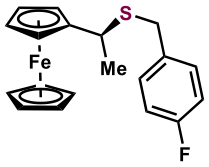
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22 (d, *J* = 8.1 Hz, 2H), 7.12 (d, *J* = 7.9 Hz, 2H), 4.21 – 4.20 (m, 1H), 4.15 – 4.14 (m, 8H), 3.69 – 3.61 (m, 3H), 2.34 (s, 3H), 1.65 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 136.4, 135.4, 129.1, 128.7, 91.5, 68.6, 67.8, 67.6, 67.4, 65.9, 38.5, 35.1, 21.3, 21.1.

HRMS (ESI-TOF) m/z: $[M]^+$ Calcd for $C_{20}H_{22}FeS$ 350.0786; Found: 350.0790.

Chiral HPLC: The ee value was 97%, t_R (minor) = 6.1 min, t_S (major) = 6.9 min (Chiralpak IF, λ = 254 nm, 3% isopropanol/hexanes, flow rate = 0.8mL/min).

***(S)*-1-((4-fluorobenzyl)thio)ethylferrocene (7)**



TLC: R_f = 0.46 (petroleum ether/Ethyl acetate = 20/1); 66 mg, yield: 93%; yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 – 7.24 (m, 2H), 7.00 – 6.95 (m, 2H), 4.19 – 4.17 (m, 1H), 4.15 – 4.10 (m, 8H), 3.67 – 3.58 (m, 3H), 1.63 (dd, *J* = 6.9, 1.6 Hz, 3H).

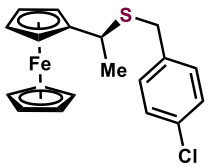
^{13}C NMR (101 MHz, $CDCl_3$) δ 162.9, 160.5, 134.2, 134.2, 130.3, 130.2, 115.3, 115.1, 91.3, 68.7, 67.8, 67.7, 67.5, 65.9, 38.7, 34.6, 21.2.

^{19}F NMR (376 MHz, $CDCl_3$) δ -115.83.

HRMS (ESI-TOF) m/z: $[M]^+$ Calcd for $C_{19}H_{19}FFeS$ 354.0535; Found: 354.0537.

Chiral HPLC: The ee value was 99%, t_R (minor) = 7.1 min, t_S (major) = 7.9 min (Chiralpak IA, λ = 254 nm, 3% isopropanol/hexanes, flow rate = 0.8 mL/min).

***(S)*-1-((4-chlorobenzyl)thio)ethylferrocene (8)**



TLC: R_f = 0.57 (petroleum ether/Ethyl acetate = 20/1); 74 mg, yield: 98%; yellow oil.

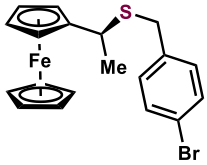
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 – 7.22 (m, 4H), 4.18 – 4.09 (m, 9H), 3.65 – 3.57 (m, 3H), 1.63 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 137.1, 132.4, 130.1, 128.5, 91.2, 68.6, 67.8, 67.7, 67.4, 65.8, 38.6, 34.7, 21.2.

HRMS (ESI-TOF) m/z: $[M]^+$ Calcd for $C_{19}H_{19}ClFeS$ 370.0240; Found: 370.0247.

Chiral HPLC: The ee value was 98%, t_R (minor) = 7.5 min, t_S (major) = 8.3 min (Chiralpak IF, λ = 254 nm, 3% isopropanol/hexanes, flow rate = 0.8 mL/min).

***(S)*-1-((4-bromobenzyl)thio)ethylferrocene (9)**



TLC: R_f = 0.66 (petroleum ether/Ethyl acetate = 20/1); 79 mg, yield: 96%; yellow oil.

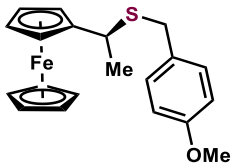
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 – 7.40 (m, 2H), 7.21 – 7.17 (m, 2H), 4.22 – 4.07 (m, 9H), 3.67 – 3.56 (m, 3H), 1.64 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 137.6, 131.5, 130.5, 120.5, 91.2, 68.6, 67.8, 67.7, 67.5, 65.8, 38.7, 34.7, 21.2.

HRMS (ESI-TOF) m/z: $[M]^+$ Calcd for $C_{19}H_{19}BrFeS$ 413.9734; Found: 413.9737.

Chiral HPLC: The ee value was 90%, t_R (minor) = 7.3 min, t_S (major) = 9.4 min (Chiralpak IF, λ = 254 nm, 3% isopropanol/hexanes, flow rate = 0.8 mL/min).

***(S)*-1-((4-methoxybenzyl)thio)ethylferrocene (10)**



TLC: R_f = 0.5 (petroleum ether/Ethyl acetate = 20/1); 67 mg, yield: 92%; yellow oil.

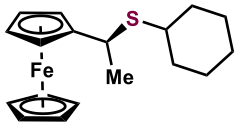
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27 – 7.17 (m, 2H), 6.89 – 6.77 (m, 2H), 4.22 – 4.07 (m, 9H), 3.79 (s, 3H), 3.68 – 3.58 (m, 3H), 1.64 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 158.4, 130.4, 129.8, 113.8, 91.5, 68.6, 67.8, 67.6, 67.4, 65.8, 55.2, 38.5, 34.8, 21.3.

HRMS (ESI-TOF) m/z: $[M]^+$ Calcd for $C_{20}H_{22}FeOS$ 366.0735; Found: 366.0734.

Chiral HPLC: The ee value was 96%, t_R (minor) = 8.8 min, t_S (major) = 10.3 min (Chiralpak IA, λ = 254 nm, 3% isopropanol/hexanes, flow rate = 0.8 mL/min).

***(S)*-1-(cyclohexylthio)ethylferrocene (11)**



TLC: R_f = 0.47 (petroleum ether/Ethyl acetate = 20/1); 61 mg, yield: 93%; yellow solid.

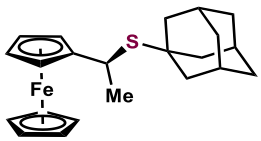
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.20 – 4.13 (m, 9H), 3.81 (q, *J* = 6.9 Hz, 1H), 2.66 – 2.59 (m, 1H), 1.94 (dd, *J* = 3.9, 1.8 Hz, 1H), 1.86 (dd, *J* = 3.9, 1.8 Hz, 1H), 1.77 – 1.72 (m, 2H), 1.65 (d, *J* = 6.9 Hz, 3H), 1.61 – 1.59 (m, 1H), 1.32 – 1.23 (m, 5H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 92.2, 68.6, 67.6, 67.6, 67.4, 65.7, 42.5, 37.0, 34.0, 33.8, 26.1, 25.8, 21.9.

HRMS (ESI-TOF) m/z: $[M]^+$ Calcd for $C_{20}H_{22}FeS$ 328.0942; Found: 328.0943.

Chiral HPLC: The ee value was 99%, t_S (major) = 11.1 min, t_R (minor) = 13.3 min (Chiralpak IF, λ = 254 nm, 0.5% isopropanol/hexanes, flow rate = 0.4 mL/min).

***(S)*-1-(((3*s*,5*s*,7*s*)-adamantan-1-yl)thio)ethylferrocene (12)**



TLC: R_f = 0.40 (PE); 64 mg, yield: 84%; yellow solid.

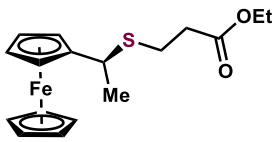
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.25 – 4.08 (m, 9H), 3.74 (q, *J* = 7.0 Hz, 1H), 2.05 (s, 3H), 1.91 (s, 6H), 1.71 (d, *J* = 7.0 Hz, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 93.8, 68.5, 67.5, 67.5, 67.4, 66.9, 45.9, 44.0, 36.3, 33.9, 29.7, 25.1.

HRMS (ESI-TOF) m/z: $[M]^+$ Calcd for $C_{22}H_{28}FeS$ 380.1255; Found: 380.1254.

Chiral HPLC: The ee value was 98%, t_R (minor) = 8.0 min, t_S (major) = 9.2 min (Chiralpak IE, λ = 254 nm, 2% isopropanol/hexanes, flow rate = 0.6 mL/min).

***(S)*-1-(3-ethoxy-3-oxopropylthio)ethylferrocene (13)**



TLC: R_f = 0.2 (petroleum ether/Ethyl acetate = 20/1); 62 mg, yield: 88%; yellow oil.

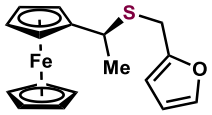
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.19 – 4.10 (m, 11H), 3.77 (q, *J* = 6.9 Hz, 1H), 2.71 (t, *J* = 7.7 Hz, 2H), 2.48 (t, *J* = 7.5 Hz, 2H), 1.66 (d, *J* = 6.9 Hz, 3H), 1.25 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 172.0, 91.3, 68.6, 67.8, 67.7, 67.6, 65.7, 60.6, 39.0, 34.9, 25.7, 21.3, 14.2.

HRMS (ESI-TOF) m/z: $[M]^+$ Calcd for $C_{17}H_{22}FeO_2S$ 346.0684; Found: 346.0684.

Chiral HPLC: The ee value was 97%, t_R (minor) = 5.7 min, t_S (major) = 6.4 min (Chiralpak IA, λ = 254 nm, 10% isopropanol/hexanes, flow rate = 1.0 mL/min).

***(S)*-2-(((1-(ferrocene-2-yl)ethyl)thio)methyl)furan (14)**



TLC: R_f = 0.5 (petroleum ether/Ethyl acetate=20/1); 42 mg, yield: 64%; yellow oil.

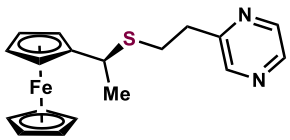
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (d, *J* = 1.3 Hz, 1H), 6.32 (dd, *J* = 3.2, 1.9 Hz, 1H), 6.17 (d, *J* = 2.9 Hz, 1H), 4.22 – 4.13 (m, 9H), 3.74 (q, *J* = 6.9 Hz, 1H), 3.66 (s, 2H), 1.65 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 152.2, 141.9, 110.4, 91.1, 68.7, 68.6, 67.9, 67.8, 67.5, 65.8, 38.7, 27.5, 21.1.

HRMS (ESI-TOF) m/z: $[M]^+$ Calcd for $C_{17}H_{18}FeOS$ 326.0422; Found: 326.0421.

Chiral HPLC: The ee value was 96%, t_R (minor) = 6.9 min, t_S (major) = 9.3 min (Chiralpak IA, λ = 254 nm, 3% isopropanol/hexanes, flow rate = 0.8 mL/min).

***(S)*-2-2-((1-(ferrocene-2-yl)ethyl)thio)ethyl)pyrazine (15)**



TLC: R_f = 0.26 (petroleum ether/Ethyl acetate = 5/1); 59 mg, yield: 84%; yellow oil.

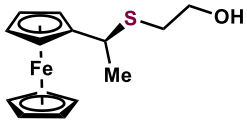
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (d, *J* = 28.3 Hz, 3H), 4.15 (d, *J* = 8.5 Hz, 9H), 3.75 (q, *J* = 6.9 Hz, 1H), 2.95 (t, *J* = 7.3 Hz, 2H), 2.85 (t, *J* = 7.1 Hz, 2H), 1.65 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.8, 144.7, 144.1, 142.4, 91.3, 68.6, 67.9, 67.7, 67.5, 65.6, 39.1, 35.5, 29.7, 21.2.

HRMS (ESI-TOF) m/z: $[M]^+$ Calcd for $C_{18}H_{20}FeN_2S$ 352.0691; Found: 352.0691.

Chiral HPLC: The ee value was 99%, t_R (minor) = 11.7 min, t_S (major) = 12.5 min (Chiralpak IA, λ = 254 nm, 10% isopropanol/hexanes, flow rate = 1.0 mL/min).

***(S)*-1-(2-hydroxyethylthio)ethylferrocene (16)**



TLC: R_f = 0.23 (petroleum ether/Ethyl acetate=5/1); 51 mg, yield: 88%; yellow oil.

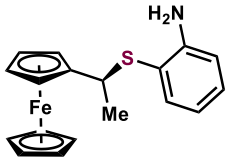
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.18 – 4.15 (m, 9H), 3.78 (q, *J* = 6.9 Hz, 1H), 3.60 (t, *J* = 6.1 Hz, 2H), 2.66 (t, *J* = 6.0 Hz, 2H), 1.67 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 91.2, 68.6, 67.9, 67.8, 67.6, 65.6, 60.7, 38.6, 33.8, 21.4.

HRMS (ESI-TOF) m/z: $[M]^+$ Calcd for $C_{14}H_{18}FeOS$ 290.0422; Found: 290.0420.

Chiral HPLC: The ee value was 99%, t_R (minor) =11.2 min, t_S (major) =13.7 min (Chiralpak Ia, λ = 254 nm, 10% isopropanol/hexanes, flow rate = 1.0 mL/min).

***(S)*-2-((1-(ferrocene)ethyl)thio)aniline (17)**



TLC: R_f = 0.21 (petroleum ether/Ethyl acetate = 20:1); 64 mg, yield: 95%; yellow oil.

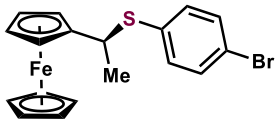
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.15 – 7.11 (m, 1H), 6.71 – 6.63 (m, 2H), 4.16 – 4.07 (m, 9H), 3.97 (q, *J* = 6.9 Hz, 2H), 3.93 – 3.92(m, 1H), 1.62 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 149.2, 137.8, 130.1, 118.2, 117.3, 114.8, 91.0, 68.5, 68.0, 67.6, 67.6, 65.4, 43.3, 20.8.

HRMS (ESI-TOF) m/z: $[M]^+$ Calcd for $C_{18}H_{19}FeNS$ 337.0582; Found: 337.0582.

Chiral HPLC: The ee value was 99%, t_R (minor) = 8.5 min, t_S (major) = 11.3 min (Chiralpak IA, λ = 254 nm, 15% isopropanol/hexanes, flow rate = 1.0 mL/min).

***(S)*-1-((4-bromophenyl)thio)ethylferrocene (18)**



TLC: R_f = 0.61 (petroleum ether/Ethyl acetate=20/1); 69 mg, yield: 86%; yellow oil.

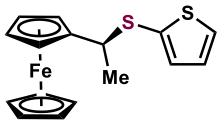
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.38 (m, 2H), 7.22 – 7.18 (m, 2H), 4.17 – 4.11 (m, 9H), 4.03 – 4.02 (m, 1H), 1.63 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 134.8, 134.1, 131.7, 121.5, 90.4, 68.7, 67.9, 67.8, 67.6, 66.0, 43.8, 21.0.

HRMS (ESI-TOF) m/z: $[M]^+$ Calcd for $C_{18}H_{17}BrFeS$ 399.9578; Found: 399.9577.

Chiral HPLC: The ee value was 99%, t_R (minor) = 6.5 min, t_S (major) = 7.2 min (Chiralpak IF, λ = 254 nm, 2% isopropanol/hexanes, flow rate = 0.8 mL/min).

***(S)*-2-(1-(thiophen-2-ylthio)ethyl)ferrocene (19)**



TLC: R_f = 0.68 (petroleum ether/Ethyl acetate = 20/1); 61 mg, yield: 93%; yellow oil.

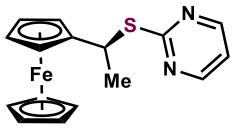
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (dd, *J* = 5.3, 1.3 Hz, 1H), 7.02 – 6.93 (m, 2H), 4.17 – 4.11 (m, 8H), 4.06 – 4.05 (m, 1H), 3.99 (q, *J* = 6.9 Hz, 1H), 1.64 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ135.5, 133.1, 130.1, 127.4, 90.0, 68.6, 68.1, 67.7, 67.6, 65.9, 46.7, 20.7.

HRMS (ESI-TOF) m/z: $[M]^+$ Calcd for $C_{16}H_{16}FeS_2$ 328.0037; Found: 328.0036.

Chiral HPLC: The ee value was 95%, t_R (minor) = 5.6 min, t_S (major) = 6.5 min (Chiralpak IF, λ = 254 nm, 3% isopropanol/hexanes, flow rate = 0.8 mL/min).

***(S)*-2-((1-(ferrocene-2-yl)ethyl)thio)pyrimidine (20)**



TLC: R_f = 0.31 (petroleum ether/Ethyl acetate = 8/1); 42 mg, yield: 65%; yellow solid.

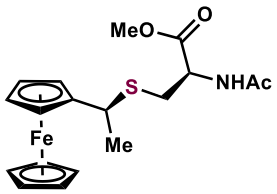
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 (d, *J* = 4.8 Hz, 2H), 6.95 (t, *J* = 4.8 Hz, 1H), 4.86 (q, *J* = 6.8 Hz, 1H), 4.31 – 4.26 (m, 2H), 4.23 (d, *J* = 0.6 Hz, 5H), 4.18 – 4.13 (m, 2H), 1.80 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 172.7, 157.2, 116.3, 89.8, 68.7, 67.8, 67.8, 67.7, 66.8, 39.7, 21.6.

HRMS (ESI-TOF) m/z: $[M]^+$ Calcd for $C_{16}H_{16}FeN_2S$ 324.0378; Found: 324.0376.

Chiral HPLC: The ee value was 98%, t_S (major) = 8.4 min, t_R (minor) = 11.2 min (Chiralpak IA, λ = 254 nm, 10% isopropanol/hexanes, flow rate = 1.0 mL/min).

methyl N-acetyl-S-(*(S)*-1-(ferrocene-2-yl)ethyl)-L-cysteinate (21)



TLC: R_f = 0.33 (petroleum ether/Ethyl acetate = 1/1); 75.0 mg, yield: 96%; yellow oil.

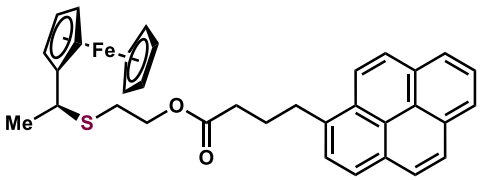
^{1}H NMR (400 MHz, $CDCl_3$) δ 6.15 (d, *J* = 7.7 Hz, 1H), 4.74 – 4.69 (m, 1H), 4.15 – 4.13 (m, 9H), 3.76 – 3.69 (m, 4H), 2.90 – 2.81 (m, 2H), 1.98 (s, 3H), 1.62 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.3, 169.9, 90.8, 68.7, 67.8, 67.7, 65.6, 52.5, 51.6, 39.4, 32.3, 23.1, 21.1.

HRMS (ESI-TOF) m/z: $[M]^+$ Calcd for $C_{18}H_{23}FeNO_3S$ 389.0742; Found: 389.0741.

Chiral HPLC: The ee value was 99%, t_S (major) = 9.1 min, t_R (minor) = 11.3 min (Chiralpak IA, λ = 254 nm, 20% isopropanol/hexanes, flow rate = 1.0 mL/min).

***(S)*-2-((1-(ferrocene-2-yl)ethyl)thio)ethyl 4-(pyren-1-yl)butanoate (22)**



TLC: R_f = 0.43 (petroleum ether/Ethyl acetate = 8/1); 72 mg, yield: 64%; yellow oil.

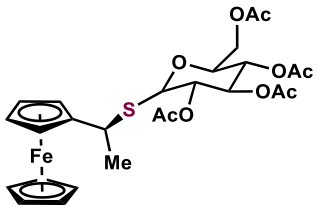
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, *J* = 9.3 Hz, 1H), 8.18 (dd, *J* = 7.6, 3.0 Hz, 2H), 8.14 (d, *J* = 2.4 Hz, 1H), 8.11 (s, 1H), 8.04 (s, 2H), 8.01 (t, *J* = 7.6 Hz, 1H), 7.87 (d, *J* = 7.8 Hz, 1H), 4.15 – 4.10 (m, 11H), 3.79 (q, *J* = 6.9 Hz, 1H), 3.42 – 3.38 (m, 2H), 2.67 (t, *J* = 7.1 Hz, 2H), 2.47 (t, *J* = 7.3 Hz, 2H), 2.21 (dt, *J* = 15.1, 7.3 Hz, 2H), 1.66 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 173.2, 135.6, 131.3, 130.8, 129.9, 128.7, 127.4, 127.4, 126.7, 125.8, 125.0, 124.9, 124.9, 124.8, 124.7, 123.3, 91.1, 68.6, 67.9, 67.8, 67.6, 65.6, 63.5, 39.0, 33.7, 32.7, 29.0, 26.7, 21.3.

HRMS (ESI-TOF) m/z: $[M]^+$ Calcd for $C_{34}H_{32}FeO_2S$ 560.1467; Found: 560.1470.

Chiral HPLC: The ee value was 97%, t_S (major) = 21.3 min, t_R (minor) = 29.8 min (Chiralcel OD-H, λ = 254 nm, 15% isopropanol/hexanes, flow rate = 1.0 mL/min).

(2S,3S,4R,5S)-2-(acetoxymethyl)-6-(((*S*)-1-((ferrocene-2-yl)ethyl)thio)tetrahydro-2H-pyran-3,4,5-triyl triacetate (23)



TLC: R_f = 0.41 (petroleum ether/Ethyl acetate = 2/1); 86 mg, yield: 75%; yellow oil.

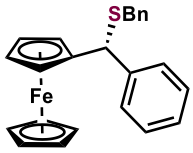
^{1}H NMR (400 MHz, $CDCl_3$) δ 5.15 – 5.09 (m, 1H), 5.05 – 5.00 (m, 1H), 4.99 – 4.93 (m, 1H), 4.35 (dd, *J* = 20.7, 10.2 Hz, 1H), 4.23 – 3.99 (m, 12H), 3.60 – 3.53 (m, 1H), 2.10 (d, *J* = 12.5 Hz, 3H), 2.00 – 1.96 (m, 9H), 1.68 (dd, *J* = 13.3, 6.9 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ170.6, 170.5, 170.2, 169.3, 169.30, 169.27, 90.3, 89.8, 82.9, 82.7, 75.5, 75.4, 73.9, 73.8, 69.9, 69.7, 68.8, 68.7, 68.4, 68.3, 68.2, 68.1, 68.0, 67.9, 67.7, 67.5, 66.2, 65.6, 62.4, 62.2, 39.5, 39.0, 22.2, 21.6, 20.8, 20.7, 20.6, 20.5.

HRMS (ESI-TOF) m/z: $[M+K]^+$ Calcd for $C_{26}H_{32}FeO_9SK$ 615.0743; Found: 615.0751.

Chiral HPLC: The ee value was 97%, t_S (major) = 10.2 min, t_R (minor) = 12.5 min (Chiralpak IA, λ = 254 nm, 10% isopropanol/hexanes, flow rate = 1.0 mL/min).

***(S)*-2-((benzylthio)(phenyl)methyl)ferrocene (24)**



TLC: R_f = 0.67 (petroleum ether/Ethyl acetate=20/1); 67 mg yield: 85%; yellow oil.

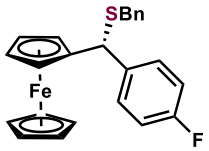
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 – 7.41 (m, 2H), 7.38 – 7.35 (m, 2H), 7.34 – 7.28 (m, 3H), 7.25 – 7.22 (m, 3H), 4.60 (s, 1H), 4.11 – 4.03 (m, 9H), 3.50 (d, *J* = 13.5 Hz, 1H), 3.40 (d, *J* = 13.5 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 142.1, 138.3, 129.0, 128.5, 128.4, 128.3, 127.2, 126.8, 89.8, 68.9, 68.1, 67.9, 67.5, 67.4, 48.9, 36.3.

HRMS (ESI-TOF) m/z: $[M+K]^+$ Calcd for $C_{24}H_{22}FeSK$ 437.0418; Found: 437.0413.

Chiral HPLC: The ee value was 80%, t_S (major) = 4.2 min, t_R (minor) = 5.2 min (Chiralpak IA, λ = 254 nm, 10% isopropanol/hexanes, flow rate =1.0 mL/min).

***(S)*-2-((benzylthio)(4-fluorophenyl)methyl)ferrocene (25)**



TLC: R_f = 0.4 (petroleum ether/Ethyl acetate=20/1); 65 mg, yield: 78%; yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 – 7.38 (m, 2H), 7.34 – 7.31 (m, 2H), 7.27 – 7.24 (m, 3H), 7.06 (t, *J* = 8.6 Hz, 2H), 4.60 (s, 1H), 4.10 – 4.05 (m, 9H), 3.53 (d, *J* = 13.6 Hz, 1H), 3.41 (d, *J* = 13.6 Hz, 1H).

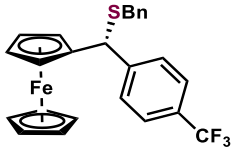
^{13}C NMR (101 MHz, $CDCl_3$) δ 163.0, 160.6, 138.1, 137.9, 137.9, 130.03, 129.9, 128.9, 128.4, 126.9, 115.2, 115.0, 89.7, 68.9, 67.9, 67.9, 67.5, 67.3, 48.1, 36.3.

^{19}F NMR (376 MHz, $CDCl_3$) δ -115.05.

HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{24}H_{22}FFeS$ 417.0765; Found: 417.0809.

Chiral HPLC: The ee value was 71%, t_R (minor) = 4.5 min, t_S (major) = 5.3 min, (Chiralpak IA, λ = 254 nm, 10% isopropanol/hexanes, flow rate =1.0 mL/min).

***(S)*-2-((benzylthio)(4-(trifluoromethyl)phenyl)methyl)ferrocene (26)**



TLC: R_f = 0.4 (petroleum ether/Ethyl acetate=20/1); 64 mg, yield: 69%; yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.1 Hz, 2H), 7.53 (d, *J* = 8.1 Hz, 2H), 7.34 – 7.30 (m, 2H), 7.27 – 7.23 (m, 3H), 4.64 (s, 1H), 4.09 (d, *J* = 7.0 Hz, 8H), 4.04 – 4.03 (m, 1H), 3.55 (d, *J* = 13.7 Hz, 1H), 3.39 (d, *J* = 13.7 Hz, 1H).

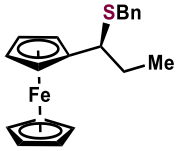
^{13}C NMR (101 MHz, $CDCl_3$) δ 146.4, 137.9, 129.5, 129.2, 128.9, 128.8, 128.5, 127.0, 125.3, 125.3, 125.3, 125.2, 88.9, 69.0, 68.1, 67.82, 67.7, 67.4, 48.5, 36.3.

^{19}F NMR (376 MHz, $CDCl_3$) δ -62.18.

HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{25}H_{21}F_3FeS$ 489.0552; Found: 489.0574.

Chiral HPLC: The ee value was 92%, t_R (minor) = 6.3 min, t_S (major) = 7.5 min (Chiralpak IA, λ = 254 nm, 3% isopropanol/hexanes, flow rate = 0.8 mL/min).

***(S)*-1-(benzylthio)propylferrocene (27)**



TLC: R_f = 0.45 (petroleum ether/Ethyl acetate = 20/1); 68 mg, yield: 97%; yellow oil.

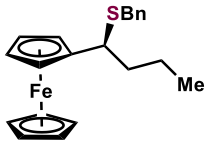
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 – 7.28 (m, 4H), 7.25 – 7.21 (m, 1H), 4.14 – 4.12 (m, 9H), 3.67 – 3.58 (m, 2H), 3.40 (dd, *J* = 9.1, 4.2 Hz, 1H), 2.20 – 2.09 (m, 1H), 1.83 – 1.72 (m, 1H), 1.09 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 138.6, 128.9, 128.3, 126.7, 91.6, 68.7, 67.7, 67.4, 67.3, 66.6, 46.3, 34.9, 28.0, 12.2.

HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{20}H_{23}FeS$ 351.0859; Found: 351.0853.

Chiral HPLC: The ee value was 90%, t_R (minor) = 12.4 min, t_S (major) = 15.2 min (Chiralpak OJ-H, λ = 254 nm, 3% isopropanol/hexanes, flow rate = 0.8 mL/min).

***(S)*-1-(benzylthio)butylferrocene (28)**



TLC: R_f = 0.43 (petroleum ether/Ethyl acetate = 20/1); 70 mg, yield: 96%; yellow oil.

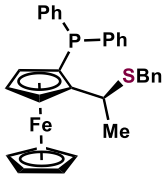
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 – 7.25 (m, 4H), 7.24 – 7.18 (m, 1H), 4.13 – 4.09 (m, 9H), 3.63 – 3.54 (m, 2H), 3.45 (dd, *J* = 9.5, 4.1 Hz, 1H), 2.07 – 1.99 (m, 1H), 1.78 – 1.69 (m, 1H), 1.66 – 1.55 (m, 1H), 1.51 – 1.43 (m, 1H), 0.92 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 138.6, 128.9, 128.3, 126.7, 91.8, 68.7, 67.7, 67.4, 67.3, 66.5, 44.0, 37.0, 34.9, 20.5, 13.9.

HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{21}H_{25}FeS$ 365.1015; Found: 365.1018.

Chiral HPLC: The ee value was 94%, t_S (major) = 6.7 min, t_R (minor) = 7.6 min (Chiralpak OD-H, λ = 254 nm, 3% isopropanol/hexanes, flow rate = 0.8 mL/min).

(*S*,$_p$*R*)-2-(1-Benzylthio)-1-diphenylphosphino-ferrocene (29)



TLC: R_f = 0.41 (petroleum ether/Ethyl acetate=20/1); 42 mg, yield: 40%; yellow oil.

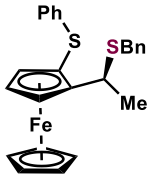
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 – 7.59 (m, 2H), 7.39 – 7.37 (m, 3H), 7.28 – 7.22 (m, 5H), 7.18 – 7.14 (m, 3H), 7.01 – 6.98 (m, 2H), 4.44 – 4.42 (m, 1H), 4.36 (t, *J* = 2.5 Hz, 1H), 4.18 – 4.12 (m, 1H), 4.00 – 3.99 (m, 1H), 3.91 (s, 5H), 3.54 (d, *J* = 12.7 Hz, 1H), 3.44 (d, *J* = 12.7 Hz, 1H), 1.73 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 140.4, 140.4, 138.3, 138.2, 138.1, 135.5, 135.3, 132.7, 129.1, 128.9, 128.2, 128.0, 128.0, 127.6, 127.5, 126.6, 97.7, 97.4, 74.6, 74.5, 71.6, 71.5, 69.6, 69.2, 68.6, 68.6, 38.4, 38.3, 35.6, 22.1.

HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{31}H_{30}FePS$ 521.1144; Found: 521.1169.

Chiral HPLC: The ee value was 99%, t_S (major) = 6.1 min, t_R (minor) = 6.7 min (Chiralpak IA, λ = 254 nm, 10% isopropanol/hexanes, flow rate = 1.0 mL/min).

(*S*,$_p$*R*)-2-(1-Benzylthio)-1-phenylthio-ferrocene (30)



TLC: R*f* = 0.5 (petroleum ether/Ethyl acetate=20/1); 77 mg yield: 87%; yellow oil.

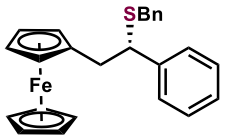
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23 – 7.16 (m, 7H), 7.11 – 7.07 (m, 1H), 7.06 – 7.02 (m, 2H), 4.54 (dd, *J* = 2.2, 1.7 Hz, 1H), 4.40 – 4.39 (m, 2H), 4.22 (s, 5H), 3.94 (q, *J* = 7.0 Hz, 1H), 3.58 – 3.48 (m, 2H), 1.73 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 140.2, 138.0, 128.7, 128.3, 128.1, 126.6, 125.9, 124.6, 95.0, 75.6, 74.0, 70.2, 68.7, 67.4, 37.0, 36.0, 22.2.

HRMS (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{25}H_{24}FeS_2Na$ 467.0555; Found: 467.0563.

Chiral HPLC: The ee value was 99%, t_S (major) = 6.2 min, t_R (minor) = 7.4 min (Chiralpak IA, λ = 254 nm, 10% isopropanol/hexanes, flow rate = 1.0 mL/min).

***(S)*-2-(benzylthio)-2-phenylethylferrocene (31)**



TLC: R_f = 0.65 (petroleum ether/Ethyl acetate = 8/1); 44 mg, yield: 53%; yellow oil.

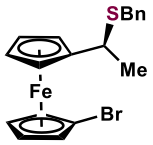
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.32 (m, 4H), 7.30 – 7.25 (m, 1H), 4.53 – 4.40 (m, 3H), 4.28 – 4.27 (m, 1H), 4.21 – 4.20 (m, 1H), 4.19 – 4.15 (m, 2H), 4.13 (s, 5H), 1.61 (d, *J* = 6.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 142.3, 138.3, 128.9, 128.3, 128.3, 128.2, 127.1, 126.8, 85.3, 69.1, 69.0, 68.5, 67.3, 67.3, 50.6, 37.6, 35.7.

HRMS (ESI-TOF) m/z: $[M+Na]^+$ $C_{25}H_{24}FeSNa$ Calcd for 435.0834; Found: 435.0849.

Chiral HPLC: The ee value was 50%, t_R (minor) = 9.3 min, t_S (major) = 12.4 min (Chiralpak OJ-H, λ = 254 nm, 10% isopropanol/hexanes, flow rate = 1.0 mL/min).

***(S)*-1-(1-(benzylthio)ethyl)-1'-bromoferrocene (32)**



TLC: R_f = 0.68 (petroleum ether/Ethyl acetate=20/1); 68 mg yield: 82%; yellow oil.

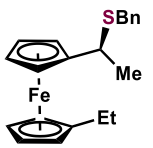
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.28 (m, 4H), 7.25 – 7.21 (m, 1H), 4.37 – 4.35 (m, 2H), 4.21 – 4.18 (m, 2H), 4.14 – 4.12 (m, 2H), 4.09 – 4.06 (m, 2H), 3.73 – 3.64 (m, 3H), 1.65 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 138.4, 128.8, 128.4, 126.8, 93.0, 77.9, 70.8, 70.7, 70.5, 70.4, 68.6, 68.3, 67.8, 67.8, 37.9, 35.5, 21.3.

HRMS (ESI-TOF) m/z: $[M]^+$ Calcd for $C_{19}H_{19}BrFeS$ 413.9734; Found: 413.9731.

Chiral HPLC: The ee value was 95%, t_R (minor) = 27 min, t_S (major) = 37.4 min (Chiralpak OJ-H, λ = 254 nm, 3% isopropanol/hexanes, flow rate = 0.8 mL/min).

***(S)*-1-(1-(benzylthio)ethyl)-1'-ethylferrocene (33)**



TLC: R_f = 0.7 (petroleum ether/Ethyl acetate=20/1); 62 mg yield: 85%; yellow oil.

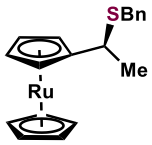
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 – 7.29 (m, 4H), 7.26 – 7.22 (m, 1H), 4.15 – 4.12 (m, 1H), 4.10 – 4.01 (m, 7H), 3.73 – 3.62 (m, 3H), 2.35 – 2.29 (m, 2H), 1.66 – 1.63 (m, 3H), 1.20 – 1.13 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 138.6, 128.8, 128.4, 126.8, 91.3, 69.2, 68.5, 68.4, 68.3, 68.3, 68.1, 67.9, 67.8, 66.2, 38.5, 35.4, 22.1, 21.3, 14.8.

HRMS (ESI-TOF) m/z: $[M]^+$ Calcd for $C_{21}H_{24}FeS$ 364.0942; Found: 364.0991.

Chiral HPLC: The ee value was 95%, t_R (minor) = 13.4 min, t_S (major) = 15.2 min (Chiralpak OJ-H, λ = 254 nm, 3% isopropanol/hexanes, flow rate = 0.8 mL/min).

***(S)*-1-(benzylthio)ethylruthenocene (34)**



TLC: R_f = 0.68 (petroleum ether/Ethyl acetate = 8/1); 64 mg, yield: 84%; colorless oil.

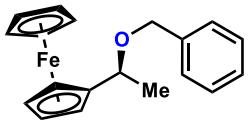
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 – 7.28 (m, 4H), 7.25 – 7.21 (m, 1H), 4.66 – 4.65 (m, 1H), 4.56 – 4.53 (m, 6H), 4.52 – 4.51 (m, 1H), 4.50 – 4.48 (m, 1H), 3.72 (d, *J* = 2.7 Hz, 2H), 3.44 (q, *J* = 6.9 Hz, 1H), 1.47 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 138.5, 128.8, 128.4, 126.8, 95.4, 70.8, 70.6, 70.0, 69.4, 68.7, 38.0, 35.8, 22.3.

HRMS (ESI-TOF) m/z: $[M+Na]^+$ $C_{19}H_{20}RuSNa$ Calcd for 405.0221; Found: 405.0225.

Chiral HPLC: The ee value was 93%, t_S (major) = 5.8 min, t_R (minor) = 6.4 min (Chiralpak IC, λ = 254 nm, 3% isopropanol/hexanes, flow rate = 0.8 mL/min).

***(S)*-1-(benzyloxy)ethylferrocene (35)**



TLC: R_f = 0.68 (petroleum ether/Ethyl acetate = 8:1); 38 mg, yield: 59%; yellow oil.

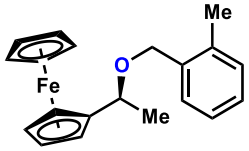
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.32 (m, 4H), 7.30 – 7.25 (m, 1H), 4.53 – 4.40 (m, 3H), 4.28 – 4.27 (m, 1H), 4.21 – 4.20 (m, 1H), 4.19 – 4.15 (m, 2H), 4.13 (s, 5H), 1.61 (d, *J* = 6.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 139.0, 128.3, 127.5, 127.3, 89.4, 72.7, 69.5, 68.7, 68.6, 68.0, 67.6, 65.9, 20.6.

HRMS (ESI-TOF) m/z: $[M]^+$ Calcd for $C_{19}H_{20}FeO$ 320.0858; Found: 320.0864.

Chiral HPLC: The ee value was 98%, t_R (minor) = 14.0 min, t_S (major) = 14.7 min (Chiralpak OJ-H, λ = 254 nm, 3% isopropanol/hexanes, flow rate = 0.8 mL/min).

***(S)*-1-((2-methylbenzyl)oxy)ethylferrocene (36)**



TLC: R_f = 0.71 (petroleum ether/Ethyl acetate = 8/1); 50 mg, yield: 75%; yellow oil.

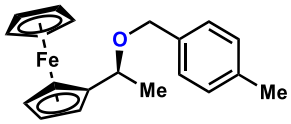
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.34 (m, 1H), 7.22 – 7.16 (m, 3H), 4.53 – 4.42 (m, 3H), 4.30 (s, 1H), 4.25 (s, 1H), 4.22 – 4.19 (m, 2H), 4.17 (s, 5H), 2.31 (s, 3H), 1.65 (d, *J* = 6.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 136.7, 136.6, 130.1, 128.5,127.5, 125.7, 89.4, 72.9, 68.7, 68.6, 68.2, 68.0, 67.5, 65.9, 20.6, 18.8.

HRMS (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{20}H_{22}FeONa$ 357.0906; Found: 357.0900.

Chiral HPLC: The ee value was 97%, t_R (minor) = 5.6 min, t_S (major) = 6.2 min (Chiralpak IF, λ = 254 nm, 3% isopropanol/hexanes, flow rate = 0.8 mL/min).

***(S)*-1-((4-methylbenzyl)oxy)ethylferrocene (37)**



TLC: R_f = 0.68 (petroleum ether/Ethyl acetate = 8/1); 49 mg, yield: 74%; yellow oil.

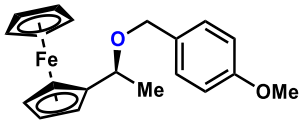
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23 (d, *J* = 8.0 Hz, 2H), 7.16 (d, *J* = 7.8 Hz, 2H), 4.50 – 4.37 (m, 3H), 4.28 (s, 1H), 4.22 (s, 1H), 4.22 – 4.14 (m, 7H), 2.35 (s, 3H), 1.60 (d, *J* = 6.5 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 136.9, 135.9, 128.9, 127.6, 89.6, 72.4, 69.4, 68.70, 68.65, 68.0, 67.6, 65.9, 21.1, 20.6.

HRMS (ESI-TOF) m/z: $[M]^+$ Calcd for $C_{20}H_{22}FeO$ 334.1014; Found: 334.1018.

Chiral HPLC: The ee value was 92%, t_S (major) = 6.4 min, t_R (minor) = 7.4 min (Chiralpak IA, λ = 254 nm, 3% isopropanol/hexanes, flow rate = 0.8 mL/min).

***(S)*-1-((4-methoxybenzyl)oxy)ethylferrocene (38)**



TLC: R_f = 0.52 (petroleum ether/Ethyl acetate = 8/1); 56 mg, yield: 80%; yellow oil.

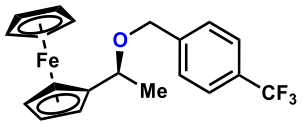
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 (d, *J* = 8.6 Hz, 2H), 6.87 (d, *J* = 8.6 Hz, 2H), 4.46 – 4.36 (m, 3H), 4.27 – 4.26 (m, 1H), 4.21 – 4.19 (m, 1H), 4.18 – 4.11 (m, 7H), 3.80 (s, 3H), 1.59 (d, *J* = 6.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 158.9, 131.1, 129.1, 113.7, 89.6, 72.4, 69.2, 68.7, 68.6, 67.9, 67.6, 65.9, 55.2, 20.6.

HRMS (ESI-TOF) m/z: $[M]^+$ Calcd for $C_{20}H_{22}FeO_2$ 350.0963; Found: 350.0968.

Chiral HPLC: The ee value was 96%, t_S (major) = 8.7 min, t_R (minor) = 10.1 min (Chiralpak IA, λ = 254 nm, 3% isopropanol/hexanes, flow rate = 0.8 mL/min).

***(S)*-1-((4-(trifluoromethyl)benzyl)oxy)ethylferrocene (39)**



TLC: R_f = 0.64 (petroleum ether/Ethyl acetate = 8/1); 39 mg, yield: 50%; yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.1 Hz, 2H), 7.43 (d, *J* = 8.0 Hz, 2H), 4.51 (q, *J* = 12.6 Hz, 2H), 4.42 (q, *J* = 6.5 Hz, 1H), 4.29 – 4.27(m, 1H), 4.21 – 4.18 (m, 3H), 4.15 (s, 5H), 1.63 (d, *J* = 6.4 Hz, 3H).

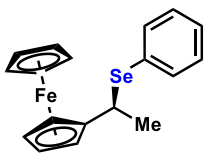
^{13}C NMR (101 MHz, $CDCl_3$) δ 143.2, 127.4, 125.6, 125.2, 125.2, 125.2, 125.1, 122.8, 88.9, 73.33, 68.7, 68.7, 68.7, 68.2, 67.7, 65.9, 20.6.

^{19}F NMR (376 MHz, $CDCl_3$) δ -62.3

HRMS (ESI-TOF) m/z: $[M]^+$ Calcd for $C_{20}H_{19}F_3FeO$ 388.0732; Found: 388.0737.

Chiral HPLC: The ee value was 99%, t_S (major) = 6.4 min, t_R (minor) = 7.2 min (Chiralpak IA, λ = 254 nm, 3% isopropanol/hexanes, flow rate = 0.8 mL/min).

***(S)*-1-(phenylselanyl)ethylferrocene (40)**



TLC: R_f = 0.57 (PE); 34 mg, yield: 46%; yellow oil.

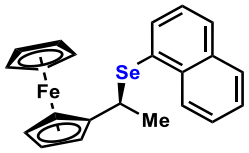
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 – 7.47 (m, 2H), 7.29 – 7.23 (m, 3H), 4.26 (q, *J* = 7.0 Hz, 1H), 4.14 – 4.09 (m, 8H), 4.01 (dt, *J* = 2.5, 1.3 Hz, 1H), 1.76 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 135.6, 130.0, 128.7, 127.6, 91.5, 68.6, 67.9, 67.7, 67.5, 65.7, 38.5, 21.8.

HRMS (ESI-TOF) m/z: $[M+K]^+$ Calcd for $C_{18}H_{18}FeSeK$ 408.9549; Found: 408.9542.

Chiral HPLC: The ee value was 78%, t_R (minor) = 10.5 min, t_S (major) = 12.3 min (Chiralpak OJ-H, λ = 254 nm, 3% isopropanol/hexanes, flow rate = 0.8 mL/min).

***(S)*-1-(naphthalen-1-ylselanyl)ethylferrocene (41)**



TLC: R_f = 0.37 (PE); 37 mg, yield: 44%; yellow oil.

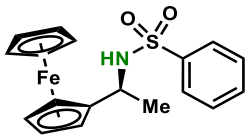
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (d, *J* = 7.4 Hz, 1H), 7.84 (d, *J* = 8.9 Hz, 2H), 7.78 (d, *J* = 7.0 Hz, 1H), 7.56 – 7.49 (m, 2H), 7.37 – 7.34 (m, 1H), 4.29 (q, *J* = 7.0 Hz, 1H), 4.18 – 4.17 (m, 1H), 4.15 – 4.10 (m, 6H), 4.05 – 4.04 (m, 1H), 3.92 – 3.90 (m, 1H), 1.72 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 135.9, 134.0, 130.0, 129.3, 128.8, 128.6, 126.7, 126.2, 125.7, 91.7, 68.7, 68.0, 67.8, 67.7, 65.8, 38.8, 22.0.

HRMS (ESI-TOF) m/z: $[M]^+$ Calcd for $C_{22}H_{20}FeSe$ 420.0080; Found: 420.0078.

Chiral HPLC: The ee value was 56%, t_R (minor) = 13.3 min, t_S (major) = 16.8 min (Chiralpak OJ-H, λ = 254 nm, 3% isopropanol/hexanes, flow rate = 0.8 mL/min).

***(S)*-N-(1-(ferrocene-2-yl)ethyl)benzenesulfonamide (42)**



TLC: R_f = 0.45 (petroleum ether/Ethyl acetate = 5/1); 60 mg, yield: 81%; yellow solid.

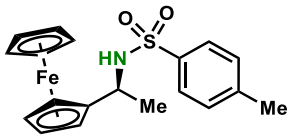
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 – 7.91 (m, 2H), 7.62 – 7.51 (m, 3H), 4.82 (d, *J* = 7.4 Hz, 1H), 4.20 – 4.17 (m, 1H), 4.13 – 4.10 (m, 5H), 4.08 – 4.05 (m, 2H), 3.94 – 3.93 (m, 1H), 3.88 – 3.87 (m, 1H), 1.42 (d, *J* = 6.6 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 140.9, 132.6, 129.1, 127.0, 90.8, 68.5, 68.1, 68.0, 67.0, 65.6, 48.5, 22.1.

HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{18}H_{20}FeNO_2S$ 370.0553; Found: 370.0601.

Chiral HPLC: The ee value was 92%, t_S (major) = 17.4 min, t_R (minor) = 19.1 min (Chiralpak IA, λ = 254 nm, 15% isopropanol/hexanes, flow rate = 1.0 mL/min).

***(S)*-4-methyl-N-(1-(ferrocene-2-yl)ethyl)benzenesulfonamide (43)**



TLC: R_f = 0.27 (petroleum ether/Ethyl acetate = 5:1); 70 mg, yield: 91%; yellow solid.

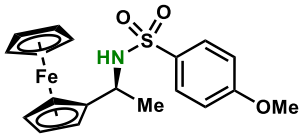
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 – 7.78 (m, 2H), 7.33 – 7.30 (m, 2H), 4.80 (d, J = 7.3 Hz, 1H), 4.18–4.12 (m, 6H), 4.09 – 4.07 (m, 2H), 3.96 – 3.95 (m, 1H), 3.92 –3.91(m, 1H), 2.44 (s, 3H), 1.40 (d, J = 6.7 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 143.2, 137.9, 129.7, 127.0, 90.9, 68.5, 68.0, 67.9, 66.9, 65.6, 48.3, 22.1, 21.5.

HRMS (ESI-TOF) m/z: $[M+K]^+$ Calcd for $C_{19}H_{21}FeNO_2SK$ 422.0268; Found: 422.0271.

Chiral HPLC: The ee value was 95%, t_R (minor) = 14.2 min, t_S (major) = 18.7 min (Chiralpak IF, λ = 254 nm, 15% isopropanol/hexanes, flow rate = 1.0 mL/min).

***(S)*-4-methoxy-N-(1-(ferrocene-2-yl)ethyl)benzenesulfonamide (44)**



TLC: R_f = 0.21 (petroleum ether/Ethyl acetate = 5/1); 70 mg, yield: 88%; yellow solid.

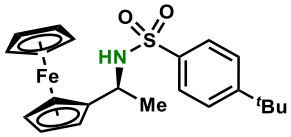
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 – 7.83 (m, 2H), 7.00 – 6.96 (m, 2H), 4.83 (d, *J* = 7.3 Hz, 1H), 4.14 – 4.11 (m, 6H), 4.08 (t, *J* = 1.9 Hz, 2H), 3.96 (q, *J* = 1.6 Hz, 1H), 3.90 (q, *J* = 1.7 Hz, 1H), 3.87 (s, 3H), 1.40 (d, *J* = 6.6 Hz, 3H).

^{13}C NMR 162.7, 132.5, 129.1, 114.2, 91.0, 68.5, 68.0, 67.9, 67.0, 65.6, 55.6, 48.3, 22.1.

HRMS (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{19}H_{21}FeNO_3SNa$ 422.0478; Found: 422.0485.

Chiral HPLC: The ee value was 97%, t_S (major) = 34.1 min, t_R (minor) = 45.2 min (Chiralpak IF, λ = 254 nm, 15% isopropanol/hexanes, flow rate = 1.0 mL/min).

***(S)*-4-(tert-butyl)-N-(1-(ferrocene-2-yl)ethyl)benzenesulfonamide (45)**



TLC: R_f = 0.43 (petroleum ether/Ethyl acetate = 5/1); 76 mg, yield: 89%; yellow solid.

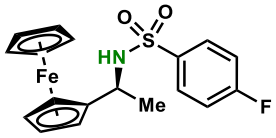
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 – 7.82 (m, 2H), 7.54 – 7.50 (m, 2H), 4.91 (d, *J* = 7.4 Hz, 1H), 4.21 – 4.15 (m, 1H), 4.11 (s, 5H), 4.07 – 4.04 (m, 2H), 3.96 – 3.95 (m, 1H), 3.90 – 3.88 (m, 1H), 1.41 (d, *J* = 6.7 Hz, 3H), 1.34 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 156.3, 137.8, 126.8, 126.0, 90.9, 68.5, 67.9, 67.9, 66.9, 65.6, 48.4, 35.1, 31.1, 22.2.

HRMS (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{22}H_{27}FeNO_2SNa$ 448.0998; Found: 448.1006.

Chiral HPLC: The ee value was 93%, t_R (minor) = 14.2 min, t_S (major) = 17.3 min (Chiralpak IA, λ = 254 nm, 15% isopropanol/hexanes, flow rate = 1.0 mL/min).

***(S)*-4-fluoro-N-(1-(ferrocene-2-yl)ethyl)benzenesulfonamide (46)**



TLC: R_f = 0.37 (petroleum ether/Ethyl acetate = 5/1); 53 mg, yield: 69%; yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 – 7.89 (m, 2H), 7.22 – 7.16 (m, 2H), 4.92 (d, *J* = 7.5 Hz, 1H), 4.19 (q, *J* = 6.9 Hz, 1H), 4.13 (s, 5H), 4.09 – 4.07 (m, 2H), 3.96 – 3.94 (m, 1H), 3.89 – 3.88 (m, 1H), 1.42 (d, *J* = 6.7 Hz, 3H).

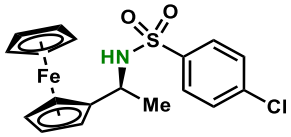
^{13}C NMR (101 MHz, CDCl3) δ 166.1, 163.6, 137.1, 137.1, 129.7, 129.6, 116.4, 116.1, 90.5, 68.5, 68.1, 68.0, 67.1, 65.5, 48.6, 22.0.

^{19}F NMR (376 MHz, $CDCl_3$) δ -105.29.

HRMS (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{18}H_{18}FFeNO_2SNa$ 410.0278; Found: 410.0279.

Chiral HPLC: The ee value was 97%, t_S (major) = 11.7 min, t_R (minor) = 16.1 min (Chiralpak IF, λ = 254 nm, 25% isopropanol/hexanes, flow rate = 1.0 mL/min).

***(S)*-4-chloro-N-(1-(ferrocene-2-yl)ethyl)benzenesulfonamide (47)**



TLC: R_f = 0.4 (petroleum ether/Ethyl acetate = 5/1); 60 mg, yield: 74%; yellow solid.

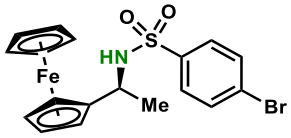
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 – 7.80 (m, 2H), 7.52 – 7.44 (m, 2H), 4.86 (d, *J* = 7.5 Hz, 1H), 4.20 (q, *J* = 7.0 Hz, 1H), 4.14 (s, 5H), 4.09 (dd, *J* = 2.5, 1.3 Hz, 2H), 3.97 – 3.94 (m, 1H), 3.92 – 3.89 (m, 1H), 1.43 (d, *J* = 6.7 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 139.6, 138.9, 129.3, 128.5, 90.6, 68.6, 68.2, 68.1, 67.1, 65.5, 48.6, 22.1.

HRMS (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{18}H_{18}ClFeNO_2SNa$ 425.9982; Found: 425.9988.

Chiral HPLC: The ee value was 95%, t_S (major) = 12.1 min, t_R (minor) = 16.8 min (Chiralpak IF, λ = 254 nm, 25% isopropanol/hexanes, flow rate = 1.0 mL/min).

***(S)*-4-bromo-N-(1-(ferrocene-2-yl)ethyl)benzenesulfonamide (48)**



TLC: R_f = 0.38 (petroleum ether/Ethyl acetate = 5/1); 45 mg, yield: 50%; yellow solid.

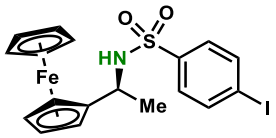
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 – 7.74 (m, 2H), 7.67 – 7.63 (m, 2H), 4.91 (d, *J* = 7.5 Hz, 1H), 4.19 (dd, *J* = 7.8, 6.2 Hz, 1H), 4.14 (s, 5H), 4.11 – 4.08 (m, 3H),3.96 – 3.95 (m, 1H), 3.91 – 3.90 (m, 1H), 1.42 (d, *J* = 6.6 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 140.1, 132.3, 128.5, 127.4, 90.5, 68.5, 68.2, 68.1, 67.1, 65.5, 48.6, 22.1.

HRMS (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{18}H_{18}BrFeNO_2SNa$ 469.9477; Found: 469.9482.

Chiral HPLC: The ee value was 97%, t_S (major) = 12.9 min, t_R (minor) = 18.2 min (Chiralpak IF, λ = 254 nm, 25% isopropanol/hexanes, flow rate = 1.0 mL/min).

***(S)*-4-iodo-N-(1-(ferrocene-2-yl)ethyl)benzenesulfonamide (49)**



TLC: R_f = 0.4 (petroleum ether/Ethyl acetate = 5/1); 49 mg, yield: 49%; yellow solid.

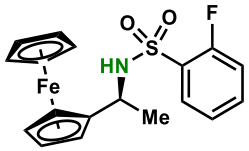
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 – 7.85 (m, 2H), 7.62 – 7.59 (m, 2H), 4.87 (d, *J* = 7.5 Hz, 1H), 4.21 – 4.17 (m, 1H), 4.14 (s, 5H), 4.11 – 4.09 (m, 2H), 3.96 – 3.95 (m, 1H), 3.92 – 3.91 (m, 1H), 1.42 (d, *J* = 6.6 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 140.8, 138.3, 128.4, 100.0, 90.5, 68.5, 68.2, 68.1, 67.1, 65.5, 48.6, 22.1.

HRMS (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{18}H_{18}FeINO_2SNa$ 517.9339; Found: 517.9323.

Chiral HPLC: The ee value was 93%, t_R (minor) = 21.9 min, t_S (major) = 24.6 min (Chiralpak IA, λ = 254 nm, 15% isopropanol/hexanes, flow rate = 1.0 mL/min).

***(S)*-2-fluoro-N-(1-(ferrocene-2-yl)ethyl)benzenesulfonamide (50)**



TLC: R_f = 0.35 (petroleum ether/Ethyl acetate = 5/1); 34 mg, yield: 44%; yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 – 7.90 (m, 1H), 7.59 – 7.53 (m, 1H), 7.29 – 7.25 (m, 1H), 7.21 – 7.16 (m, 1H), 4.97 (d, *J* = 7.8 Hz, 1H), 4.28 – 4.21 (m, 1H), 4.14 (s, 5H), 4.10 – 4.08 (m, 1H), 4.05 – 4.03 (m, 2H), 3.90 – 3.88 (m, 1H), 1.44 (d, *J* = 6.7 Hz, 3H).

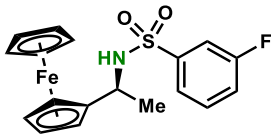
^{13}C NMR (101 MHz, $CDCl_3$) δ 160.0, 157.5, 134.8, 134.7, 130.0, 129.3, 129.1, 124.4, 124.4, 117.0, 116.8, 90.3, 68.5, 68.1, 68.0, 67.3, 65.3, 48.8, 21.8.

^{19}F NMR (376 MHz, $CDCl_3$) δ -110.26.

HRMS (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{18}H_{18}FFeNO_2SNa$ 410.0278; Found: 410.0290.

Chiral HPLC: The ee value was 93%, t_S (major) = 16.0 min, t_R (minor) = 22.5 min (Chiralpak IA, λ = 254 nm, 15% isopropanol/hexanes, flow rate = 1.0 mL/min).

3-fluoro-N-(1-(ferrocene-2-yl)ethyl)benzenesulfonamide (51)



TLC: R_f = 0.35 (petroleum ether/Ethyl acetate = 5/1); 49 mg, yield: 64%; yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 – 7.69 (m, 1H), 7.63 – 7.59 (m, 1H), 7.54 – 7.48 (m, 1H), 7.31 – 7.26 (m, 1H), 4.95 (d, J = 7.6 Hz, 1H), 4.26 – 4.19 (m, 1H), 4.13 (s, 5H), 4.10 – 4.07 (m, 2H), 3.96 – 3.95 (m, 1H), 3.91 – 3.90 (m, 1H), 1.43 (d, J = 6.7 Hz, 3H).

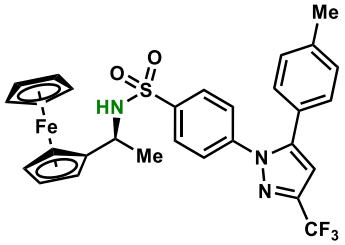
^{13}C NMR (101 MHz, $CDCl_3$) δ 163.6, 161.1, 143.2, 143.1, 130.9, 130.9, 122.7, 122.7, 119.8, 119.6, 114.5, 114.3, 90.5, 68.5, 68.1, 68.1, 67.1, 65.5, 48.7, 22.1.

^{19}F NMR (376 MHz, $CDCl_3$) δ -109.44.

HRMS (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{18}H_{18}FFeNO_2SNa$ 410.0278; Found: 410.0277.

Chiral HPLC: The ee value was 93%, t_R (minor) = 12.2 min, t_S (major) = 13.5 min (Chiralpak IA, λ = 254 nm, 15% isopropanol/hexanes, flow rate = 1.0 mL/min).

***(S)*-N-(1-(ferrocene-2-yl)ethyl)-4-(5-(p-tolyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl)benzenesulfonamide (52)**



TLC: R_f = 0.27 (petroleum ether/Ethyl acetate = 5/1); 65 mg, yield: 55%; yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 – 7.88 (m, 2H), 7.49 – 7.46 (m, 2H), 7.16 (d, *J* = 7.9 Hz, 2H), 7.09 (d, *J* = 8.2 Hz, 2H), 6.75 (s, 1H), 4.91 (d, *J* = 7.5 Hz, 1H), 4.20 (q, *J* = 6.8 Hz, 1H), 4.14 (s, 5H), 4.10 (t, *J* = 1.9 Hz, 2H), 3.96 – 3.93 (m, 2H), 2.38 (s, 3H), 1.43 (d, *J* = 6.6 Hz, 3H).

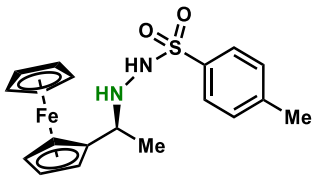
^{13}C NMR (101 MHz, CDCl3) δ 145.2, 144.6, 144.2, 143.8, 143.2, 142.3, 140.5, 139.7, 129.7, 128.7, 128.0, 125.7, 125.5, 125.1, 122.4, 119.7, 117.0, 106.3, 90.5, 68.6, 68.2, 68.1, 67.1, 65.5, 48.7, 22.0, 21.3.

^{19}F NMR (376 MHz, $CDCl_3$) δ -62.26.

HRMS (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{29}H_{26}F_3FeN_3O_2SNa$ 616.0933; Found: 616.0936.

Chiral HPLC: The ee value was 92%, t_R (minor) =13.5 min, t_S (major) = 17.0 min (Chiralpak IA, λ = 254 nm, 25% isopropanol/hexanes, flow rate = 1.0 mL/min).

***(S)*-4-methyl-N'-(1-(ferrocene-2-yl)ethyl)benzenesulfonohydrazide (53)**



TLC: R_f = 0.32 (petroleum ether/Ethyl acetate = 5/1); 39 mg, yield: 49%; yellow solid.

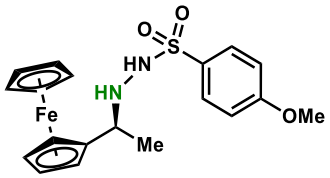
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (d, *J* = 8.0 Hz, 2H), 7.18 (d, *J* = 7.9 Hz, 2H), 4.14 – 4.09 (m, 8H), 3.99 (q, *J* = 7.1 Hz, 1H), 3.93 (s, 1H), 2.39 (s, 3H), 1.69 (d, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.3, 133.0, 129.6, 129.0, 70.7, 68.7, 68.6, 68.4, 66.9, 62.3, 21.6, 13.9.

HRMS (ESI-TOF) m/z: $[M+K]^+$ Calcd for $C_{19}H_{22}FeN_2O_2SK$ 437.0378; Found: 437.0404.

Chiral HPLC: The ee value was 88%, t_R (minor) = 14.3 min, t_S (major) =14.8 min (Chiralpak IA, λ = 254 nm, 10% isopropanol/hexanes, flow rate = 1.0 mL/min).

***(S)*-4-methoxy-N'-(1-(ferrocene-2-yl)ethyl)benzenesulfonohydrazide (54)**



TLC: R_f = 0.3 (petroleum ether/Ethyl acetate = 5/1); 33 mg, yield: 40%; yellow solid.

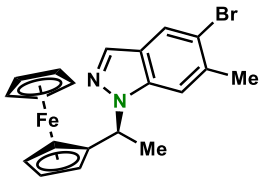
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 – 7.39 (m, 2H), 6.86 – 6.83 (m, 2H), 4.14 – 4.10 (m, 8H), 3.98 (q, *J* = 7.1 Hz, 1H), 3.93 (s, 1H), 3.83 (s, 3H), 1.69 (d, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.5, 131.7, 126.2, 113.6, 81.4, 70.7, 68.7, 68.6, 68.4, 66.9, 62.4, 55.5, 14.0.

HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{19}H_{23}FeN_2O_3S$ 415.0768; Found: 415.0748.

Chiral HPLC: The ee value was 90%, t_R (minor) = 38.8 min, t_S (major) = 42.9 min (Chiralpak IF, λ = 254 nm, 10% isopropanol/hexanes, flow rate = 1.0 mL/min).

***(S)*-5-bromo-6-methyl-1-(1-(ferrocene-2-yl)ethyl)-1H-indazole (55)**



TLC: R_f = 0.46 (petroleum ether/Ethyl acetate = 8/1); 65 mg, yield: 77%; yellow solid.

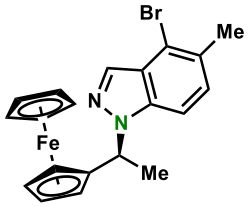
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (s, 1H), 7.87 (s, 1H), 7.28 (s, 1H), 5.67 (q, *J* = 7.0 Hz, 1H), 4.29 (d, *J* = 1.9 Hz, 1H), 4.16 (t, *J* = 2.1 Hz, 2H), 4.13 (s, 6H), 2.51 (s, 3H), 1.92 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 138.0, 135.2, 131.5, 124.0, 117.1, 110.4, 89.1, 68.8, 68.4, 67.8, 67.6, 66.5, 54.6, 24.2, 20.0.

HRMS (ESI-TOF) m/z: $[M+K]^+$ Calcd for $C_{20}H_{19}BrFeN_2K$ 460.9707; Found: 460.9708.

Chiral HPLC: The ee value was 99%, t_S (major) = 6.7 min, t_R (minor) = 12.8 min (Chiralcel OD-H, λ = 254 nm, 15% isopropanol/hexanes, flow rate = 1.0 mL/min).

***(S)*-4-bromo-5-methyl-1-(1-(ferrocene-2-yl)ethyl)-1H-indazole (56)**



TLC: R_f = 0.49 (petroleum ether/Ethyl acetate = 8/1); 62 mg, yield: 73%; yellow solid.

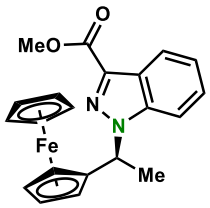
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (s, 1H), 7.24 (d, *J* = 8.5 Hz, 1H), 7.16 (d, *J* = 8.5 Hz, 1H), 5.69 (q, *J* = 7.0 Hz, 1H), 4.30 (s, 1H), 4.16 (s, 2H), 4.13 (s, 6H), 2.47 (s, 3H), 1.93 (d, *J* = 7.0 Hz, 3H)

^{13}C NMR (101 MHz, $CDCl_3$) δ 137.7, 132.5, 129.1, 128.8, 125.9, 115.5, 108.6, 89.0, 68.8, 68.4, 67.8, 67.6, 66.5, 55.2, 21.4, 20.0.

HRMS (ESI-TOF) m/z: $[M]^+$ Calcd for $C_{20}H_{19}BrFeN_2$ 422.0075; Found: 422.0074.

Chiral HPLC: The ee value was 96%, t_R (minor) = 5.7 min, t_S (major) = 6.0 min (Chiralpak IF, λ = 254 nm, 15% isopropanol/hexanes, flow rate = 1.0 mL/min).

methyl *(S)*-1-(1-(ferrocene-2-yl)ethyl)-1H-indazole-3-carboxylate (57)



TLC: R_f = 0.31 (petroleum ether/Ethyl acetate = 8/1); 63 mg, yield: 81%; yellow oil.

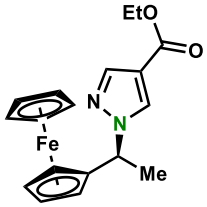
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (d, *J* = 7.3 Hz, 1H), 7.35 (d, *J* = 8.0 Hz, 1H), 7.30 – 7.21 (m, 2H), 5.97 (q, *J* = 7.1 Hz, 1H), 4.38 (s, 1H), 4.21 – 4.17 (m, 2H), 4.13 (s, 6H), 4.03 (s, 3H), 1.96 (d, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.2, 139.0, 133.8, 126.2, 124.3, 122.9, 122.1, 110.8, 87.4, 68.9, 68.8, 68.4, 67.6, 66.6, 57.4, 51.9, 19.4.

HRMS (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{21}H_{20}FeN_2O_2Na$ 411.0760; Found: 411.0768.

Chiral HPLC: The ee value was 96%, t_S (major) = 11.6 min, t_R (minor) = 14.7 min (Chiralpak IF, λ = 254 nm, 10% isopropanol/hexanes, flow rate = 0.8 mL/min).

ethyl *(S)*-1-(1-(ferrocene-2-yl)ethyl)-1H-pyrazole-4-carboxylate (58)



TLC: R_f = 0.53 (petroleum ether/Ethyl acetate = 5/1); 53mg, yield: 76%; yellow solid.

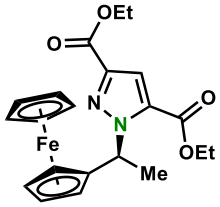
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (s, 1H), 7.73 (s, 1H), 5.35 (q, *J* = 7.0 Hz, 1H), 4.27 – 4.20 (m, 4H), 4.18 – 4.15 (m, 7H), 1.83 (d, *J* = 7.0 Hz, 3H), 1.30 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.1, 140.3, 130.3, 114.5, 87.4, 68.9, 68.8, 68.2, 68.0, 66.1, 60.0, 58.0, 21.1, 14.3.

HRMS (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{18}H_{20}FeN_2O_2Na$ 375.0760; Found: 375.0766;

Chiral HPLC: The ee value was 99%, t_R (minor) = 7.6 min, t_S (major) = 9.8 min (Chiralpak IA, λ = 254 nm, 15% isopropanol/hexanes, flow rate = 1.0 mL/min).

diethyl *(S)*-1-(1-(ferrocene-2-yl)ethyl)-1H-pyrazole-3,5-dicarboxylate (59)



TLC: R_f = 0.43 (petroleum ether/Ethyl acetate = 8/1); 73 mg, yield: 86%; yellow solid.

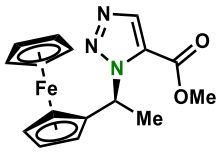
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (s, 1H), 6.49 (q, J = 7.0 Hz, 1H), 4.41 – 4.33 (m, 4H), 4.25 (s, 2H), 4.11 (s, 7H), 1.92 (d, J = 7.0 Hz, 3H), 1.42 – 1.34 (m, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.8, 159.5, 141.9, 132.8, 113.9, 89.6, 68.8, 68.0, 67.6, 67.5, 66.8, 61.3, 60.9, 55.7, 20.8, 14.3, 14.2.

HRMS (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{21}H_{24}FeN_2O_4Na$ 447.0972; Found: 447.0975.

Chiral HPLC: The ee value was 99%, t_S (major) = 5.5 min, t_R (minor) = 8.0 min (Chiralpak IF, λ = 254 nm, 15% isopropanol/hexanes, flow rate = 1.0 mL/min).

methyl *(S)*-1-(1-(ferrocene-2-yl)ethyl)-1H-1,2,3-triazole-5-carboxylate (60)



TLC: R_f = 0.31 (petroleum ether/Ethyl acetate = 8/1); 39 mg, yield: 58%; yellow solid.

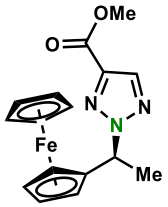
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (s, 1H), 5.75 (q, *J* = 7.1 Hz, 1H), 4.31 – 4.29 (m, 1H), 4.27 – 4.26 (m, 1H), 4.18 – 4.17 (m, 1H), 4.15 – 4.14 (m, 1H), 4.09 (s, 5H), 3.94 (s, 3H), 1.93 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.2, 138.7, 136.6, 87.5, 68.8, 68.6, 68.0, 67.5, 66.5, 61.9, 52.3, 20.6.

HRMS (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{16}H_{17}FeN_3O_2Na$ 362.0556; Found: 362.0567.

Chiral HPLC: The ee value was 96%, t_R (minor) = 8.4 min, t_S (major) = 9.3 min (Chiralpak IF, λ = 254 nm, 15% isopropanol/hexanes, flow rate = 1.0 mL/min).

methyl *(S)*-2-(1-(ferrocene-2-yl)ethyl)-2H-1,2,3-triazole-4-carboxylate (61)



TLC: R_f = 0.39 (petroleum ether/Ethyl acetate = 8/1); 38.6 mg, yield: 57%; yellow solid.

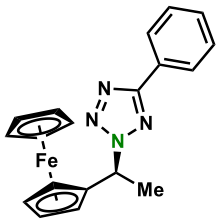
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (s, 1H), 5.75 (q, *J* = 7.0 Hz, 1H), 4.30 – 4.26 (m, 2H), 4.18 – 4.14 (m, 2H), 4.10 (s, 5H), 3.94 (s, 3H), 1.94 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.3, 138.8, 136.6, 87.6, 68.8, 68.6, 68.0, 67.5, 66.5, 61.9, 52.3, 20.6.

HRMS (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{16}H_{17}FeN_3O_2Na$ 362.0556; Found: 362.0565.

Chiral HPLC: The ee value was 95%, t_R (minor) = 8.8 min, t_S (major) =10.0 min (Chiralpak IF, λ = 254 nm, 15% isopropanol/hexanes, flow rate = 1.0 mL/min).

***(S)*-5-phenyl-2-(1-(ferrocene-2-yl)ethyl)-2H-tetrazole (62)**



TLC: R_f = 0.47 (petroleum ether/Ethyl acetate = 8/1); 51 mg, yield: 71%; yellow solid.

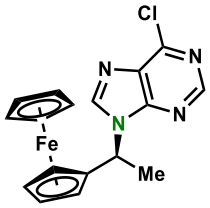
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (dd, *J* = 7.8, 1.9 Hz, 2H), 7.48 (d, *J* = 7.5 Hz, 3H), 5.95 (q, *J* = 7.0 Hz, 1H), 4.30 (d, *J* = 7.2 Hz, 2H), 4.19 – 4.17 (m, 2H), 4.11 (s, 5H), 2.01 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 164.6, 130.3, 129.0, 127.8, 126.9, 87.7, 69.0, 68.7, 68.2, 67.3, 66.8, 60.0, 21.2.

HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{19}H_{19}FeN_4$ 359.0948; Found: 359.0963.

Chiral HPLC: The ee value was 91%, t_R (minor) = 8.8 min, t_S (major) = 10.2 min (Chiralpak IF, λ = 254 nm, 15% isopropanol/hexanes, flow rate = 1.0 mL/min).

***(S)*-6-chloro-9-(1-(ferrocene-2-yl)ethyl)-9H-purine (63)**



TLC: R_f = 0.13 (petroleum ether/Ethyl acetate = 5/1); 51 mg, yield: 70%; yellow oil.

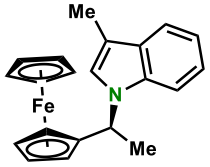
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.76 (s, 1H), 7.92 (s, 1H), 5.80 (q, *J* = 7.0 Hz, 1H), 4.38 (d, *J* = 1.3 Hz, 1H), 4.27 (d, *J* = 1.3 Hz, 1H), 4.19 (s, 6H), 4.16 (dd, *J* = 2.4, 1.2 Hz, 1H), 1.94 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.6, 151.1, 150.8, 143.5, 131.6, 86.5, 69.2, 69.0, 68.5, 68.1, 66.0, 51.0, 20.7.

HRMS (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{17}H_{15}ClFeN_4Na$ 389.0221; Found: 389.0211.

Chiral HPLC: The ee value was 98%, t_R (minor) = 27.0 min, t_S (major) = 32.1 min (Chiralpaks IE, λ = 254 nm, 15% isopropanol/hexanes, flow rate = 1.0 mL/min).

***(S)*-3-methyl-1-(1-(ferrocene-2-yl)ethyl)-1H-indole (64)**



TLC: R_f = 0.72 (petroleum ether/Ethyl acetate = 10:1); 41 mg, yield: 60%; yellow solid.

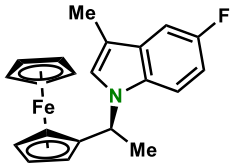
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 7.8 Hz, 1H), 7.44 (d, *J* = 8.2 Hz, 1H), 7.26 – 7.22 (m, 1H), 7.15 – 7.11(m, 1H), 6.81 (s, 1H), 5.53 (q, *J* = 6.9 Hz, 1H), 4.34 – 4.33 (m, 1H), 4.22 – 4.15 (m, 8H), 2.31 (d, *J* = 1.1 Hz, 3H), 1.83 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 135.7, 128.6, 122.4, 121.1, 119.0, 118.4, 110.1, 109.1, 89.6, 68.8, 68.4, 68.1, 67.5, 66.4, 50.4, 20.6, 9.7.

HRMS (ESI-TOF) m/z: $[M]^+$ Calcd for $C_{21}H_{21}FeN$ 343.1018; Found: 343.1021.

Chiral HPLC: The ee value was 95%, t_R (minor) = 19.0 min, t_S (major) = 21.1 min (Chiralpak IA, λ = 254 nm, 1% isopropanol/hexanes, flow rate = 0.2 mL/min).

***(S)*-5-fluoro-3-methyl-1-(1-(ferrocene-2-yl)ethyl)-1H-indole (65)**



TLC: R_f = 0.65 (petroleum ether/Ethyl acetate = 10/1); 45 mg, yield: 62%; yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 (dd, *J* = 8.9, 4.3 Hz, 1H), 7.17 (dd, *J* = 9.6, 2.5 Hz, 1H), 6.97 – 6.92 (m, 1H), 6.82 (d, *J* = 1.2 Hz, 1H), 5.47 – 5.42 (m, 1H), 4.32 – 4.11 (m, 9H), 2.22 (d, *J* = 1.0 Hz, 3H), 1.80 (d, *J* = 6.9 Hz, 3H).

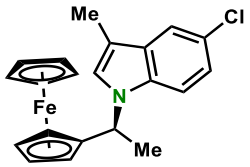
^{13}C NMR (101 MHz, $CDCl_3$) δ 158.5, 156.2, 132.3, 128.8, 124.2, 110.1, 110.1, 109.8, 109.7, 109.5, 109.2, 103.9, 103.7, 89.5, 68.9, 68.5, 68.0, 67.6, 66.4, 50.8, 20.6, 9.6.

^{19}F NMR (376 MHz, $CDCl_3$) δ -125.80.

HRMS (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{21}H_{20}FFeNNa$ 384.0816; Found: 384.0818.

Chiral HPLC: The ee value was 97%, t_R (minor) = 12.9 min, t_S (major) = 14.7 min (Chiralpak IA, λ = 254 nm, 2% isopropanol/hexanes, flow rate = 0.4 mL/min).

***(S)*-5-chloro-3-methyl-1-(1-(ferrocene-2-yl)ethyl)-1H-indole (66)**



TLC: R_f = 0.64 (petroleum ether/Ethyl acetate = 10/1); 44 mg, yield: 58%; yellow solid.

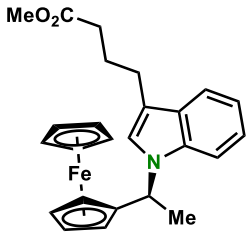
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 2.0 Hz, 1H), 7.30 (d, *J* = 8.7 Hz, 1H), 7.15 (dd, *J* = 8.7, 2.1 Hz, 1H), 6.81 (d, *J* = 1.2 Hz, 1H), 5.47–5.42 (q, *J* = 6.9 Hz, 1H), 4.33 – 4.08 (m, 9H), 2.23 (d, *J* = 1.1 Hz, 3H), 1.80 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 134.1, 129.7, 124.2, 123.9, 121.3, 118.5, 110.2, 109.9, 89.4, 68.9, 68.6, 68.0, 67.7, 66.4, 50.8, 20.6, 9.6.

HRMS (ESI-TOF) m/z: $[M+K]^+$ Calcd for $C_{21}H_{20}ClFeNK$ 416.0259; Found: 416.0225.

Chiral HPLC: The ee value was 92%, t_R (minor) = 10.3 min, t_S (major) = 11.1 min (Chiralpak IA, λ = 254 nm, 2% isopropanol/hexanes, flow rate = 0.4 mL/min).

methyl *(S)*-4-(1-(1-(ferrocene-2-yl)ethyl)-1H-indol-3-yl)butanoate (67)



TLC: R_f = 0.31 (petroleum ether/Ethyl acetate = 10/1); 49 mg, yield: 57%; yellow oil.

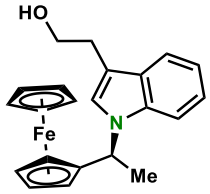
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 7.9 Hz, 1H), 7.41 (d, *J* = 8.2 Hz, 1H), 7.23 – 7.19 (m, 1H), 7.11 – 7.07 (m, 1H), 6.80 (s, 1H), 5.50 (q, *J* = 6.9 Hz, 1H), 4.31 – 4.27 (m, 1H), 4.22 – 4.10 (m, 8H), 3.65 (s, 3H), 2.76 – 2.72 (m, 2H), 2.35 (t, *J* = 7.5 Hz, 2H), 2.01 – 1.97 (m, 2H), 1.81 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 174.2, 135.9, 127.8, 122.3, 121.2, 119.1, 118.6, 114.1, 109.4, 89.6, 68.8, 68.4, 68.0, 67.5, 66.4, 51.4, 50.5, 33.7, 25.4, 24.6, 20.7.

HRMS (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{25}H_{27}FeNO_2Na$ 452.1278; Found: 452.1277.

Chiral HPLC: The ee value was 93%, t_R (minor) = 4.9 min, t_S (major) = 5.5 min (Chiralpak IA, λ = 254 nm, 15% isopropanol/hexanes, flow rate = 1.0 mL/min).

***(S)*-2-(1-(1-(ferrocene-2-yl)ethyl)-1H-indol-3-yl)ethan-1-ol (68)**



TLC: R_f = 0.35 (petroleum ether/Ethyl acetate= 3/1); 49 mg, yield: 66%; yellow solid.

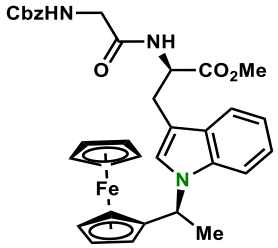
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 7.9 Hz, 1H), 7.43 (d, *J* = 7.9 Hz, 1H), 7.25 – 7.21 (m, 1H), 7.13 – 7.09 (m, 1H), 6.88 (s, 1H), 5.51 (q, *J* = 6.9 Hz, 1H), 4.30 (d, *J* = 1.3 Hz, 1H), 4.21 – 4.17 (m, 6H), 4.15 – 4.11 (m, 2H), 3.83 (t, *J* = 6.3 Hz, 2H), 2.98 – 2.94 (m, 2H), 1.82 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 136.0, 127.8, 123.3, 121.4, 119.0, 118.9, 110.6, 109.5, 89.4, 68.8, 68.5, 68.0, 67.6, 66.4, 62.6, 50.6, 28.8, 20.6.

HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{22}H_{24}FeNO$ 374.1196; Found: 374.1216.

Chiral HPLC: The ee value was 97%, t_R (minor) = 12.2 min, t_S (major) = 13.4 min (Chiralpak IC, λ = 254 nm, 10% isopropanol/hexanes, flow rate = 1.0 mL/min).

methyl (*R*)-2-(2-(((benzyloxy)carbonyl)amino)acetamido)-2-(1-((*S*)-1-(ferrocene-2-yl)ethyl)-1H-indol-3-yl)acetate (69)



TLC: R_f = 0.62 (petroleum ether/Ethyl acetate = 1/1); 89 mg, yield: 68%; yellow solid.

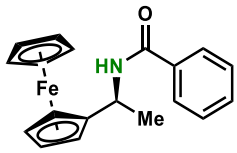
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (dd, *J* = 17.5, 8.1 Hz, 2H), 7.38-4.30 (m, 5H), 7.23 – 7.19 (m, 1H), 7.09 (t, *J* = 7.5 Hz, 1H), 6.72 (s, 1H), 6.34 – 6.28 (m, 1H), 5.49 (dd, *J* = 6.9 Hz, 1H), 5.29 – 5.26 (m, 1H), 5.09 (s, 2H), 4.85 (dd, *J* = 7.9, 4.5 Hz, 1H), 4.33 (d, *J* = 4.2 Hz, 1H), 4.17 (dd, 9H), 3.80 – 3.75 (m, 2H), 3.59 (d, *J* = 27.8 Hz, 3H), 3.24 (d, *J* = 5.8 Hz, 2H), 1.79 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.8, 168.3, 135.6, 128.5, 128.2, 128.0, 123.7, 121.5, 119.3, 118.5, 109.5, 108.2, 89.1, 68.9, 68.8, 68.6, 68.1, 67.7, 67.1, 66.4, 60.4, 53.3, 52.3, 50.7, 44.3, 27.5, 20.6, 14.2.

HRMS (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{34}H_{35}FeN_3O_5Na$ 644.1813; Found: 644.1809.

Chiral HPLC: The ee value was 98%, t_R (minor) = 13.9 min, t_S (major) = 15.0 min (Chiralpak IA, λ = 254 nm, 20% isopropanol/hexanes, flow rate = 1.0 mL/min).

***(S)*-N-(1-(ferrocene-2-yl)ethyl)benzamide (70)**



TLC: R_f = 0.17 (petroleum ether/Ethyl acetate = 8/1); 40 mg, yield: 60%; yellow solid.

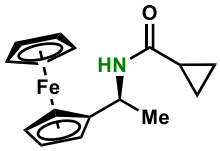
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 7.0 Hz, 2H), 7.52 – 7.42 (m, 3H), 6.41 (d, *J* = 8.2 Hz, 1H), 5.11 – 5.04 (m, 1H), 4.27 – 4.16 (m, 9H), 1.56 (d, *J* = 6.7 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.1, 134.7, 131.4, 128.6, 126.8, 91.3, 68.5, 68.1, 67.8, 67.5, 65.8, 44.1, 20.7.

HRMS (ESI-TOF) m/z: $[M]^+$ Calcd for $C_{19}H_{19}FeNO$ 333.0810; Found: 333.0823.

Chiral HPLC: The ee value was 90%, t_R (minor) = 17.4 min, t_S (major) = 21.7 min (Chiralpak IA, λ = 254 nm, 10% isopropanol/hexanes, flow rate = 1.0 mL/min).

***(S)*-N-(1-(ferrocene-2-yl)ethyl)cyclopropanecarboxamide (71)**



TLC: R_f = 0.19 (petroleum ether/Ethyl acetate = 8/1); 25 mg, yield: 42%; yellow solid.

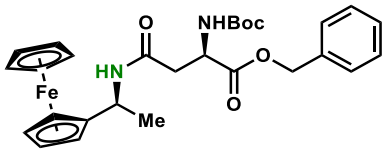
^{1}H NMR (400 MHz, $CDCl_3$) δ 5.84 (d, *J* = 8.5 Hz, 1H), 4.94 – 4.87 (m, 1H), 4.21 – 4.20 (m, 1H), 4.18 – 4.12 (m, 8H), 1.45 (d, *J* = 6.7 Hz, 3H), 1.33 – 1.25 (m, 1H), 1.00 – 0.97 (m, 2H), 0.76 – 0.71 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 172.1, 91.5, 68.5, 68.0, 67.6, 67.4, 65.8, 43.8, 20.8, 14.9, 7.1.

HRMS (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{16}H_{20}FeNONa$ 320.0702; Found: 320.0714.

Chiral HPLC: The ee value was 98%, t_R (minor) = 10.3 min, t_S (major) = 14.0 min (Chiralpak IA, λ = 254 nm, 10% isopropanol/hexanes, flow rate = 1.0 mL/min).

benzyl N^2-(*tert*-butoxycarbonyl)-N^4-((*S*)-1-(ferrocene-2-yl)ethyl)-D-asparaginate (72)



TLC: R_f = 0.22 (petroleum ether/Ethyl acetate = 2/1); 63 mg, yield: 59%; yellow solid.

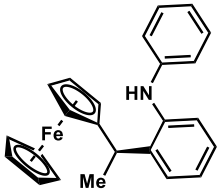
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 – 7.30 (m, 5H), 5.91 – 5.74 (m, 2H), 5.24 – 5.12 (m, 2H), 4.83 (t, *J* = 7.3 Hz, 1H), 4.52 (dd, *J* = 8.7, 4.4 Hz, 1H), 4.14 (d, *J* = 12.4 Hz, 9H), 2.86 (dd, *J* = 15.5, 4.8 Hz, 1H), 2.67 (dd, *J* = 15.6, 4.5 Hz, 1H), 1.40 (d, *J* = 10.3 Hz, 12H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.3, 171.3, 168.4, 155.7, 135.4, 135.3, 128.5, 128.2, 128.2, 128.1, 128.1, 90.8, 90.7, 79.9, 77.2, 68.5, 68.5, 68.1, 67.6, 67.3, 67.3, 67.3, 65.6, 65.6, 50.6, 50.6, 43.8, 37.9, 28.2, 20.5, 20.5.

HRMS (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{28}H_{34}FeN_2O_5Na$ 557.1703; Found: 557.1703.

Chiral HPLC: The ee value was 90%, t_R (minor) = 9.4 min, t_S (major) = 11.4 min (Chiralpak IA, λ = 254 nm, 20% isopropanol/hexanes, flow rate = 1.0 mL/min).

***(S)*-N-phenyl-2-(1-(ferrocene-2-yl)ethyl)aniline (73)**



TLC: R_f = 0.43 (petroleum ether/Ethyl acetate = 8/1); 34 mg, yield: 45%; yellow oil.

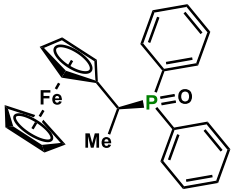
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 – 7.23 (m, 2H), 7.08 – 7.06 (m, 2H), 7.04 – 6.98 (m, 4H), 6.91 – 6.88 (m, 1H), 5.61 (s, 1H), 4.21 – 4.19 (m, 1H), 4.16 – 4.11 (m, 6H),4.10 – 4.08 (m, 1H), 4.02 – 4.02 (m, 1H), 3.82 (q, *J* = 7.2 Hz, 1H), 1.59 (d, *J* = 7.2 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 143.6, 140.8, 140.6, 129.2, 127.9, 120.4, 118.2, 117.1, 94.7, 68.5, 67.8, 67.5, 66.7, 66.3, 39.0, 22.6.

HRMS (ESI-TOF) m/z: $[M]^+$ $C_{24}H_{23}FeN$ Calcd for 381.1174; Found: 381.1179.

Chiral HPLC: The ee value was 98%, t_R (minor) = 10.2 min, t_S (major) = 12.4 min (Chiralpak IA, λ = 254 nm, 10% isopropanol/hexanes, flow rate = 1.0 mL/min).

***(S)*-diphenyl(1-(ferrocene-2-yl)ethyl)phosphine oxide (74)**



TLC: R_f = 0.17 (petroleum ether/Ethyl acetate = 1/1); 65 mg, yield: 78%; yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 – 7.74 (m, 2H), 7.54 – 7.42 (m, 6H), 7.36 – 7.31 (m, 2H), 4.11 (s, 7H), 3.93 (d, *J* = 2.6 Hz, 1H), 3.50 – 3.49 (m, 1H), 3.42 – 3.33 (m, 1H), 1.58 (dd, *J* = 15.9, 7.3 Hz, 3H).

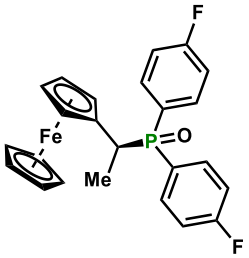
^{13}C NMR (101 MHz, $CDCl_3$) δ 132.5, 132.0, 131.9, 131.6, 131.6, 131.5, 131.4, 131.3, 130.1, 128.5, 128.4, 127.9, 127.8, 85.7, 69.4, 69.4, 68.5, 67.7, 67.5, 67.3, 36.0, 35.4, 13.9, 13.9.

^{31}P NMR (160 MHz, $CDCl_3$) δ 34.1

HRMS (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{24}H_{23}FeOPNa$ 437.0722; Found: 437.0733.

Chiral HPLC: The ee value was 92%, t_S (major) = 11.3 min, t_R (minor) = 13.6 min (Chiralpak IA, λ = 254 nm, 20% isopropanol/hexanes, flow rate = 1.0 mL/min).

***(S)*-bis(4-fluorophenyl)(1-(ferrocene-2-yl)ethyl)phosphine oxide (75)**



TLC: R_f = 0.18 (petroleum ether/Ethyl acetate = 1/1); 65 mg, yield: 72%; yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 – 7.69 (m, 2H), 7.49 – 7.43 (m, 2H), 7.18 – 7.13 (m, 2H), 7.06 – 7.01 (m, 2H), 4.13 (d, *J* = 8.2 Hz, 7H), 3.98 (s, 1H), 3.52 (s, 1H), 3.34 – 3.26 (m, 1H), 1.53 (dd, *J* = 16.1, 7.2 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.2, 163.6, 134.5, 134.4, 134.4, 134.3, 133.9, 133.8, 133.7, 116.1, 115.9, 115.9, 115.7, 115.5, 115.4, 115.3, 115.2, 85.5, 69.5, 68.8, 67.9, 67.6, 67.6, 53.4, 36.3, 35.6, 13.8, 13.8.

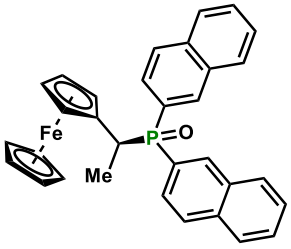
^{19}F NMR (376 MHz, $CDCl_3$) δ -106.7, -107.0.

^{31}P NMR (160 MHz, $CDCl_3$) δ 33.1.

HRMS (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{24}H_{21}F_2FeOPNa$ 473.0534; Found: 473.0542.

Chiral HPLC: The ee value was 95%, t_S (major) = 9.7 min, t_R (minor) = 12.4 min (Chiralpak IA, λ = 254 nm, 20% isopropanol/hexanes, flow rate = 1.0 mL/min).

***(S)*-di(naphthalen-2-yl)(1-(ferrocene-2-yl)ethyl)phosphine oxide (76)**



TLC: R_f = 0.15 (petroleum ether/Ethyl acetate = 1/1); 50 mg, yield: 49%; yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 (d, *J* = 12.8 Hz, 1H), 8.23 (d, *J* = 12.8 Hz, 1H), 7.95 – 7.87 (m, 3H), 7.84 – 7.78 (m, 4H), 7.60 – 7.46 (m, 5H), 4.20 – 4.08 (m, 7H), 3.87 (s, 1H), 3.63 – 3.58 (m, 1H), 3.53 (s, 1H), 1.68 (dd, *J* = 15.9, 7.3 Hz, 3H).

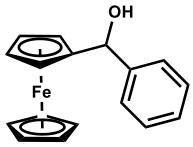
^{13}C NMR (101 MHz, $CDCl_3$) δ 134.5, 134.2, 133.5, 128.9, 128.2, 128.0, 127.9, 127.7, 127.6, 127.5, 127.4, 126.8, 126.6, 126.3, 85.6, 69.4, 68.5, 67.7, 67.6, 67.4, 36.0, 35.3, 14.0.

^{31}P NMR (160 MHz, $CDCl_3$) δ 34.48.

HRMS (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{32}H_{27}FeOPNa$ 537.1035; Found: 537.1042.

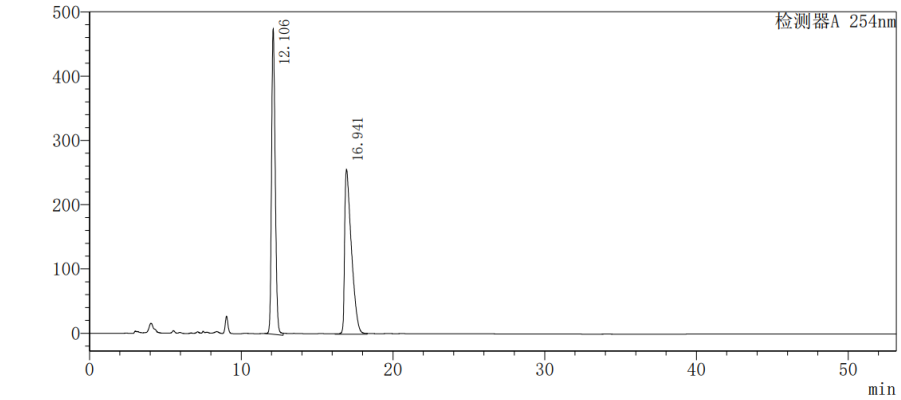
Chiral HPLC: The ee value was 90%, t_R (minor) = 9.2 min, t_S (major) = 11.5 min (Chiralpak OD-H, λ = 254 nm, 20% isopropanol/hexanes, flow rate = 1.0 mL/min).

8. Summary of Chiral HPLC analysis Spectra



(±)-S2

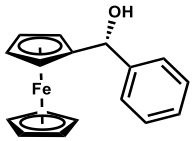
〈色谱图〉



〈峰表〉

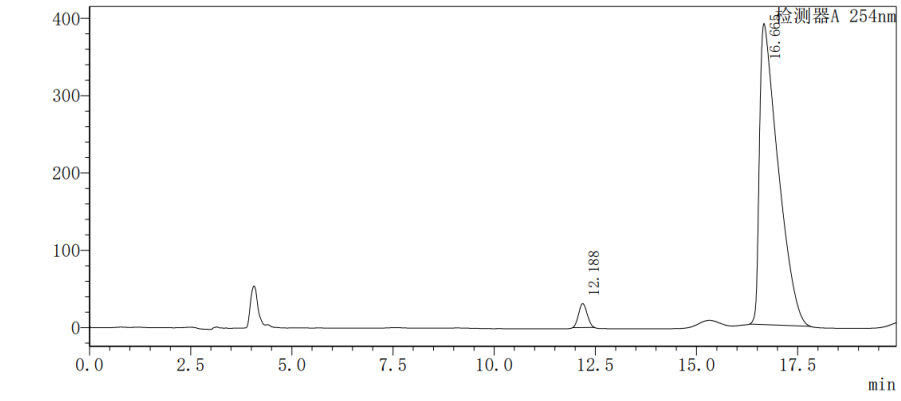
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	12.106	7957124	475023	49.840		M	
2	16.941	8008130	256641	50.160		M	
总计		15965254	731664				



(*S*)-S2

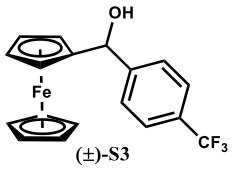
〈色谱图〉



〈峰表〉

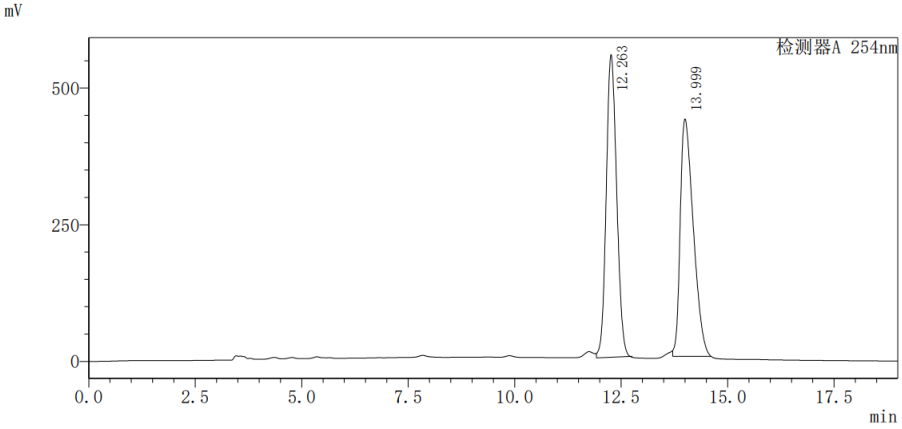
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	12.188	457517	31125	3.532		M	
2	16.665	12497019	389436	96.468		M	
总计		12954536	420561				



(±)-S3

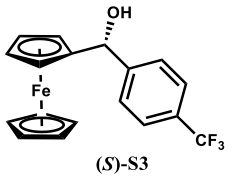
〈色谱图〉



〈峰表〉

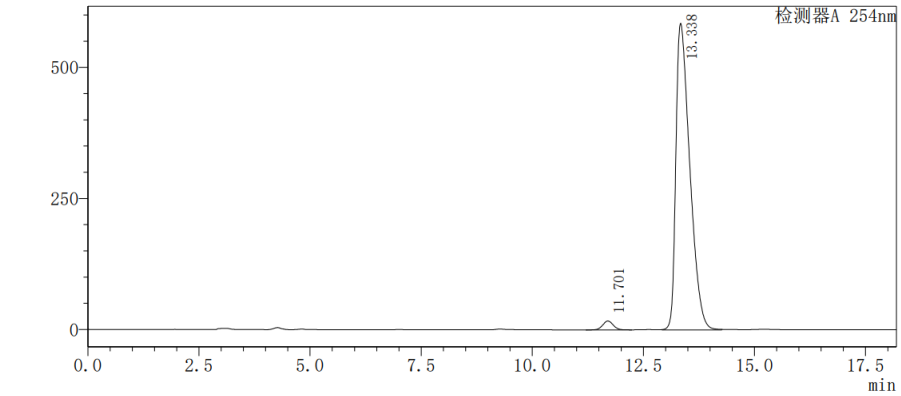
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	12.263	9422026	553294	50.398		M	
2	13.999	9273099	434150	49.602		M	
总计		18695125	987444				



(*S*)-S3

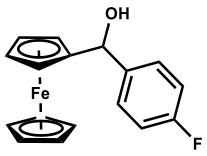
〈色谱图〉



〈峰表〉

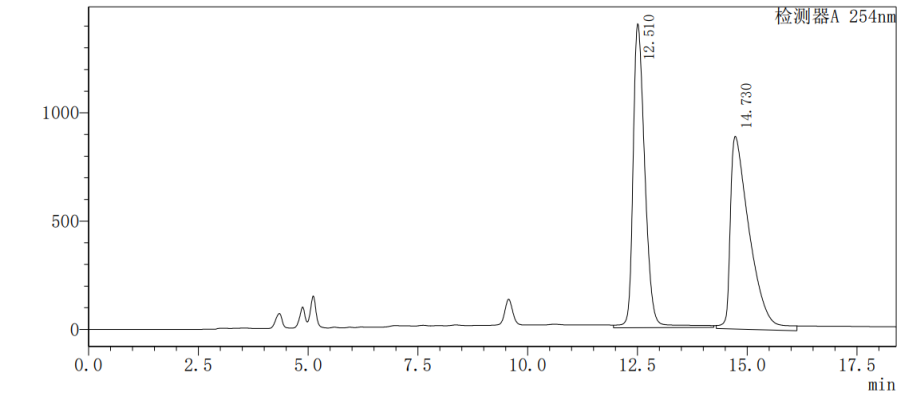
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	11.701	279762	16948	2.146			
2	13.338	12758677	584860	97.854		M	
总计		13038439	601808				



(±)-S4

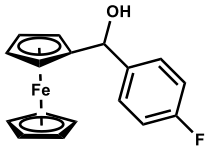
〈色谱图〉



〈峰表〉

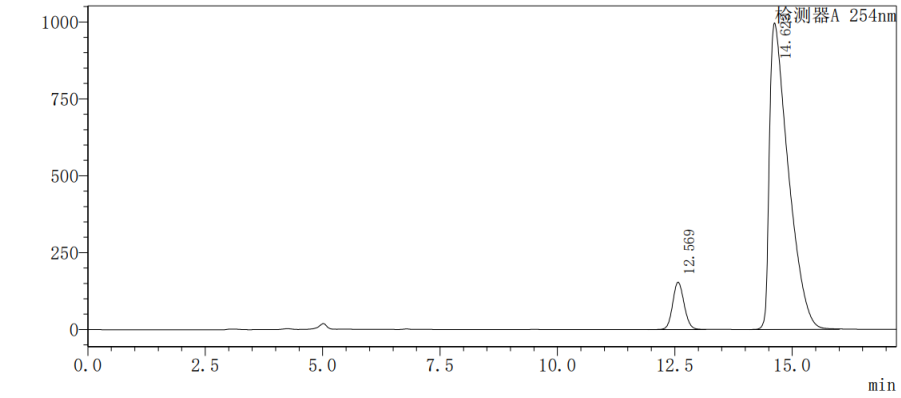
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	12.510	26537569	1402694	49.481			
2	14.730	27093817	889128	50.519		M	
总计		53631386	2291821				



(*S*)-S4

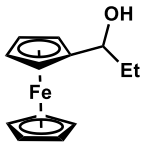
〈色谱图〉



〈峰表〉

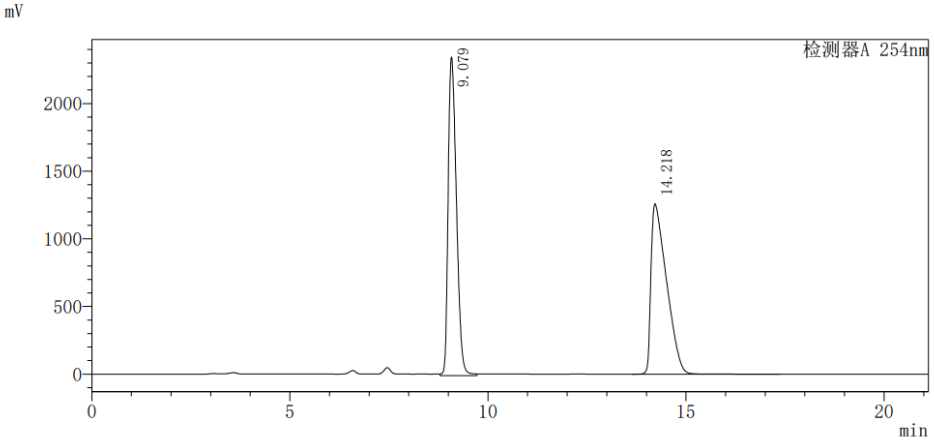
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	12.569	2609919	153833	8.539		M	
2	14.623	27954417	996294	91.461		M	
总计		30564336	1150127				



(±)-S5

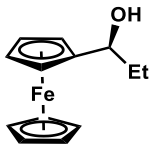
〈色谱图〉



〈峰表〉

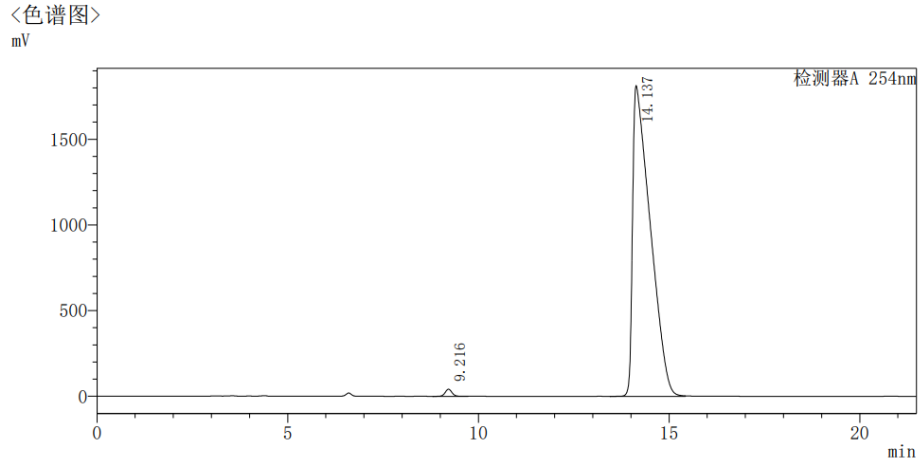
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	9.079	34231642	2352351	49.936		M	
2	14.218	34319946	1259027	50.064			
总计		68551589	3611378				



(*S*)-S5

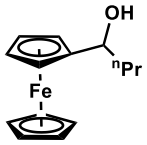
〈色谱图〉



〈峰表〉

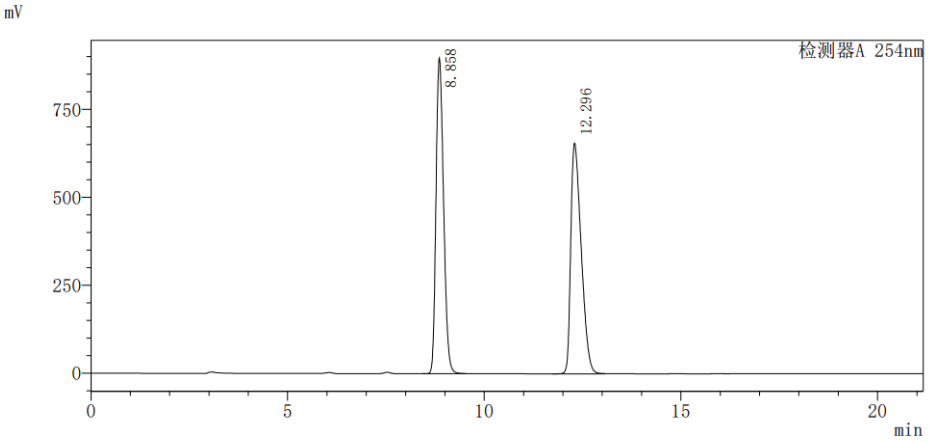
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	9.216	524261	41973	0.891			
2	14.137	58283531	1813307	99.109		M	
总计		58807793	1855279				



(±)-S6

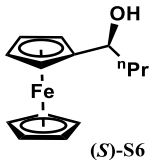
〈色谱图〉



〈峰表〉

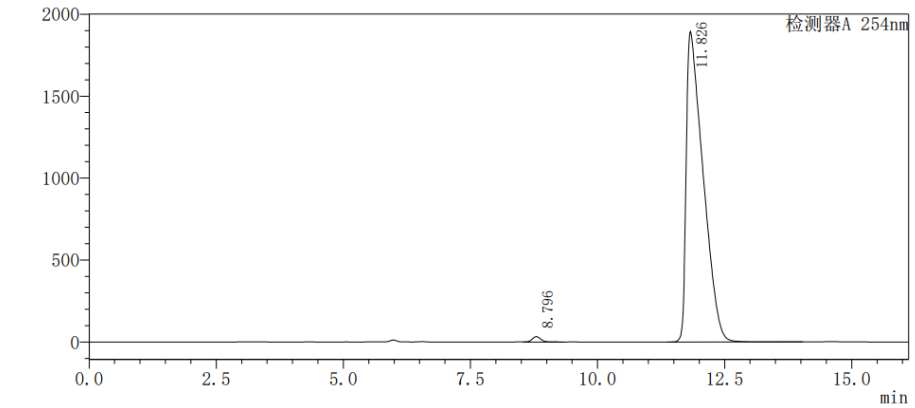
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	8.858	12054194	897063	49.965		M	
2	12.296	12071239	655326	50.035		M	
总计		24125433	1552389				



(*S*)-S6

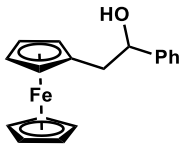
〈色谱图〉



〈峰表〉

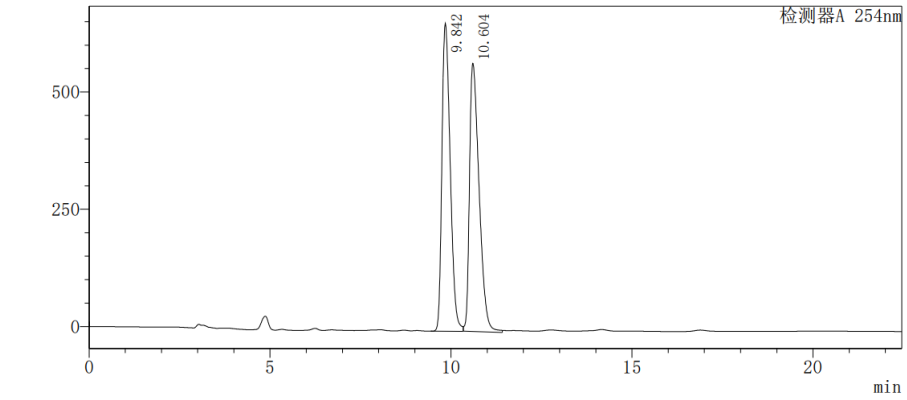
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	8.796	389486	32633	0.883			
2	11.826	43695823	1895023	99.117			
总计		44085309	1927656				



(±)-S7

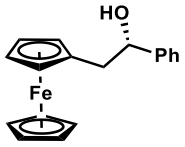
〈色谱图〉



〈峰表〉

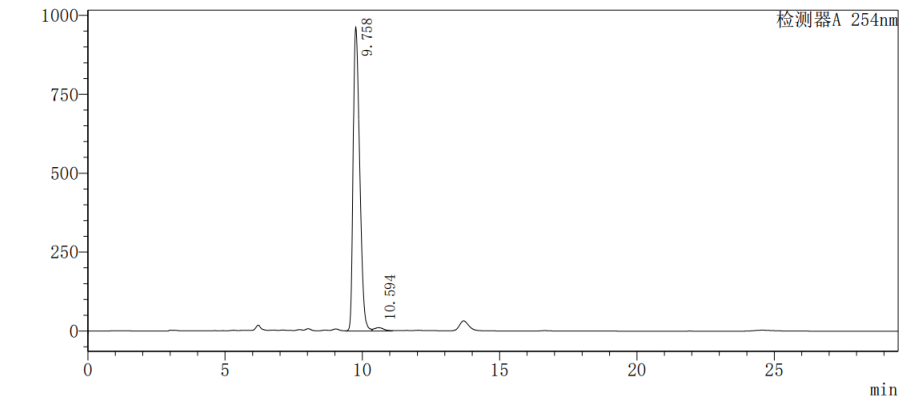
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	9.842	10436609	656400	49.638			
2	10.604	10588914	571590	50.362		M	
总计		21025523	1227990				



(*S*)-S7

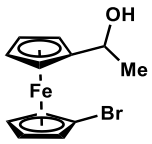
〈色谱图〉



〈峰表〉

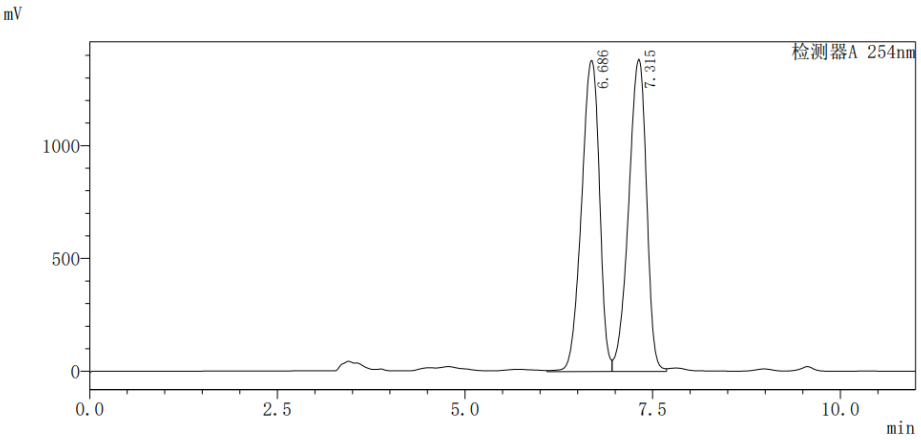
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	9.758	15968605	962150	98.311			
2	10.594	274367	10746	1.689		V	
总计		16242972	972896				



(±)-S8

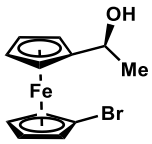
〈色谱图〉



〈峰表〉

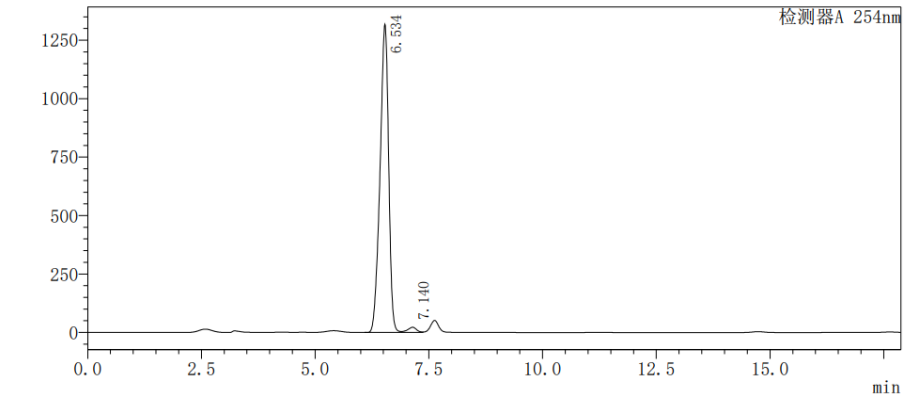
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.686	22932313	1378988	49.960			
2	7.315	22968808	1383721	50.040		V	
总计		45901121	2762710				



(*S*)-S8

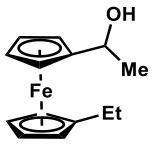
〈色谱图〉



〈峰表〉

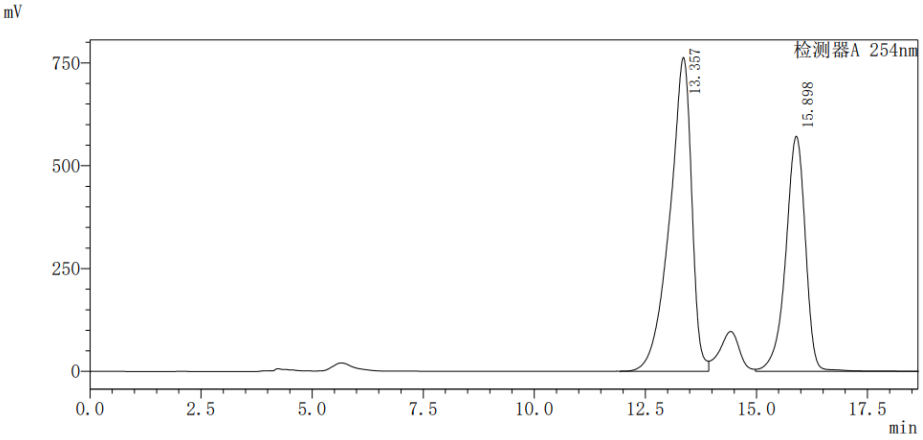
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.534	17375054	1318710	98.207			
2	7.140	317169	22410	1.793		V	
总计		17692223	1341120				



(±)-S9

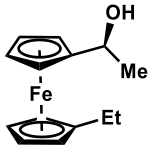
〈色谱图〉



〈峰表〉

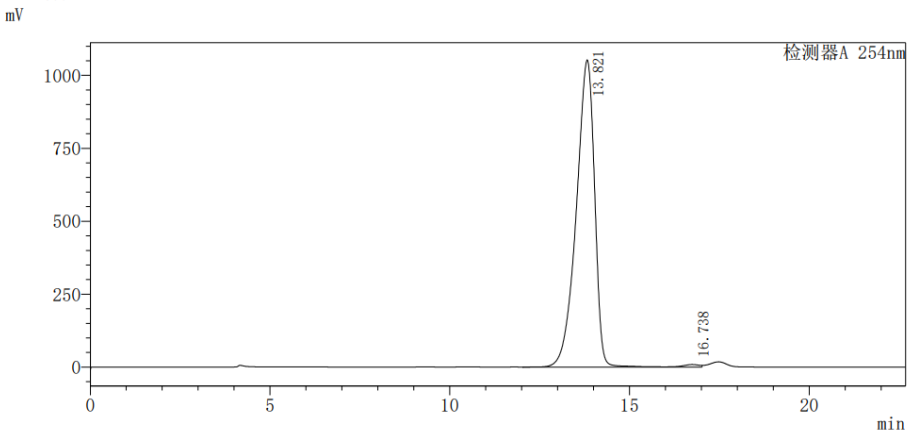
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	13.357	26204858	762982	59.848			
2	15.898	17580899	571348	40.152			
总计		43785757	1334330				



(*S*)-S9

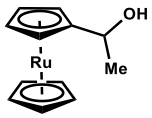
〈色谱图〉



〈峰表〉

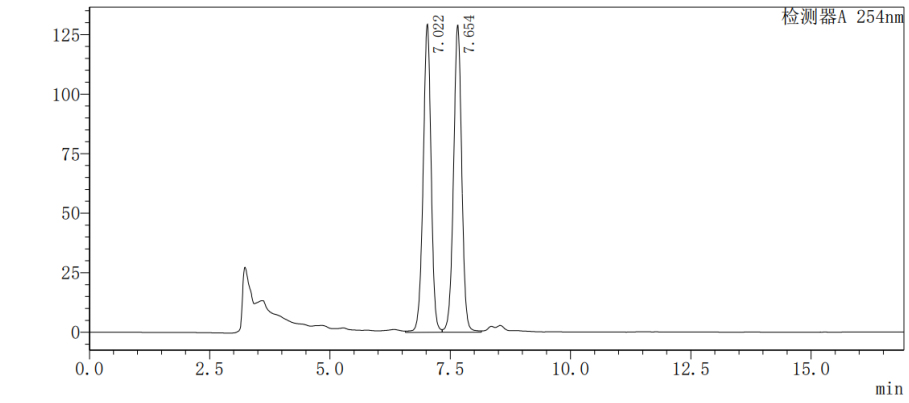
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	13.821	37315946	1052761	99.236			
2	16.738	287295	8763	0.764		V	
总计		37603241	1061524				



(±)-S12

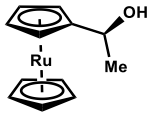
〈色谱图〉



〈峰表〉

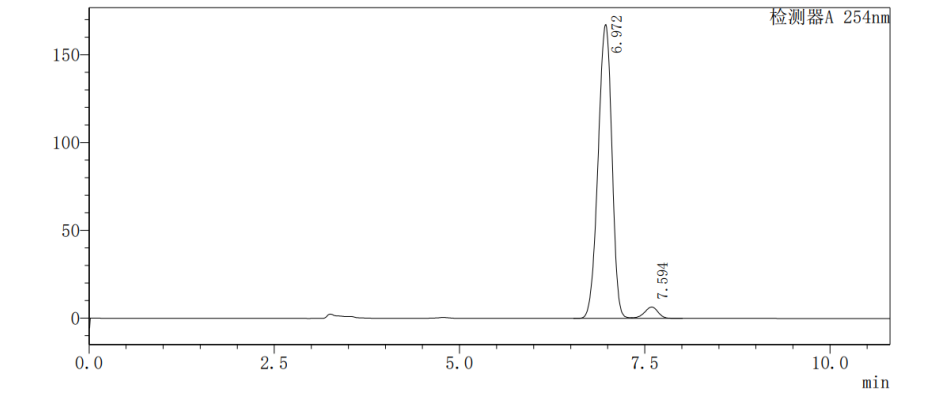
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	7.022	1489680	129352	49.302			
2	7.654	1531853	128928	50.698		V	
总计		3021533	258280				



(*S*)-S12

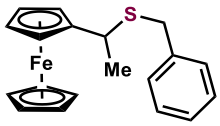
〈色谱图〉



〈峰表〉

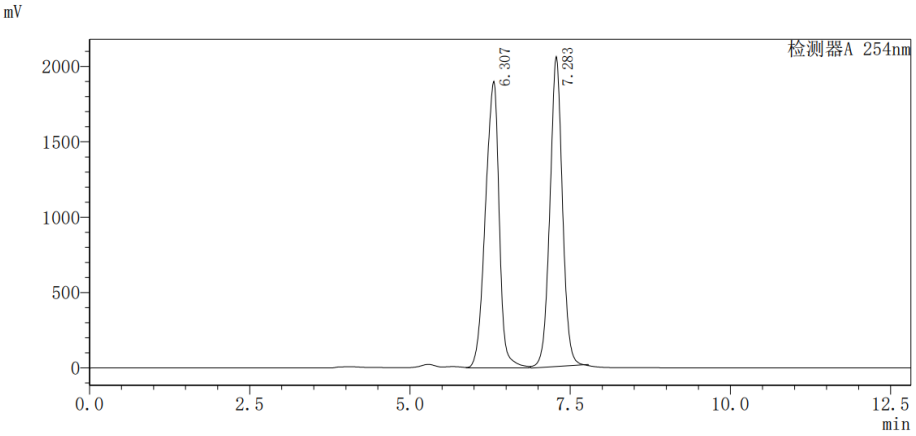
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.972	2163047	167325	96.353			
2	7.594	81867	6429	3.647		V	
总计		2244913	173754				



(±)-3

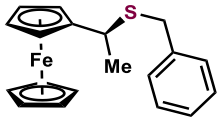
〈色谱图〉



〈峰表〉

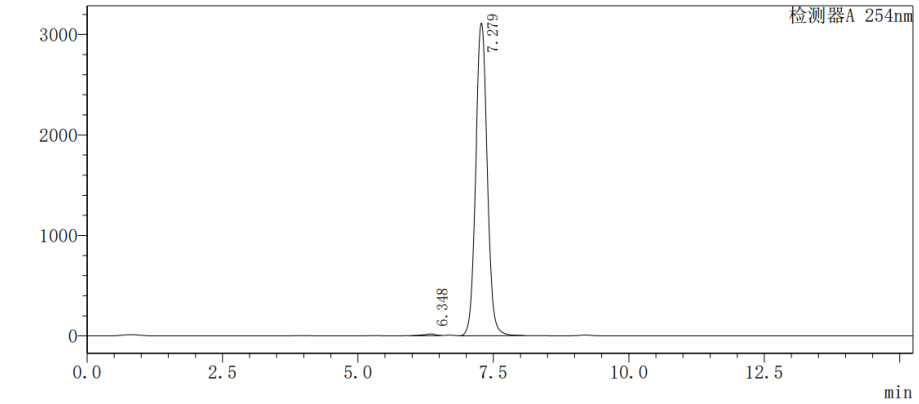
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.307	28561446	1901791	50.588			
2	7.283	27897532	2055068	49.412		M	
总计		56458978	3956859				



(*S*)-3

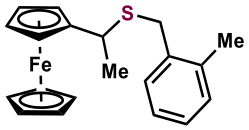
〈色谱图〉



〈峰表〉

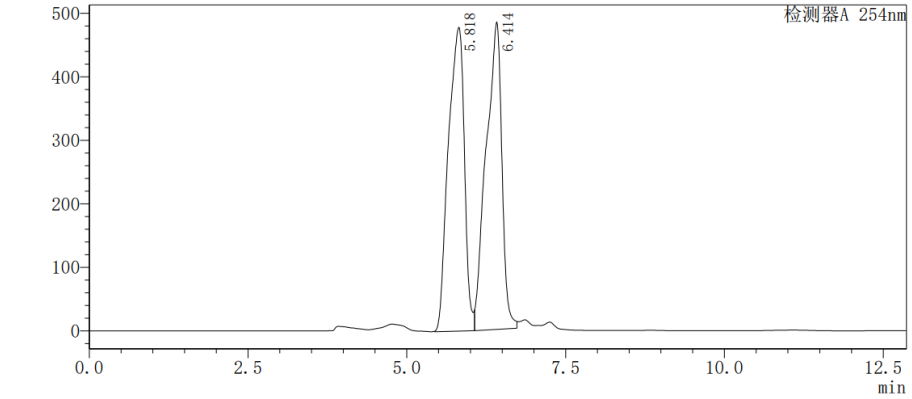
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.348	298139	18012	0.645		M	
2	7.279	45940995	3110364	99.355		M	
总计		46239135	3128375				



(±)-4

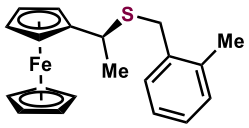
〈色谱图〉



〈峰表〉

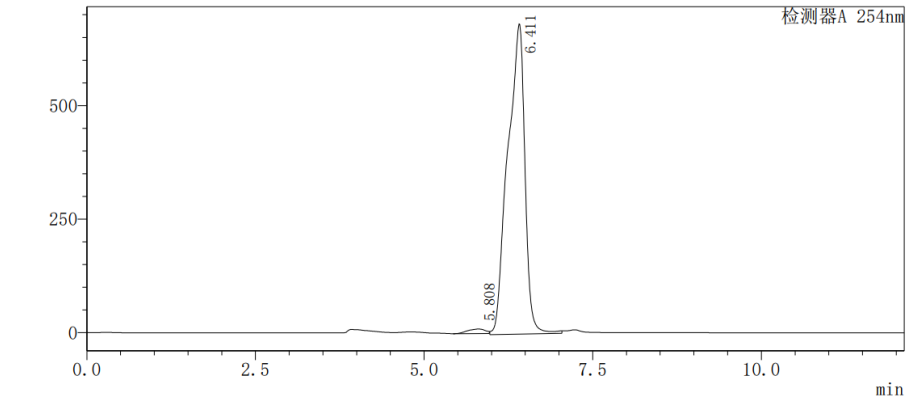
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	5.818	8405099	478198	50.109		M	
2	6.414	8368679	483476	49.891		M	
总计		16773778	961674				



(*S*)-4

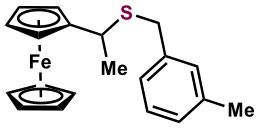
〈色谱图〉



〈峰表〉

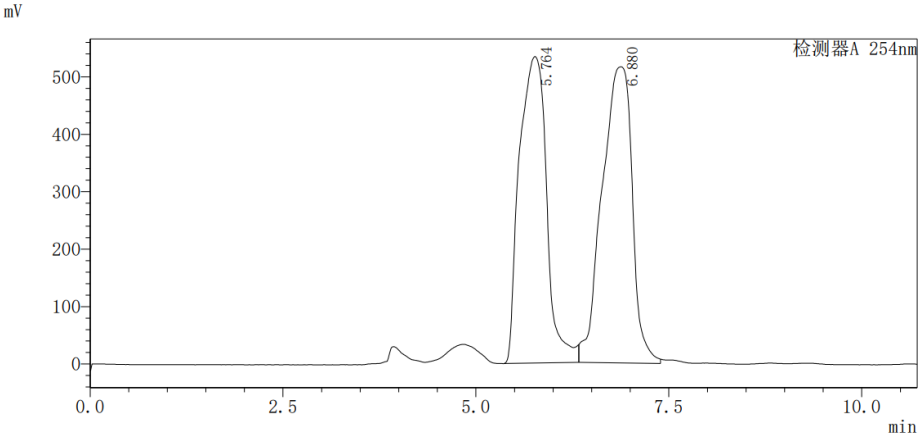
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	5.808	183331	9915	1.495			
2	6.411	12077219	682766	98.505		M	
总计		12260550	692681				



(±)-5

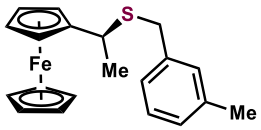
〈色谱图〉



〈峰表〉

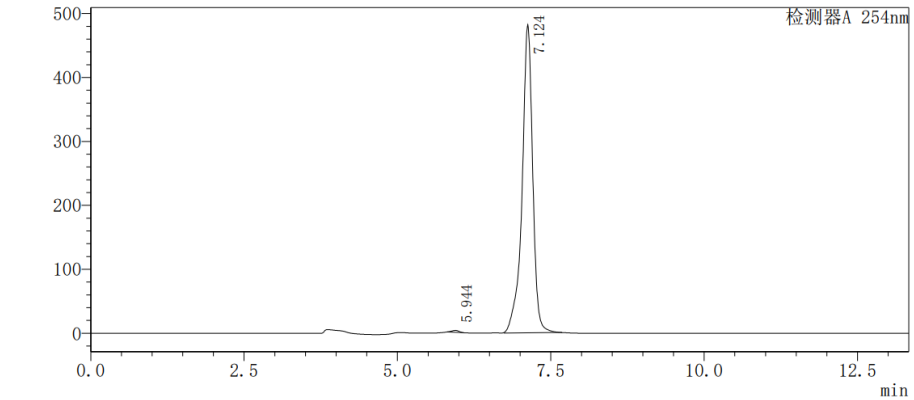
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	5.764	13175654	533891	48.449		M	
2	6.880	14019174	516013	51.551		M	
总计		27194828	1049904				



(*S*)-5

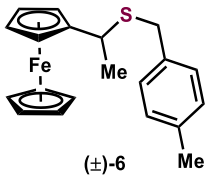
〈色谱图〉



〈峰表〉

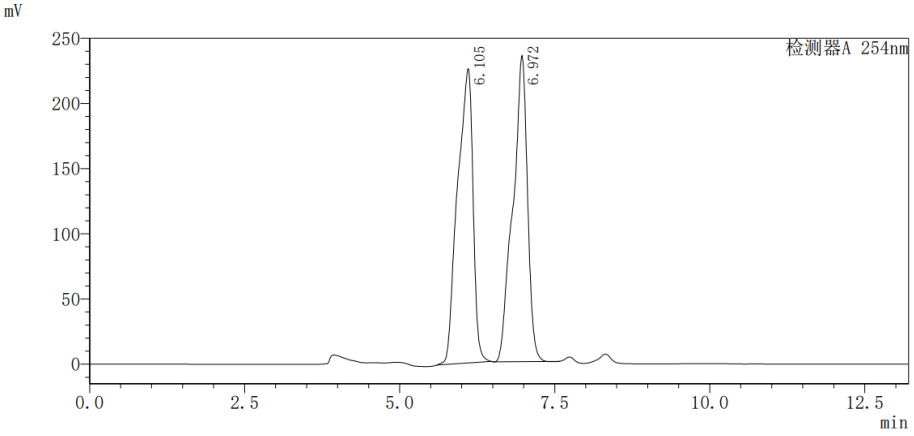
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	5.944	24252	3026	0.415		M	
2	7.124	5820710	481451	99.585		M	
总计		5844962	484477				



(±)-6

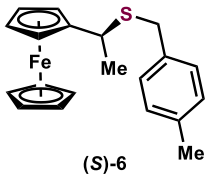
〈色谱图〉



〈峰表〉

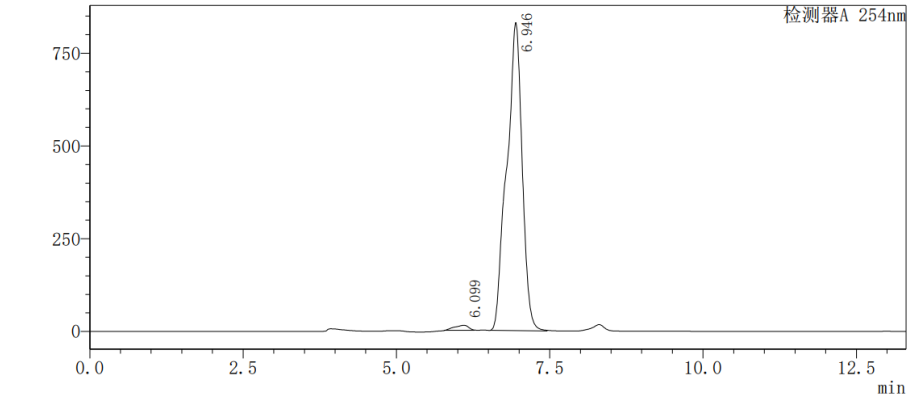
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.105	3915383	225597	50.470		M	
2	6.972	3842477	234668	49.530		M	
总计		7757861	460264				



(*S*)-6

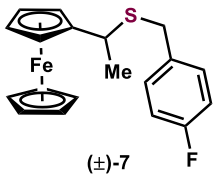
〈色谱图〉



〈峰表〉

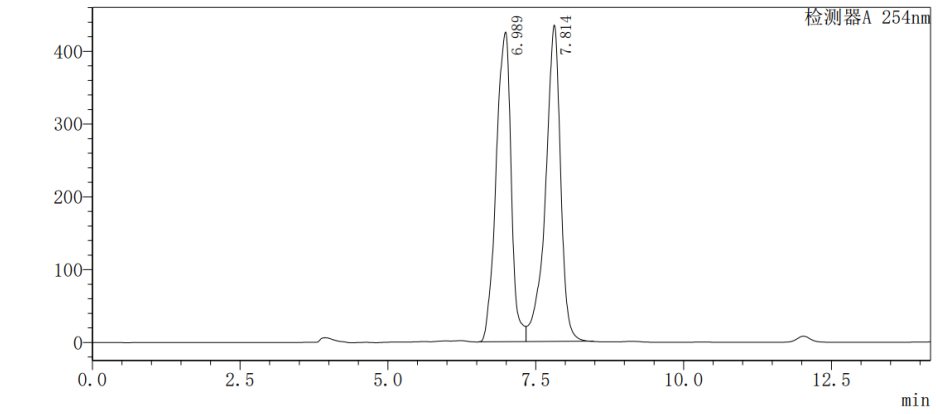
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.099	211310	13366	1.432		M	
2	6.946	14543052	829875	98.568		M	
总计		14754363	843241				



(±)-7

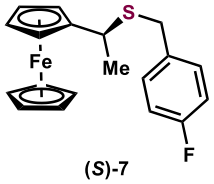
〈色谱图〉



〈峰表〉

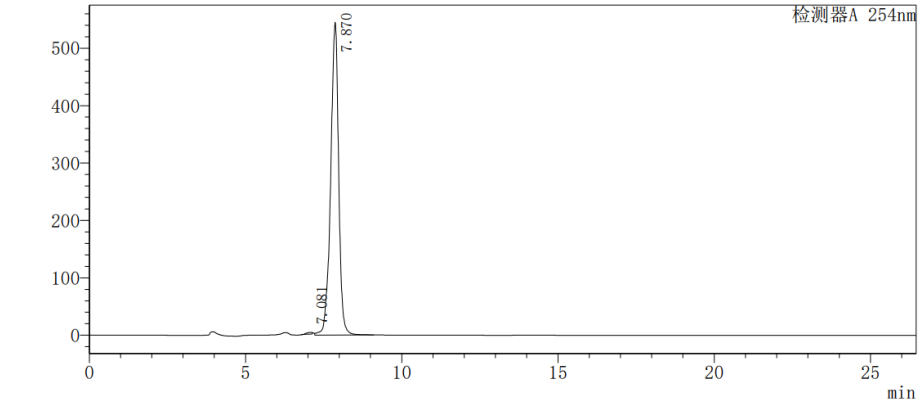
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.989	7514352	425330	49.266		M	
2	7.814	7738296	434399	50.734		V M	
总计		15252648	859729				



(*S*)-7

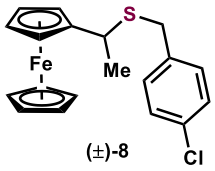
〈色谱图〉



〈峰表〉

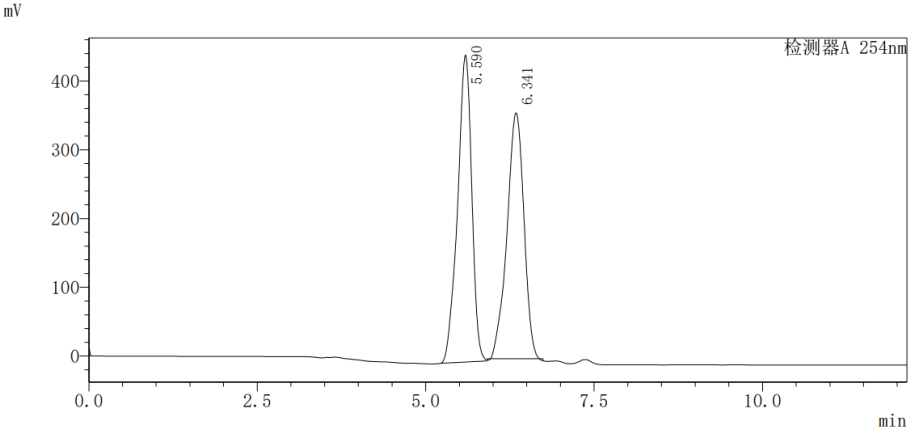
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	7.081	35953	3023	0.370		M	
2	7.870	9685564	544322	99.630		M	
总计		9721517	547345				



(±)-8

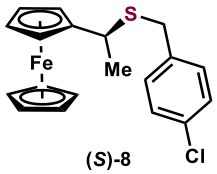
〈色谱图〉



〈峰表〉

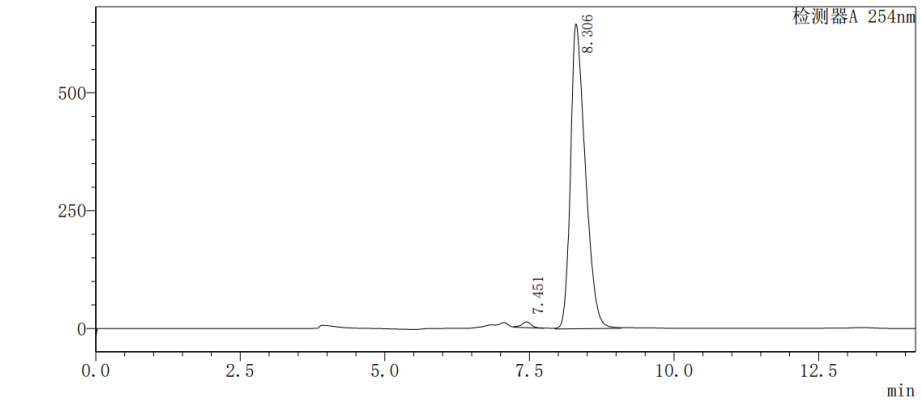
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	5.590	6538541	446298	51.171		M	
2	6.341	6239364	357638	48.829		M	
总计		12777905	803935				



(*S*)-8

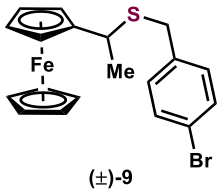
〈色谱图〉



〈峰表〉

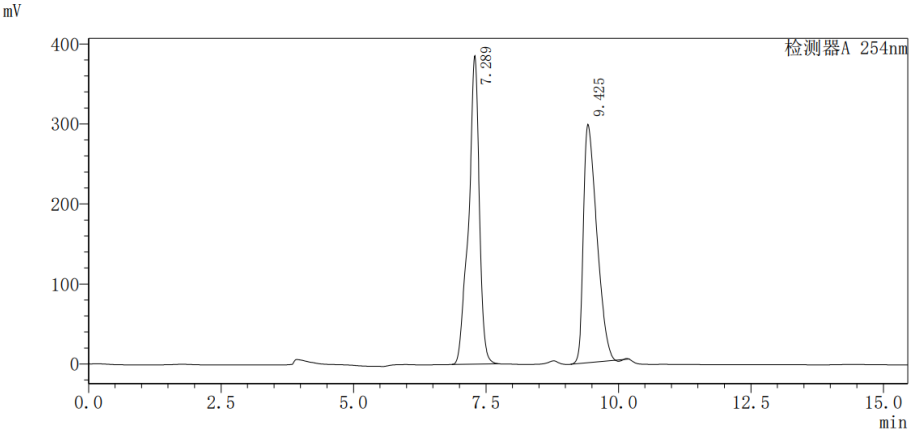
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	7.451	144204	12206	1.234		M	
2	8.306	11537580	646240	98.766		M	
总计		11681784	658446				



(±)-9

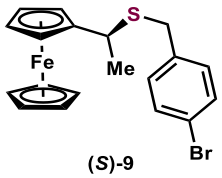
〈色谱图〉



〈峰表〉

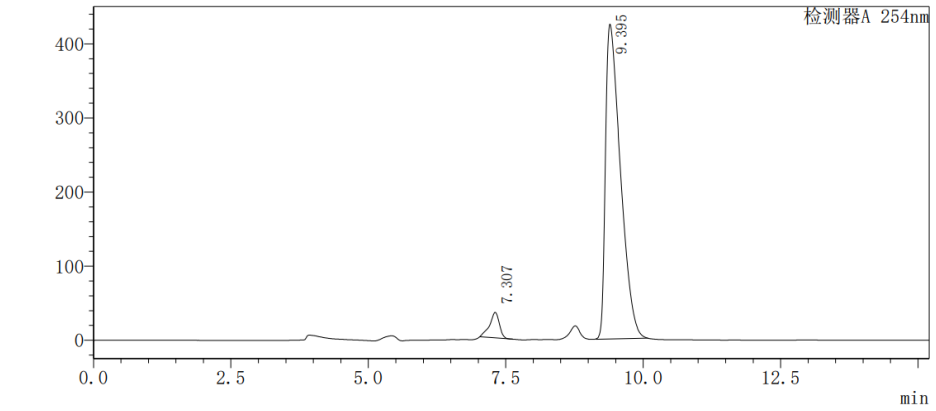
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	7.289	5428649	385382	50.760		M	
2	9.425	5266120	298146	49.240		M	
总计		10694768	683528				



(*S*)-9

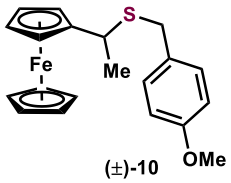
〈色谱图〉



〈峰表〉

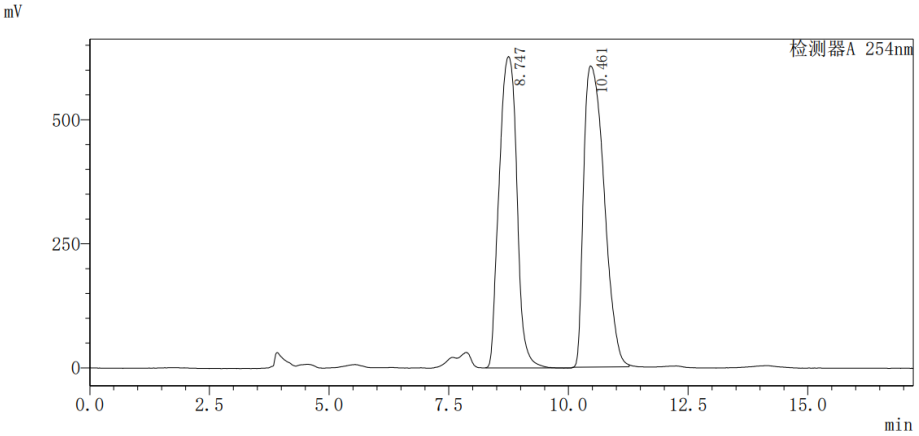
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	7.307	424608	34498	5.028		M	
2	9.395	8019898	424594	94.972		M	
总计		8444506	459092				



(±)-10

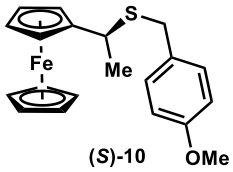
〈色谱图〉



〈峰表〉

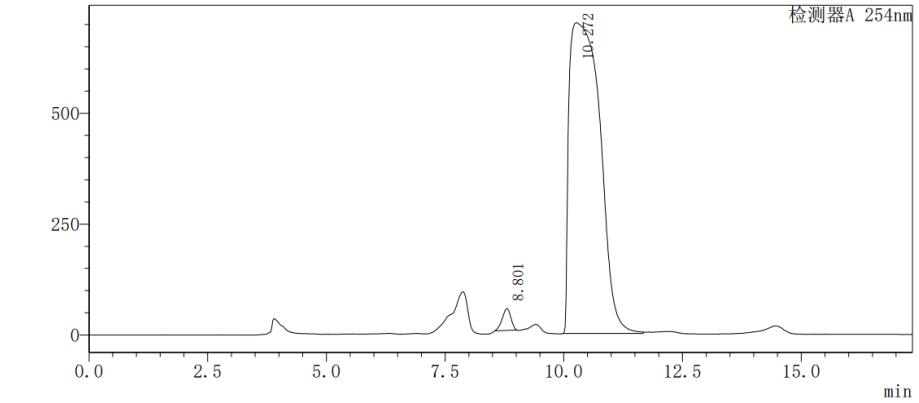
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	8.747	16217444	627537	47.285		M	
2	10.461	18079809	606671	52.715		M	
总计		34297253	1234208				



(*S*)-10

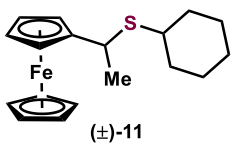
〈色谱图〉



〈峰表〉

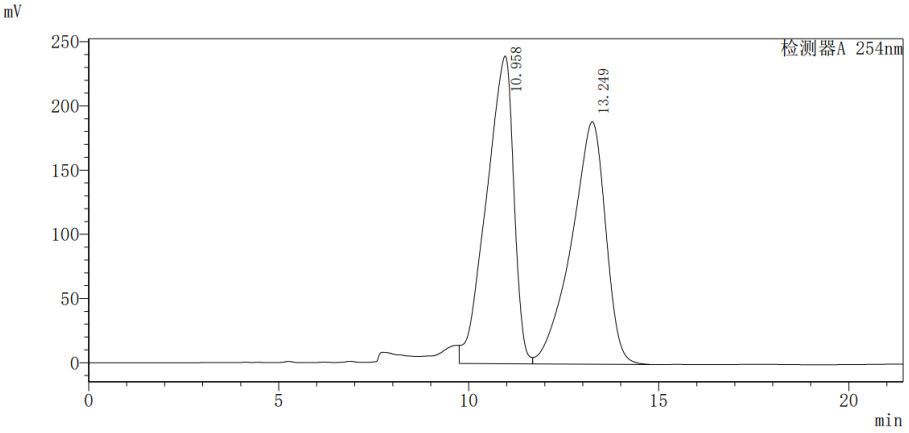
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	8.801	619259	48834	1.923		M	
2	10.272	31579908	700308	98.077		M	
总计		32199167	749142				



(±)-11

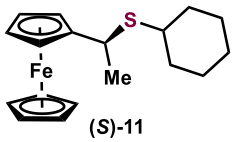
<色谱图>



<峰表>

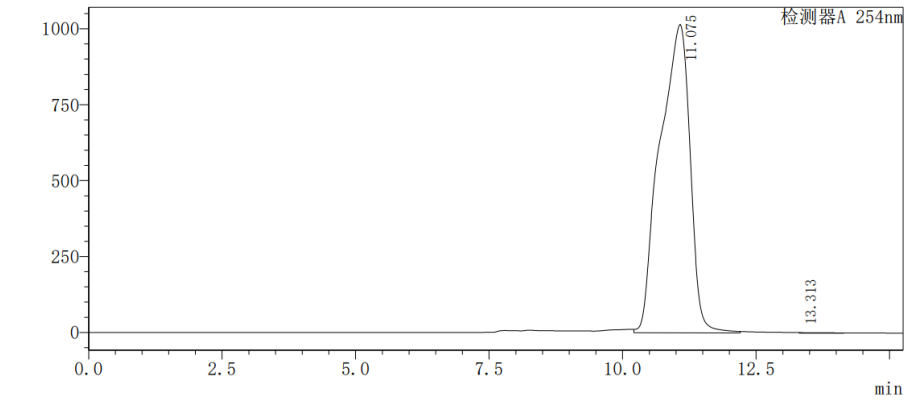
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	10.958	11957600	239696	50.256			
2	13.249	11835662	188901	49.744		V	
总计		23793262	428598				



(*S*)-11

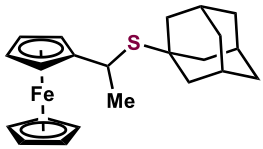
<色谱图>



<峰表>

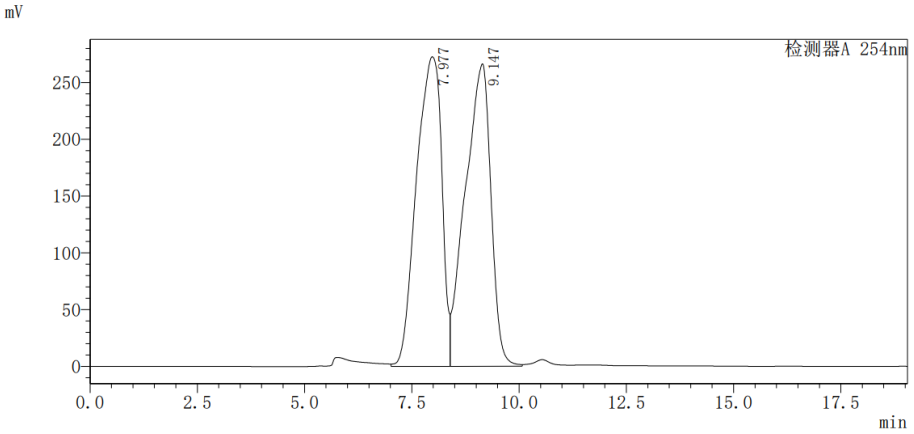
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	11.075	39882636	1015182	99.776		M	
2	13.313	89513	2323	0.224		M	
总计		39972149	1017505				



(±)-12

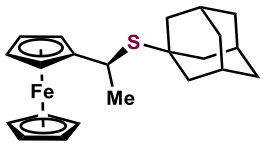
〈色谱图〉



〈峰表〉

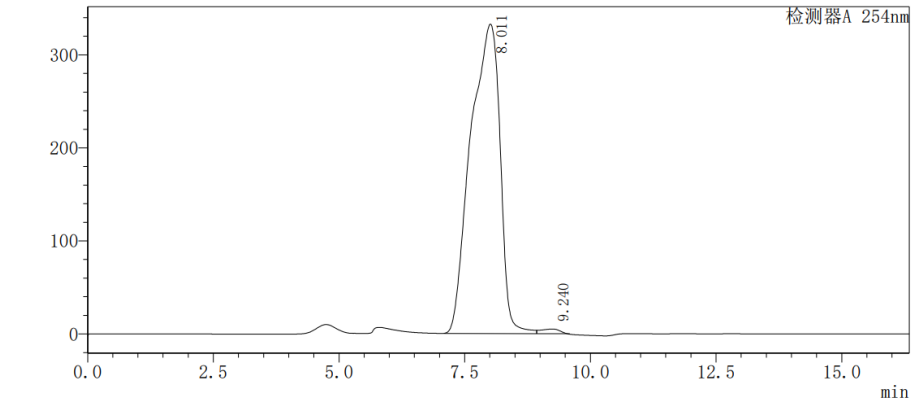
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	7.977	11184002	272577	50.220			
2	9.147	11086118	266182	49.780		V	
总计		22270120	538759				



(*S*)-12

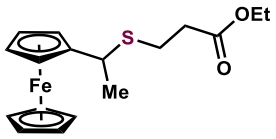
〈色谱图〉



〈峰表〉

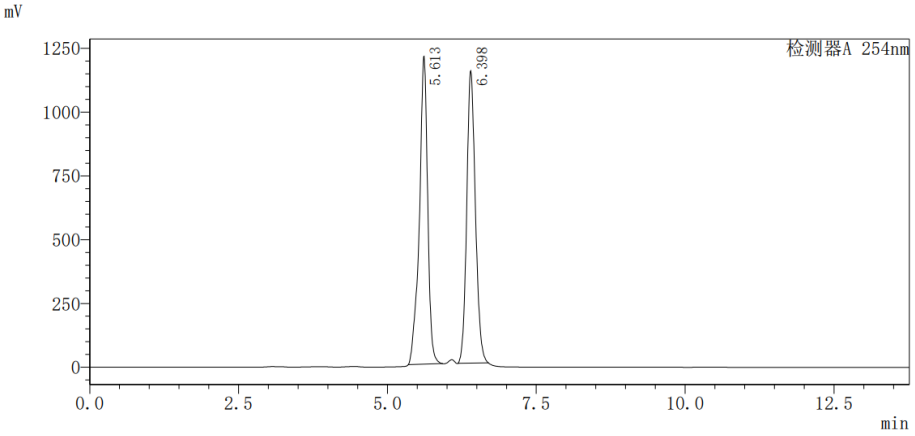
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	8.011	13589567	332620	99.058		M	
2	9.240	129186	5003	0.942		V M	
总计		13718753	337622				



(±)-13

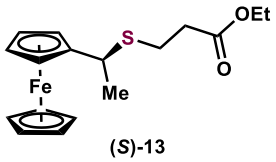
〈色谱图〉



〈峰表〉

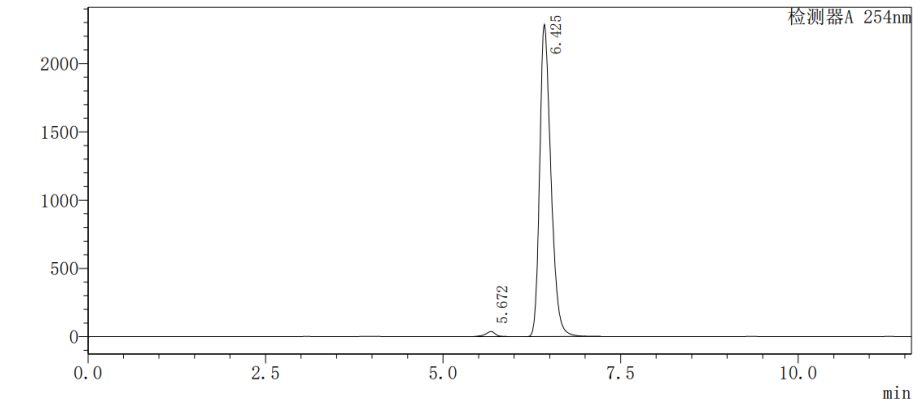
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	5.613	11750522	1206642	50.324		M	
2	6.398	11599185	1146014	49.676		M	
总计		23349707	2352656				



***(S)*-13**

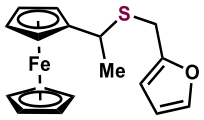
〈色谱图〉



〈峰表〉

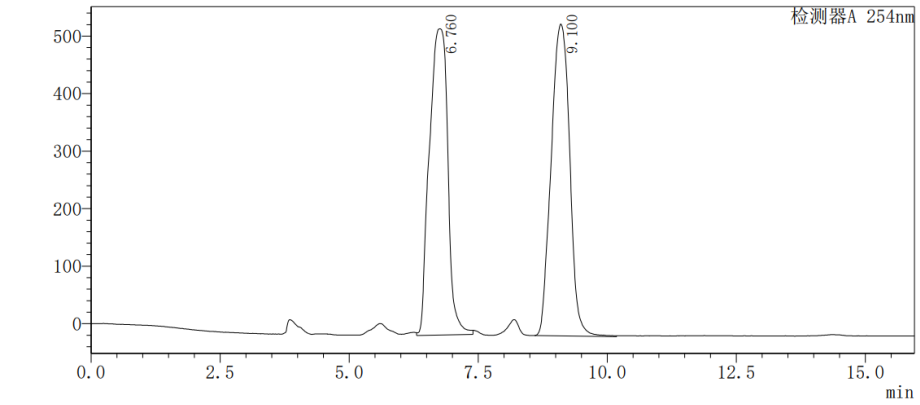
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	5.672	356513	37236	1.397		M	
2	6.425	25170096	2284118	98.603		M	
总计		25526609	2321355				



(±)-14

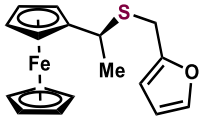
〈色谱图〉



〈峰表〉

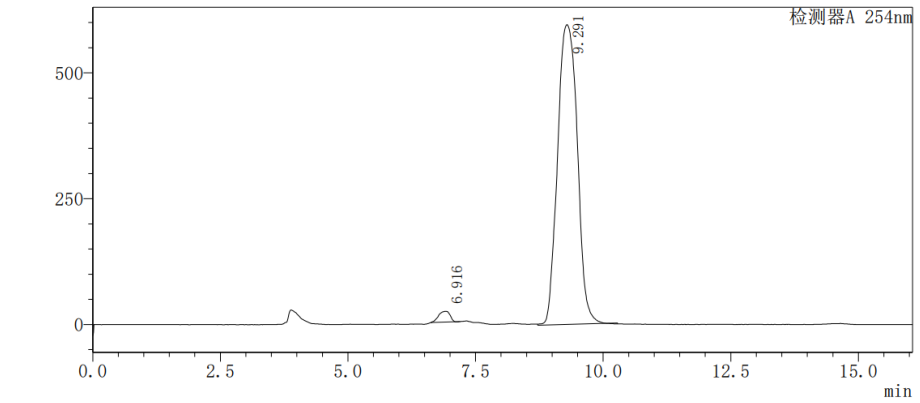
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.760	13238983	532215	49.393		M	
2	9.100	13564357	541985	50.607		M	
总计		26803339	1074201				



(*S*)-14

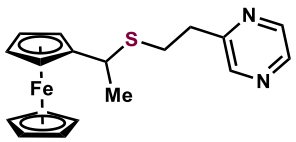
〈色谱图〉



〈峰表〉

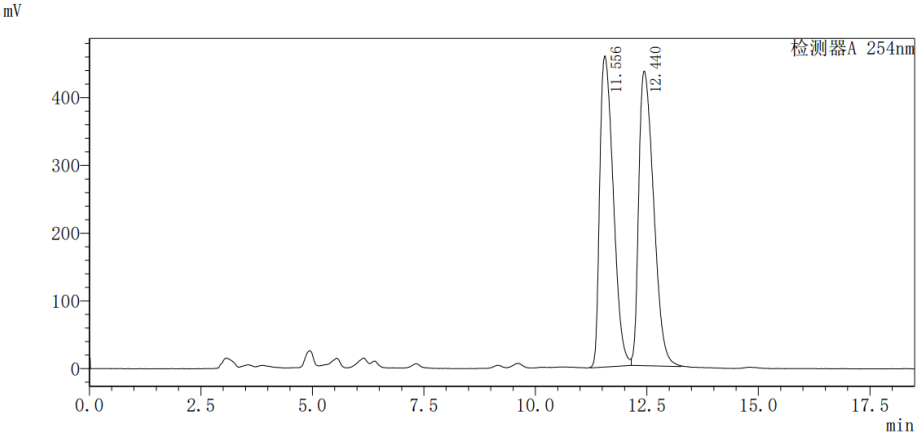
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.916	330332	21439	2.019		M	
2	9.291	16032273	595616	97.981		M	
总计		16362605	617054				



(±)-15

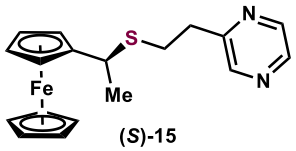
〈色谱图〉



〈峰表〉

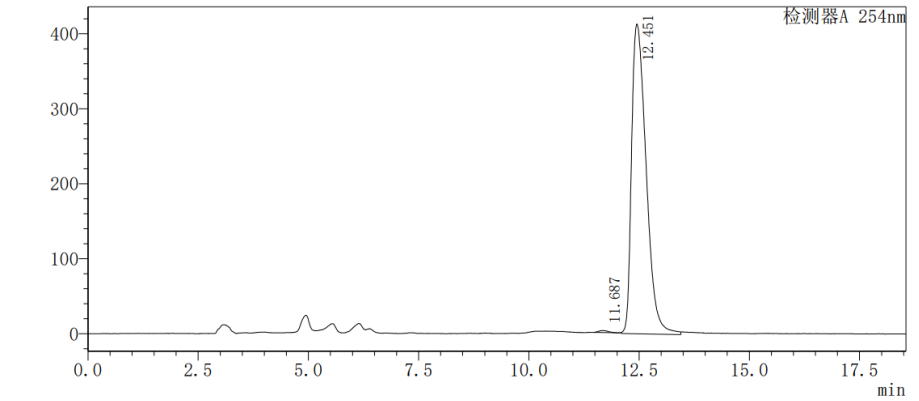
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	11.556	9690687	459331	48.956		M	
2	12.440	10103906	435201	51.044		M	
总计		19794593	894533				



(*S*)-15

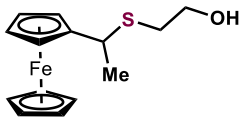
〈色谱图〉



〈峰表〉

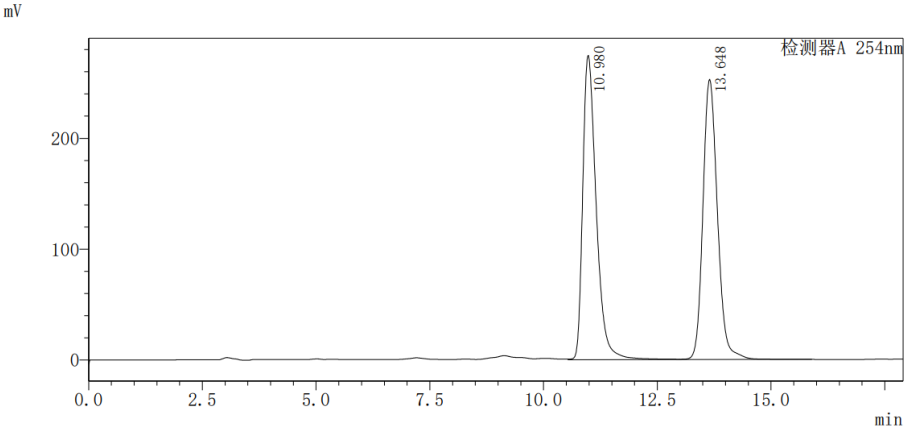
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	11.687	37536	2498	0.394		M	
2	12.451	9492963	413010	99.606		M	
总计		9530499	415508				



(±)-16

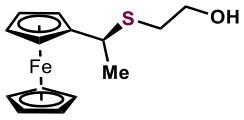
〈色谱图〉



〈峰表〉

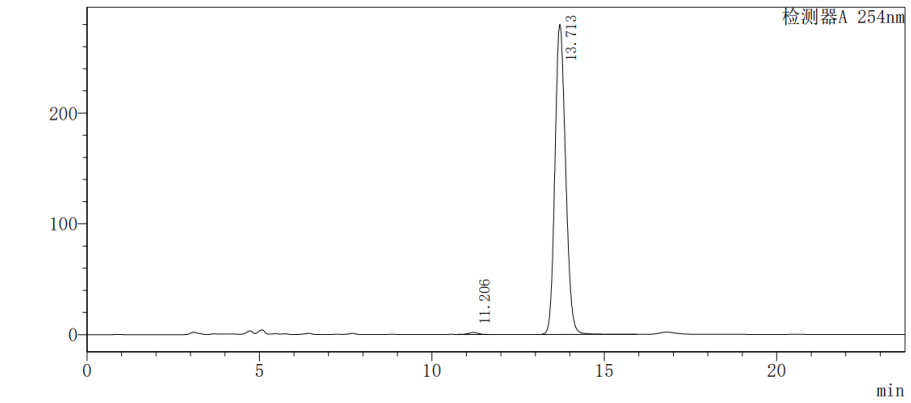
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	10.980	5676129	274421	50.270			
2	13.648	5615167	252646	49.730		V	
总计		11291296	527067				



(*S*)-16

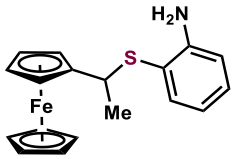
〈色谱图〉



〈峰表〉

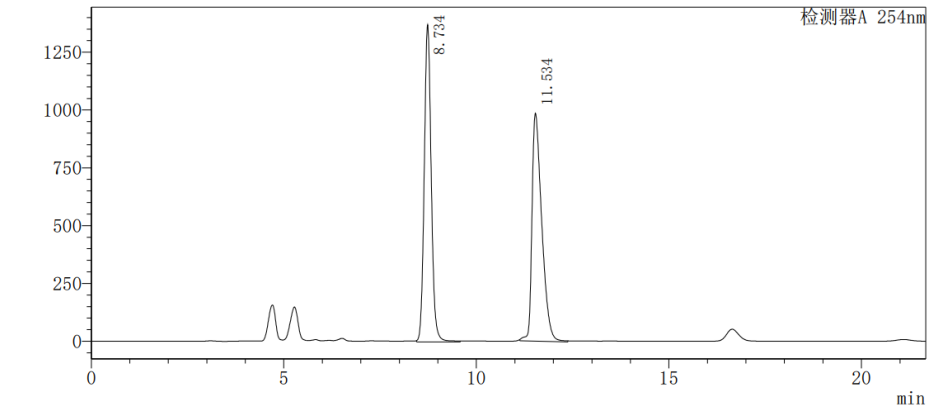
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	11.206	38256	1849	0.632			
2	13.713	6014158	279779	99.368		M	
总计		6052414	281628				



(±)-17

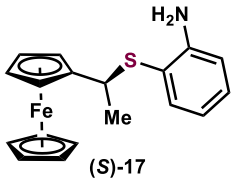
〈色谱图〉



〈峰表〉

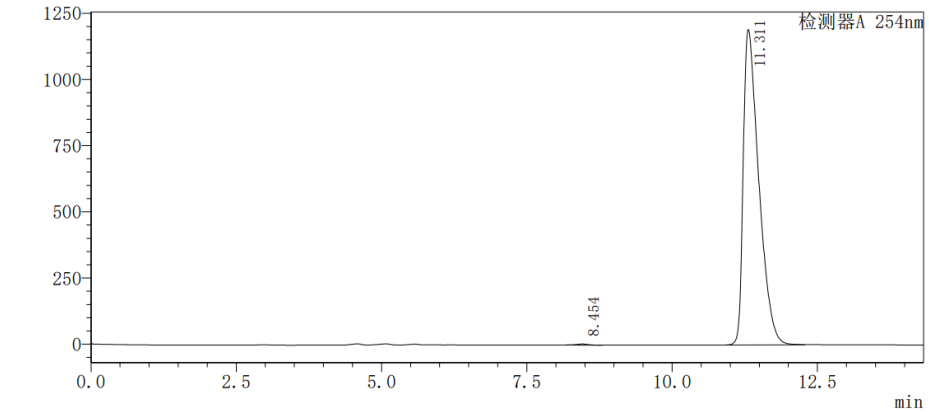
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	8.734	17356776	1371079	49.924		M	
2	11.534	17409474	985647	50.076		M	
总计		34766249	2356726				



(*S*)-17

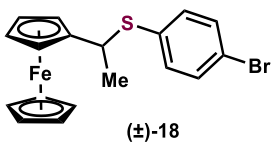
〈色谱图〉



〈峰表〉

检测器A 254nm

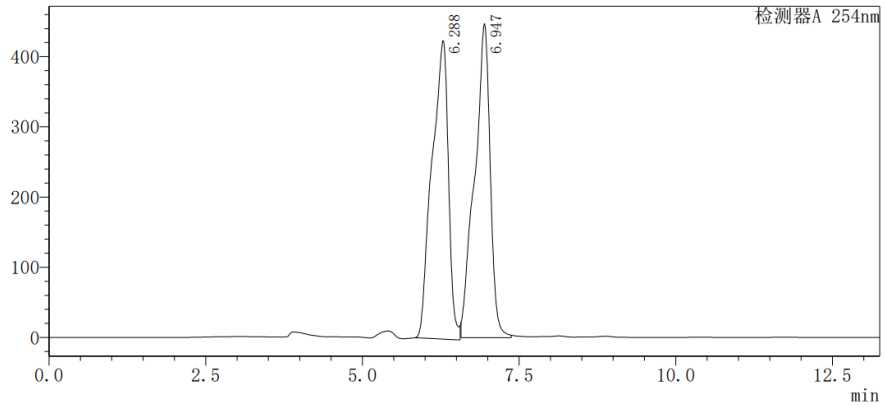
峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	8.454	67748	4344	0.304		M	
2	11.311	22223138	1191286	99.696		M	
总计		22290887	1195630				



(±)-18

〈色谱图〉

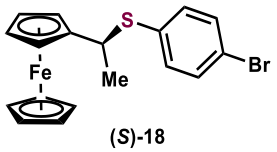
mV



〈峰表〉

检测器A 254nm

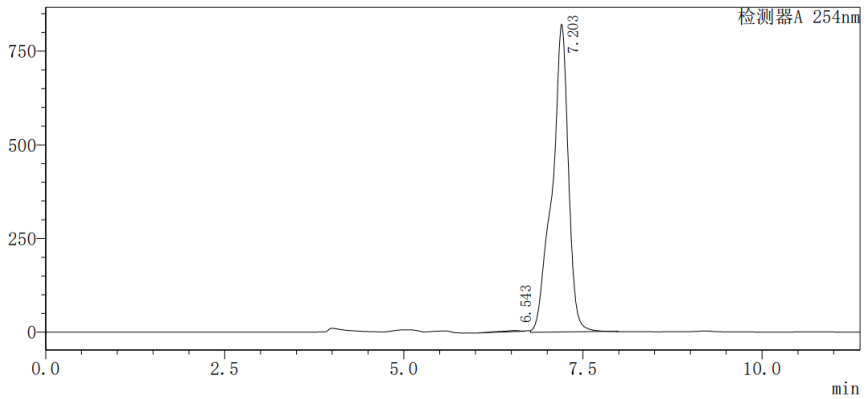
峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.288	7761315	424967	50.137		M	
2	6.947	7718838	446891	49.863		M	
总计		15480153	871858				



(*S*)-18

〈色谱图〉

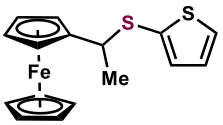
mV



〈峰表〉

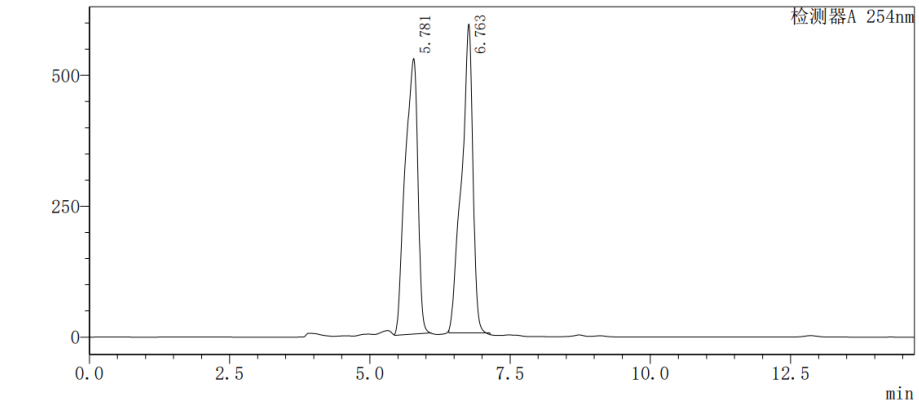
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.543	53650	3004	0.411		M	
2	7.203	13003652	820353	99.589		M	
总计		13057302	823357				



(±)-19

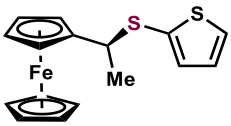
〈色谱图〉



〈峰表〉

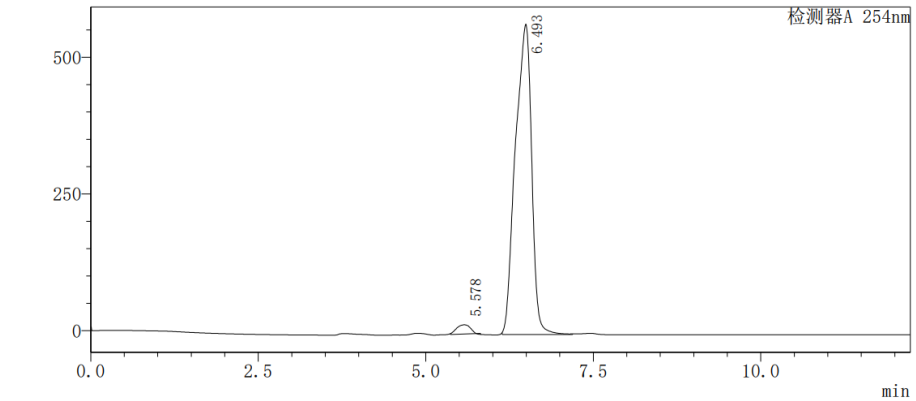
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	5.781	8322216	526338	49.982		M	
2	6.763	8328250	589475	50.018		M	
总计		16650465	1115814				



(*S*)-19

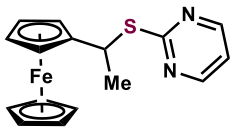
〈色谱图〉



〈峰表〉

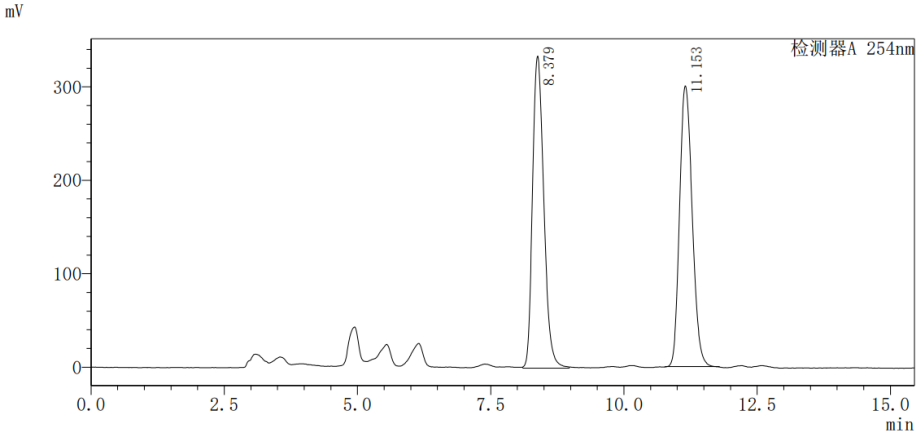
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	5.578	231956	16688	2.369		M	
2	6.493	9561329	567582	97.631		M	
总计		9793286	584270				



(±)-20

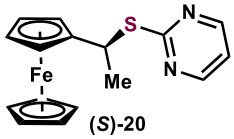
〈色谱图〉



〈峰表〉

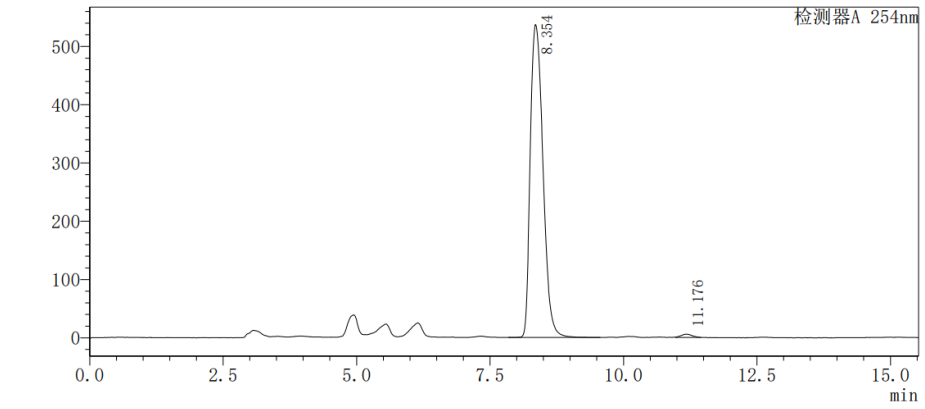
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	8.379	4926124	333705	49.925		M	
2	11.153	4940984	300344	50.075		M	
总计		9867109	634049				



(*S*)-20

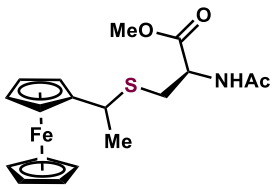
〈色谱图〉



〈峰表〉

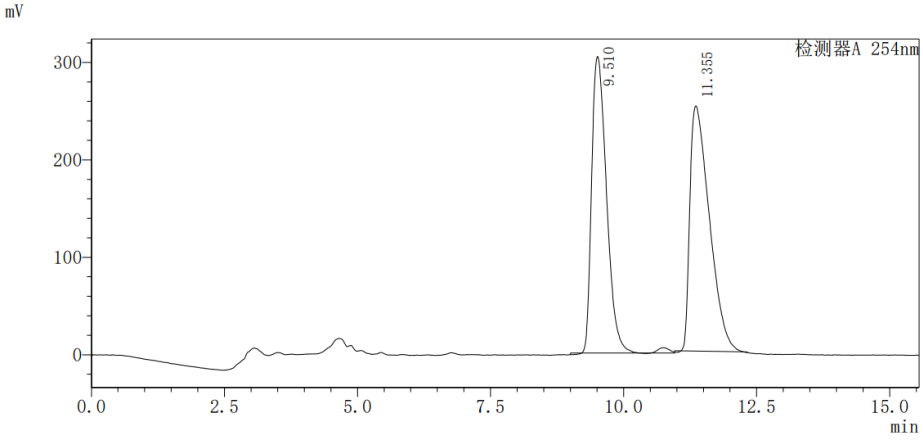
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	8.354	8897870	536845	99.108		M	
2	11.176	80101	5601	0.892		M	
总计		8977971	542445				



(±)-21

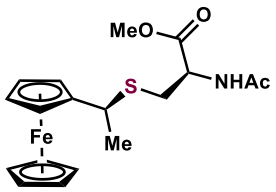
〈色谱图〉



〈峰表〉

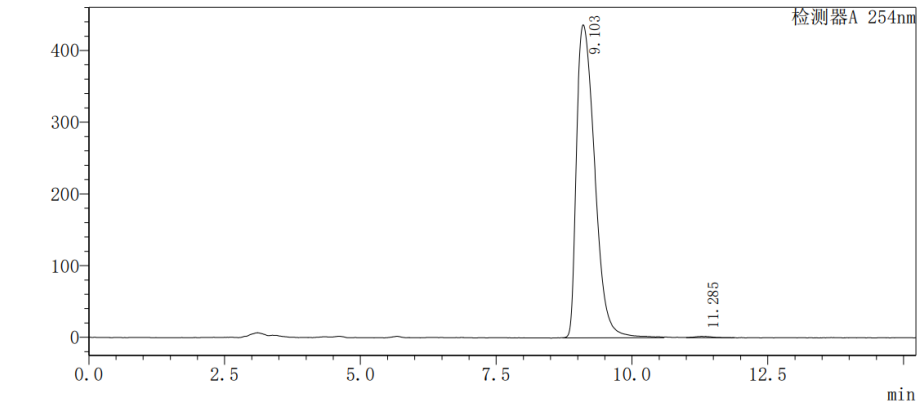
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	9.510	5994370	304368	48.300		M	
2	11.355	6416367	251628	51.700		M	
总计		12410737	555996				



***(S)*-21**

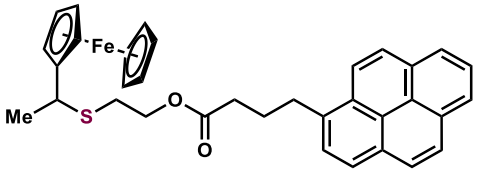
〈色谱图〉



〈峰表〉

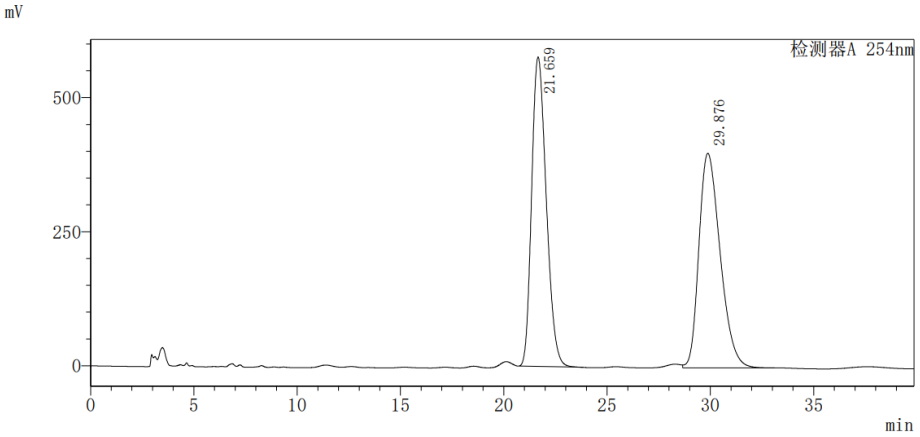
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	9.103	10192583	436499	99.676		M	
2	11.285	33108	1768	0.324		M	
总计		10225691	438267				



(±)-22

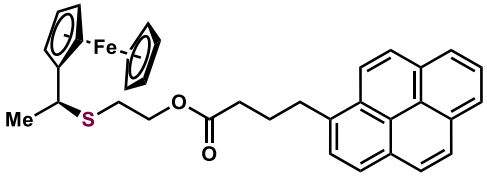
〈色谱图〉



〈峰表〉

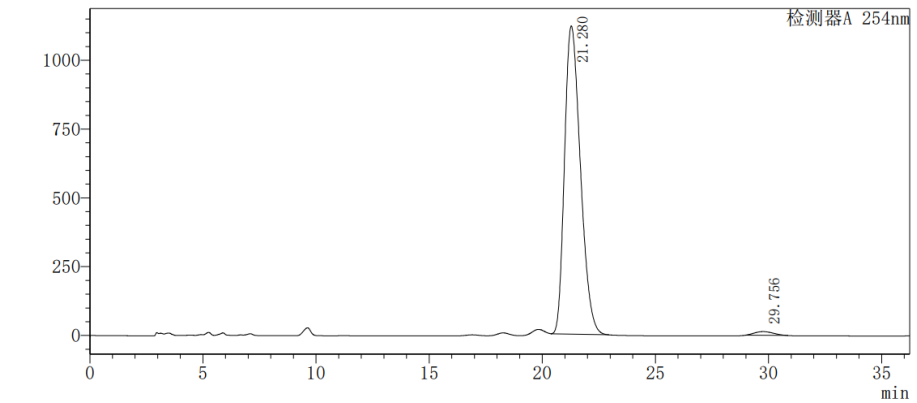
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	21.659	28333092	576740	49.756		M	
2	29.876	28611250	400179	50.244			
总计		56944341	976919				



(*S*)-22

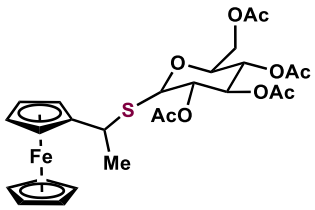
〈色谱图〉



〈峰表〉

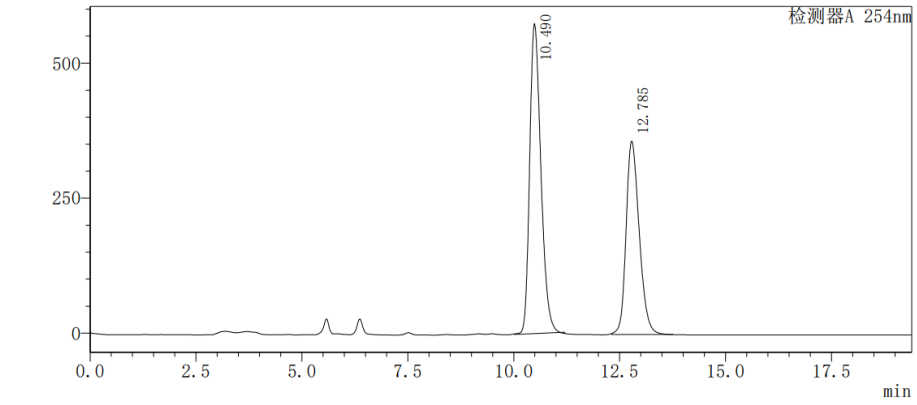
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	21.280	54724057	1119994	98.558		M	
2	29.756	800934	13708	1.442		M	
总计		55524990	1133702				



(±)-23

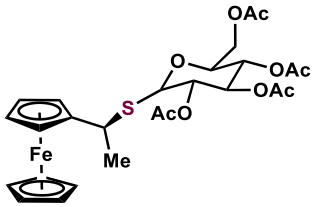
〈色谱图〉



〈峰表〉

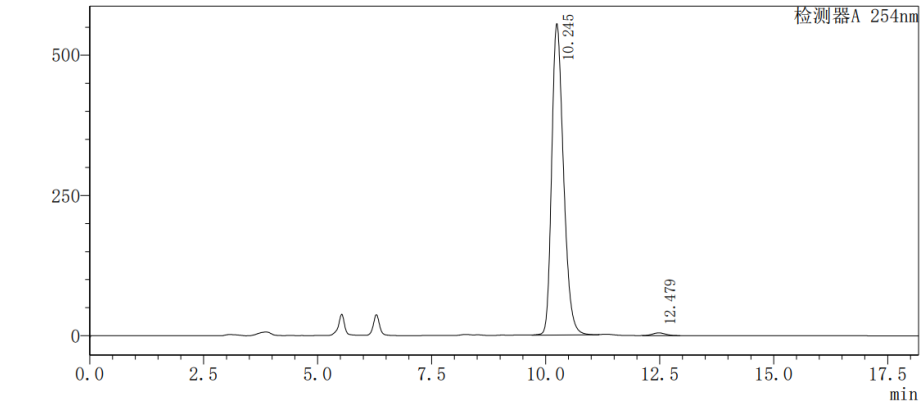
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	10.490	10537270	573461	57.738		M	
2	12.785	7713032	357924	42.262		M	
总计		18250302	931385				



***(S)*-23**

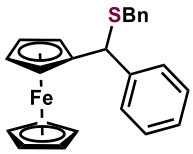
〈色谱图〉



〈峰表〉

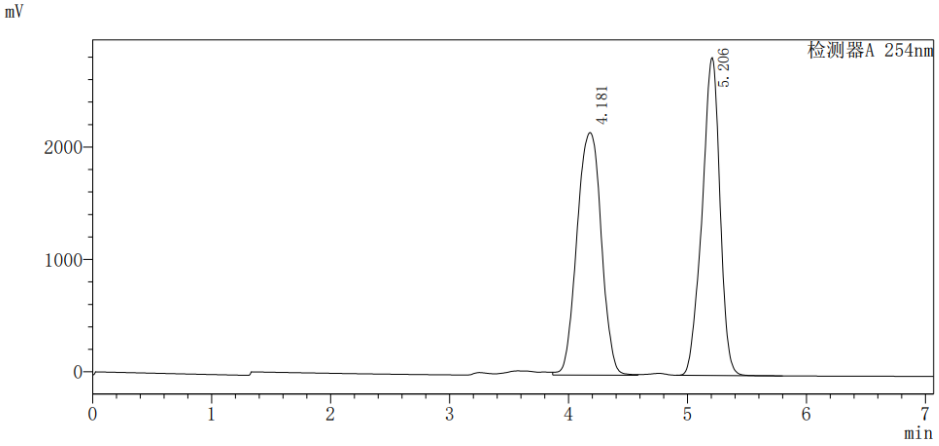
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	10.245	10012532	555183	98.926		M	
2	12.479	108715	5130	1.074		M	
总计		10121247	560313				



(±)-24

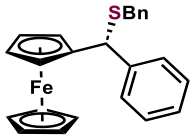
〈色谱图〉



〈峰表〉

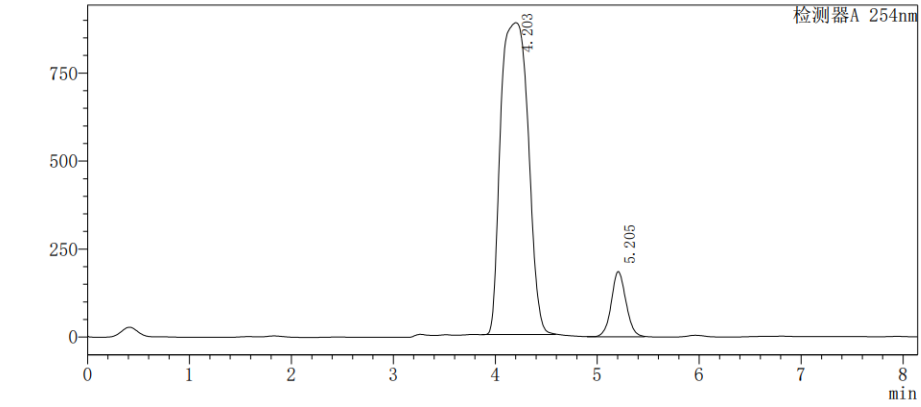
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	4.181	30764180	2157481	51.033			
2	5.206	29519147	2827498	48.967			
总计		60283327	4984979				



(*S*)-24

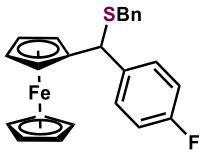
〈色谱图〉



〈峰表〉

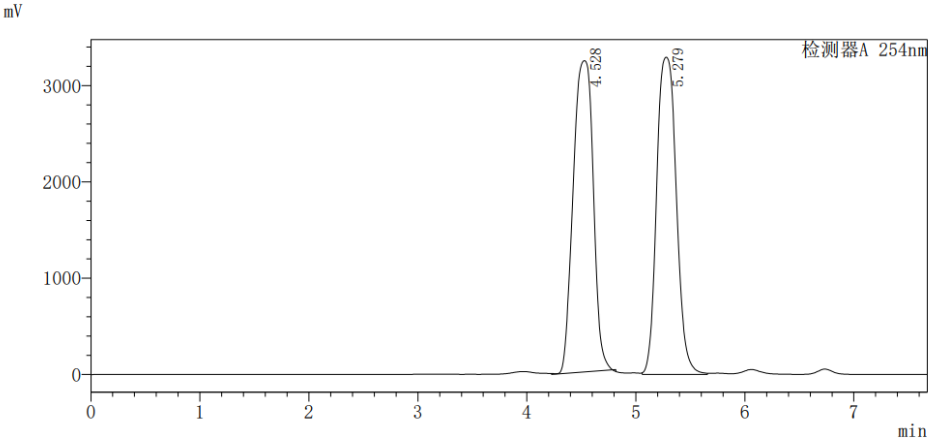
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	4.203	16643945	885648	89.964		M	
2	5.205	1856742	185276	10.036		M	
总计		18500688	1070924				



(±)-25

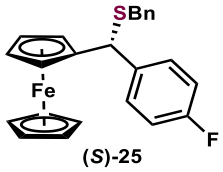
〈色谱图〉



〈峰表〉

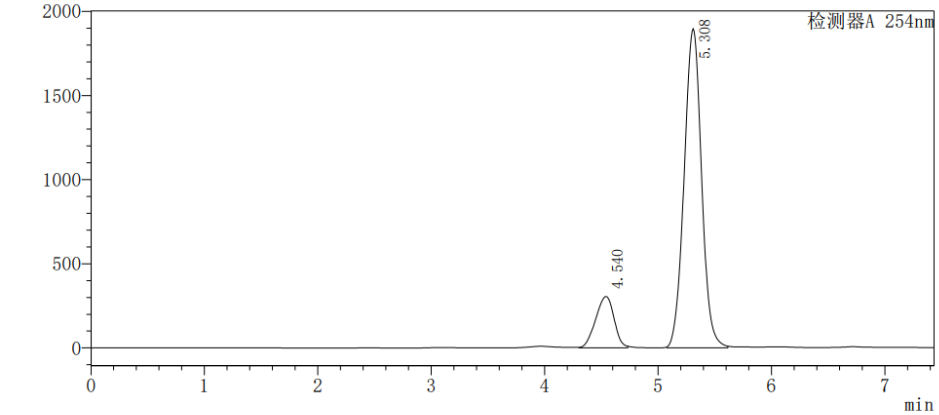
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	4.528	41421662	3231879	50.090		M	
2	5.279	41272884	3292307	49.910		M	
总计		82694546	6524185				



(*S*)-25

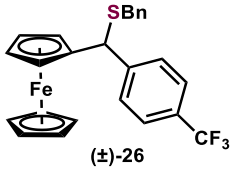
〈色谱图〉



〈峰表〉

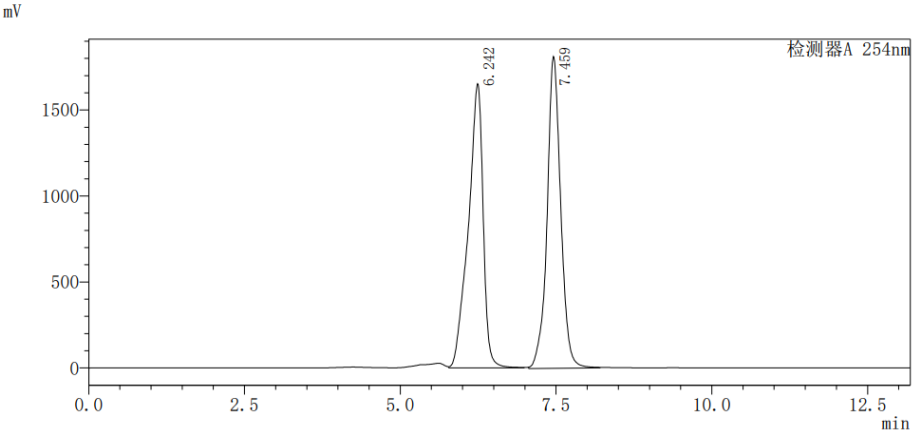
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	4.540	3424979	304600	14.471		M	
2	5.308	20243051	1895920	85.529		M	
总计		23668030	2200520				



(±)-26

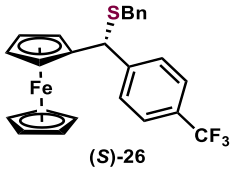
〈色谱图〉



〈峰表〉

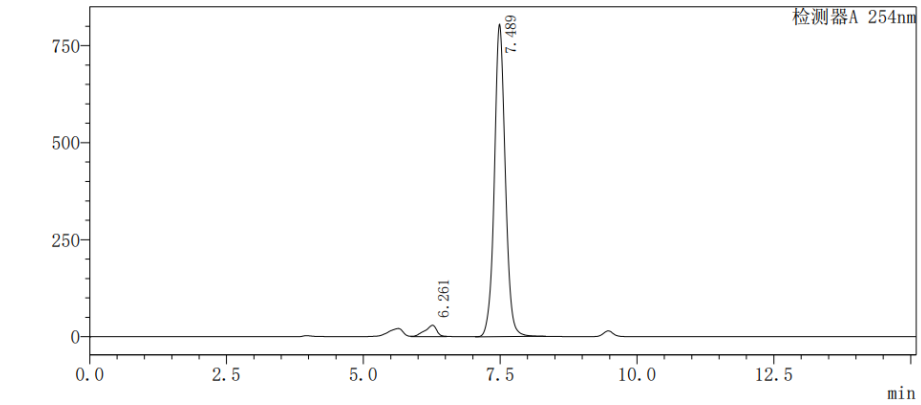
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.242	27474950	1653040	49.873			
2	7.459	27614889	1812620	50.127		M	
总计		55089839	3465659				



(*S*)-26

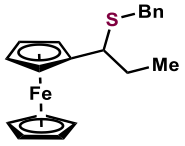
〈色谱图〉



〈峰表〉

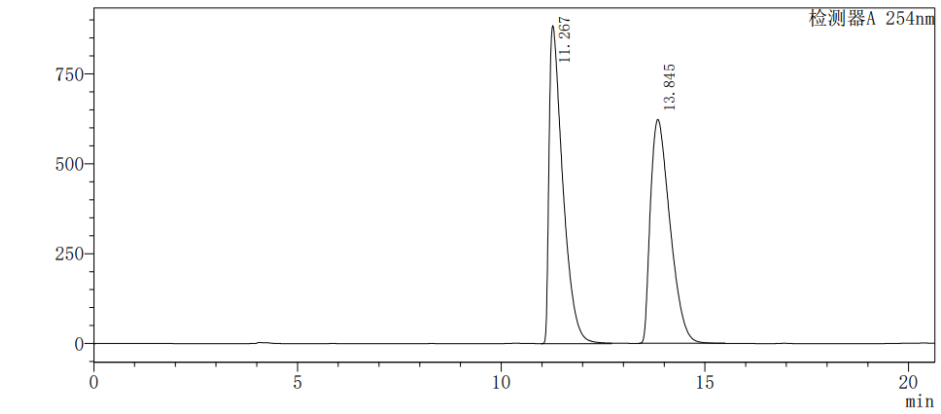
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.261	450697	29501	3.895		M	
2	7.489	11119102	804899	96.105		M	
总计		11569800	834400				



(±)-27

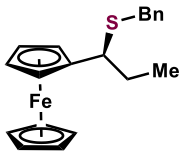
〈色谱图〉



〈峰表〉

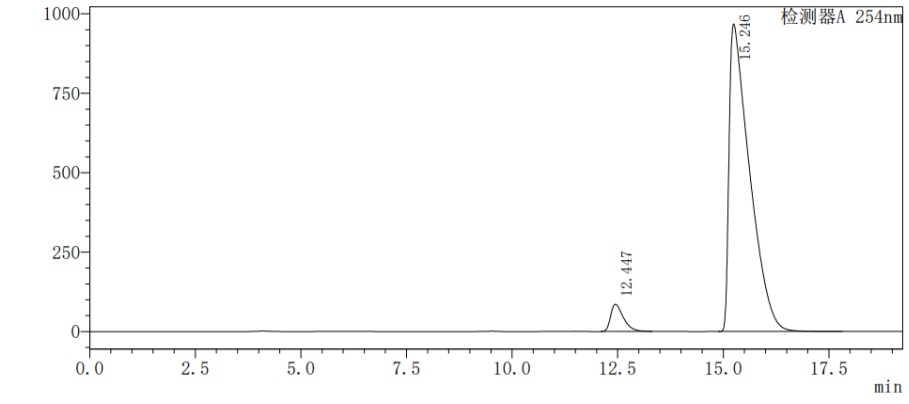
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	11.267	20772437	884218	50.099		M	
2	13.845	20690550	622364	49.901		M	
总计		41462987	1506582				



(*S*)-27

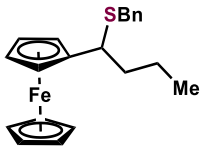
〈色谱图〉



〈峰表〉

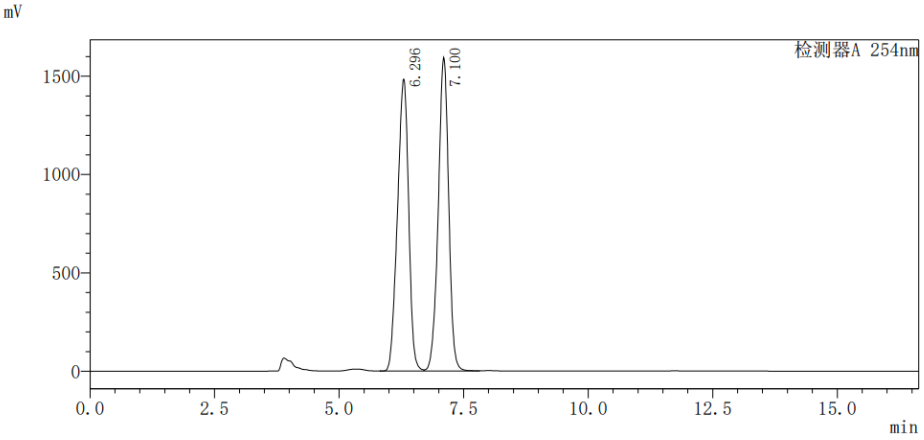
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	12.447	1796798	85532	5.215		M	
2	15.246	32655859	967813	94.785			
总计		34452658	1053345				



(±)-28

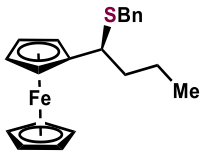
〈色谱图〉



〈峰表〉

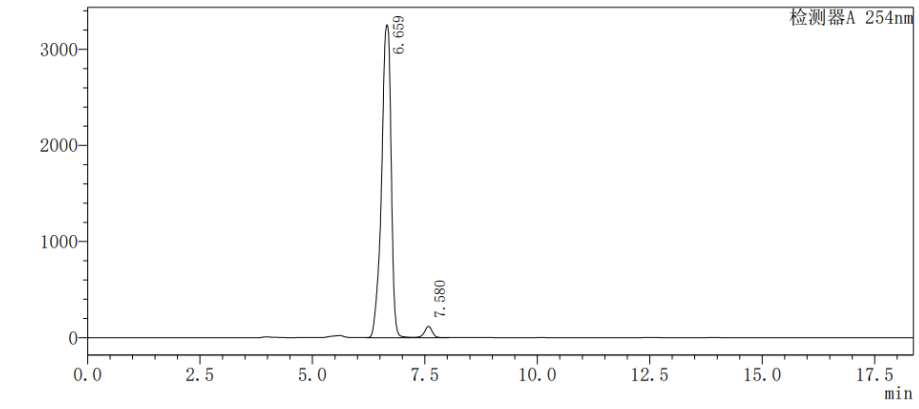
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.296	23207186	1484515	49.903			
2	7.100	23297346	1595295	50.097		V M	
总计		46504532	3079811				



(*S*)-28

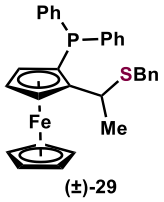
〈色谱图〉



〈峰表〉

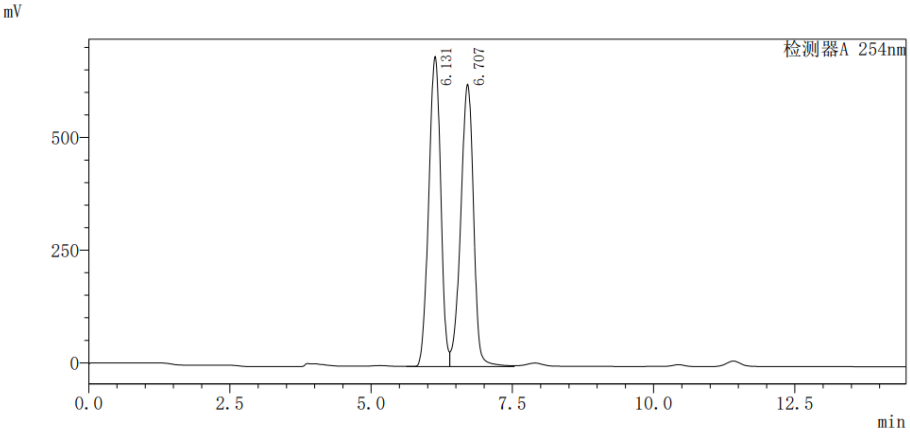
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.659	48127076	3254206	97.110			
2	7.580	1432244	118331	2.890		V	
总计		49559319	3372537				



(±)-29

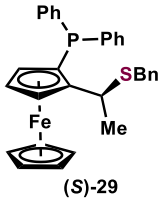
〈色谱图〉



〈峰表〉

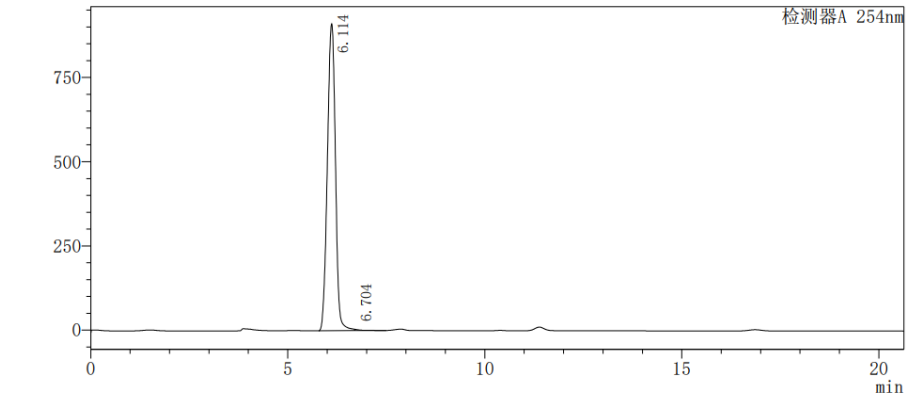
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.131	10159262	688088	50.523			
2	6.707	9948891	626849	49.477		V	
总计		20108153	1314937				



(*S*)-29

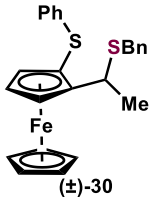
〈色谱图〉



〈峰表〉

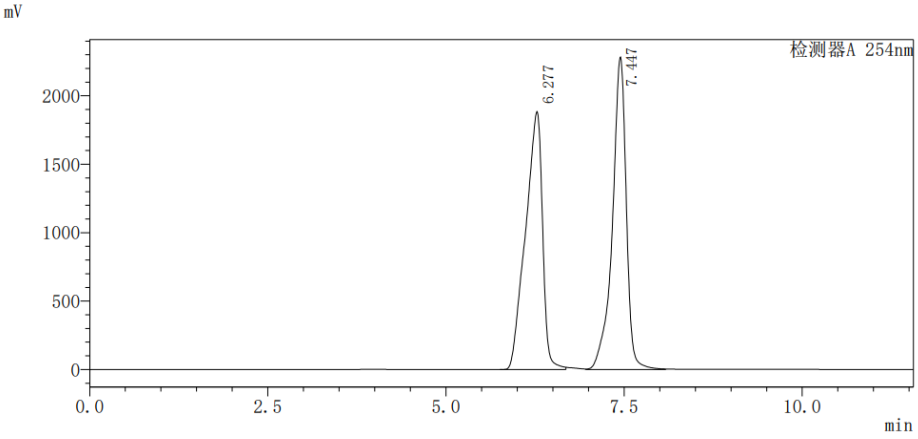
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.114	12958489	910507	99.727		M	
2	6.704	35520	3885	0.273		V M	
总计		12994009	914393				



(±)-30

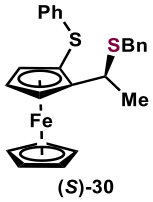
<色谱图>



<峰表>

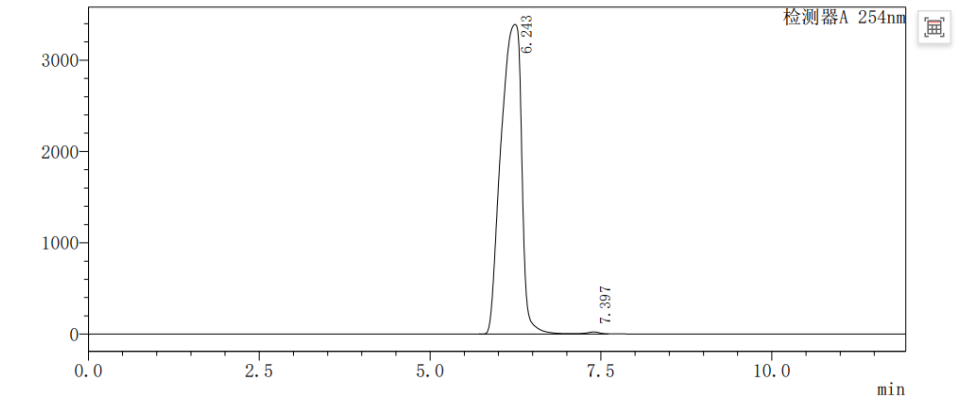
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.277	31287459	1884328	50.248		M	
2	7.447	30979123	2283002	49.752		M	
总计		62266582	4167330				



(*S*)-30

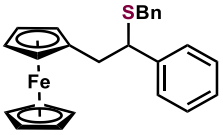
<色谱图>



<峰表>

检测器A 254nm

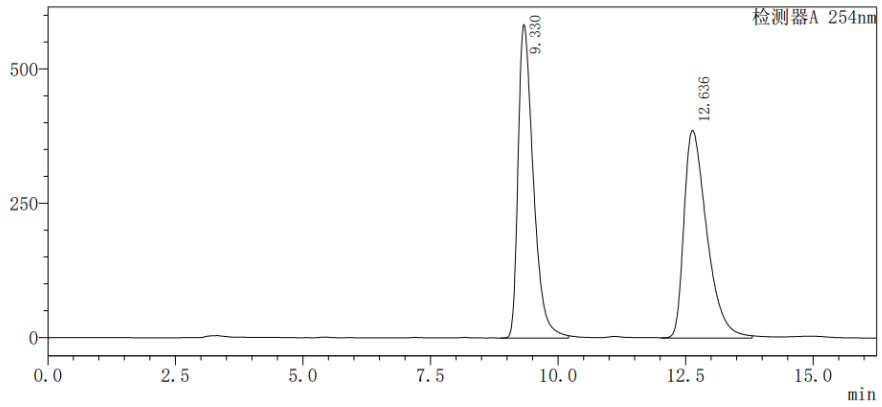
峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.243	71166270	3391047	99.491			
2	7.397	364030	23566	0.509		V M	
总计		71530299	3414613				



(±)-31

〈色谱图〉

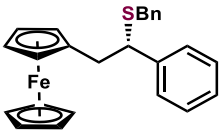
mV



〈峰表〉

检测器A 254nm

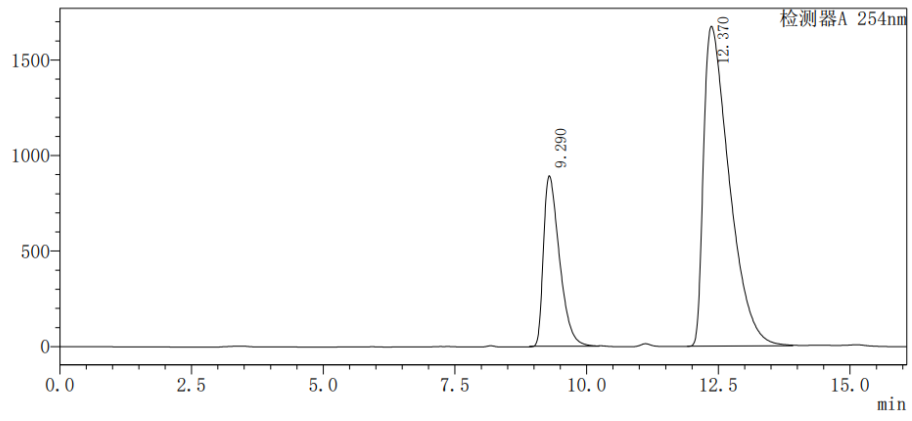
峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	9.330	12118784	583518	50.080		M	
2	12.636	12080137	386661	49.920		M	
总计		24198921	970180				



(*S*)-31

〈色谱图〉

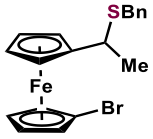
mV



〈峰表〉

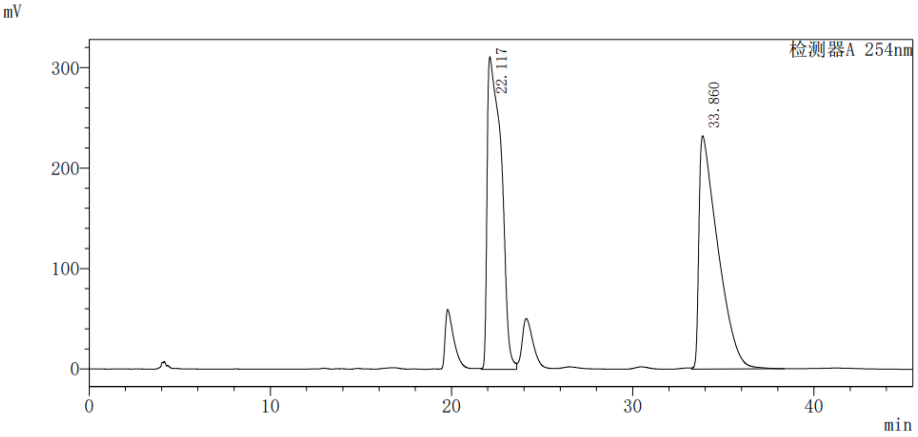
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	9.290	18801842	892711	24.828		M	
2	12.370	56925246	1673897	75.172		M	
总计		75727087	2566608				



(±)-32

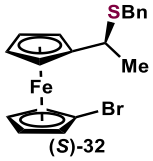
〈色谱图〉



〈峰表〉

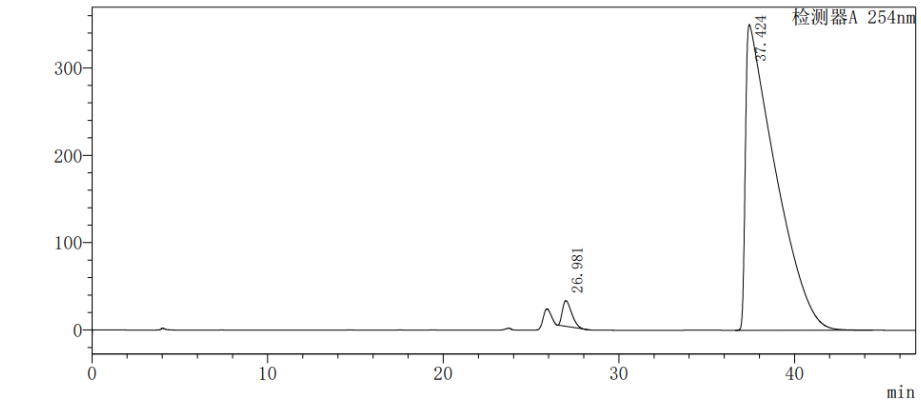
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	22.117	16756436	310946	49.808			
2	33.860	16885432	232218	50.192			
总计		33641868	543164				



(*S*)-32

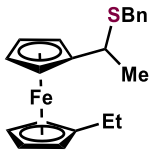
〈色谱图〉



〈峰表〉

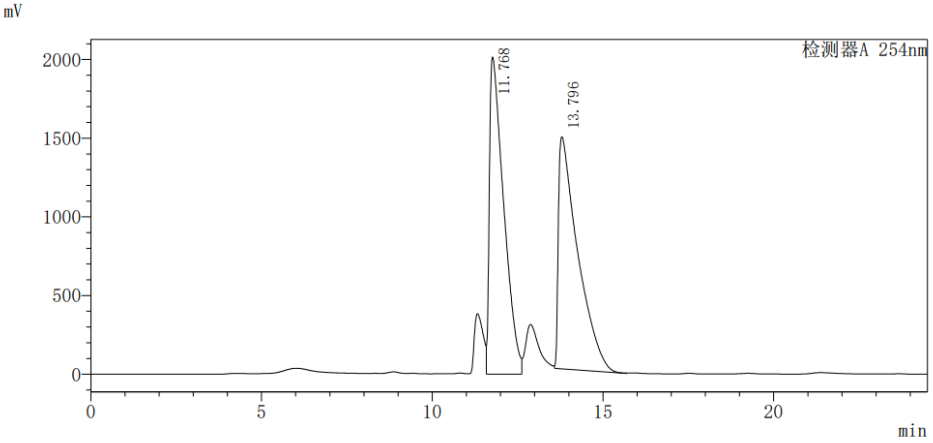
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	26.981	1072212	29389	2.524		M	
2	37.424	41407532	349919	97.476			
总计		42479743	379309				



(±)-33

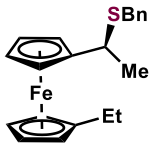
〈色谱图〉



〈峰表〉

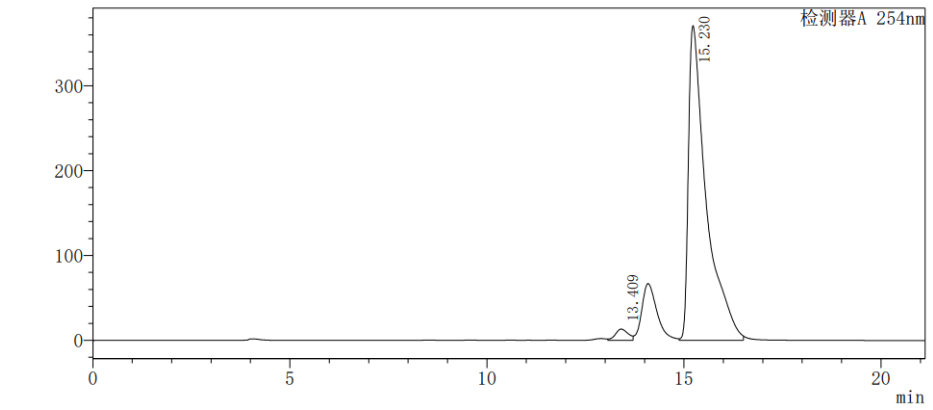
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	11.768	58644465	2014506	50.133			
2	13.796	58332971	1476034	49.867		M	
总计		116977436	3490540				



(*S*)-33

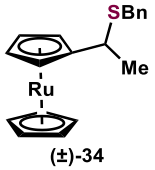
〈色谱图〉



〈峰表〉

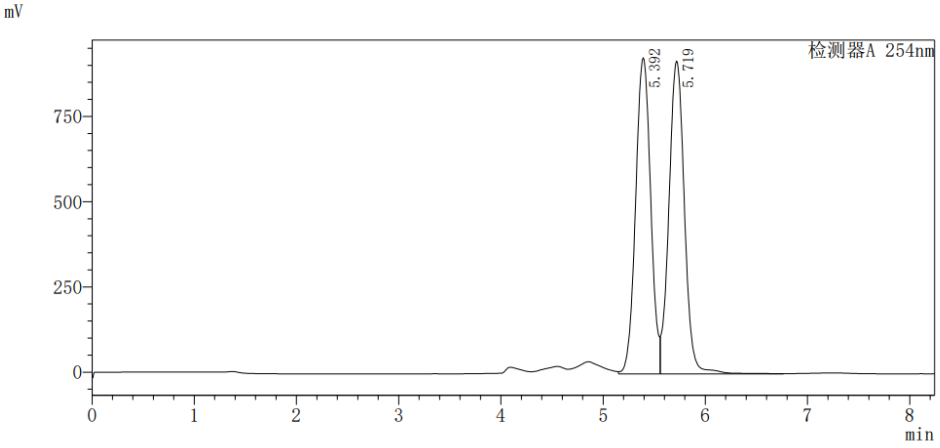
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	13.409	297589	13220	2.489			
2	15.230	11657926	370725	97.511		M	
总计		11955515	383945				



(±)-34

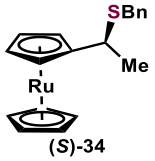
〈色谱图〉



〈峰表〉

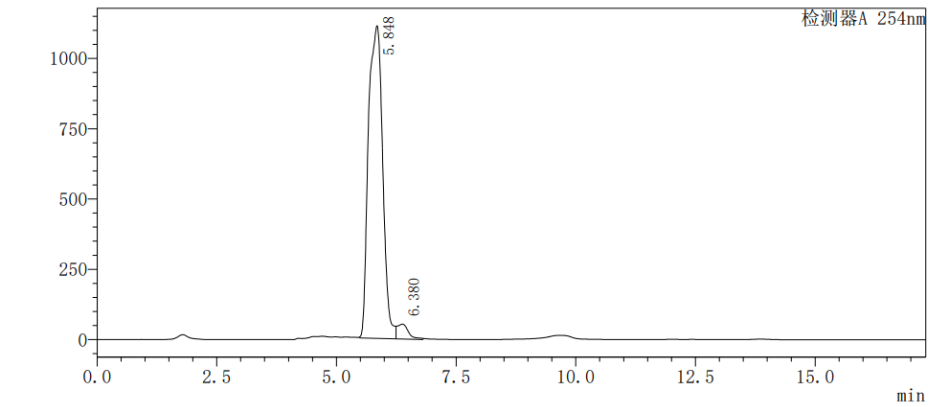
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	5.392	9472950	926309	49.491			
2	5.719	9667874	917067	50.509		V	
总计		19140824	1843376				



(*S*)-34

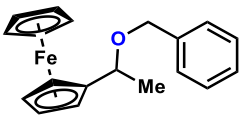
〈色谱图〉



〈峰表〉

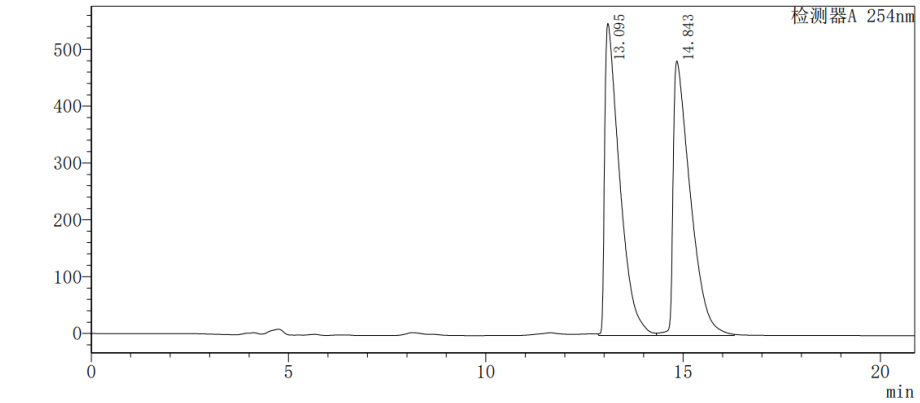
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	5.848	22957391	1111665	96.377		M	
2	6.380	862952	52824	3.623		V M	
总计		23820344	1164489				



(±)-35

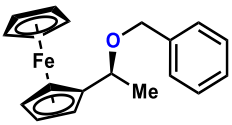
〈色谱图〉



〈峰表〉

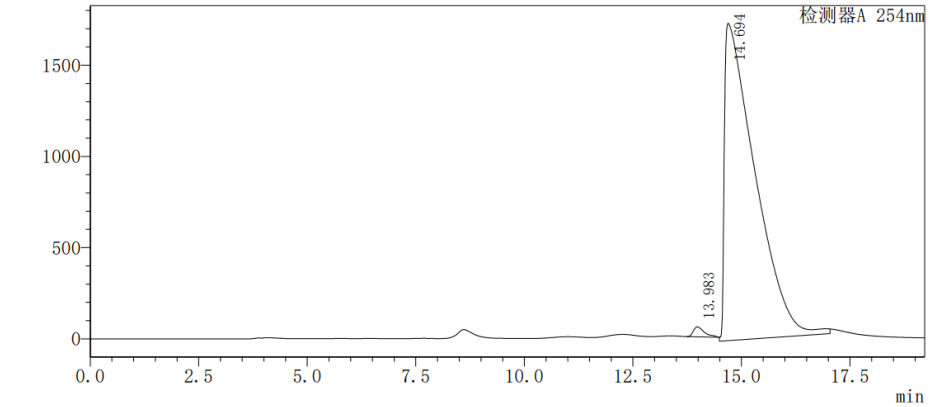
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	13.095	14533212	548903	49.700			
2	14.843	14708637	483072	50.300		V M	
总计		29241849	1031975				



(*S*)-35

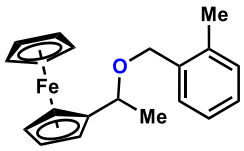
〈色谱图〉



〈峰表〉

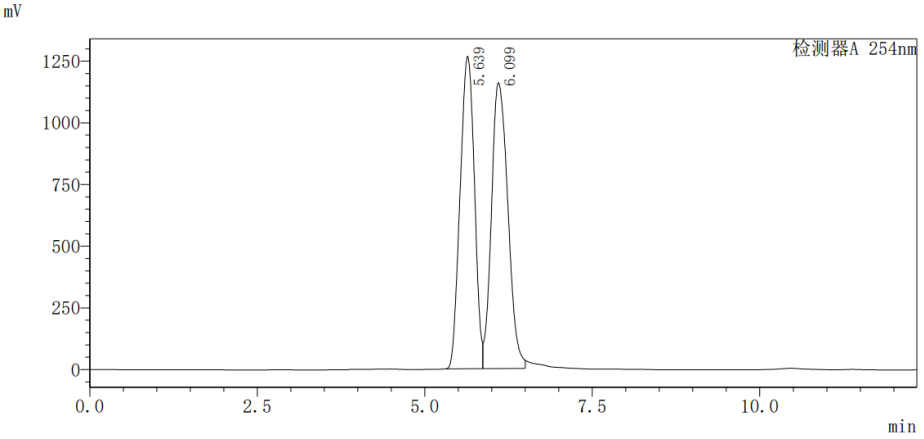
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	13.983	944299	53909	1.098		M	
2	14.694	85065396	1739460	98.902		M	
总计		86009695	1793368				



(±)-36

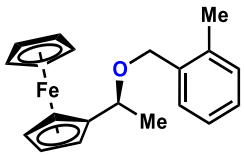
〈色谱图〉



〈峰表〉

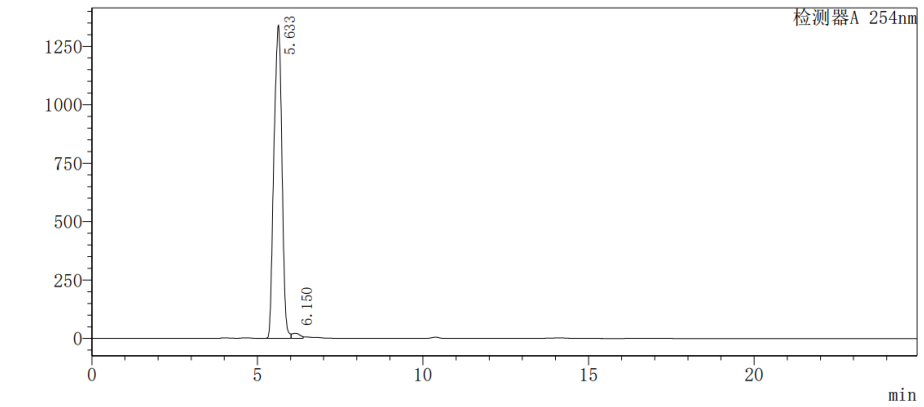
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	5.639	18831621	1266141	48.759		M	
2	6.099	19790271	1158614	51.241		V M	
总计		38621892	2424756				



(*S*)-36

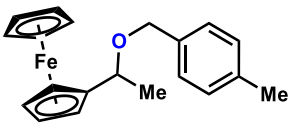
〈色谱图〉



〈峰表〉

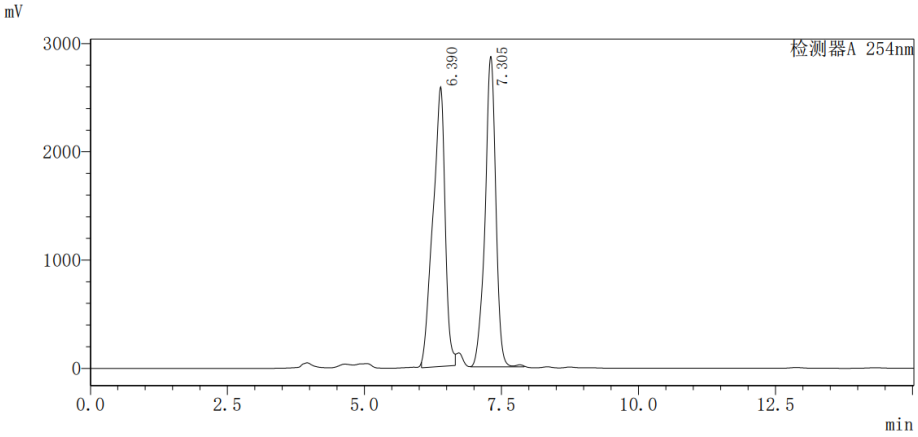
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	5.633	22534084	1339307	98.372			
2	6.150	373029	21715	1.628		V M	
总计		22907112	1361022				



(±)-37

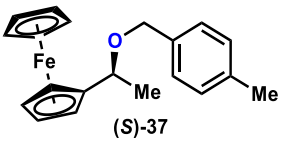
〈色谱图〉



〈峰表〉

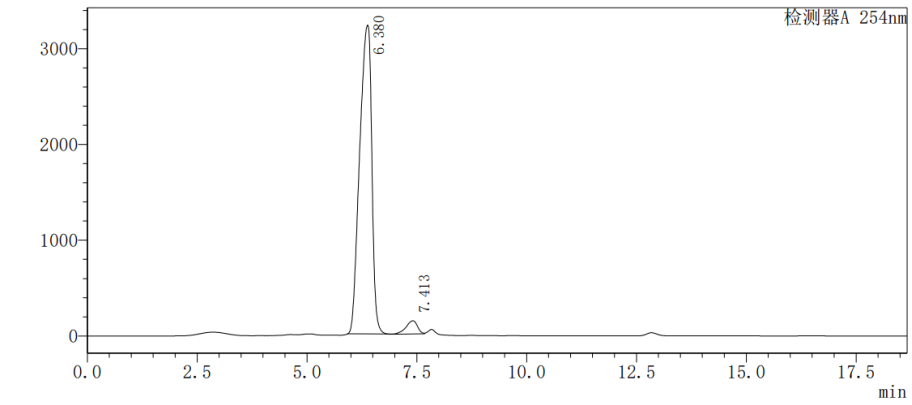
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.390	40077575	2582740	50.632		M	
2	7.305	39077026	2865613	49.368		M	
总计		79154601	5448353				



(*S*)-37

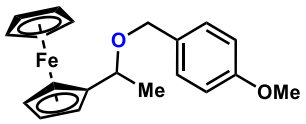
〈色谱图〉



〈峰表〉

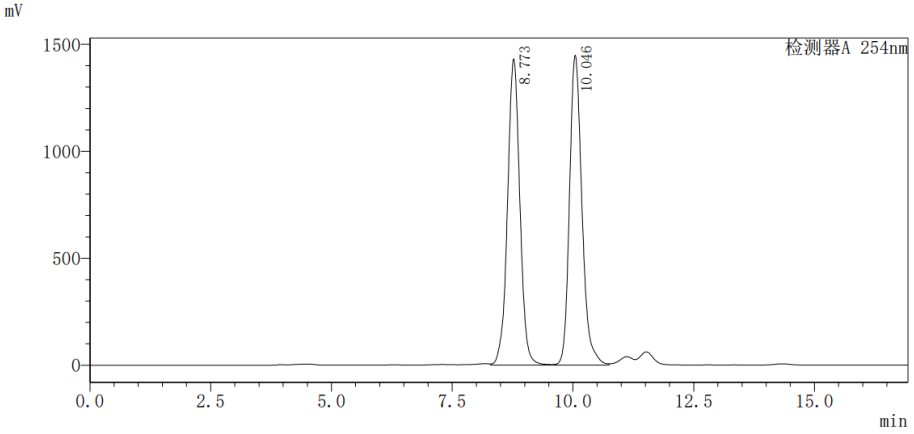
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.380	61772540	3226121	96.069		M	
2	7.413	2527591	137260	3.931		M	
总计		64300132	3363380				



(±)-38

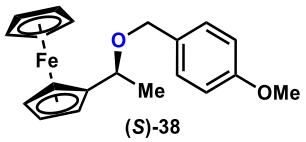
〈色谱图〉



〈峰表〉

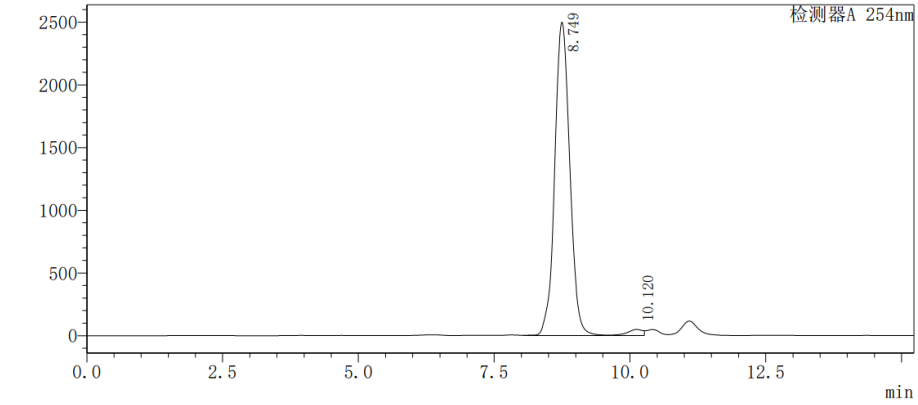
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	8.773	25481240	1431622	49.549			
2	10.046	25945303	1448245	50.451		V	
总计		51426544	2879868				



(*S*)-38

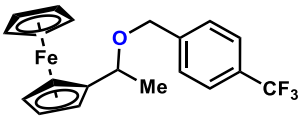
〈色谱图〉



〈峰表〉

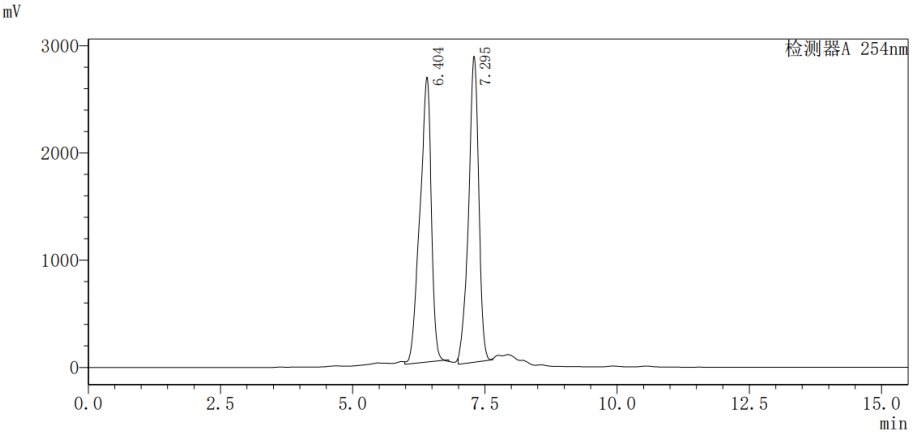
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	8.749	48487121	2498843	97.967			
2	10.120	1006433	49629	2.033		V	
总计		49493554	2548472				



(±)-39

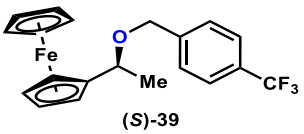
〈色谱图〉



〈峰表〉

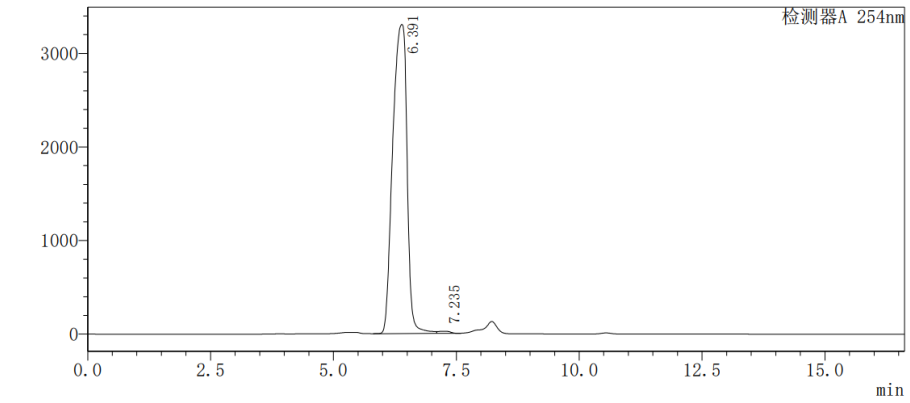
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.404	39620246	2656722	50.841		M	
2	7.295	38310128	2853571	49.159		M	
总计		77930374	5510293				



(*S*)-39

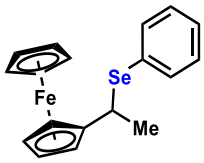
〈色谱图〉



〈峰表〉

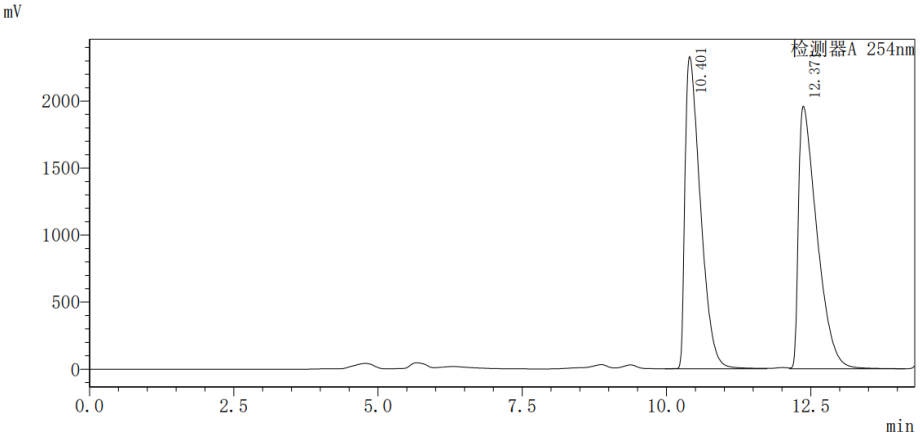
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.391	66850558	3303085	99.418		M	
2	7.235	391421	23124	0.582		V M	
总计		67241978	3326209				



(±)-40

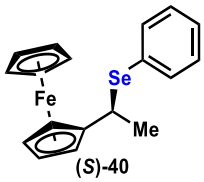
〈色谱图〉



〈峰表〉

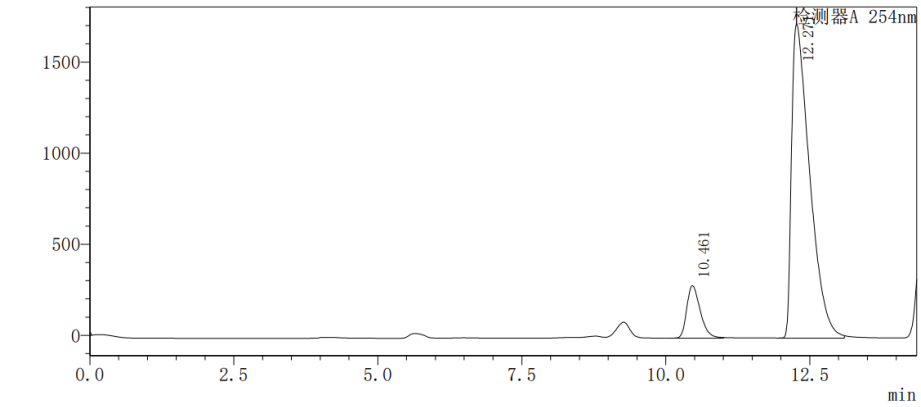
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	10.401	43526824	2329591	49.913		M	
2	12.371	43678889	1959159	50.087			
总计		87205713	4288749				



(*S*)-40

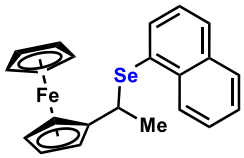
〈色谱图〉



〈峰表〉

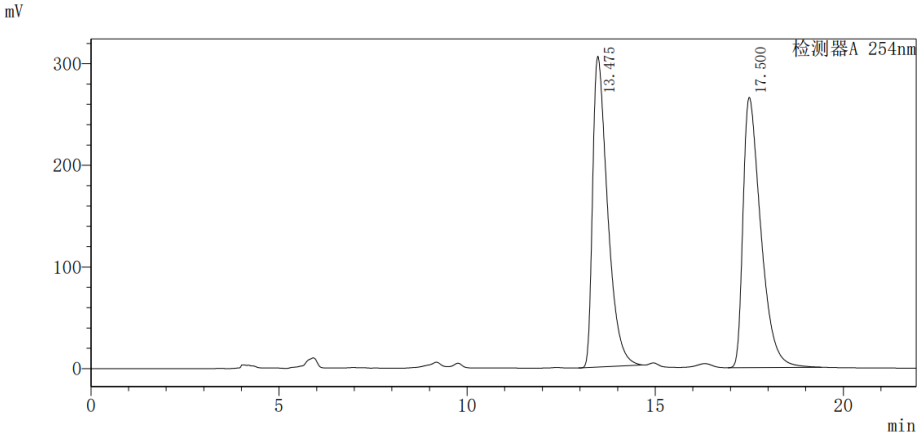
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	10.461	4705751	288099	11.075		M	
2	12.271	37785299	1721048	88.925		M	
总计		42491050	2009148				



(±)-41

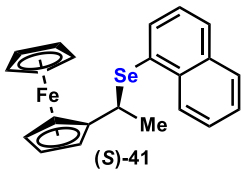
〈色谱图〉



〈峰表〉

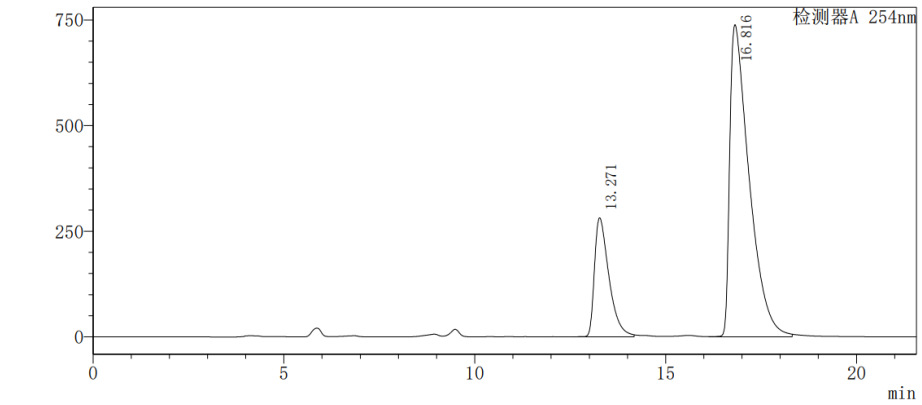
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	13.475	8461010	305592	49.163		M	
2	17.500	8749201	265858	50.837		M	
总计		17210211	571450				



(*S*)-41

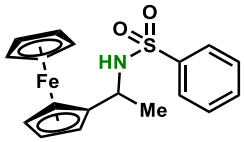
〈色谱图〉



〈峰表〉

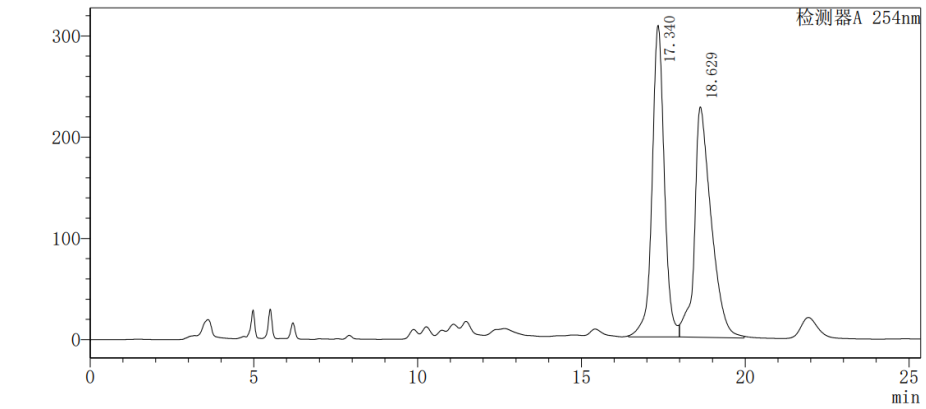
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	13.271	7442374	281835	22.120		M	
2	16.816	26202554	738570	77.880		M	
总计		33644928	1020405				



(±)-42

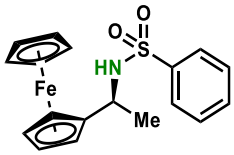
〈色谱图〉



〈峰表〉

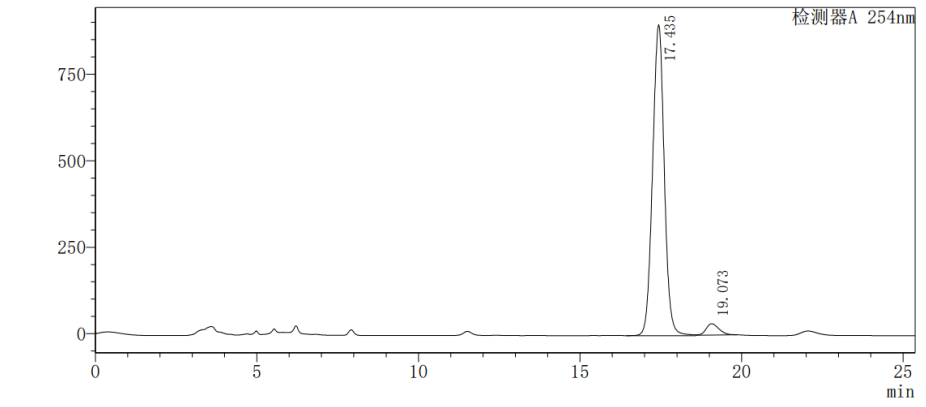
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	17.340	8015044	307672	49.673		M	
2	18.629	8120688	227552	50.327		M	
总计		16135731	535224				



(*S*)-42

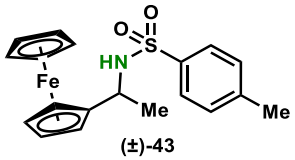
〈色谱图〉



〈峰表〉

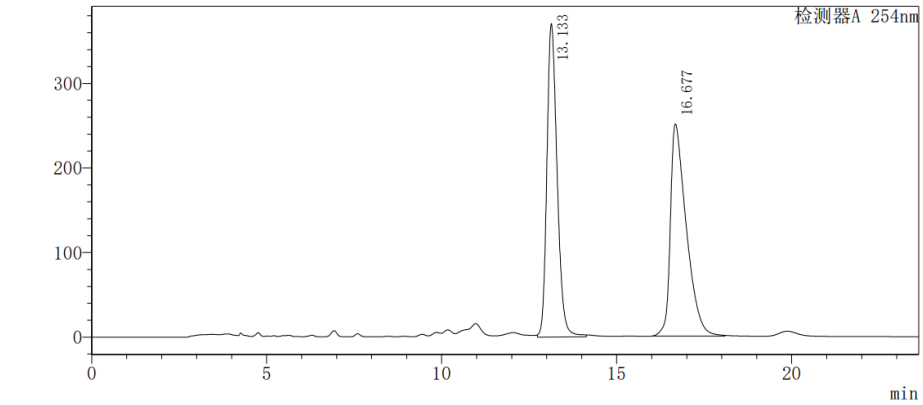
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	17.435	22607318	898389	96.109			
2	19.073	915370	32893	3.891		M	
总计		23522688	931282				



(±)-43

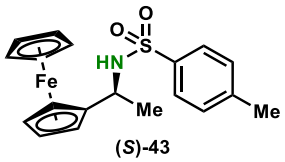
〈色谱图〉



〈峰表〉

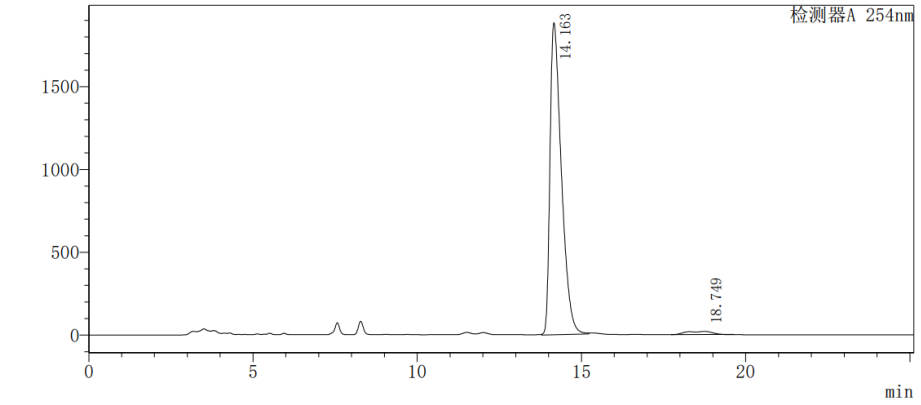
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	13.133	7551633	370404	48.741		M	
2	16.677	7941891	250940	51.259		M	
总计		15493525	621344				



(*S*)-43

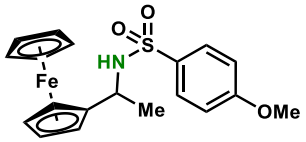
〈色谱图〉



〈峰表〉

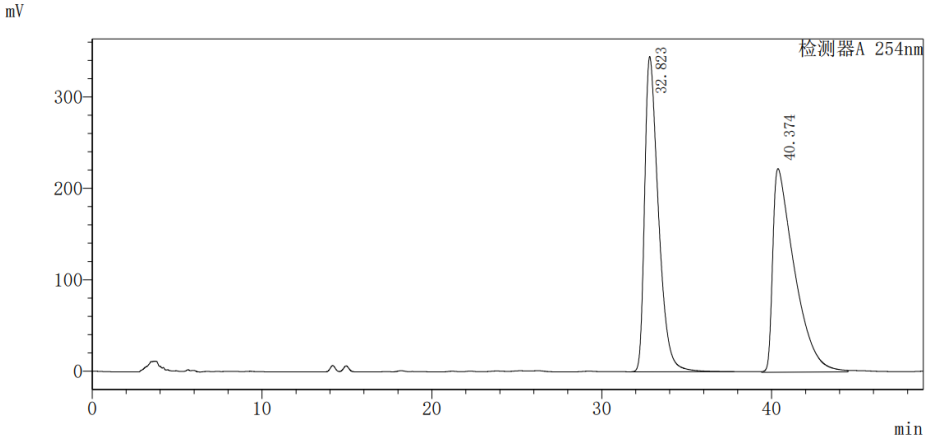
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	14.163	45370002	1883144	97.782		M	
2	18.749	1029075	19154	2.218		M	
总计		46399078	1902298				



(±)-44

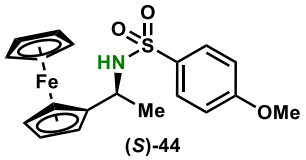
〈色谱图〉



〈峰表〉

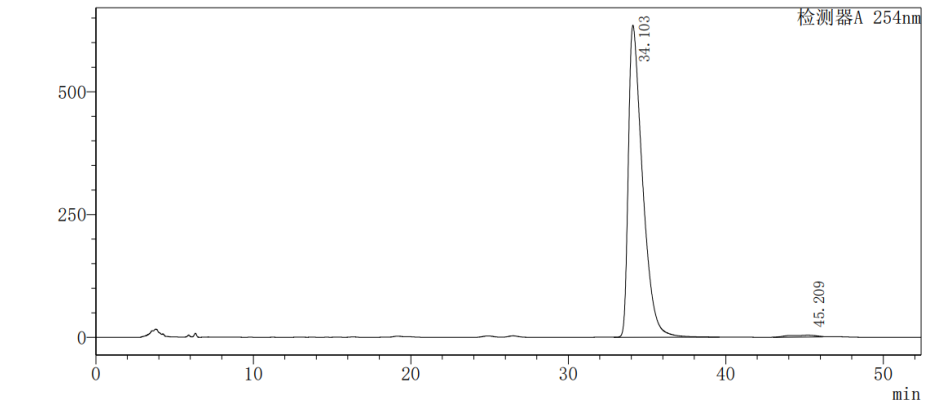
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	32.823	19456164	344858	49.553			
2	40.374	19807072	222885	50.447		M	
总计		39263236	567743				



(*S*)-44

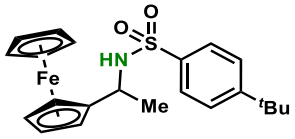
〈色谱图〉



〈峰表〉

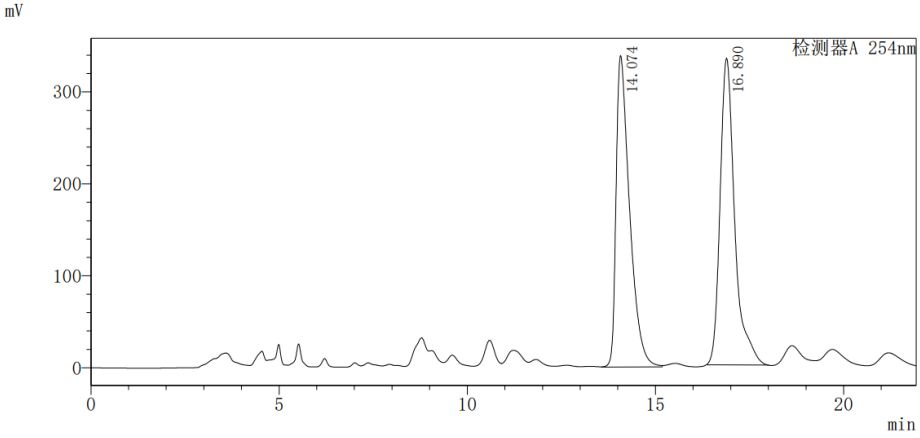
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	34.103	39632277	635317	98.762			
2	45.209	496787	3924	1.238		M	
总计		40129064	639241				



(±)-45

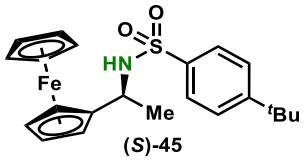
〈色谱图〉



〈峰表〉

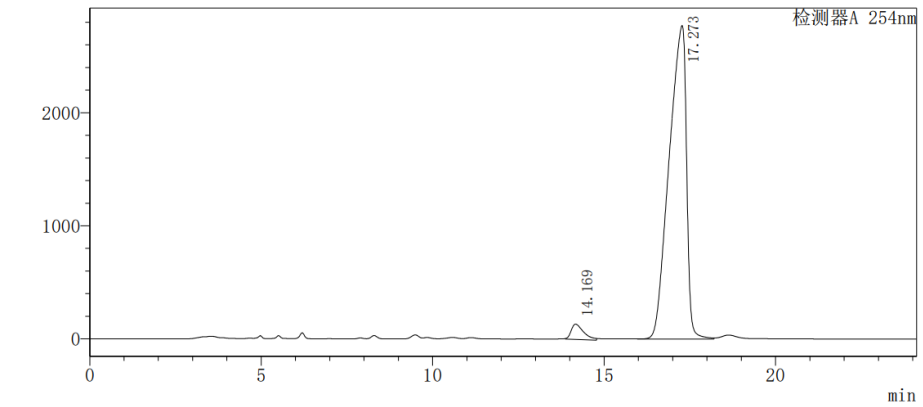
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	14.074	8449013	338514	48.403		M	
2	16.890	9006570	333503	51.597		M	
总计		17455583	672017				



(*S*)-45

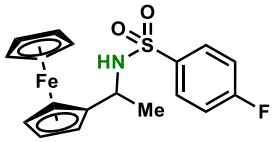
〈色谱图〉



〈峰表〉

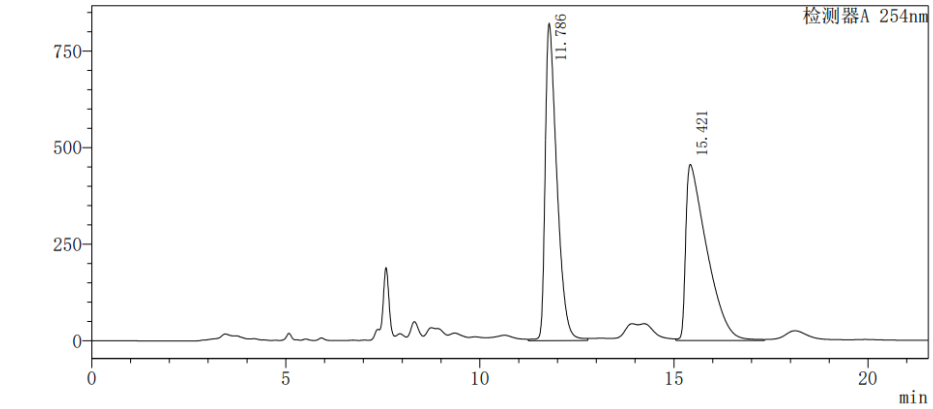
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	14.169	3432023	135691	3.393		M	
2	17.273	97706582	2771219	96.607			
总计		101138605	2906910				



(±)-46

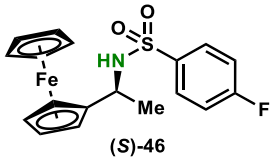
〈色谱图〉



〈峰表〉

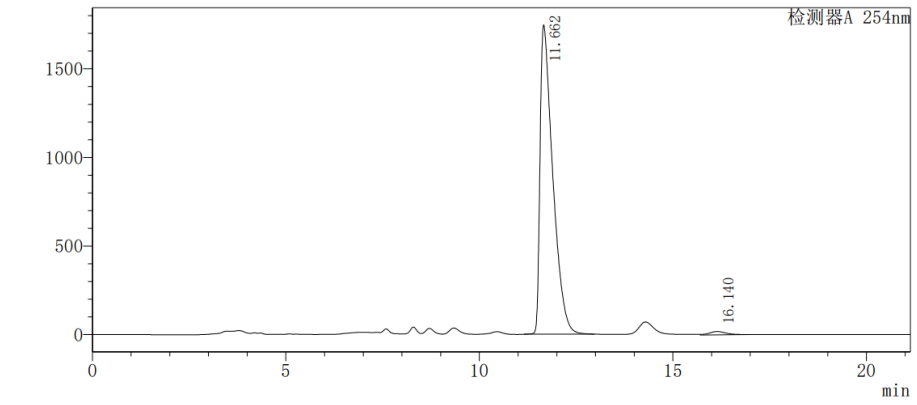
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	11.786	17199930	821117	49.980			
2	15.421	17213547	455781	50.020			
总计		34413477	1276898				



(*S*)-46

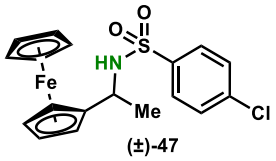
〈色谱图〉



〈峰表〉

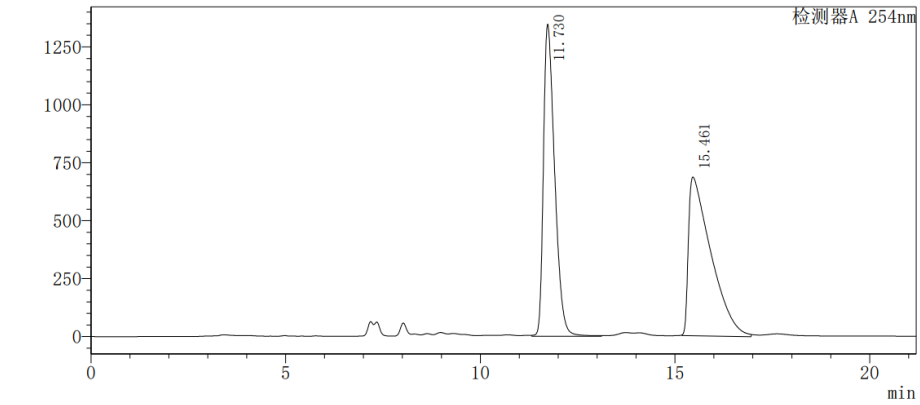
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	11.662	39857549	1744793	98.567		M	
2	16.140	579526	18978	1.433		M	
总计		40437075	1763772				



(±)-47

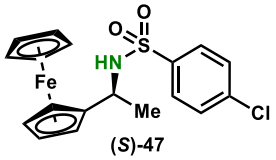
〈色谱图〉



〈峰表〉

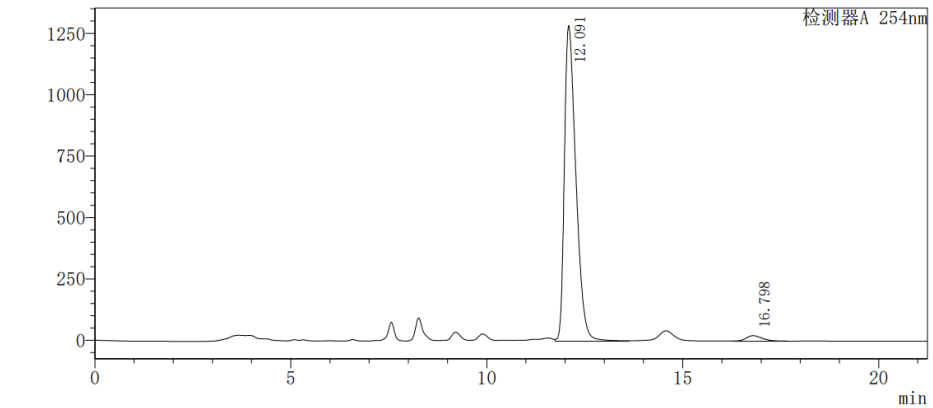
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	11.730	26992970	1345790	49.511			
2	15.461	27526156	684813	50.489		M	
总计		54519126	2030603				



(*S*)-47

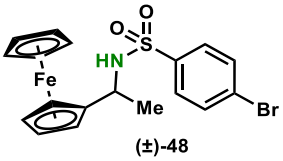
〈色谱图〉



〈峰表〉

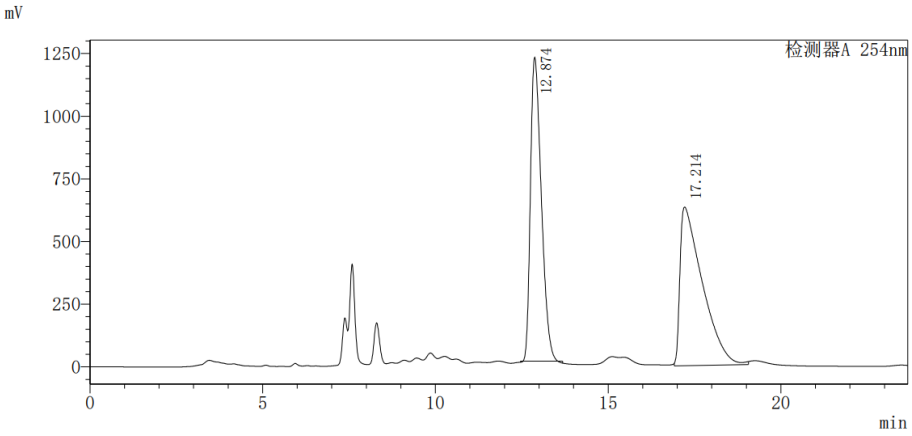
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	12.091	26284499	1284900	97.563			
2	16.798	656650	22534	2.437			
总计		26941149	1307433				



(±)-48

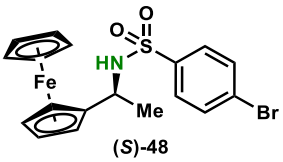
〈色谱图〉



〈峰表〉

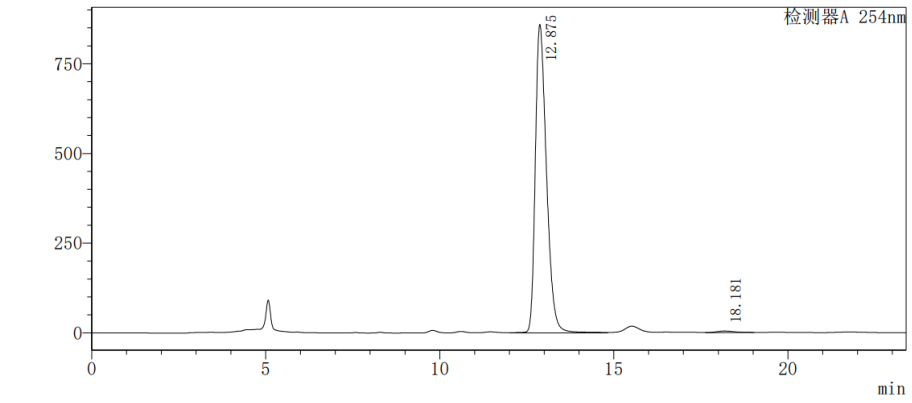
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	12.874	26448905	1211479	48.147		M	
2	17.214	28484867	632970	51.853		M	
总计		54933772	1844449				



(*S*)-48

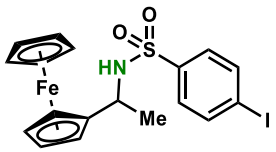
〈色谱图〉



〈峰表〉

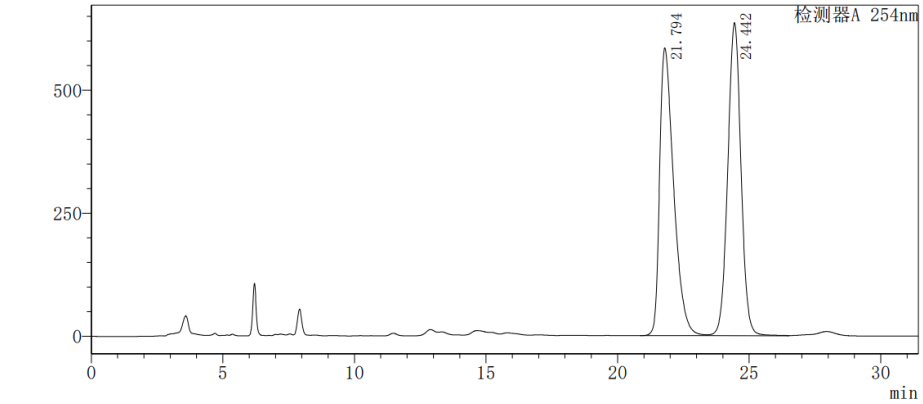
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	12.875	19210728	859873	99.188			
2	18.181	157333	4373	0.812		M	
总计		19368061	864247				



(±)-49

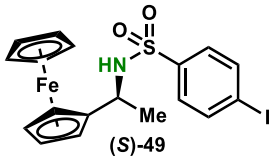
<色谱图>



<峰表>

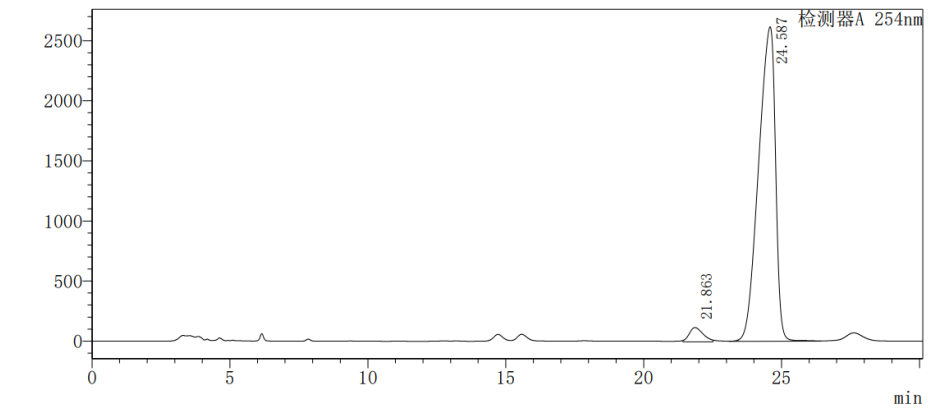
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	21.794	21664013	584532	49.345			
2	24.442	22239552	635827	50.655		V	
总计		43903564	1220360				



(*S*)-49

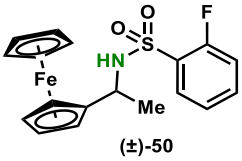
<色谱图>



<峰表>

检测器A 254nm

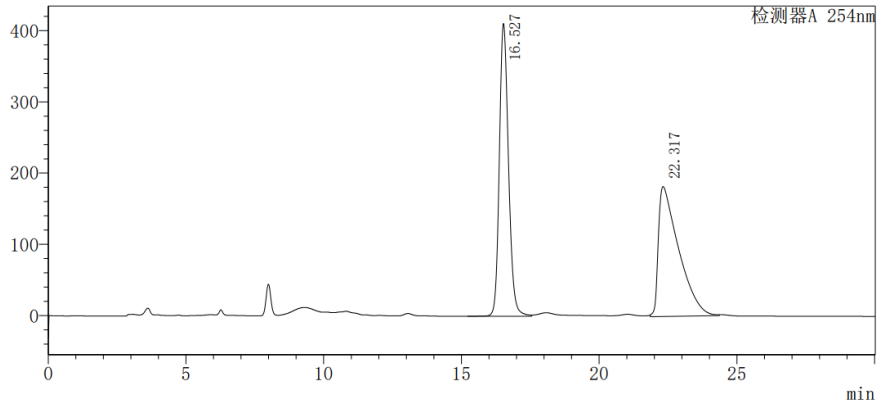
峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	21.863	4108180	118019	3.565		M	
2	24.587	111138871	2616979	96.435			
总计		115247051	2734998				



(±)-50

〈色谱图〉

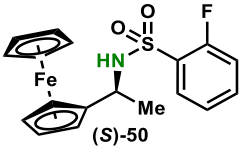
mV



〈峰表〉

检测器A 254nm

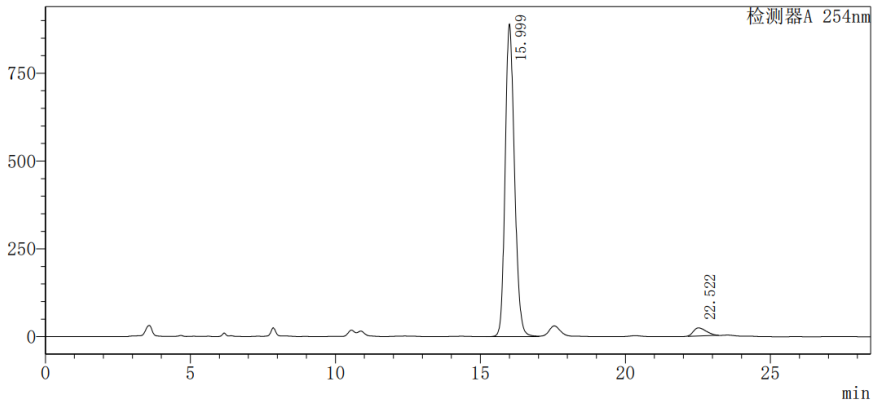
峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	16.527	9500375	410805	50.409			
2	22.317	9346208	182376	49.591		M	
总计		18846583	593181				



(*S*)-50

〈色谱图〉

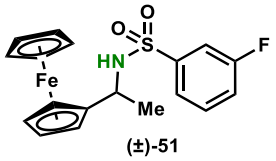
mV



〈峰表〉

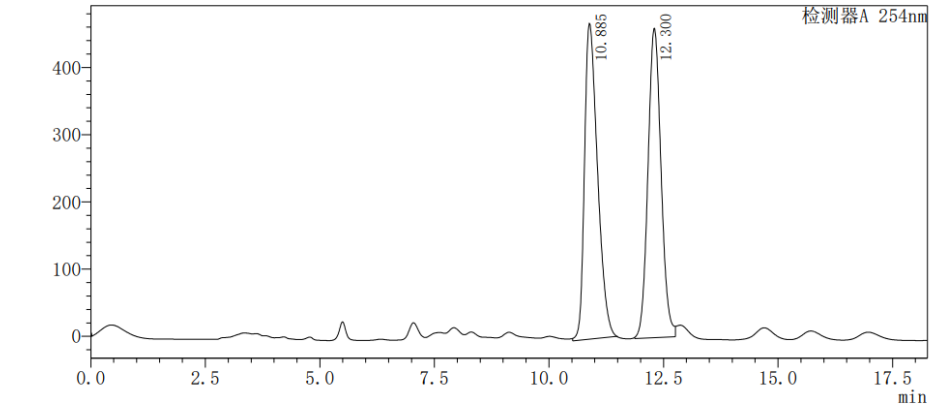
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	15.999	19979600	889789	96.550			
2	22.522	713976	23292	3.450		M	
总计		20693576	913082				



(±)-51

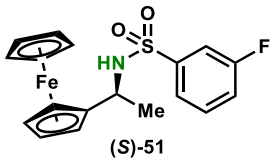
〈色谱图〉



〈峰表〉

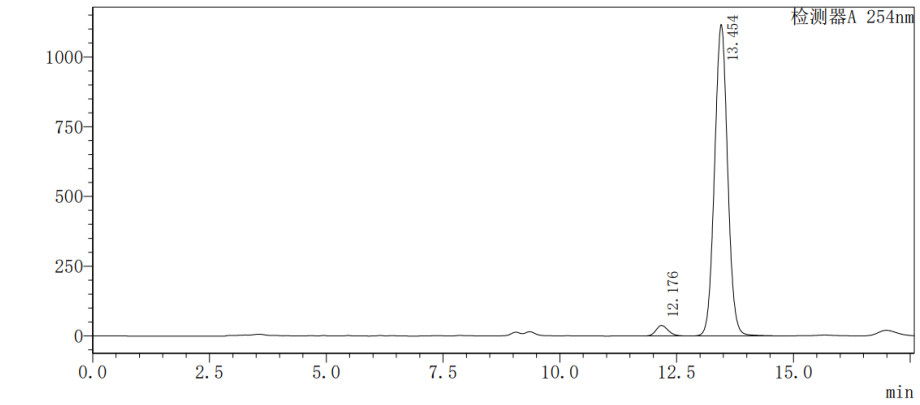
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	10.885	9282792	469846	50.381		M	
2	12.300	9142525	460526	49.619		M	
总计		18425317	930372				



(*S*)-51

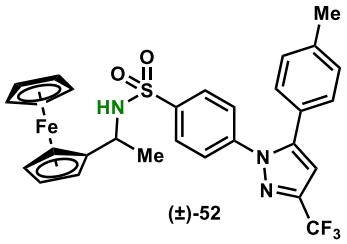
〈色谱图〉



〈峰表〉

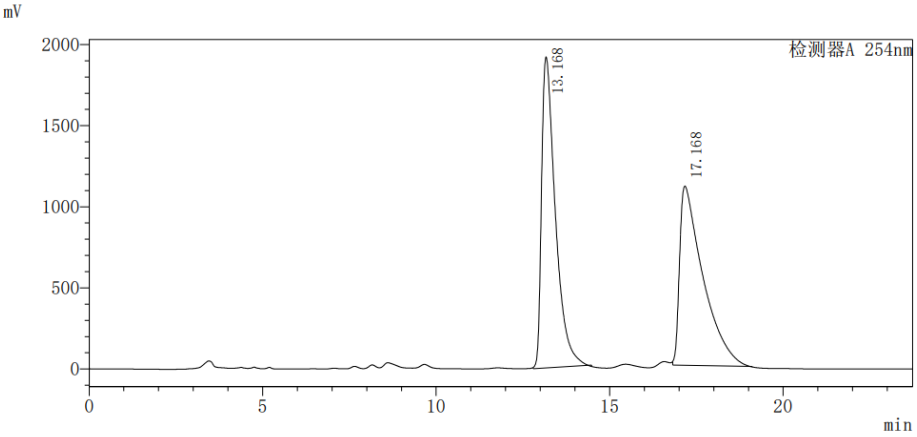
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	12.176	683818	37648	3.044		M	
2	13.454	21779222	1116718	96.956			
总计		22463040	1154365				



(±)-52

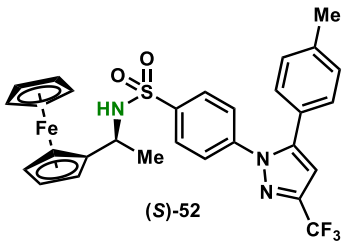
〈色谱图〉



〈峰表〉

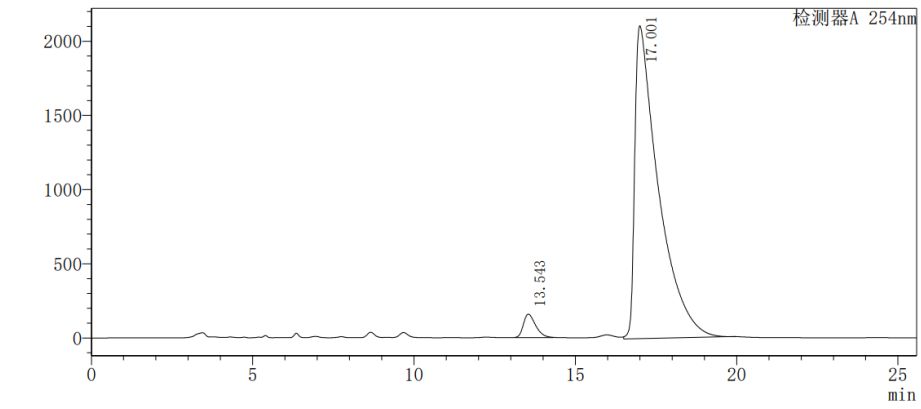
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	13.168	52995977	1916262	50.684		M	
2	17.168	51565793	1105042	49.316		M	
总计		104561770	3021304				



(*S*)-52

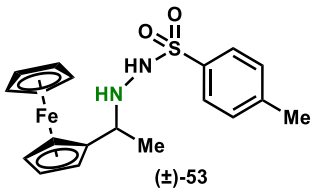
〈色谱图〉



〈峰表〉

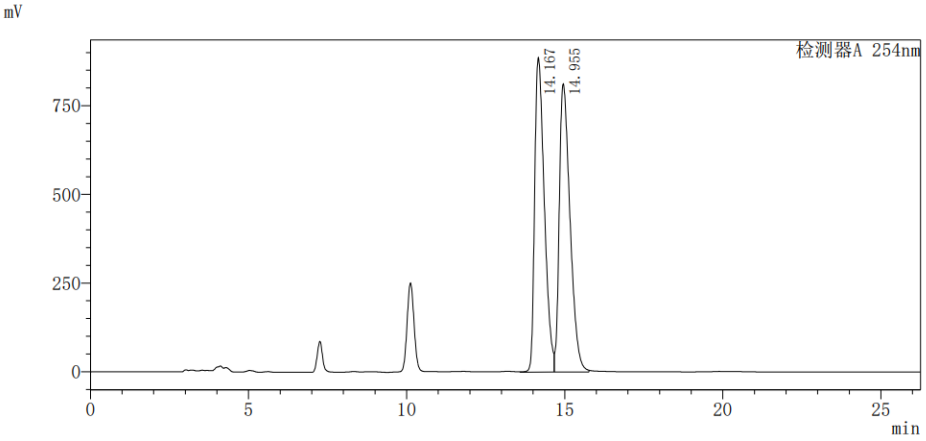
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	13.543	4211878	158639	3.769		M	
2	17.001	107529442	2107816	96.231		M	
总计		111741320	2266455				



(±)-53

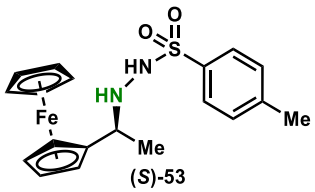
〈色谱图〉



〈峰表〉

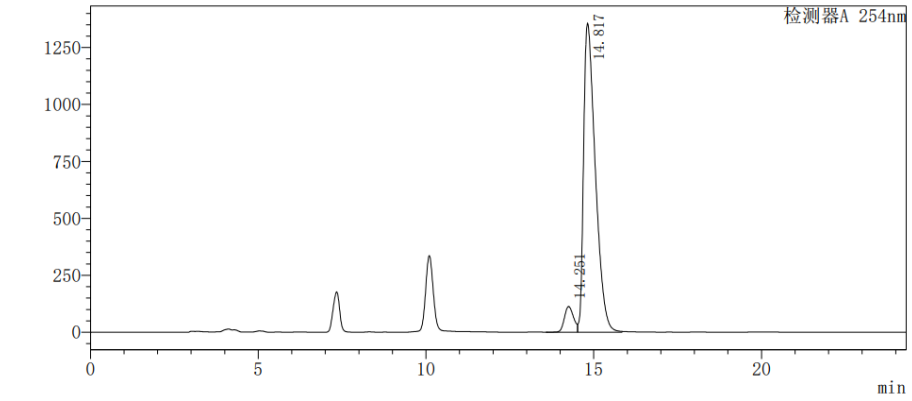
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	14.167	18875668	887060	49.530			
2	14.955	19233881	812718	50.470		V M	
总计		38109548	1699778				



(*S*)-53

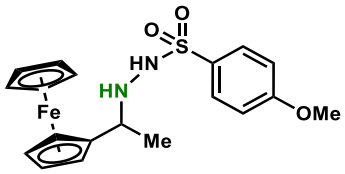
〈色谱图〉



〈峰表〉

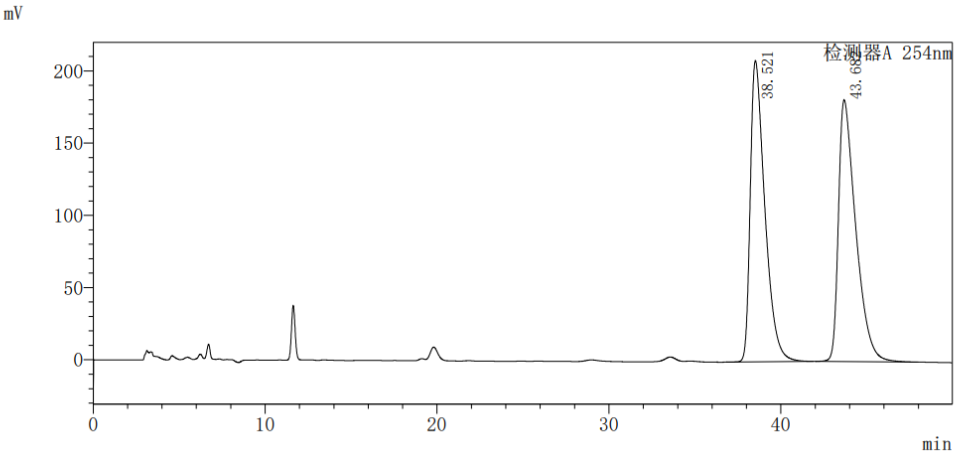
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	14.251	2165543	113304	6.150			
2	14.817	33044613	1356535	93.850		V M	
总计		35210156	1469839				



(±)-54

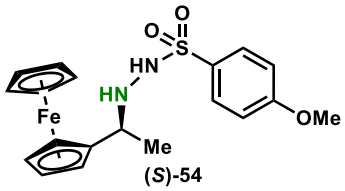
〈色谱图〉



〈峰表〉

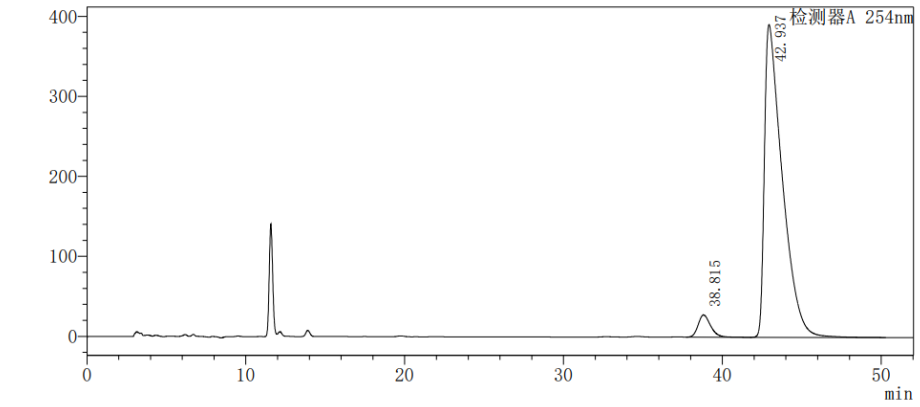
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	38.521	12307474	208624	49.265			
2	43.682	12674718	181141	50.735			
总计		24982192	389766				



(*S*)-54

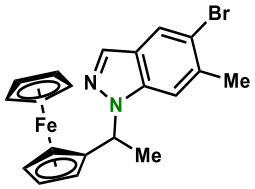
〈色谱图〉



〈峰表〉

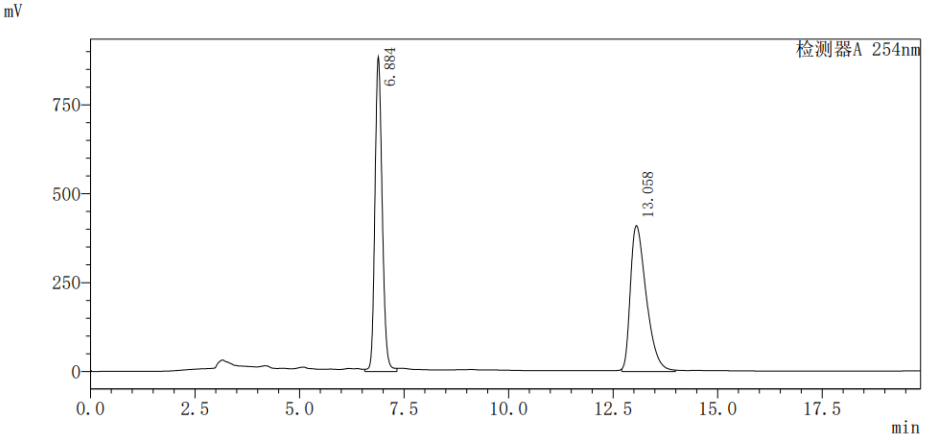
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	38.815	1534084	27849	4.775			
2	42.937	30593392	391013	95.225			
总计		32127476	418862				



(±)-55

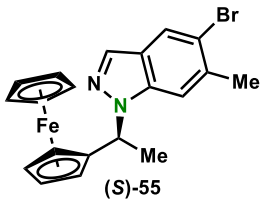
〈色谱图〉



〈峰表〉

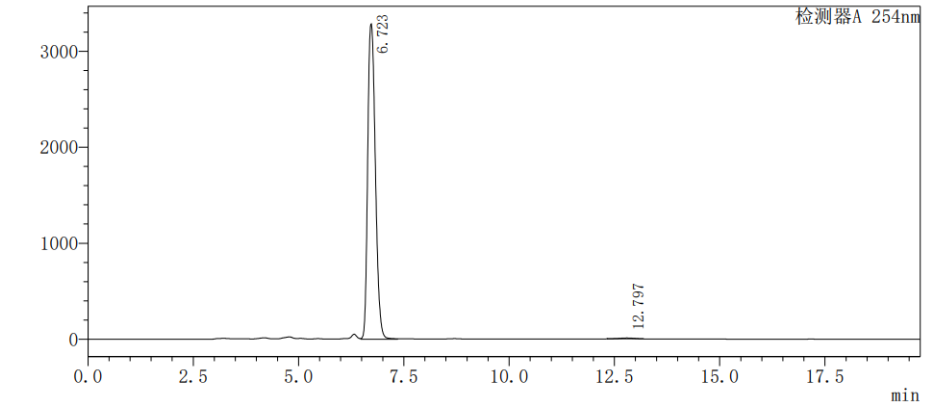
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.884	10719999	885678	49.609		M	
2	13.058	10888894	411101	50.391		M	
总计		21608894	1296779				



(*S*)-55

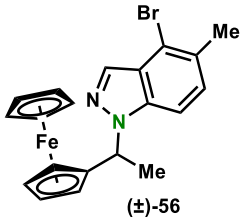
〈色谱图〉



〈峰表〉

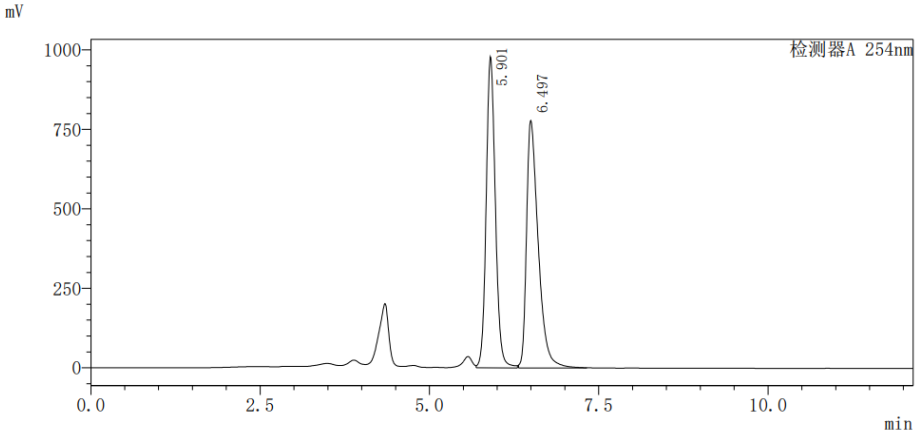
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.723	41532962	3286738	99.441		M	
2	12.797	233541	9378	0.559		M	
总计		41766503	3296116				



(±)-56

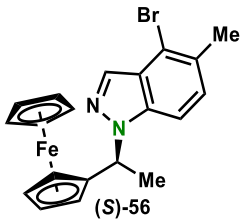
〈色谱图〉



〈峰表〉

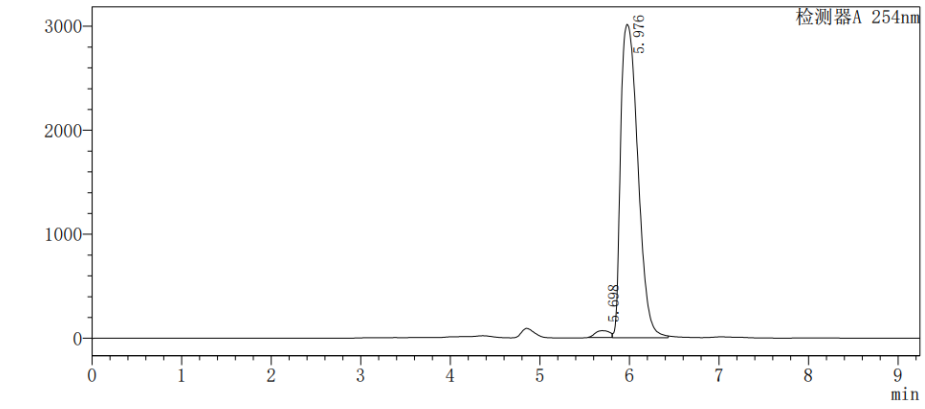
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	5.901	9222281	978512	49.665		M	
2	6.497	9346812	778237	50.335		M	
总计		18569093	1756749				



(*S*)-56

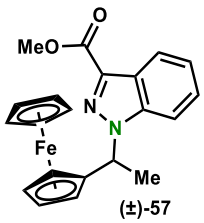
〈色谱图〉



〈峰表〉

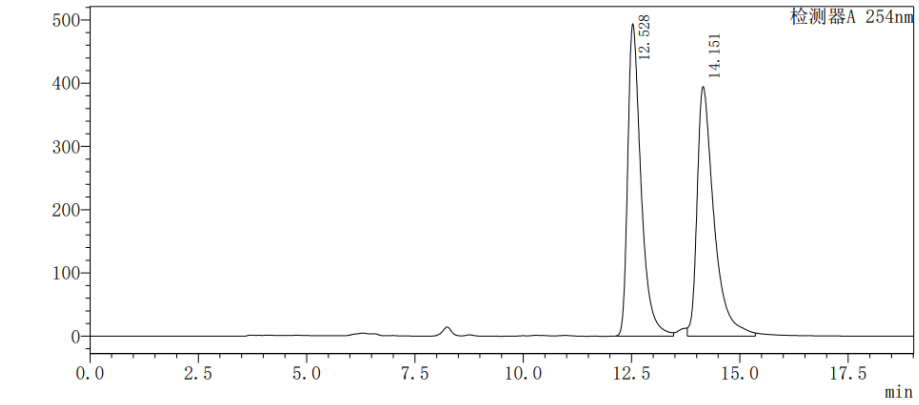
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	5.698	745265	65642	1.818		M	
2	5.976	40257302	3013190	98.182		M	
总计		41002567	3078832				



(±)-57

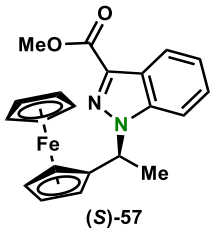
〈色谱图〉



〈峰表〉

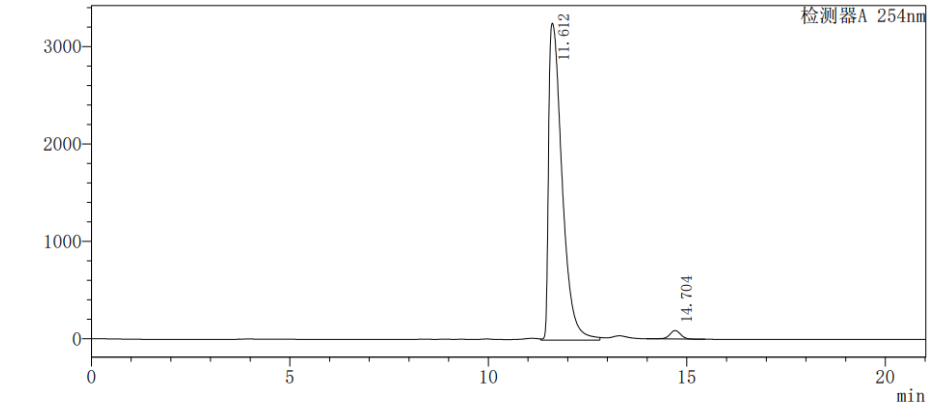
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	12.528	10533998	493774	49.595		M	
2	14.151	10706080	394863	50.405		M	
总计		21240078	888638				



(*S*)-57

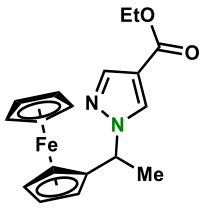
〈色谱图〉



〈峰表〉

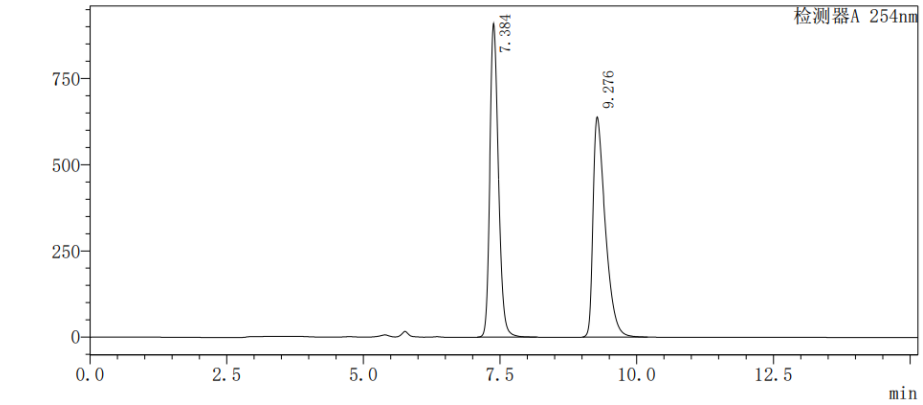
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	11.612	76943854	3254574	97.852		M	
2	14.704	1688827	86616	2.148			
总计		78632680	3341190				



(±)-58

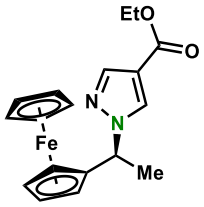
<色谱图>



<峰表>

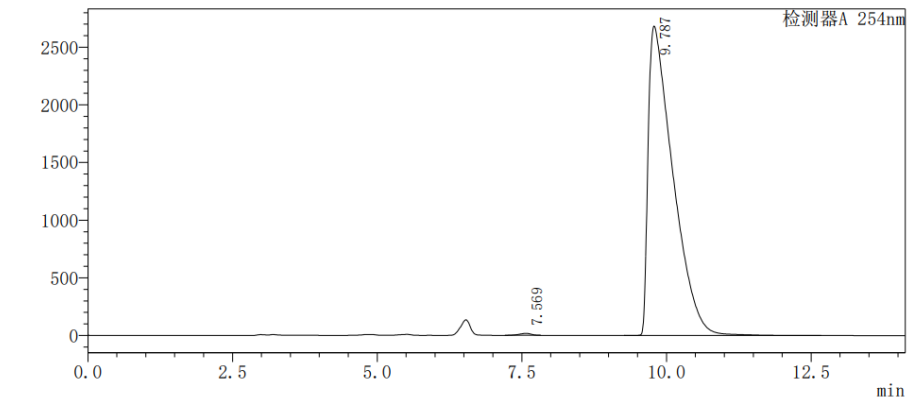
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	7.384	9994881	909360	49.997		M	
2	9.276	9996022	638899	50.003		M	
总计		19990903	1548259				



(*S*)-58

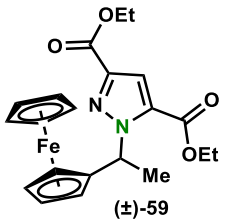
<色谱图>



<峰表>

检测器A 254nm

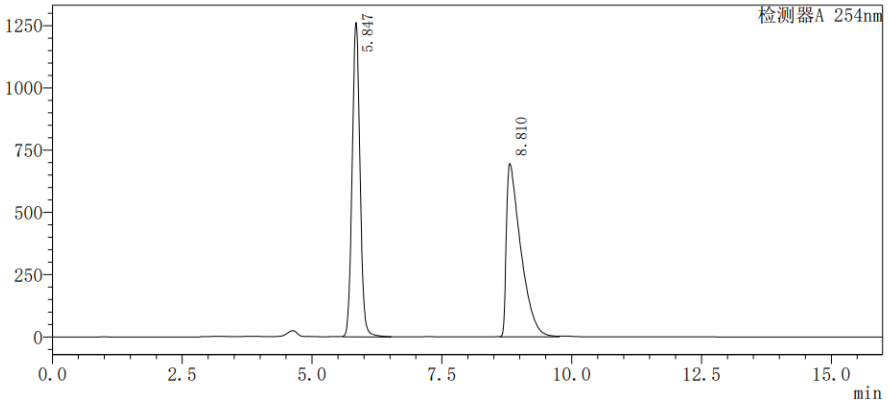
峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	7.569	236963	17275	0.296		M	
2	9.787	79901506	2682823	99.704			
总计		80138470	2700098				



(±)-59

〈色谱图〉

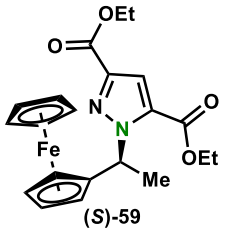
mV



〈峰表〉

检测器A 254nm

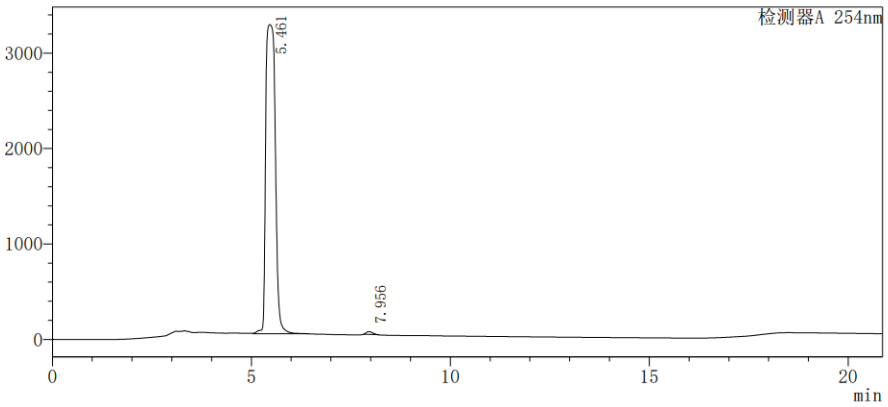
峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	5.847	13330049	1261236	49.737		M	
2	8.810	13470989	695704	50.263		M	
总计		26801038	1956940				



(*S*)-59

〈色谱图〉

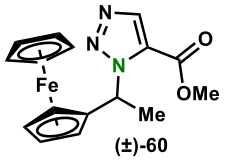
mV



〈峰表〉

检测器A 254nm

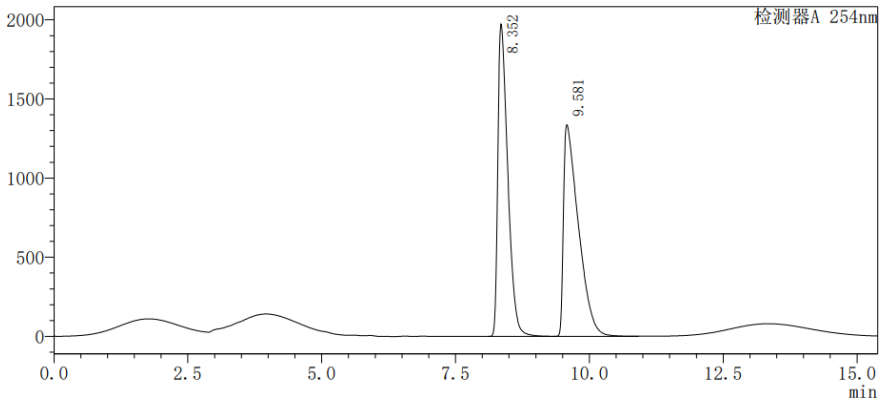
峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	5.461	54312820	3239453	99.411		M	
2	7.956	322008	28726	0.589		M	
总计		54634828	3268179				



(±)-60

〈色谱图〉

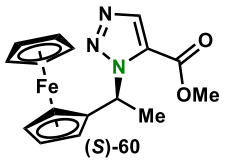
mV



〈峰表〉

检测器A 254nm

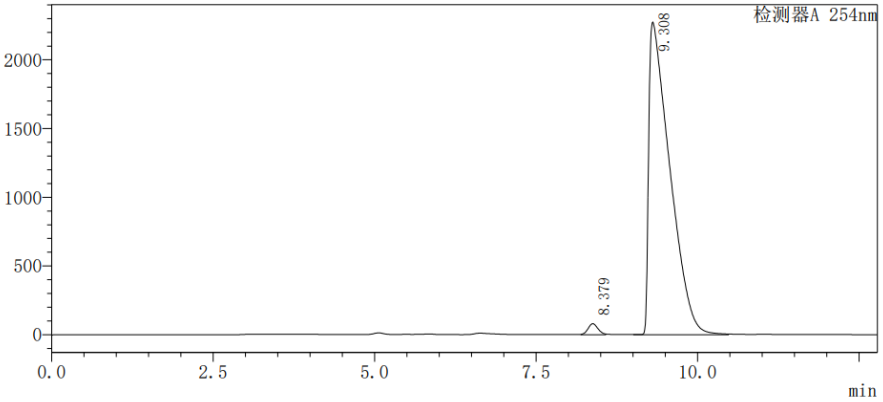
峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	8.352	25602515	1973410	49.582			
2	9.581	26033688	1337386	50.418		V	
总计		51636202	3310796				



(S)-60

〈色谱图〉

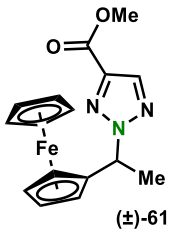
mV



〈峰表〉

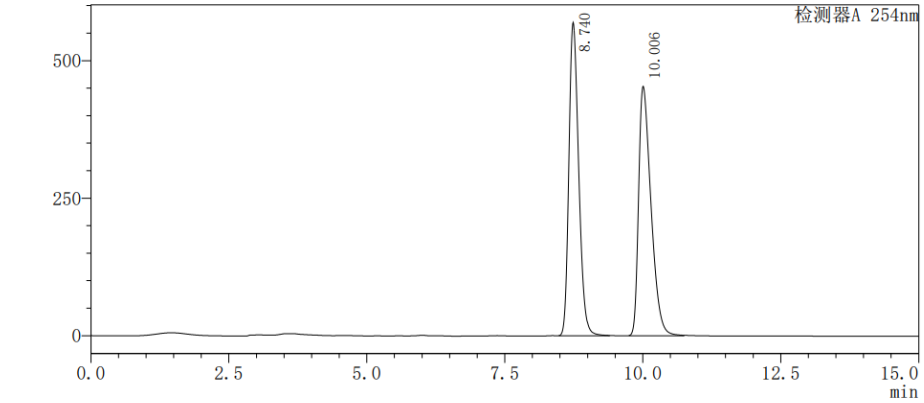
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	8.379	855649	80367	1.633		M	
2	9.308	51551266	2273748	98.367		M	
总计		52406915	2354115				



(±)-61

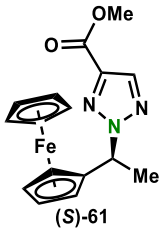
〈色谱图〉



〈峰表〉

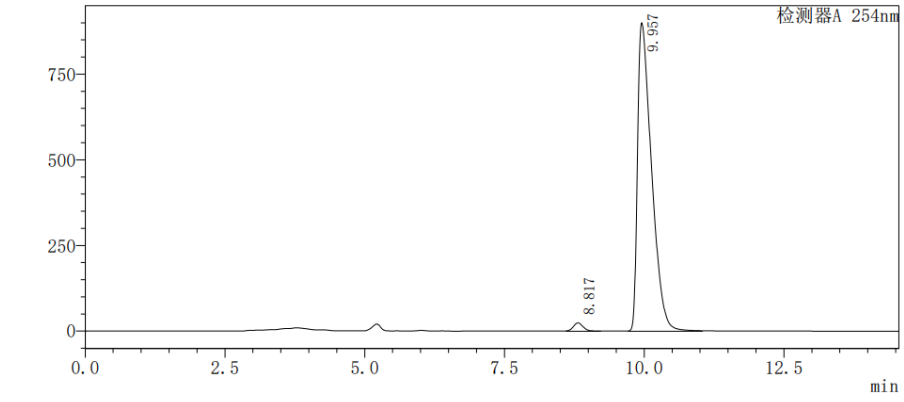
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	8.740	7061037	569800	49.906		M	
2	10.006	7087653	453809	50.094		M	
总计		14148690	1023608				



(*S*)-61

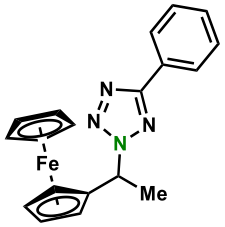
〈色谱图〉



〈峰表〉

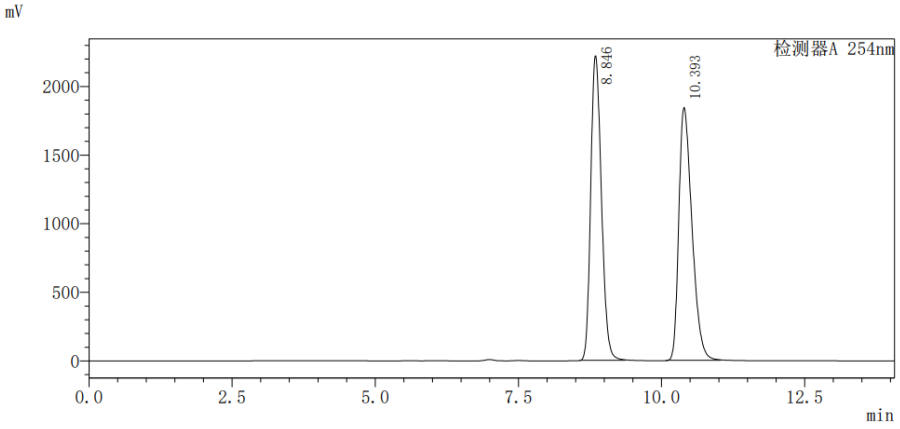
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	8.817	294798	23983	1.839		M	
2	9.957	15731357	899700	98.161		M	
总计		16026156	923683				



(±)-62

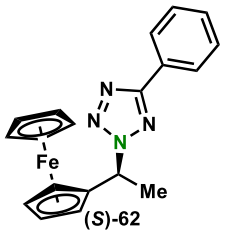
〈色谱图〉



〈峰表〉

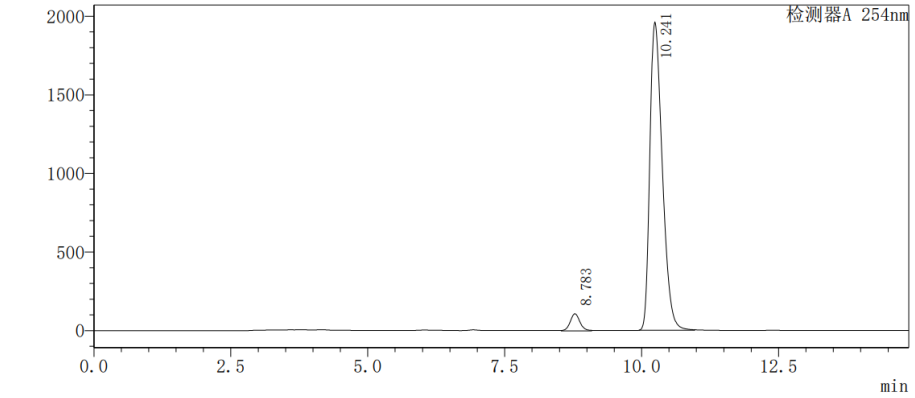
检测器A 254nm

峰号	保留时间	面积	高度	面积%	高度%
1	8.846	28806242	2217654	49.423	54.622
2	10.393	29478745	1842333	50.577	45.378
总计		58284987	4059988	100.000	100.000



(*S*)-62

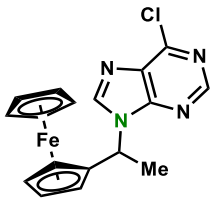
〈色谱图〉



〈峰表〉

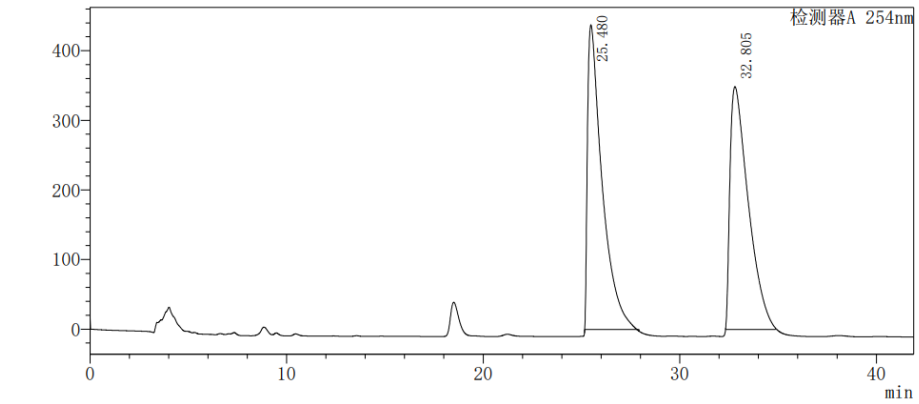
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	8.783	1344820	108641	4.169		M	
2	10.241	30912506	1959641	95.831		M	
总计		32257326	2068282				



(±)-63

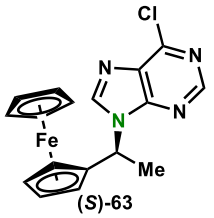
〈色谱图〉



〈峰表〉

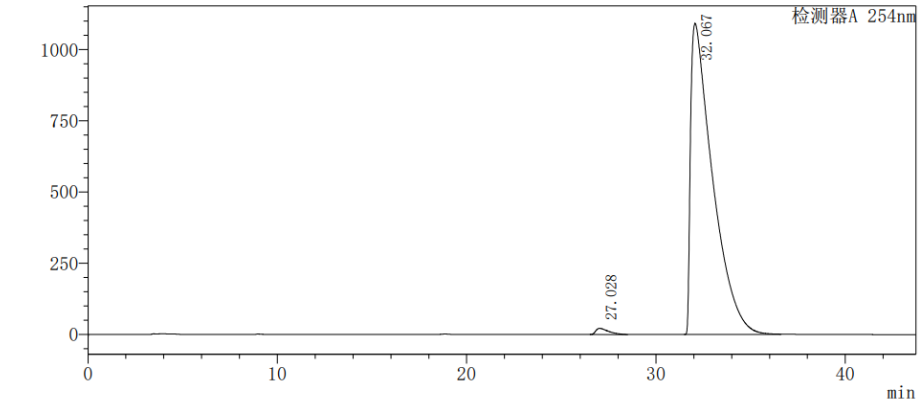
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	25.480	22672405	437619	50.112		M	
2	32.805	22571020	348848	49.888		M	
总计		45243425	786468				



(*S*)-63

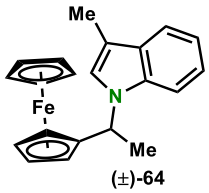
〈色谱图〉



〈峰表〉

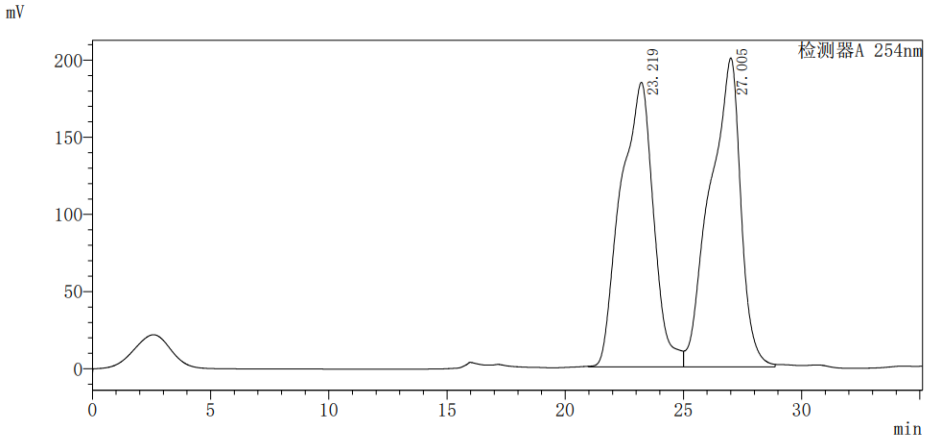
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	27.028	1022610	21600	1.143		M	
2	32.067	88427150	1091359	98.857		M	
总计		89449759	1112959				



(±)-64

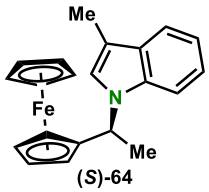
〈色谱图〉



〈峰表〉

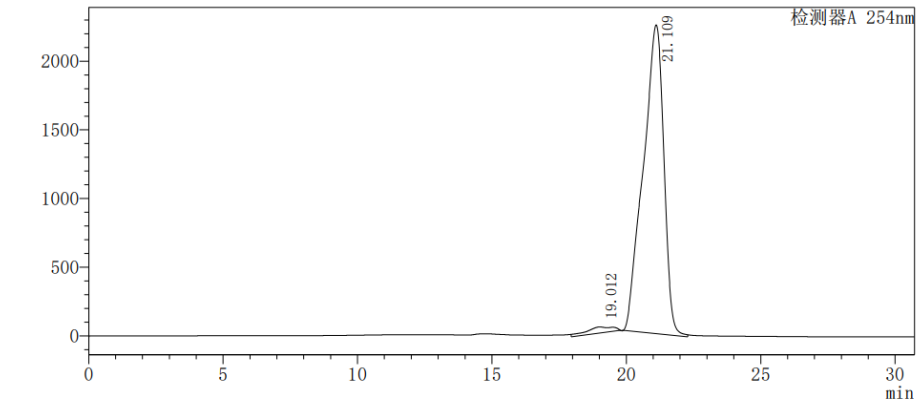
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	23.219	17845204	184460	49.596		M	
2	27.005	18135881	200245	50.404		V M	
总计		35981086	384705				



(*S*)-64

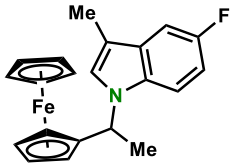
〈色谱图〉



〈峰表〉

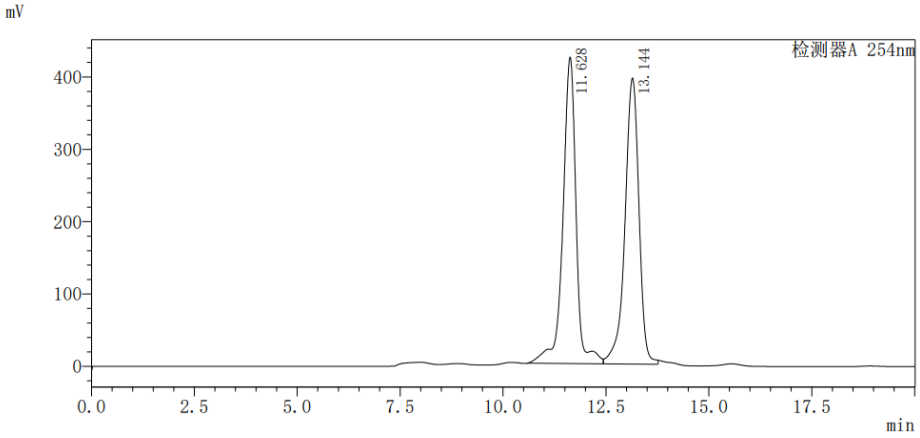
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	19.012	3105071	44865	2.525		M	
2	21.109	119874080	2248595	97.475		M	
总计		122979151	2293461				



(±)-65

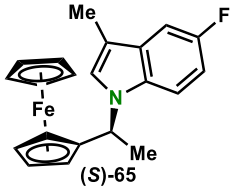
〈色谱图〉



〈峰表〉

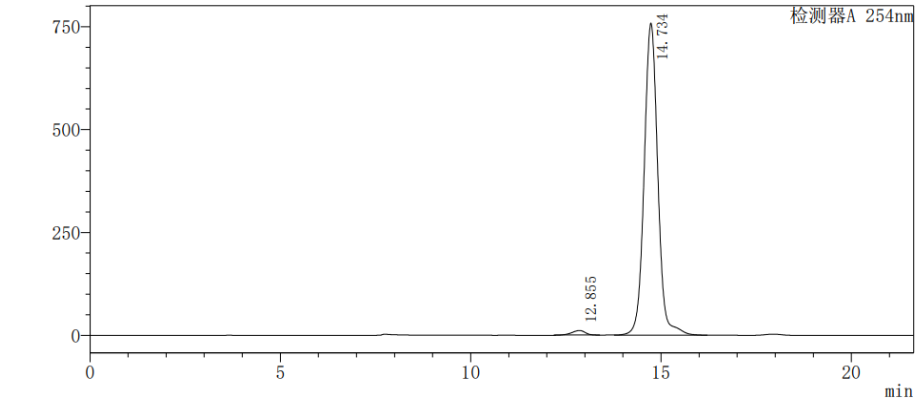
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	11.628	9405872	423365	50.092		M	
2	13.144	9371262	395291	49.908		V M	
总计		18777134	818656				



(*S*)-65

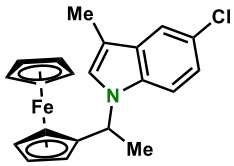
〈色谱图〉



〈峰表〉

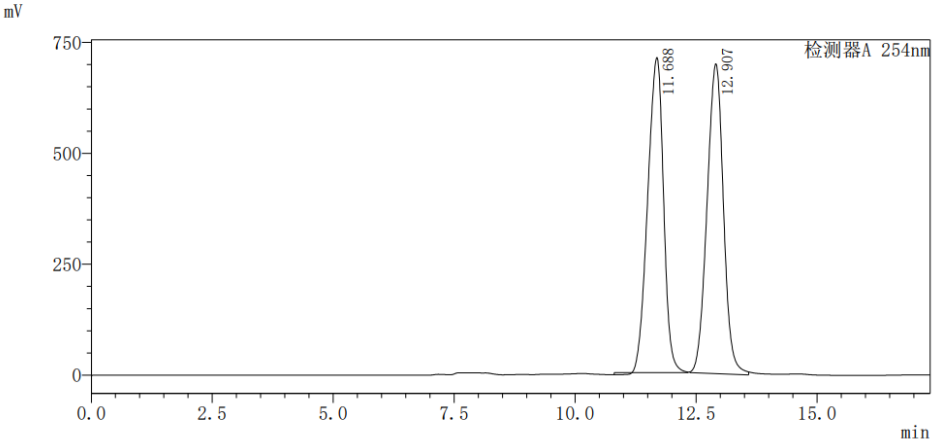
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	12.855	241124	10795	1.260		M	
2	14.734	18889811	758375	98.740		M	
总计		19130934	769170				



(±)-66

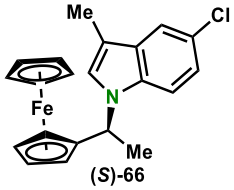
〈色谱图〉



〈峰表〉

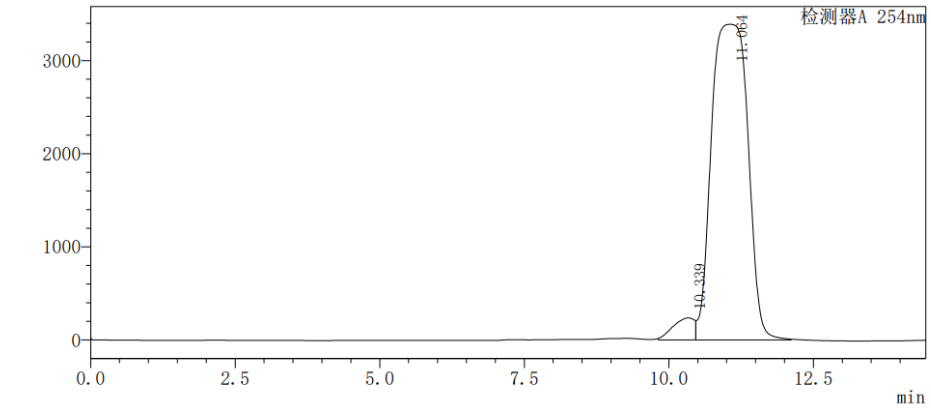
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	11.688	16084718	709820	49.398		M	
2	12.907	16476501	698504	50.602		M	
总计		32561219	1408324				



(*S*)-66

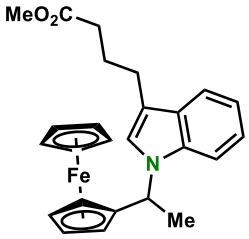
〈色谱图〉



〈峰表〉

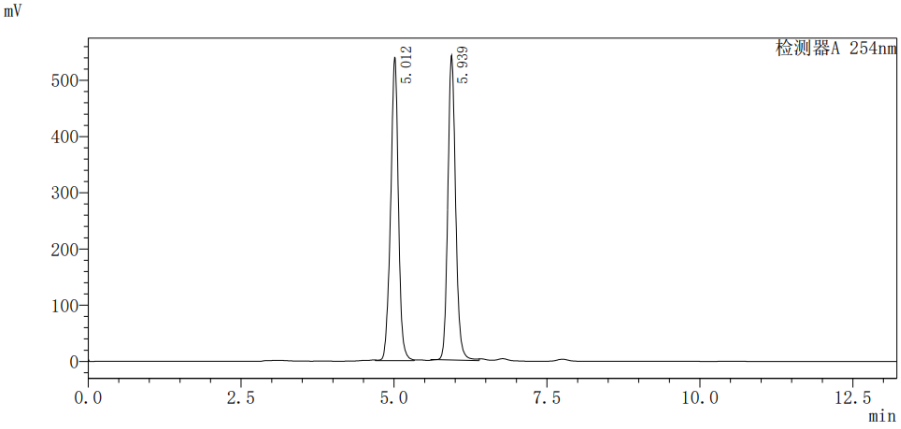
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	10.339	6080652	236224	3.938		M	
2	11.064	148335543	3389696	96.062		V M	
总计		154416194	3625920				



(±)-67

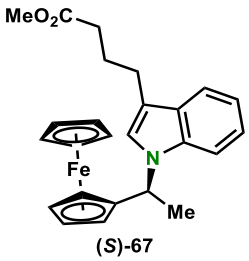
〈色谱图〉



〈峰表〉

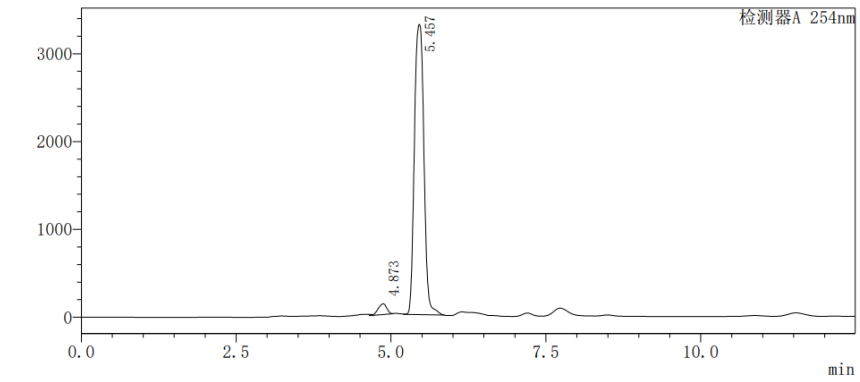
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	5.012	4785270	539659	49.895		M	
2	5.939	4805343	542259	50.105		M	
总计		9590614	1081918				



(*S*)-67

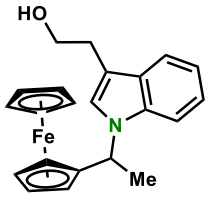
〈色谱图〉



〈峰表〉

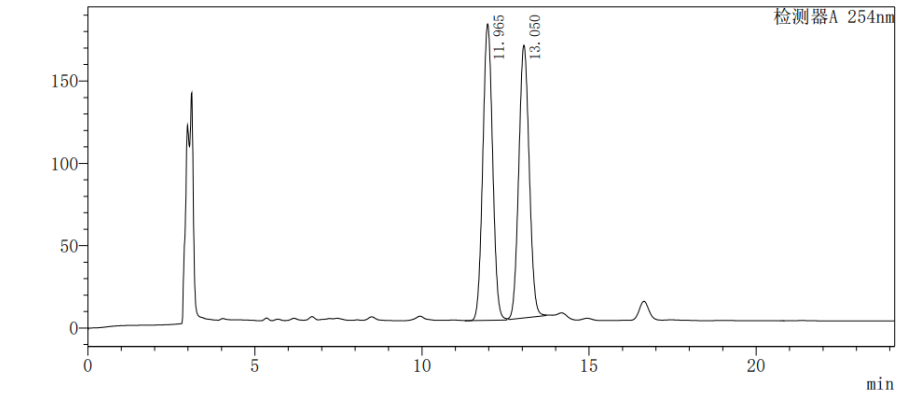
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	4.873	1212646	122820	3.328		M	
2	5.457	35226843	3303216	96.672		M	
总计		36439489	3426037				



(±)-68

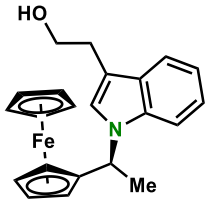
〈色谱图〉



〈峰表〉

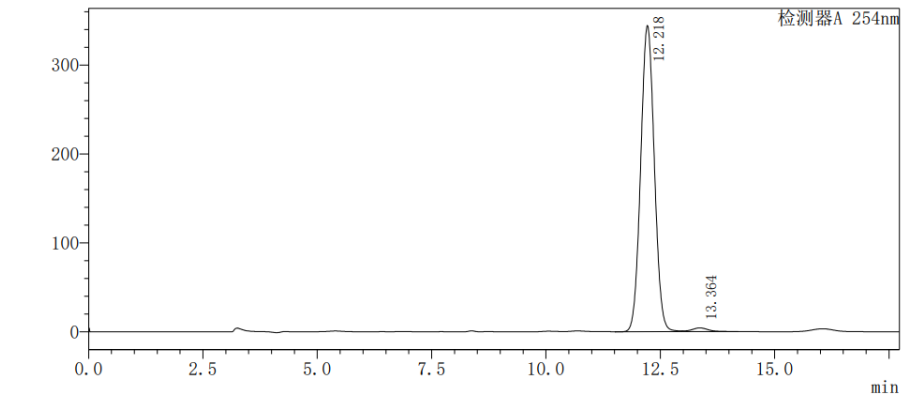
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	11.965	3684837	179942	50.541		M	
2	13.050	3605937	165592	49.459		M	
总计		7290774	345534				



(*S*)-68

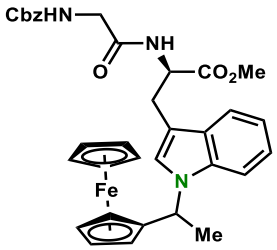
〈色谱图〉



〈峰表〉

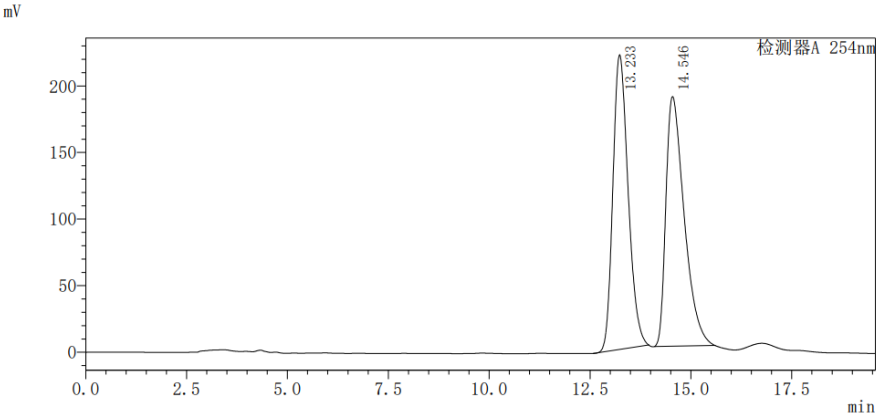
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	12.218	7155643	344432	98.542		M	
2	13.364	105878	4215	1.458		V M	
总计		7261521	348647				



(±)-69

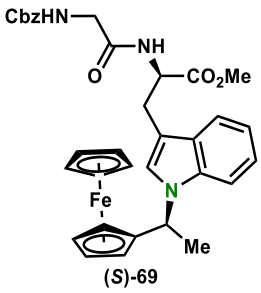
〈色谱图〉



〈峰表〉

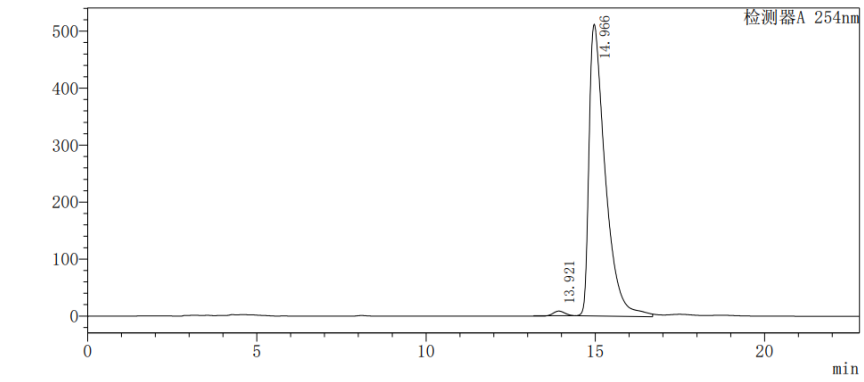
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	13.233	5812441	221233	49.570		M	
2	14.546	5913359	187449	50.430		M	
总计		11725801	408682				



(*S*)-69

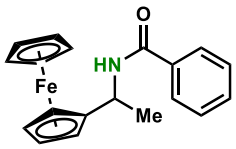
〈色谱图〉



〈峰表〉

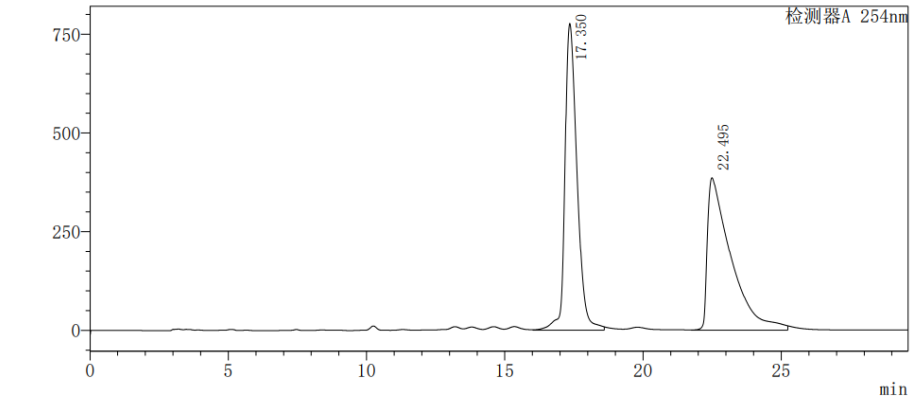
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	13.921	161624	8021	0.937		M	
2	14.966	17083461	511796	99.063		M	
总计		17245085	519817				



(±)-70

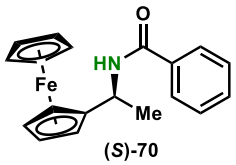
〈色谱图〉



〈峰表〉

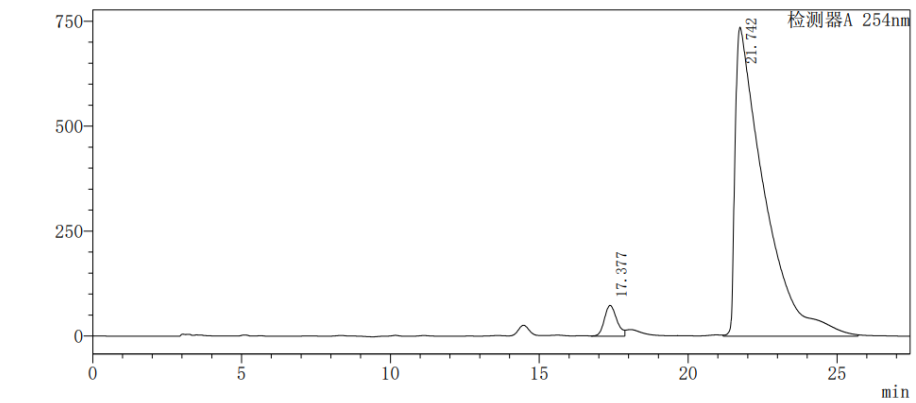
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	17.350	23609904	776620	50.725		M	
2	22.495	22934736	385943	49.275		M	
总计		46544640	1162562				



(*S*)-70

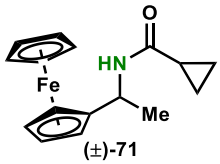
〈色谱图〉



〈峰表〉

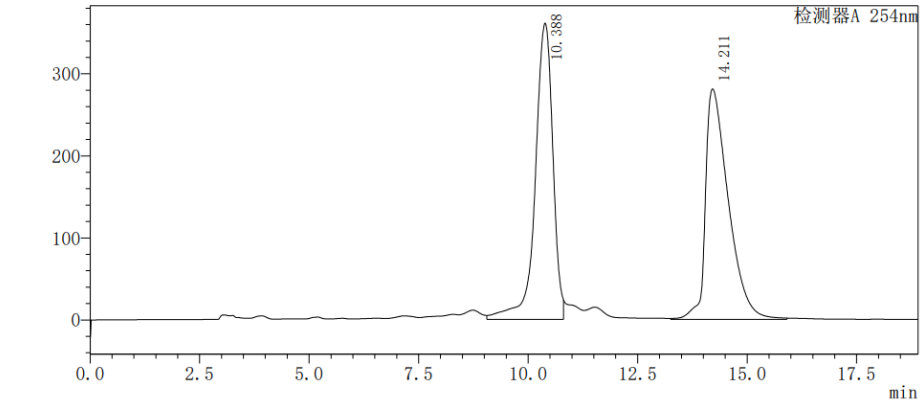
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	17.377	2140303	73261	4.120			
2	21.742	49809002	736146	95.880		M	
总计		51949304	809408				



(±)-71

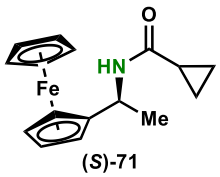
〈色谱图〉



〈峰表〉

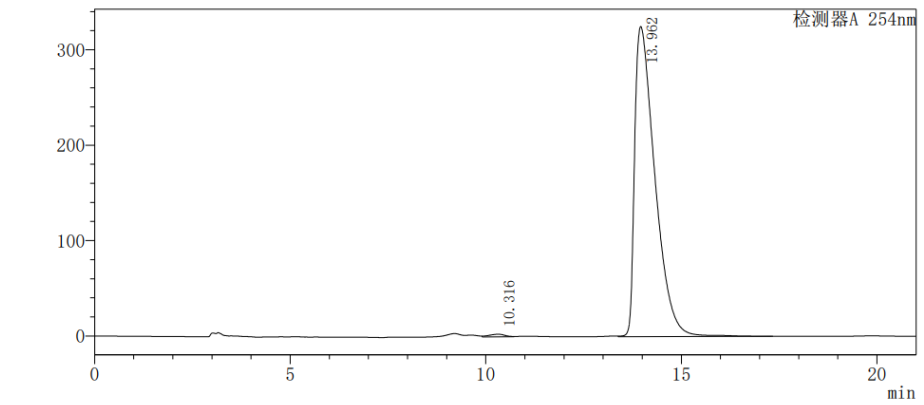
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	10.388	10143386	360992	49.746		M	
2	14.211	10246773	280968	50.254		M	
总计		20390159	641960				



(*S*)-71

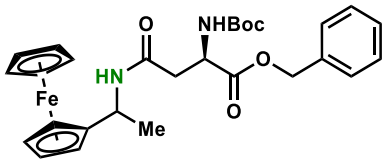
〈色谱图〉



〈峰表〉

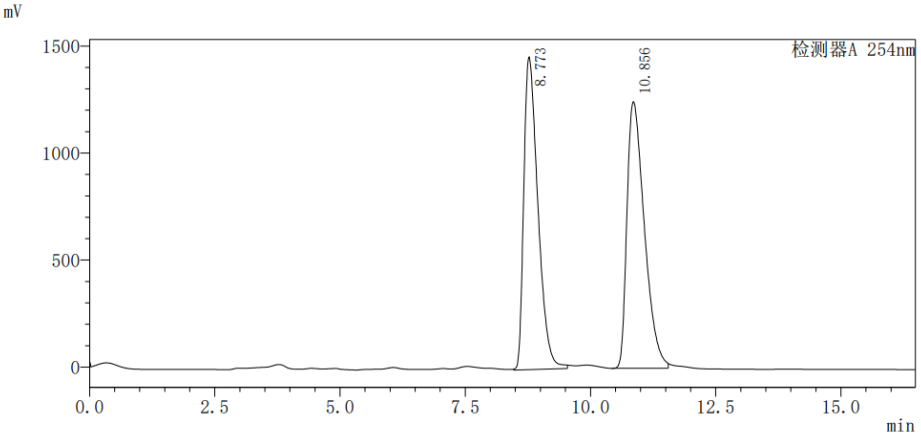
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	10.316	79101	2789	0.672			
2	13.962	11694260	324931	99.328			
总计		11773361	327720				



(±)-72

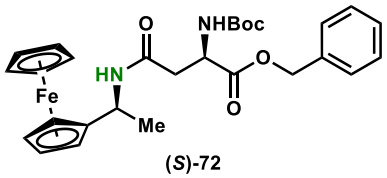
〈色谱图〉



〈峰表〉

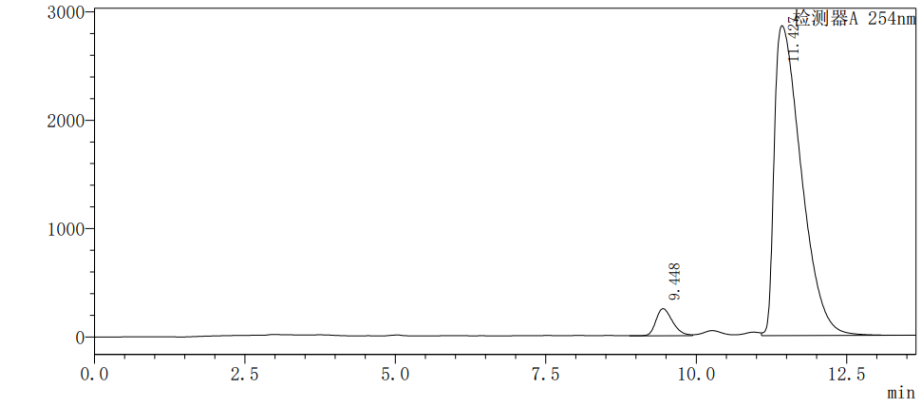
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	8.773	28646036	1460588	48.770		M	
2	10.856	30090548	1246048	51.230		M	
总计		58736584	2706636				



(*S*)-72

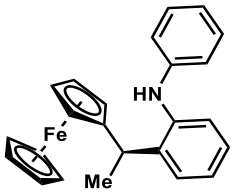
〈色谱图〉



〈峰表〉

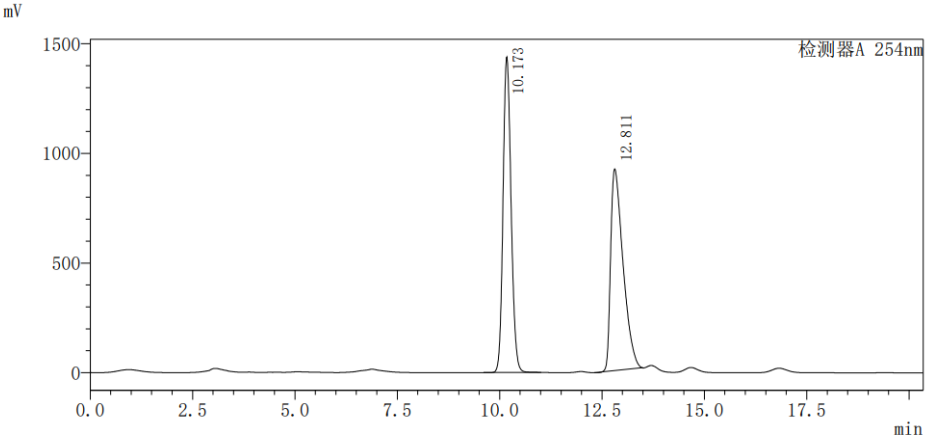
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	9.448	4854228	250744	5.158			
2	11.427	89256685	2859288	94.842			
总计		94110913	3110032				



(±)-73

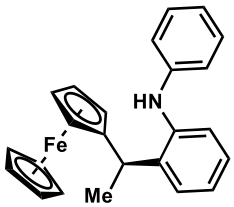
〈色谱图〉



〈峰表〉

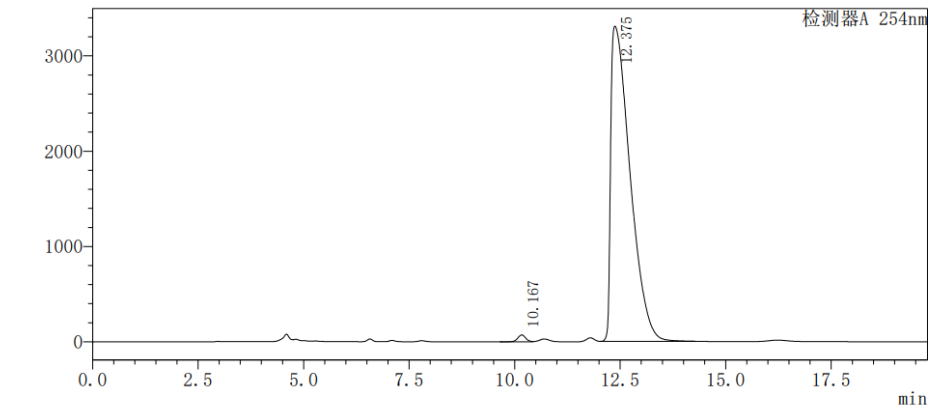
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	10.173	19658414	1438994	50.401		M	
2	12.811	19345759	920171	49.599		M	
总计		39004174	2359165				



(*S*)-73

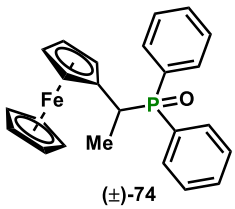
〈色谱图〉



〈峰表〉

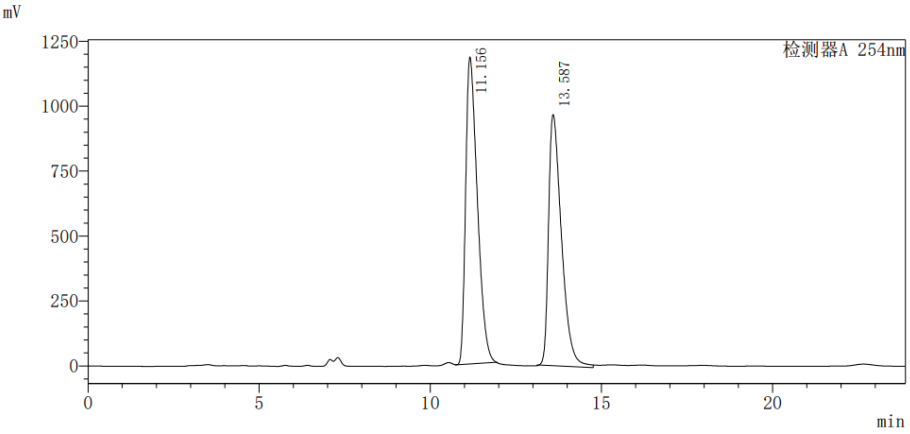
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	10.167	966886	72357	0.909			
2	12.375	105405884	3307955	99.091		M	
总计		106372770	3380311				



(±)-74

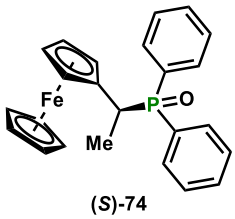
〈色谱图〉



〈峰表〉

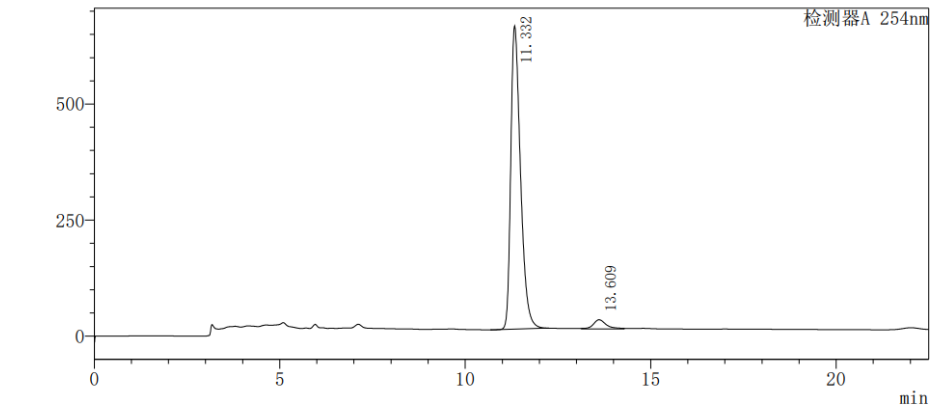
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	11.156	28006276	1181513	52.445		M	
2	13.587	25394783	967120	47.555		M	
总计		53401059	2148633				



(*S*)-74

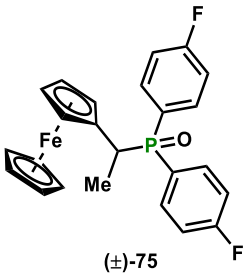
〈色谱图〉



〈峰表〉

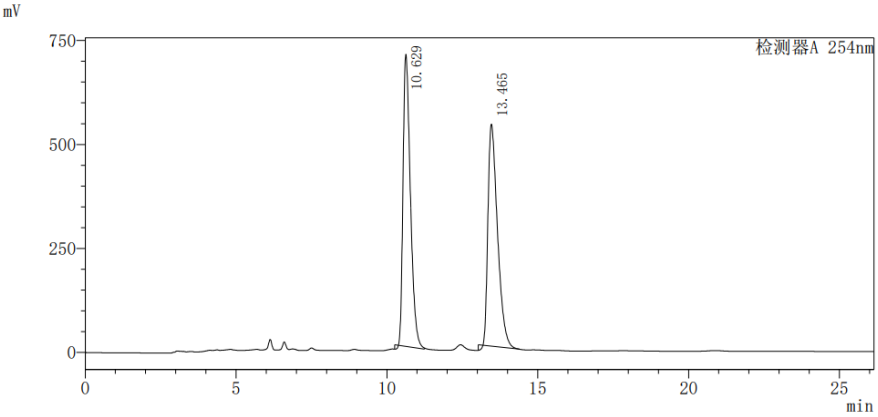
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	11.332	11915292	653388	95.971		M	
2	13.609	500176	19882	4.029		M	
总计		12415468	673270				



(±)-75

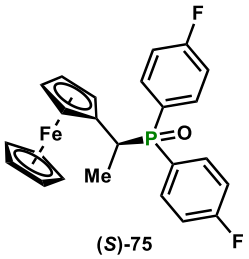
〈色谱图〉



〈峰表〉

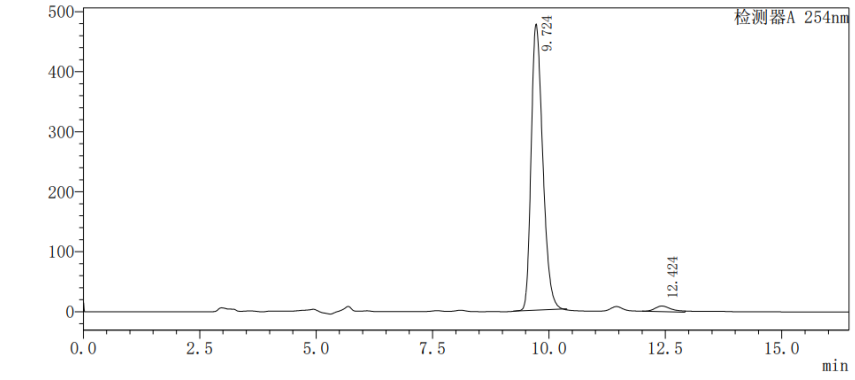
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	10.629	11855096	701494	50.465		M	
2	13.465	11636720	533199	49.535		M	
总计		23491816	1234693				



(*S*)-75

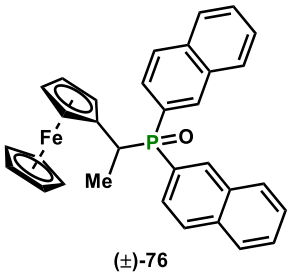
〈色谱图〉



〈峰表〉

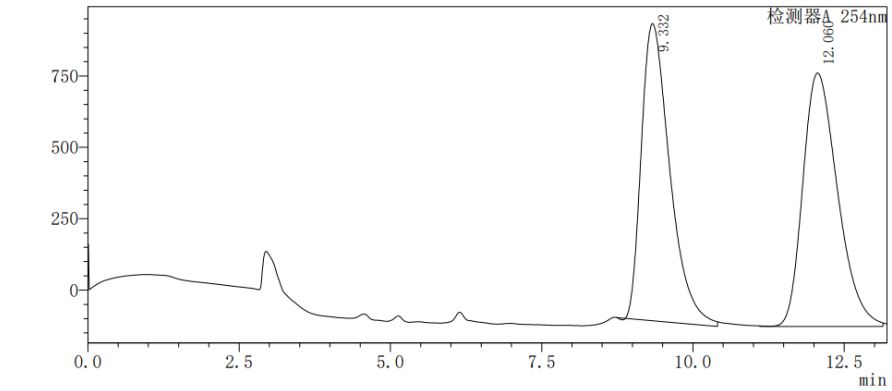
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	9.724	8242120	476510	97.205		M	
2	12.424	236992	9339	2.795		M	
总计		8479112	485849				



(±)-76

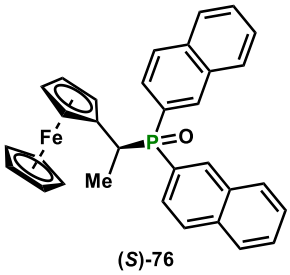
〈色谱图〉



〈峰表〉

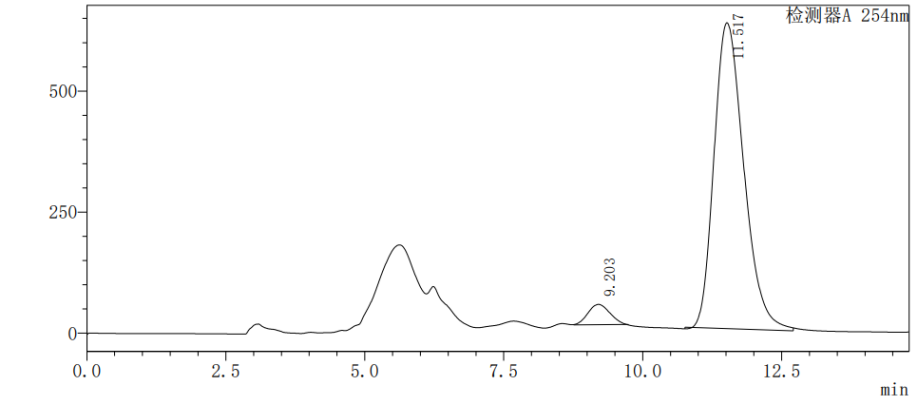
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	9.332	34129841	1041224	49.019		M	
2	12.060	35495771	888095	50.981		M	
总计		69625611	1929319				



(*S*)-76

〈色谱图〉



〈峰表〉

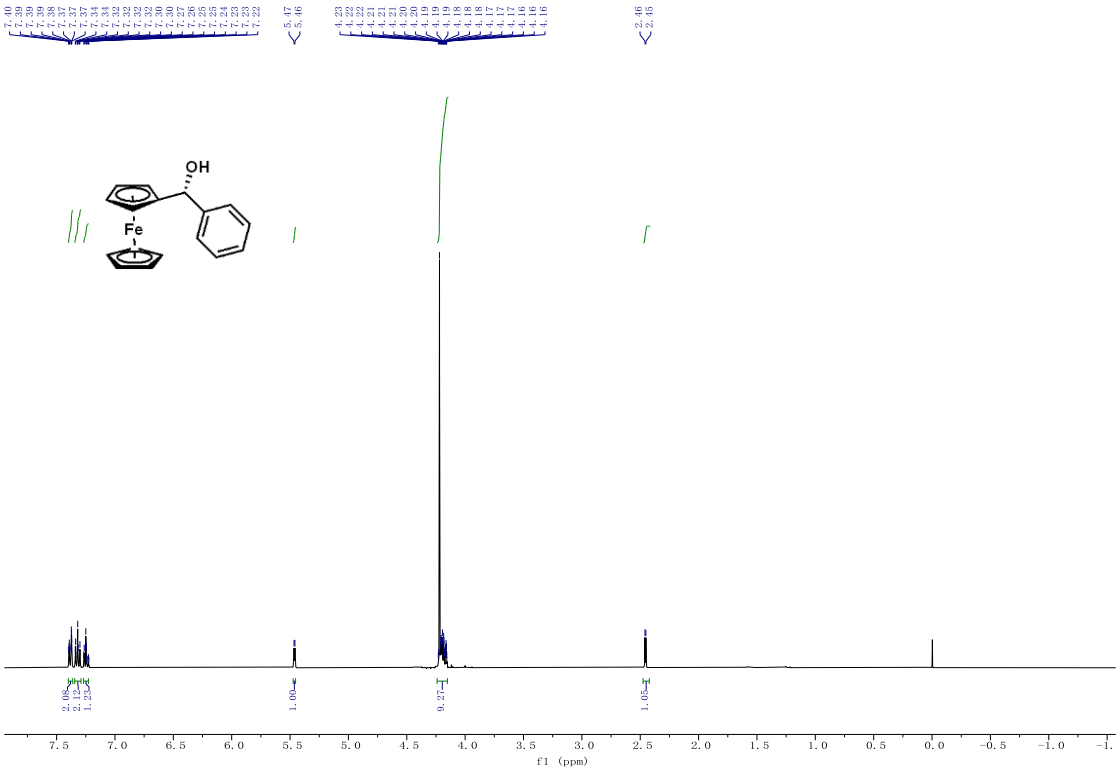
检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	9.203	1152983	42057	4.669		M	
2	11.517	23539594	631932	95.331		M	
总计		24692577	673989				

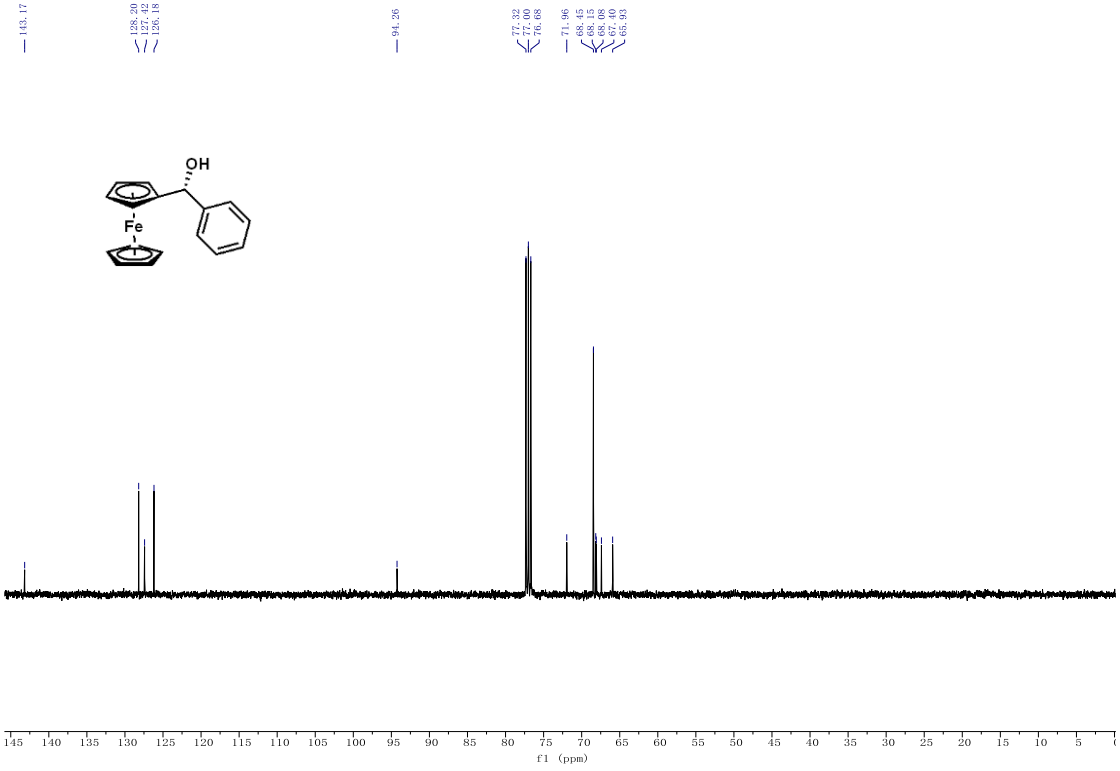
9. ^{1}H, ^{13}C, ^{19}F and ^{31}P NMR Spectra of Products

(S)-phenyl(ferrocene-2-yl)methanol (S2)

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

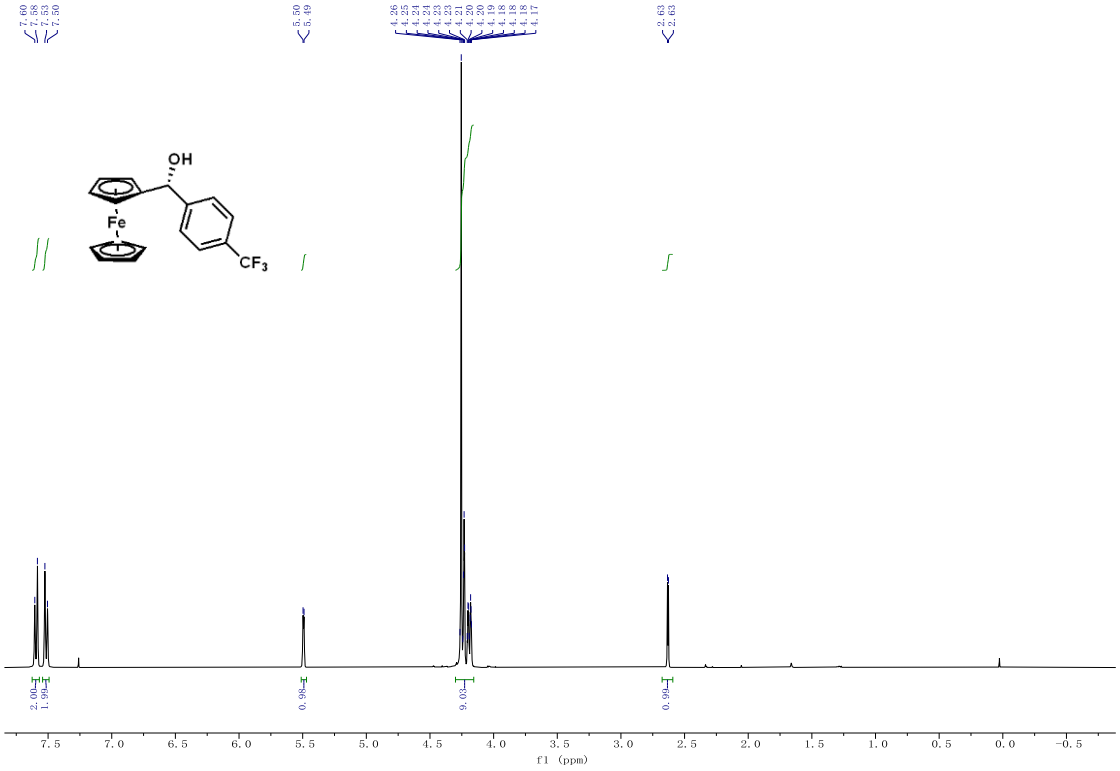


^{13}C NMR (101 MHz, $CDCl_3$)

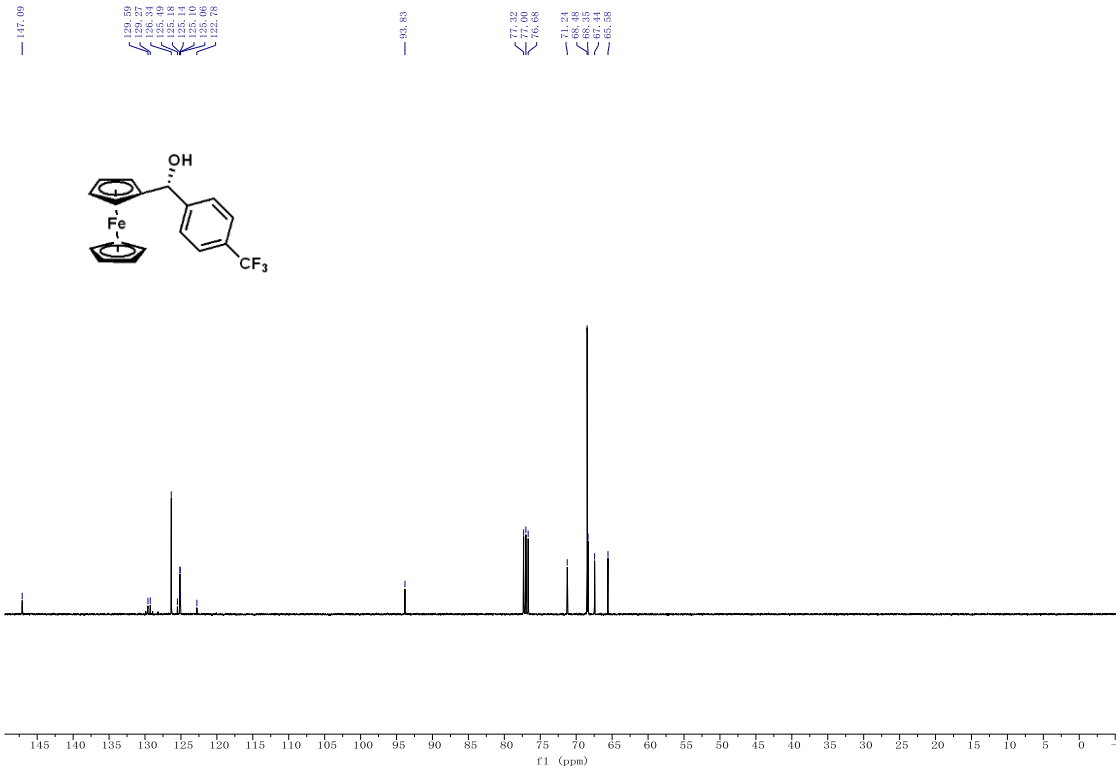


(S)-ferrocene-2-yl(4-(trifluoromethyl)phenyl)methanol (S3)

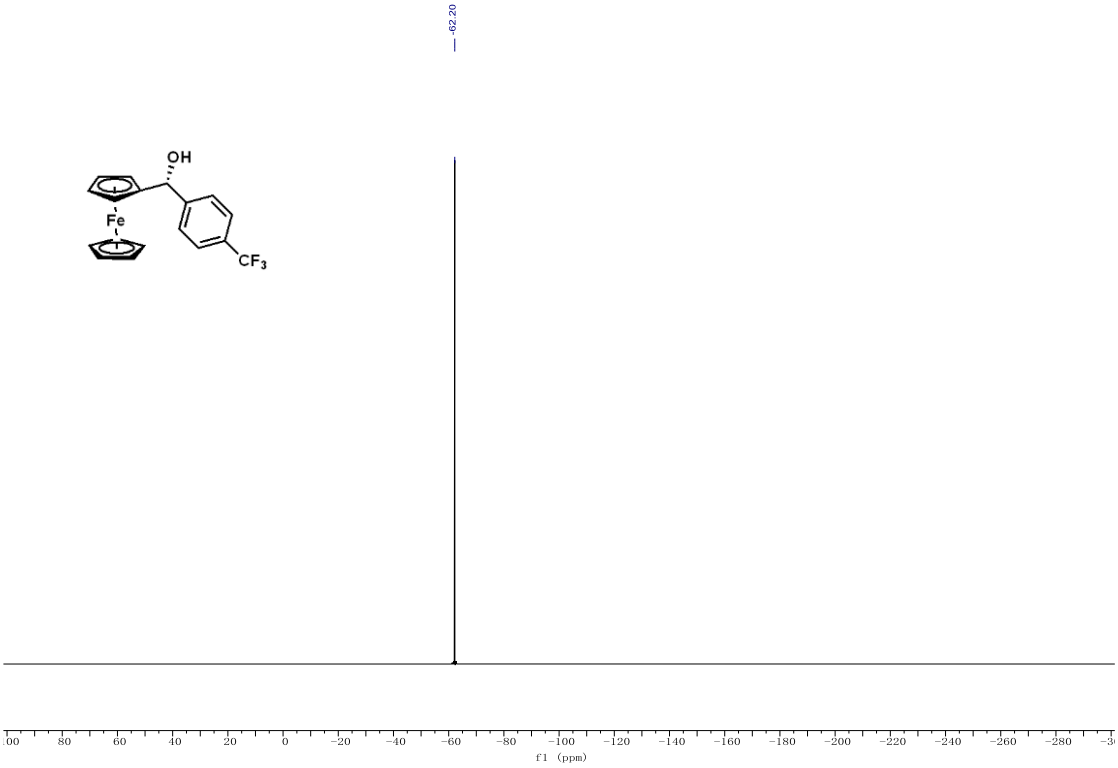
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)

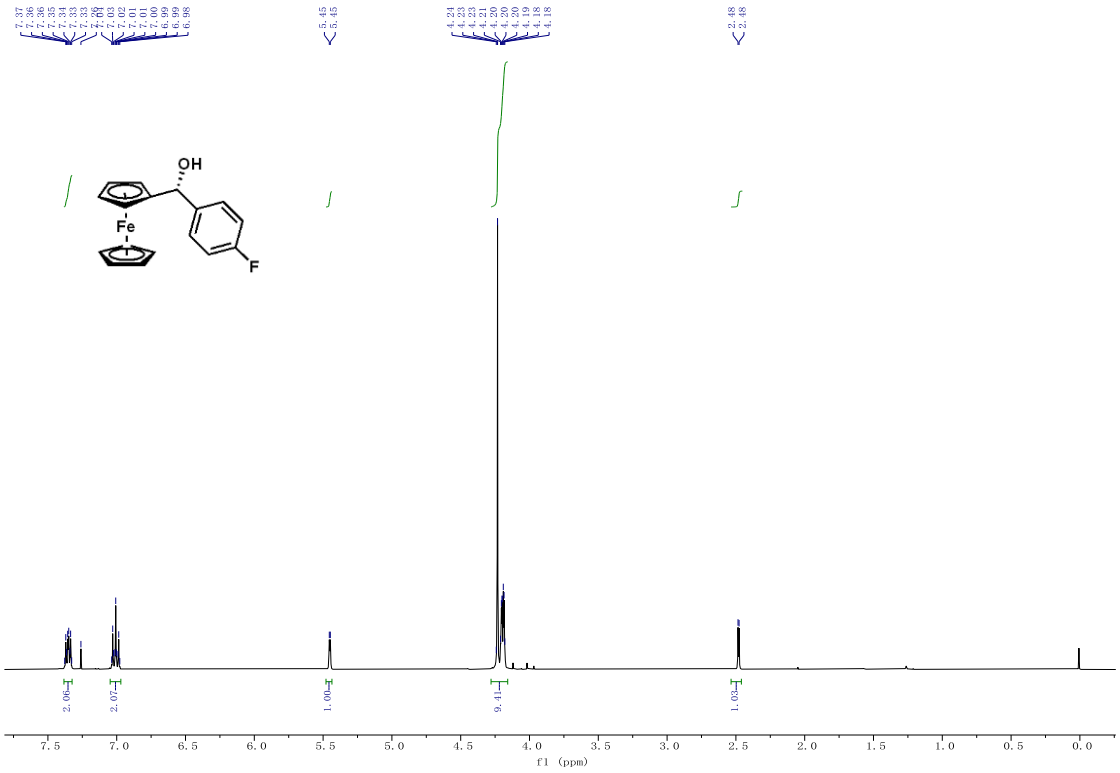


^{19}F NMR (376 MHz, $CDCl_3$)

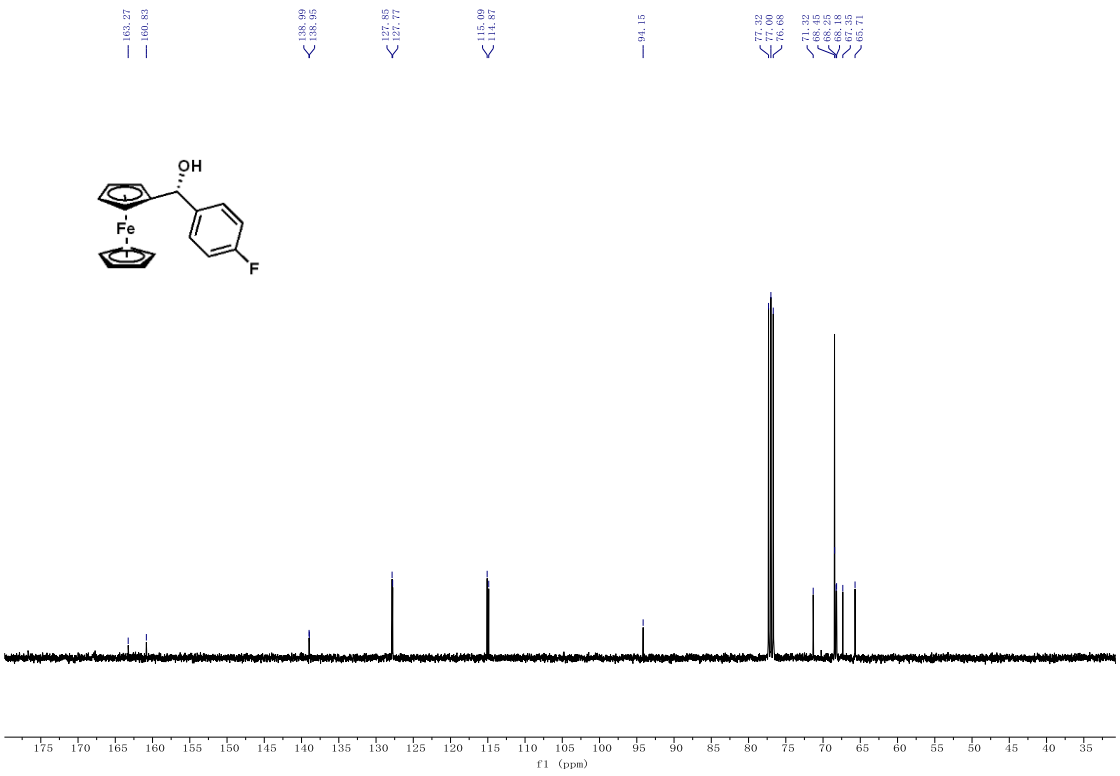


(S)-(4-fluorophenyl)(ferrocene-2-yl)methanol (S4)

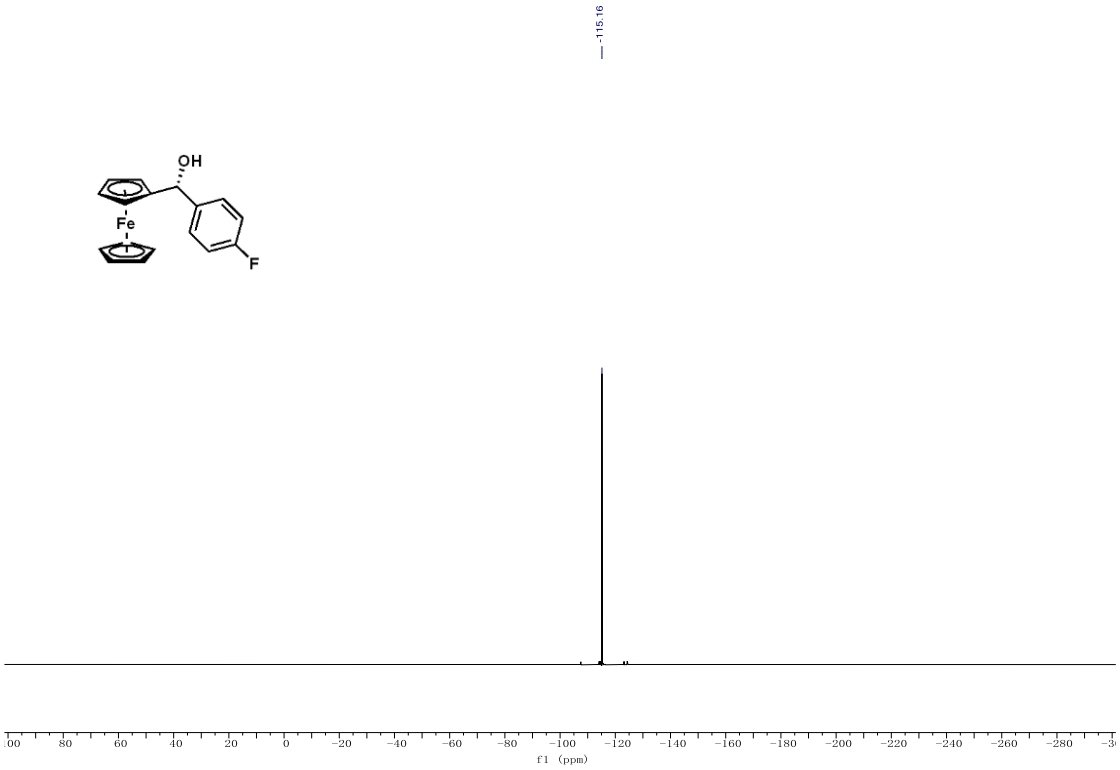
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)

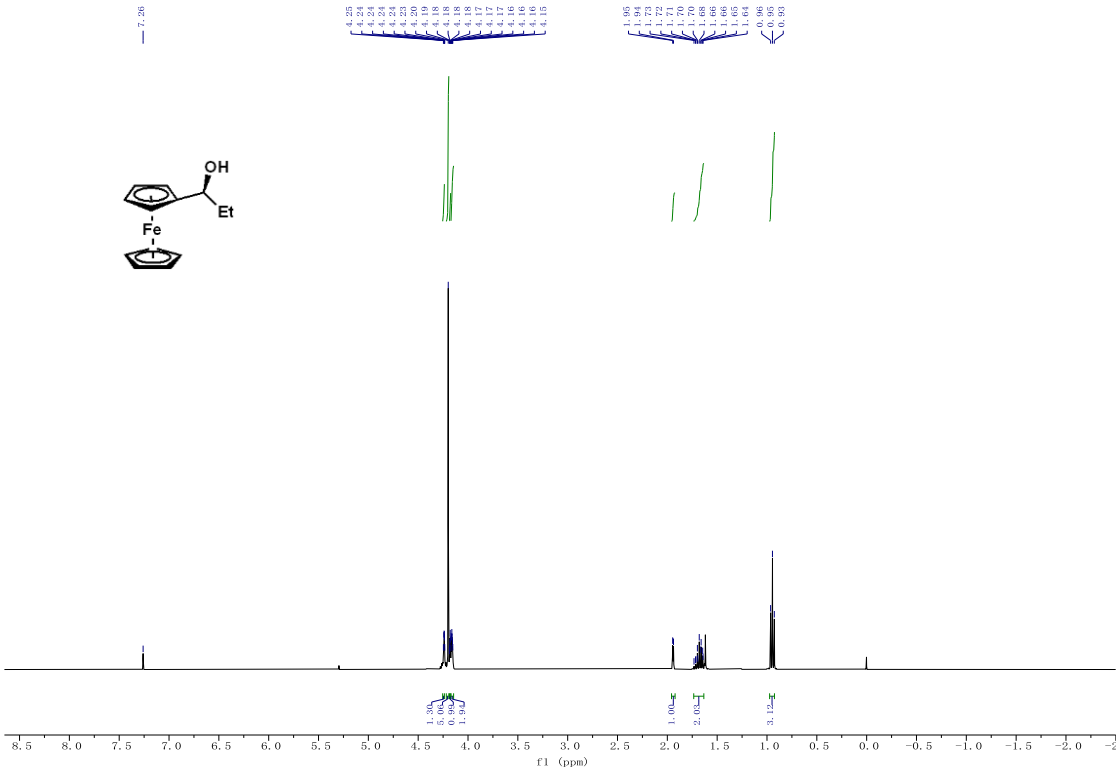


^{19}F NMR (376 MHz, $CDCl_3$)

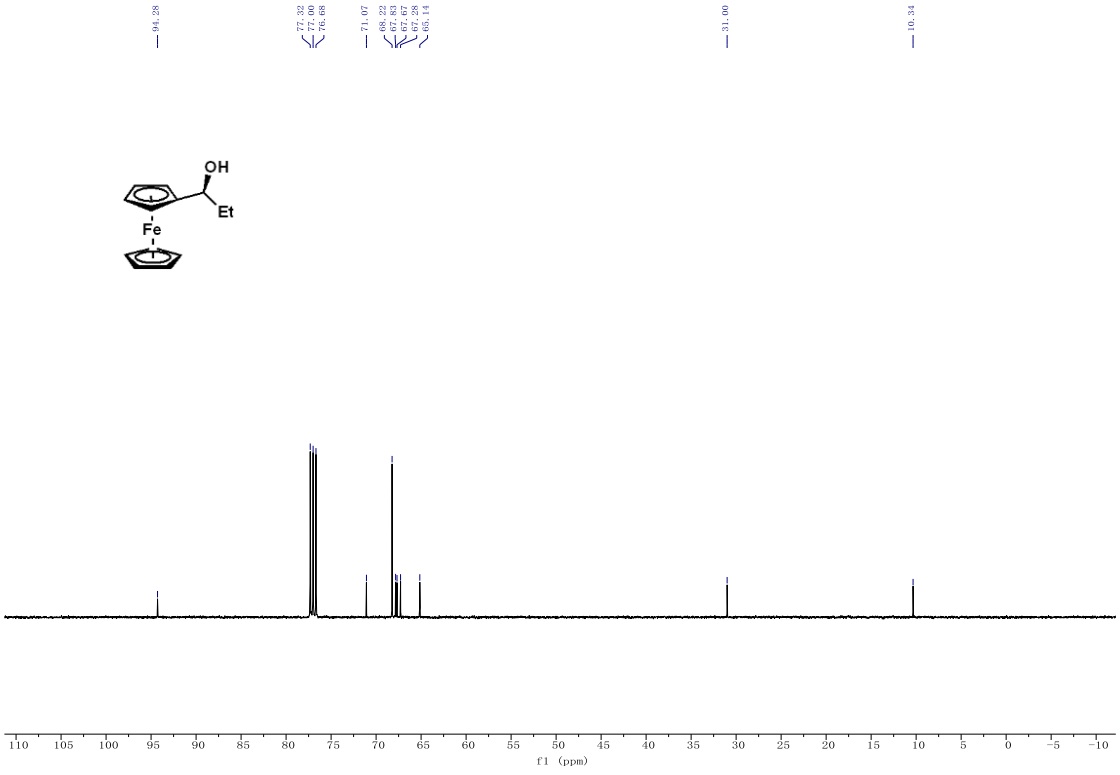


(S)-1-(ferrocene-2-yl)propan-1-ol (S5)

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

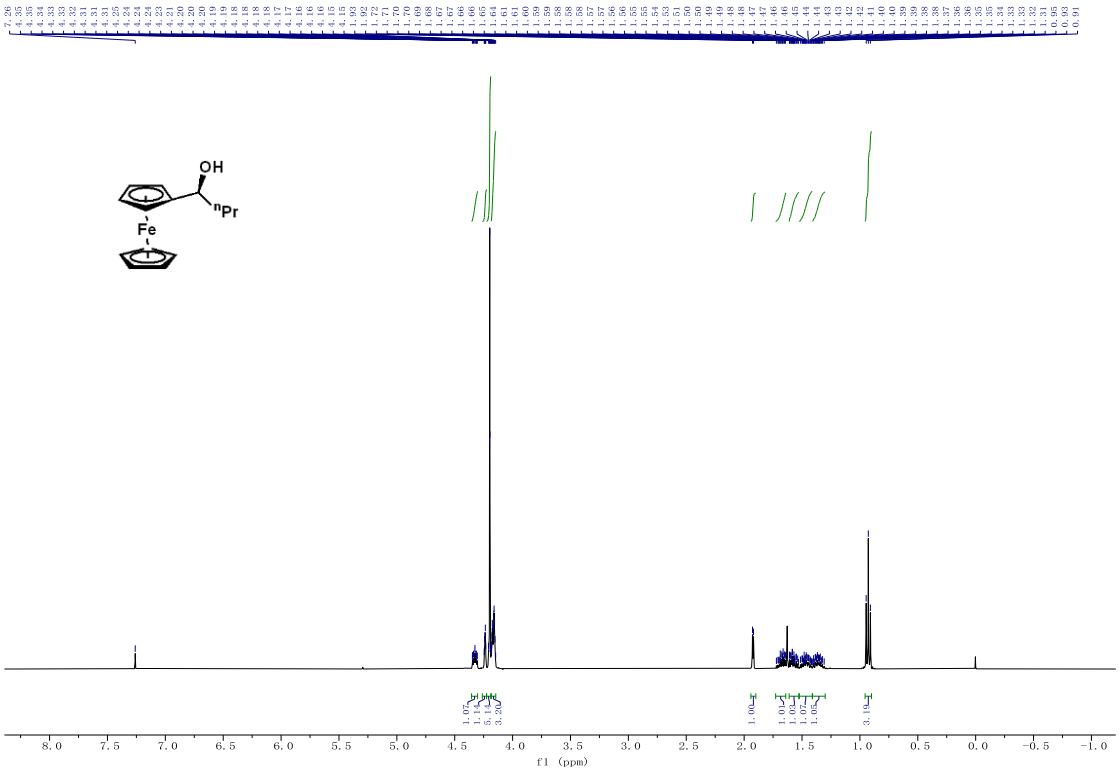


^{13}C NMR (101 MHz, $CDCl_3$)

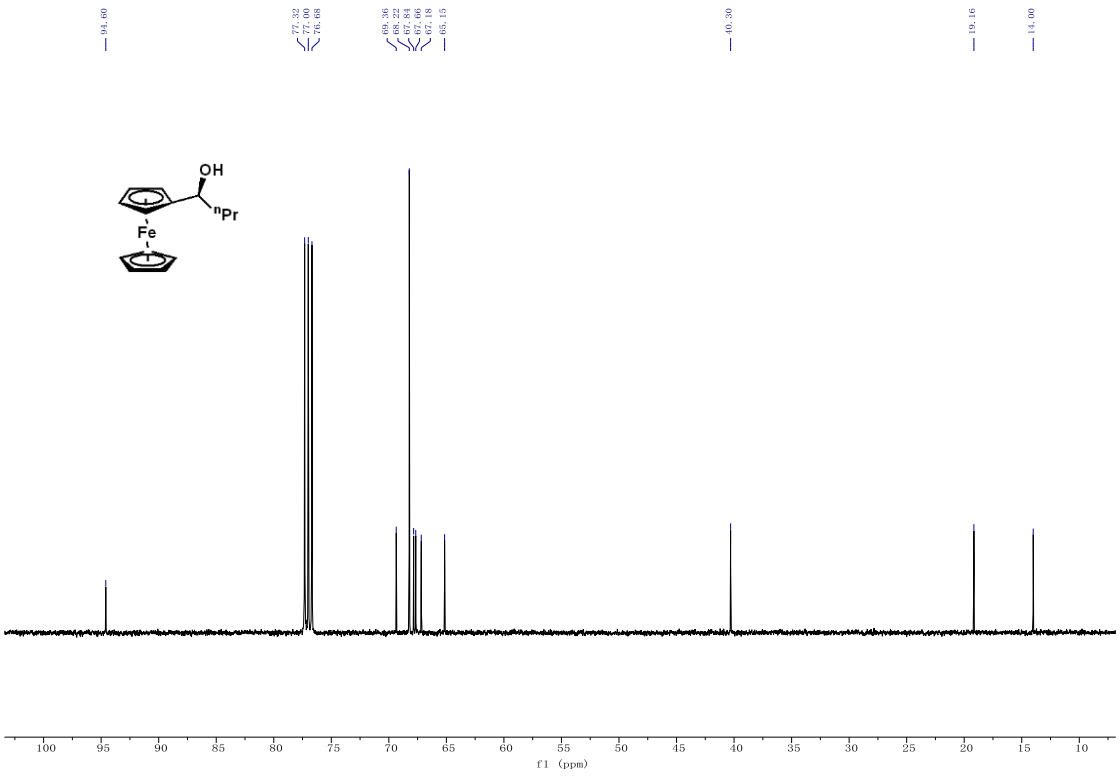


(S)-1-(ferrocene-2-yl)butan-1-ol (S6)

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

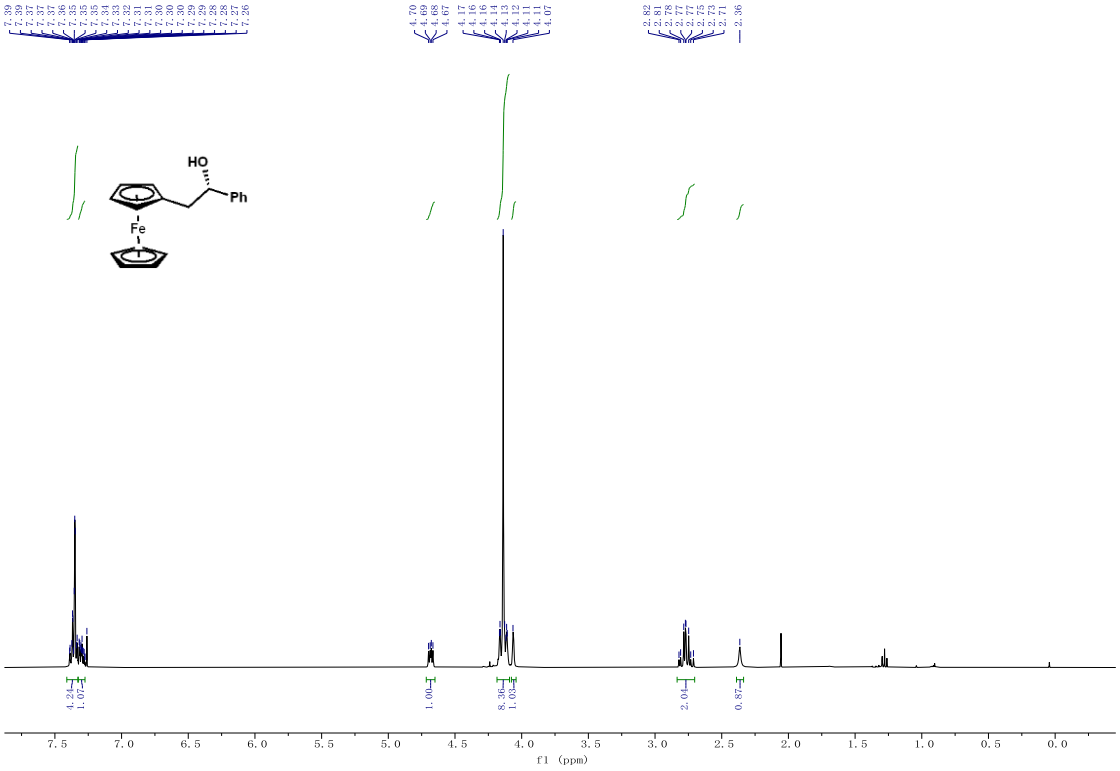


^{13}C NMR (101 MHz, $CDCl_3$)

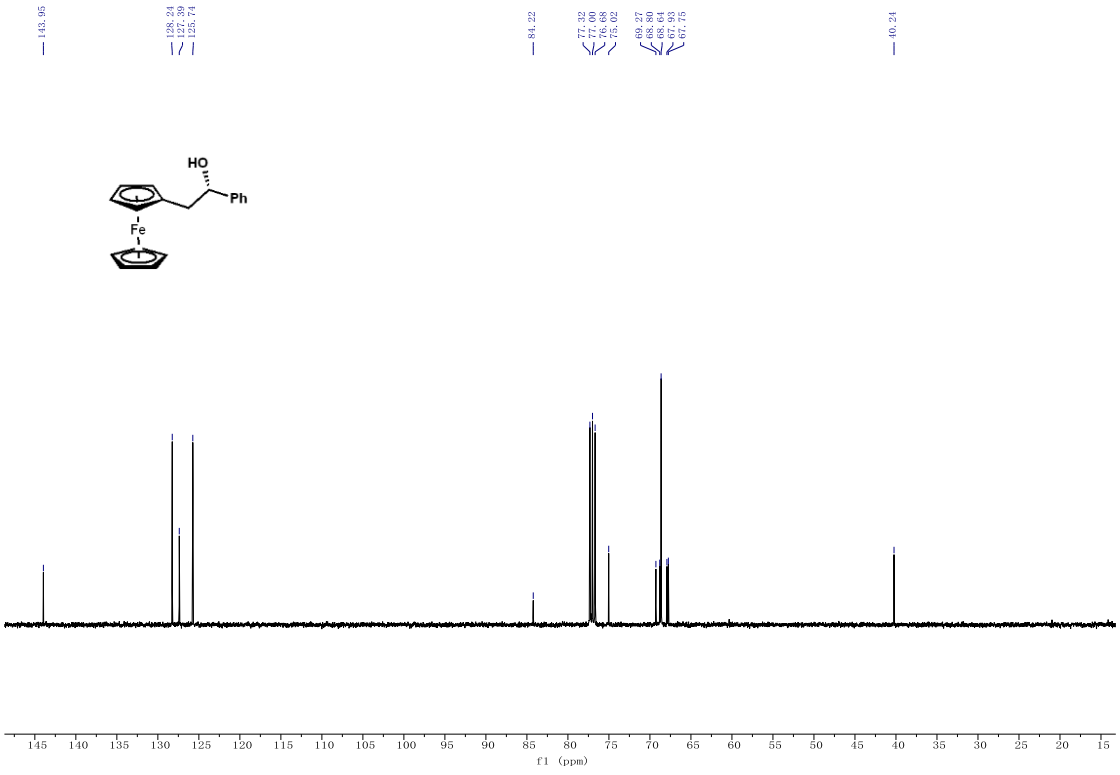


(S)-1-phenyl-2-(ferrocene-2-yl)ethan-1-ol (S7)

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

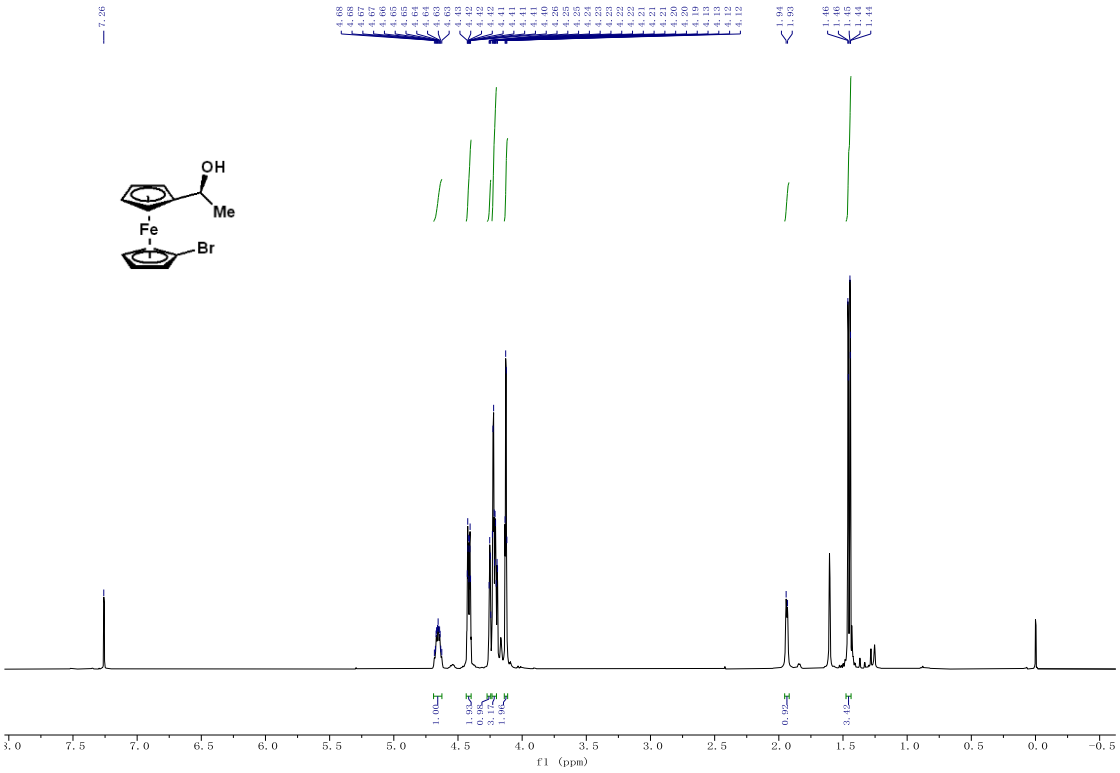


^{13}C NMR (101 MHz, $CDCl_3$)

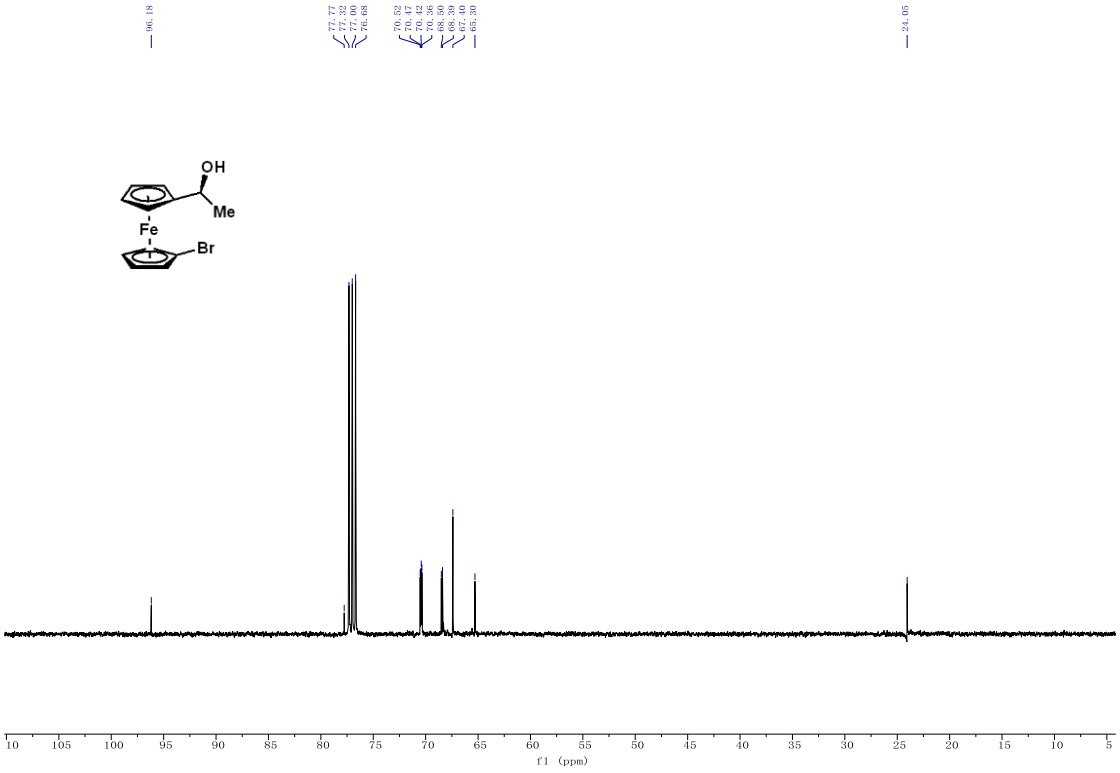


(S)-1-(1-Hydroxyethyl)-1'-bromoferrocene (S8)

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

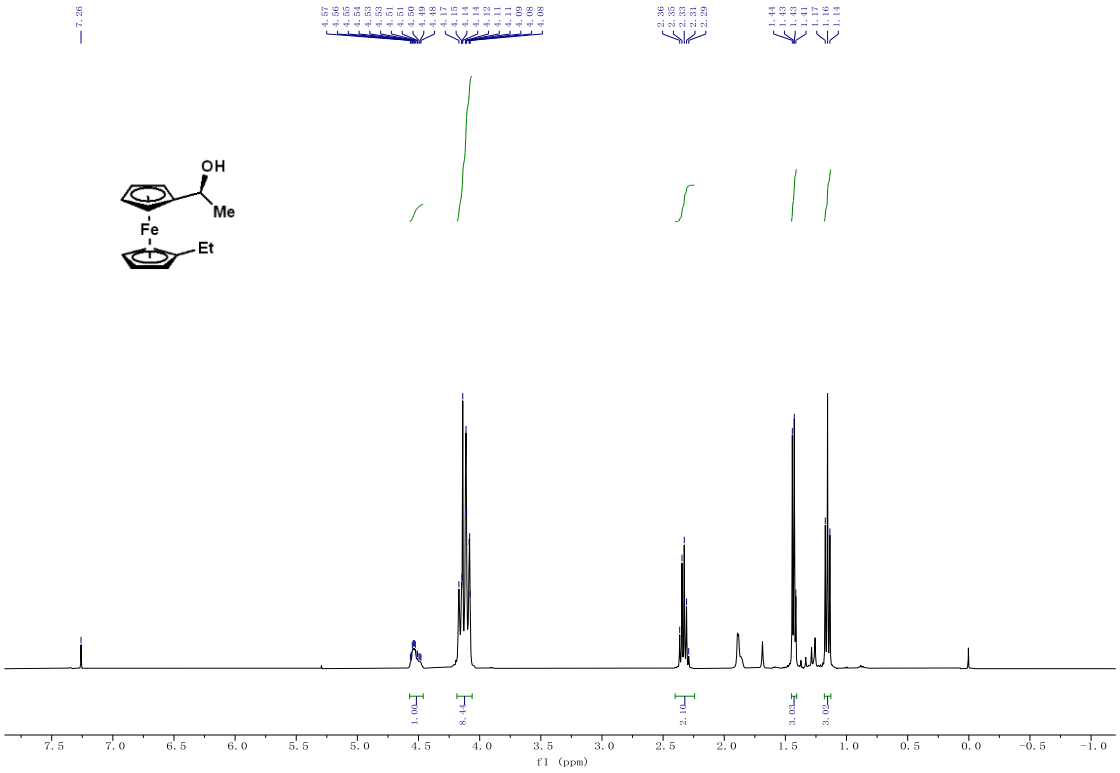


^{13}C NMR (101 MHz, $CDCl_3$)

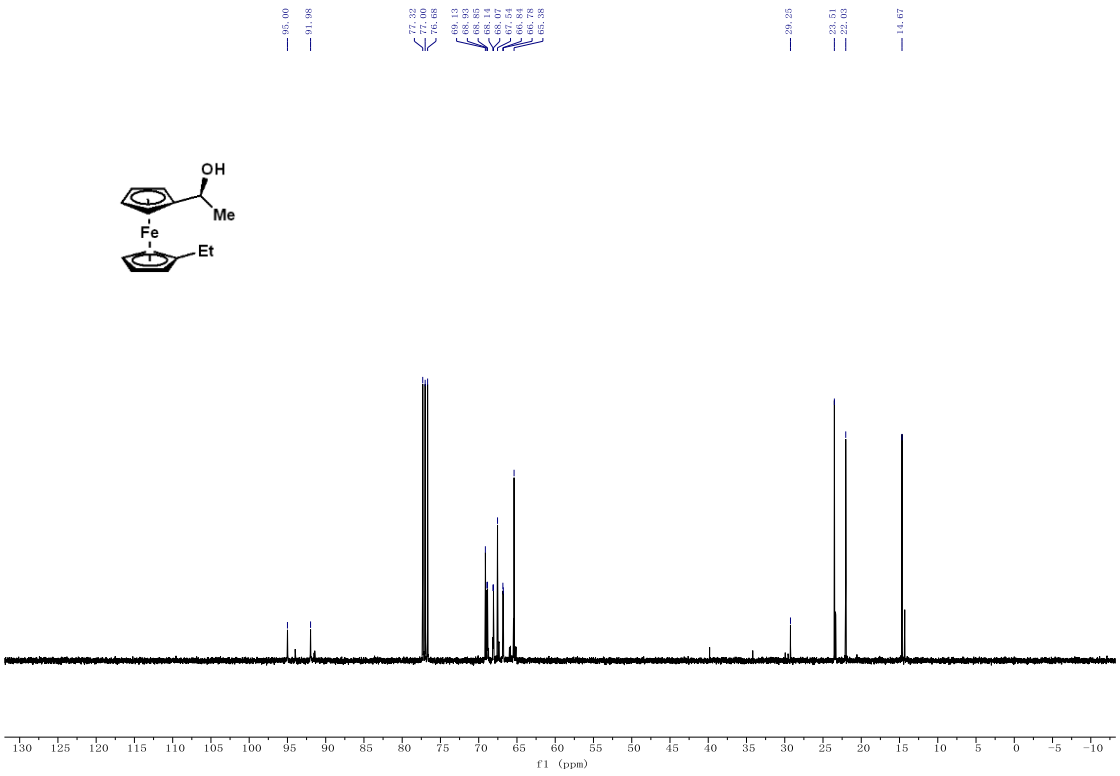


(S)-1-(1-Hydroxyethyl)-1'-ethylferrocene (S9)

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

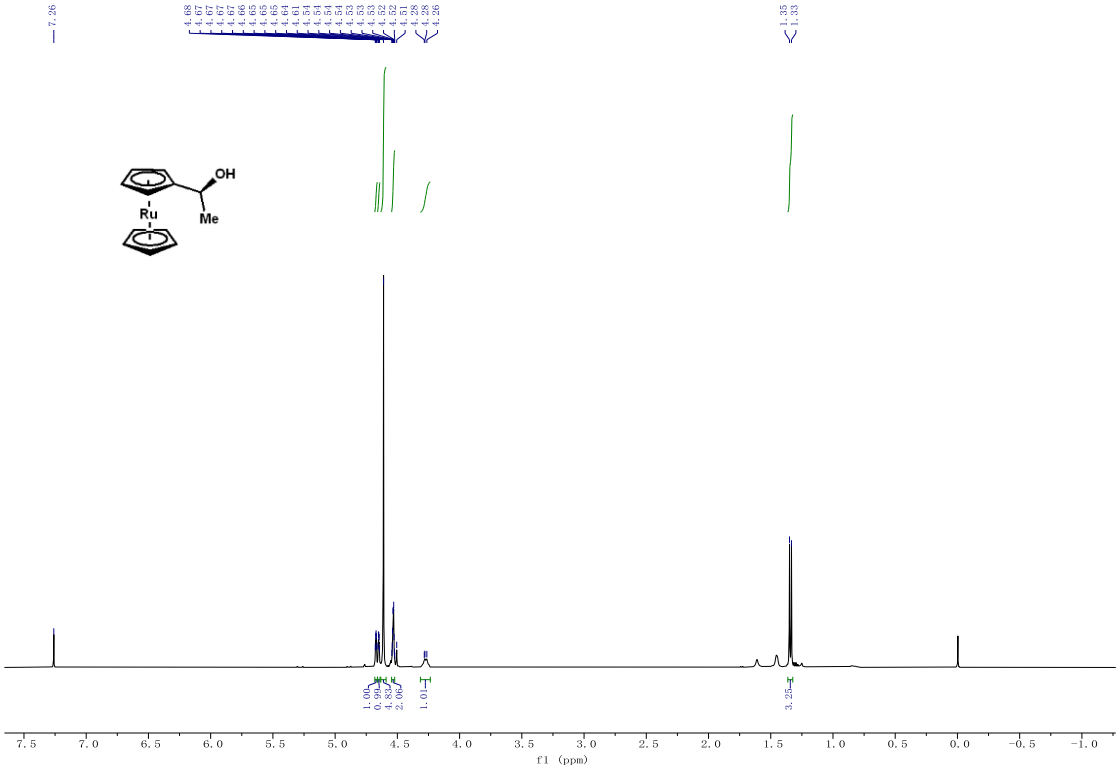


^{13}C NMR (101 MHz, $CDCl_3$)

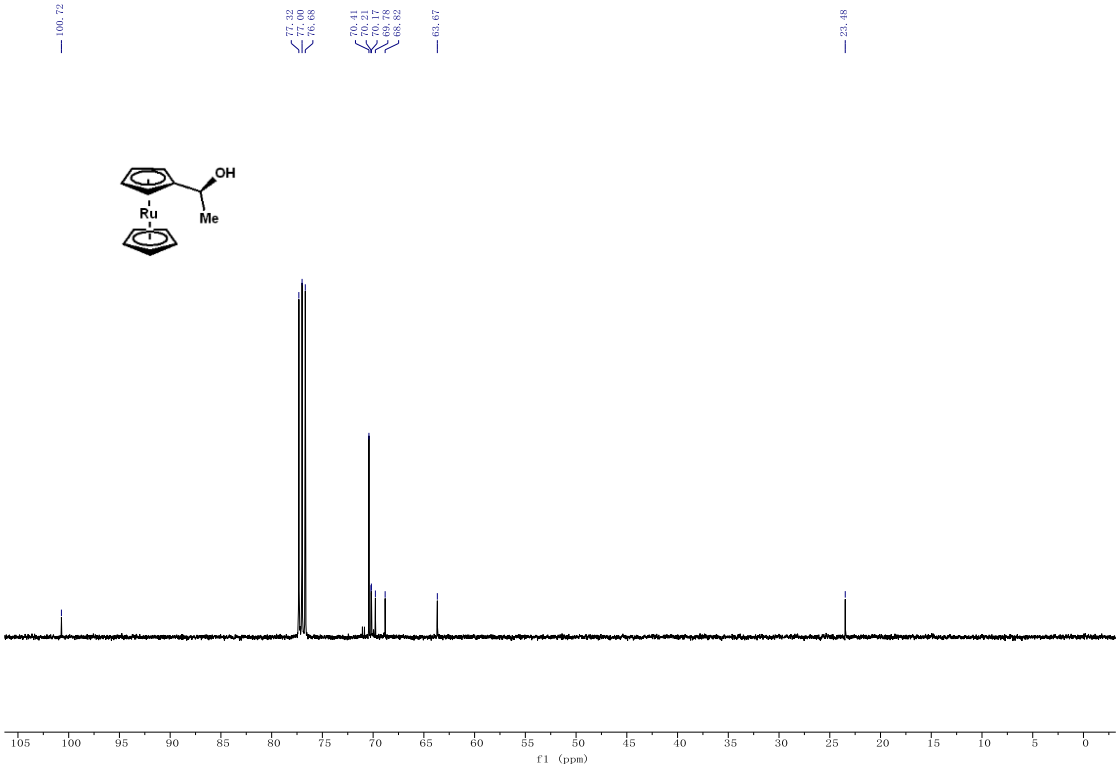


(S)-1-(ruthenocene-2-yl)ethan-1-ol (S12)

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

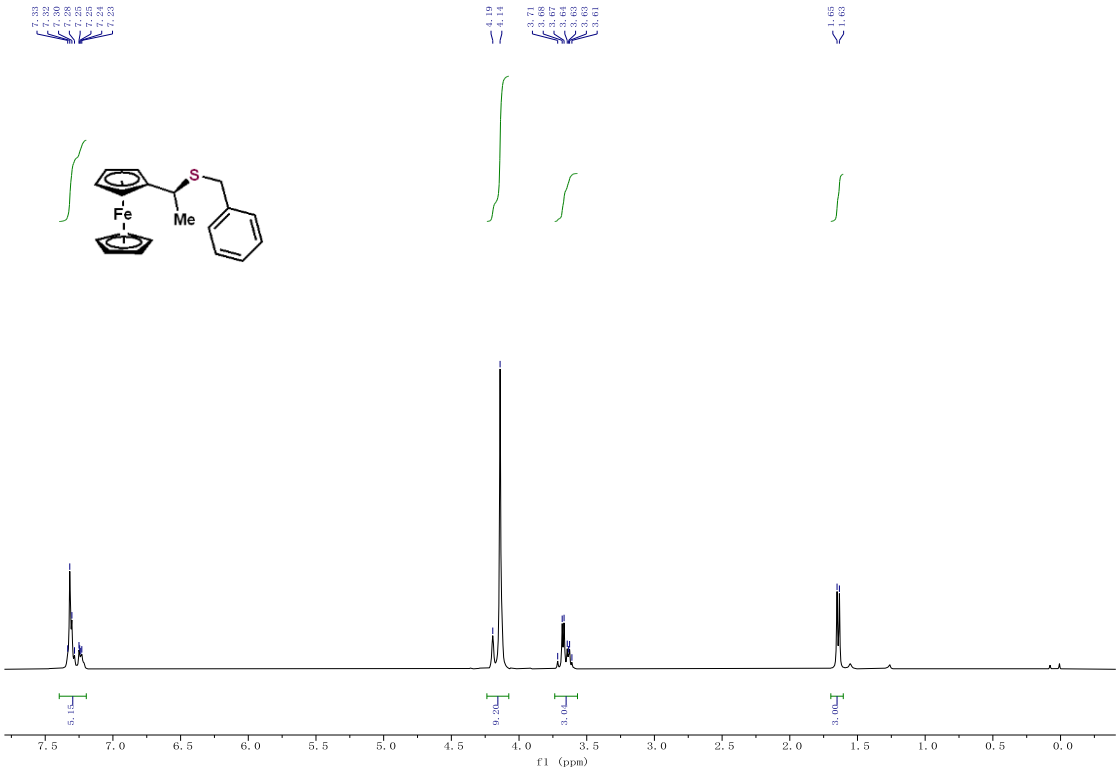


^{13}C NMR (101 MHz, $CDCl_3$)

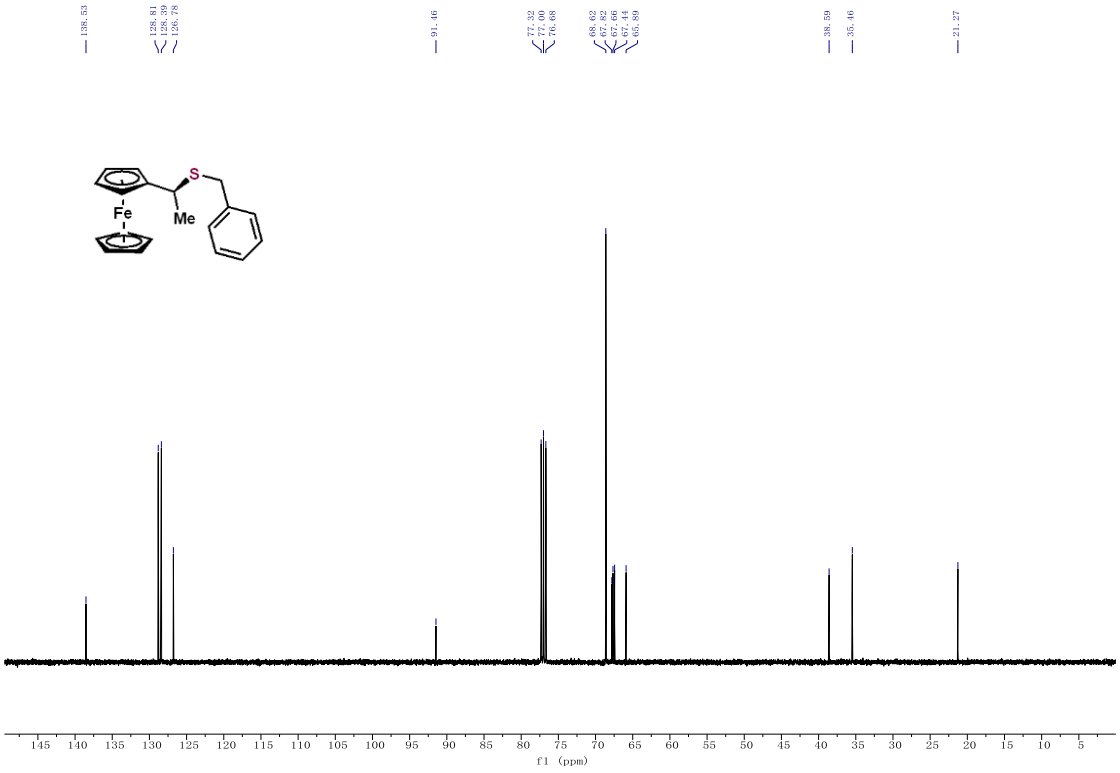


(S) -1-(benzylthio)ethylferrocene (3)

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

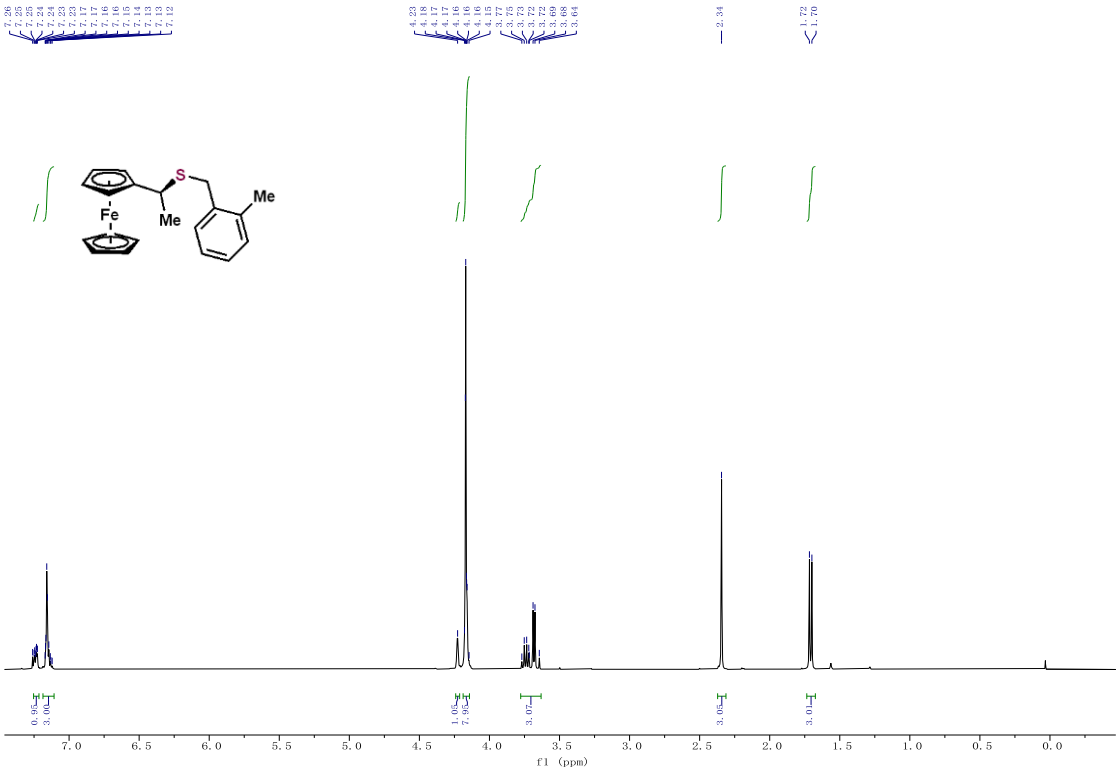


^{13}C NMR (101 MHz, $CDCl_3$)

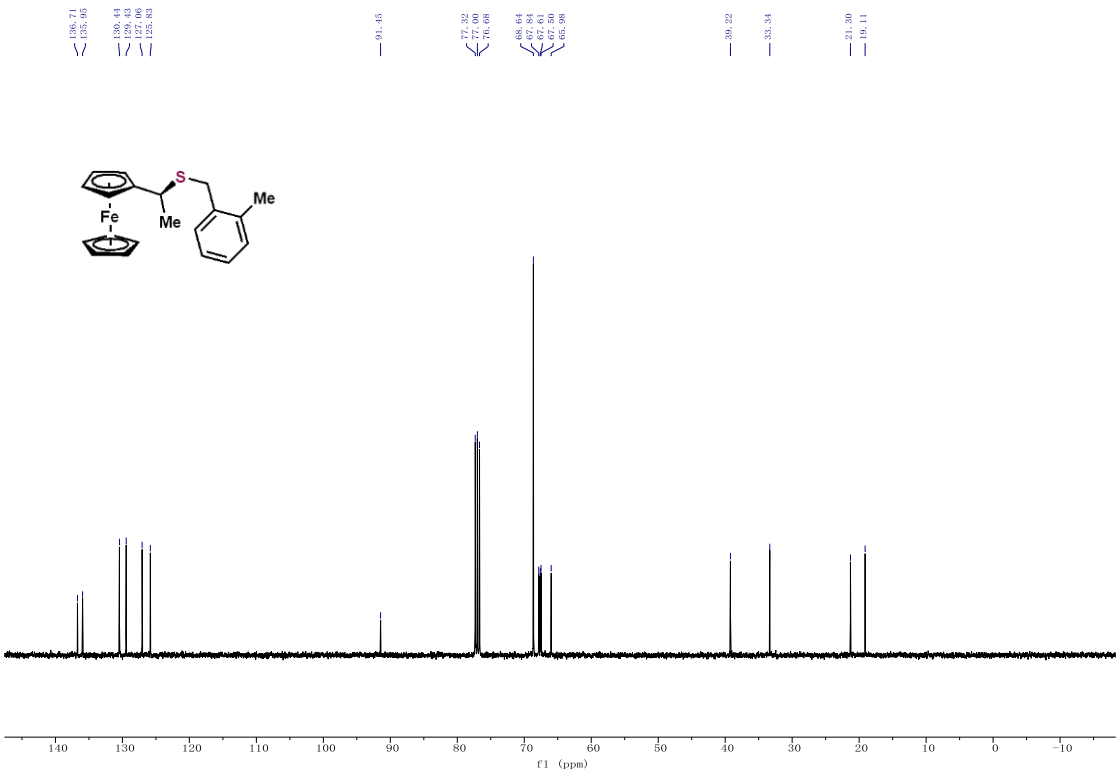


(S)-1-((2-methylbenzyl)thio)ethylferrocene (4)

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

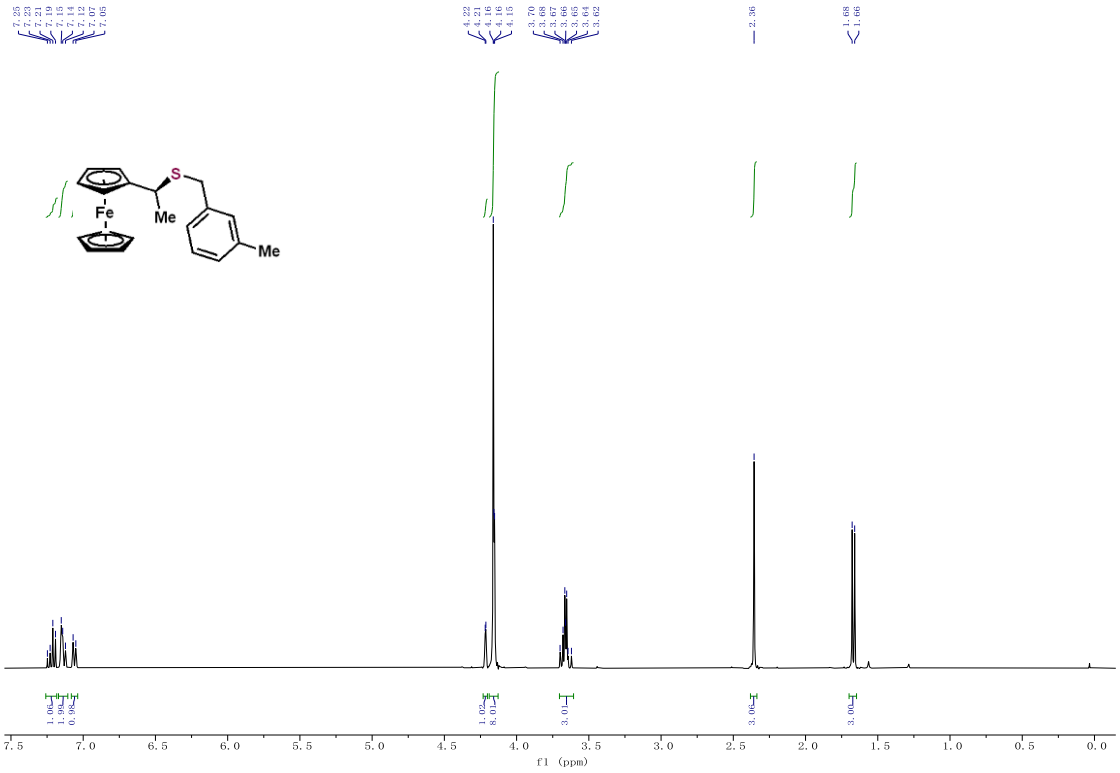


^{13}C NMR (101 MHz, $CDCl_3$)

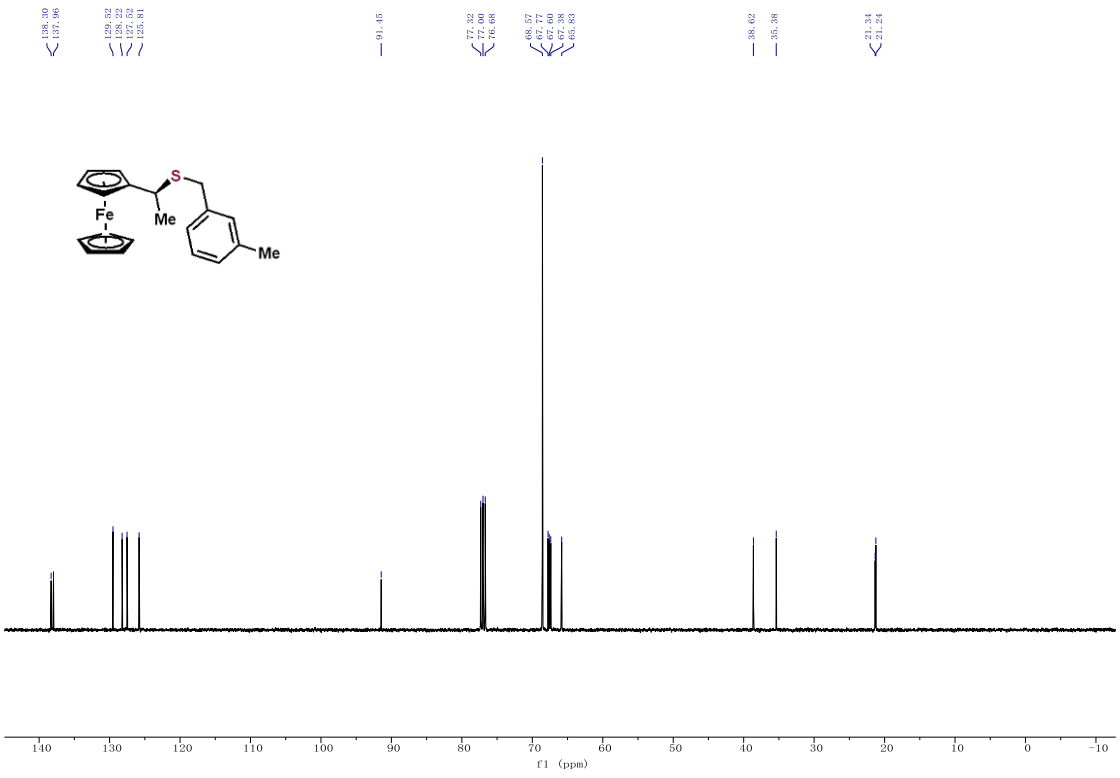


(S)-1-((3-methylbenzyl)thio)ethylferrocene (5)

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

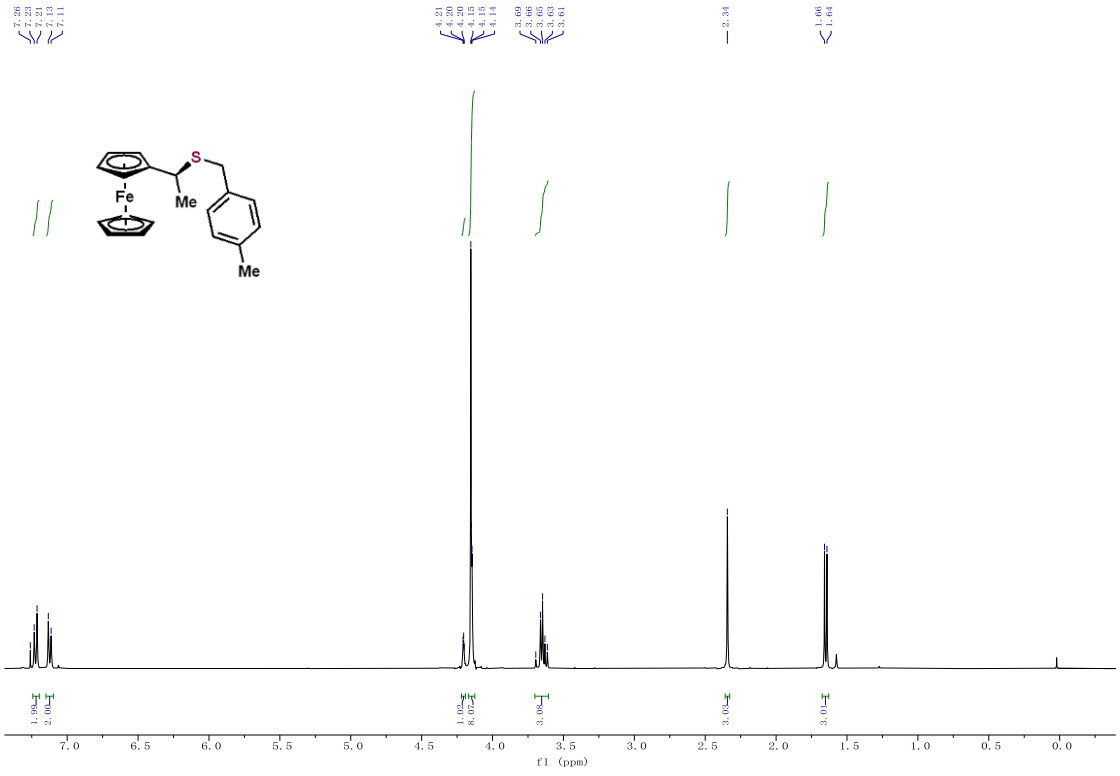


^{13}C NMR (101 MHz, $CDCl_3$)

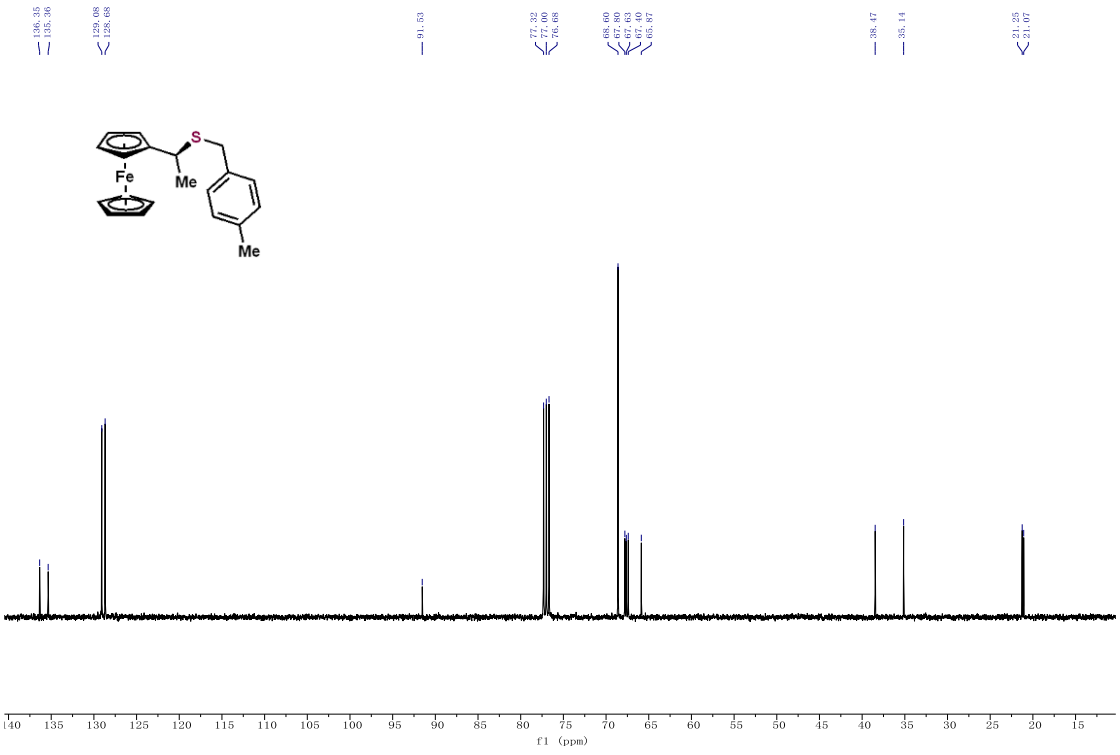


(S)-1-((4-methylbenzyl)thio)ethylferrocene (6)

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

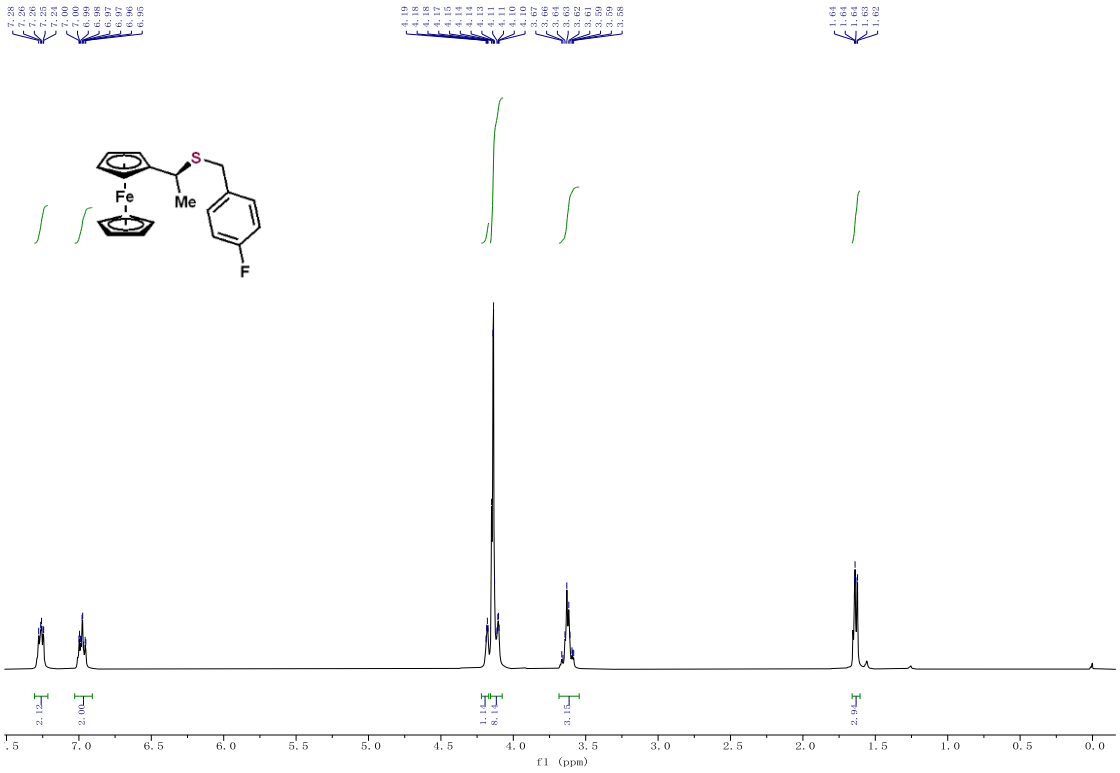


^{13}C NMR (101 MHz, $CDCl_3$)

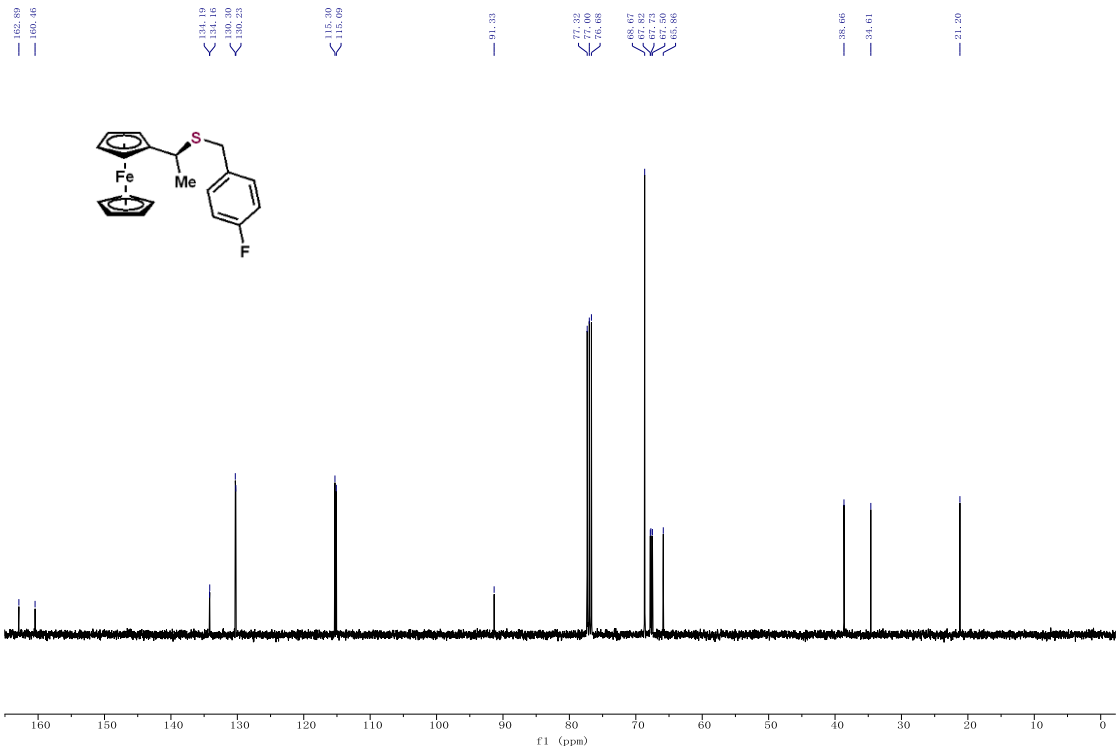


(S)-1-((4-fluorobenzyl)thio)ethylferrocene (7)

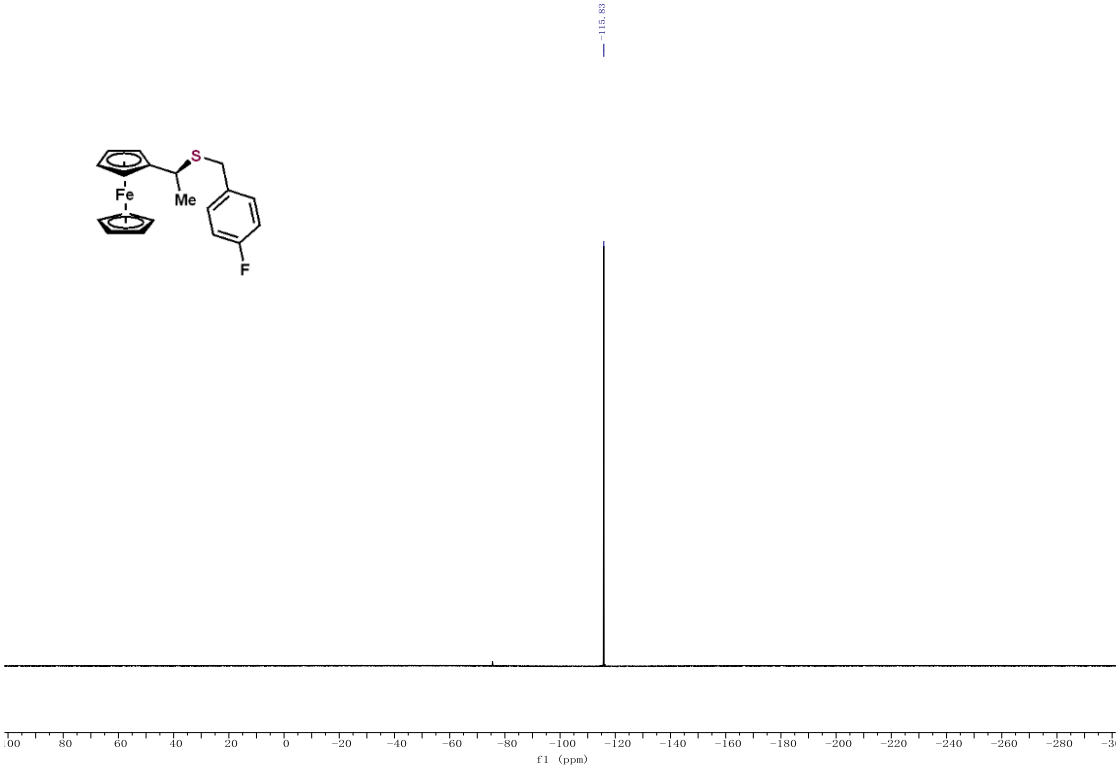
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)

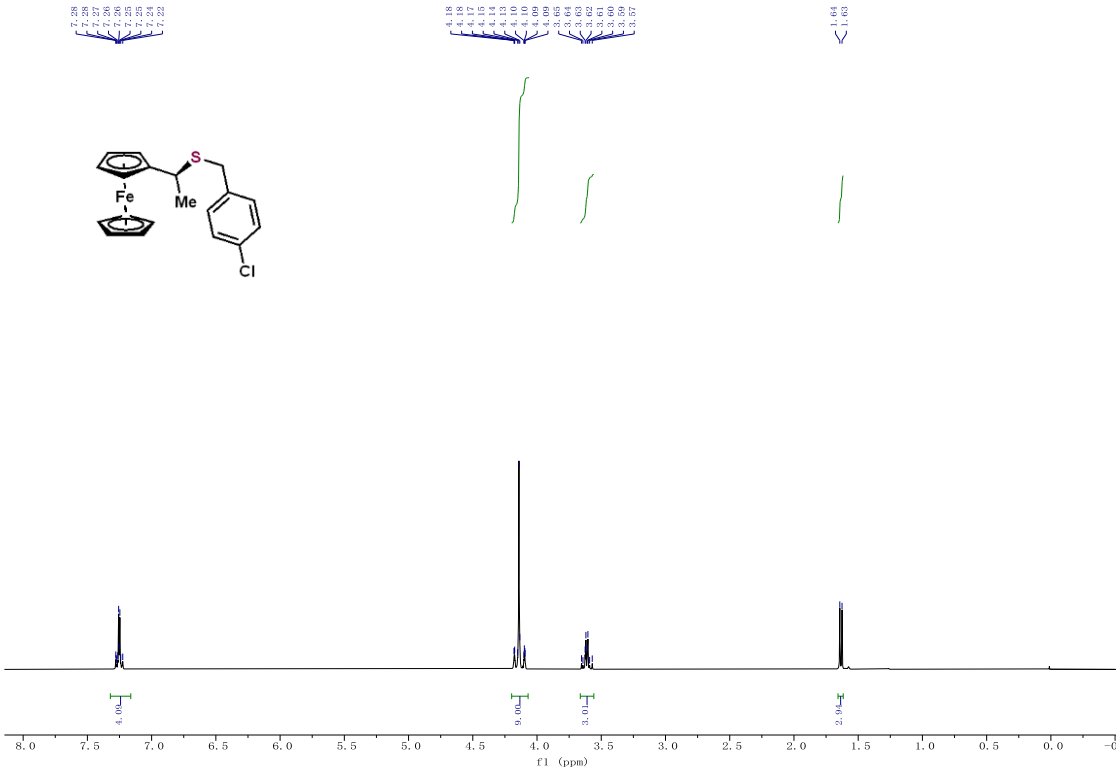


^{19}F NMR (376 MHz, $CDCl_3$)

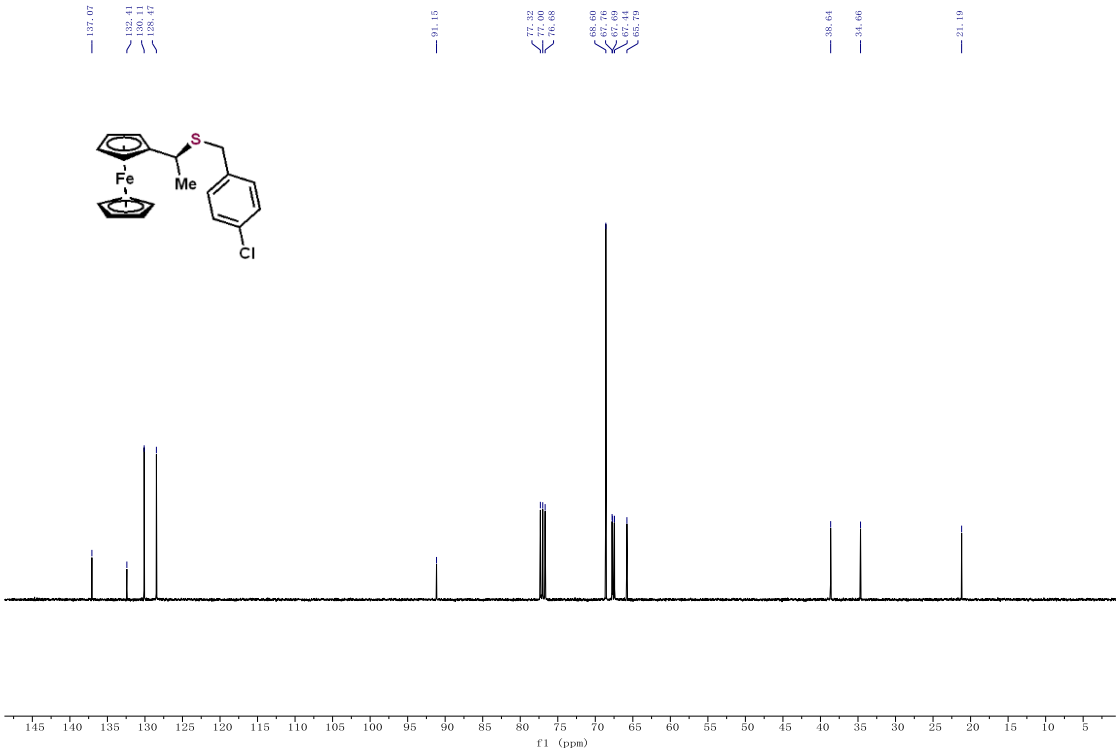


(S)-1-((4-chlorobenzyl)thio)ethylferrocene (8)

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

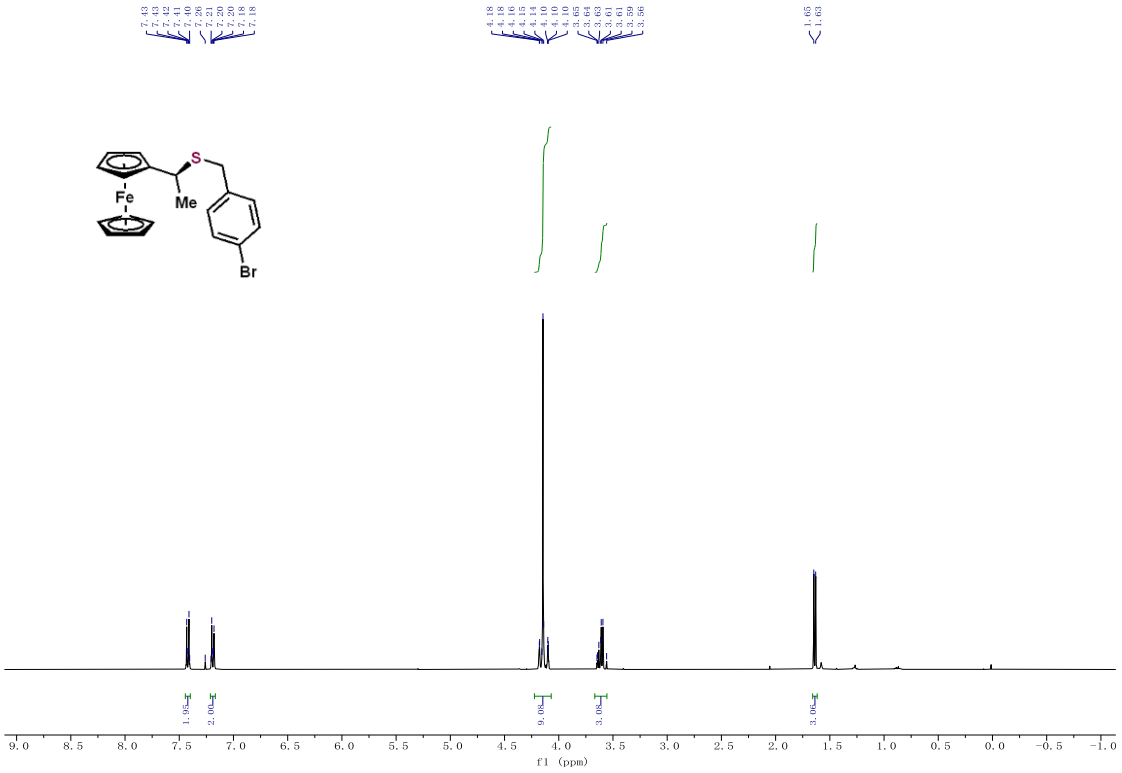


^{13}C NMR (101 MHz, $CDCl_3$)

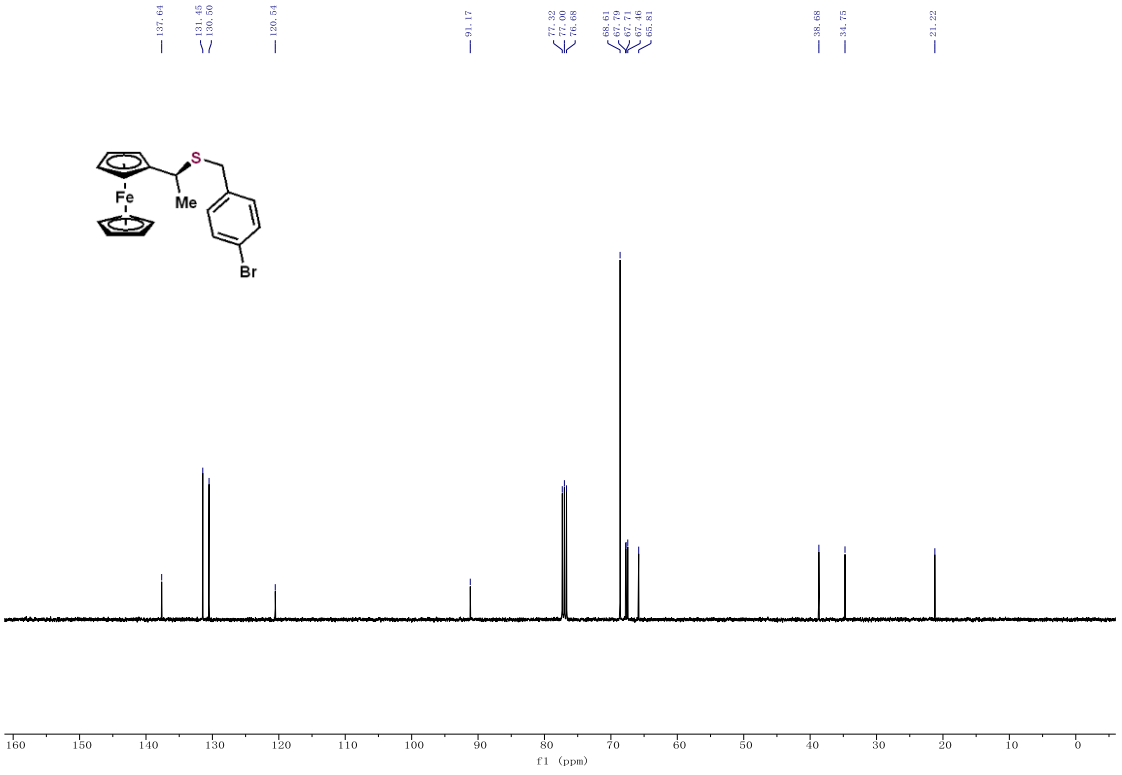


(S)-1-((4-bromobenzyl)thio)ethylferrocene (9)

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

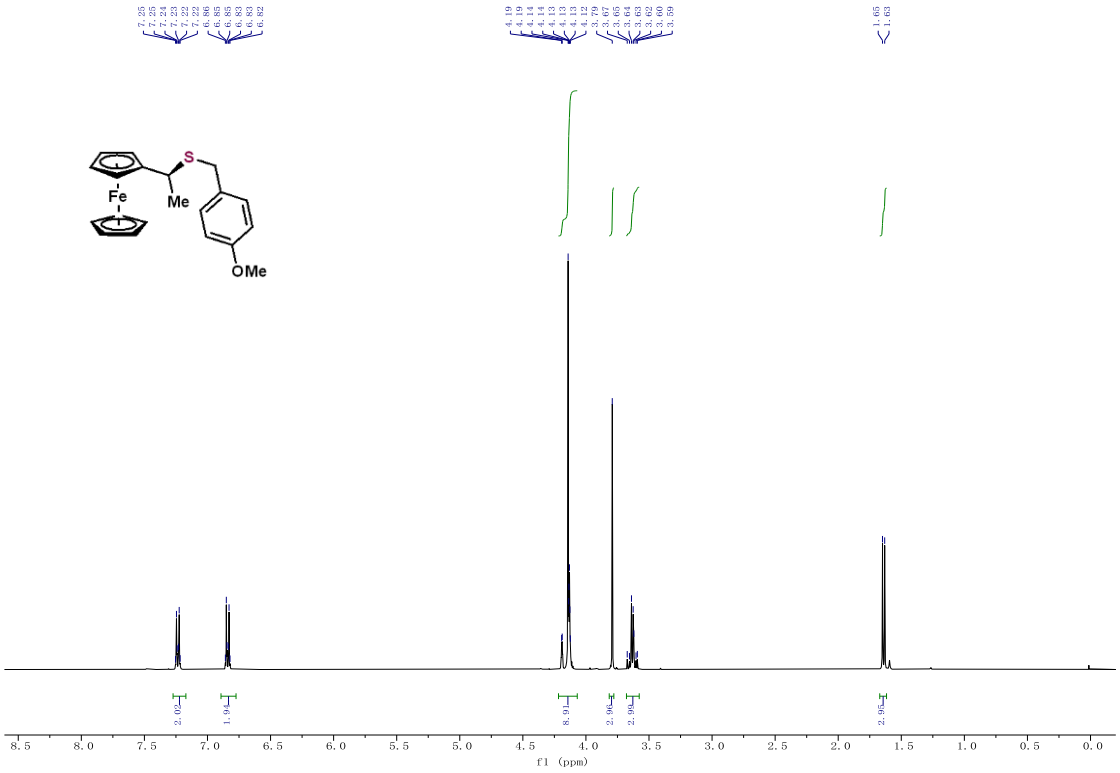


^{13}C NMR (101 MHz, $CDCl_3$)



(S)-1-((4-methoxybenzyl)thio)ethylferrocene (10)

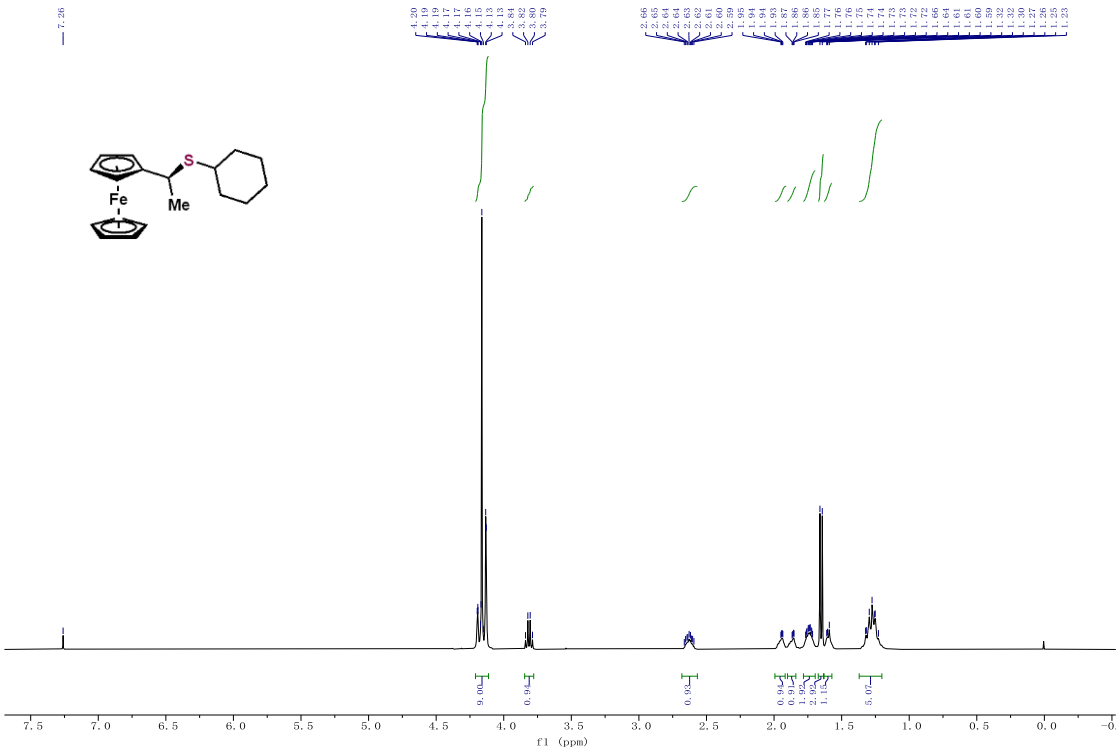
^{1}H NMR (400 MHz, $CDCl_3$)



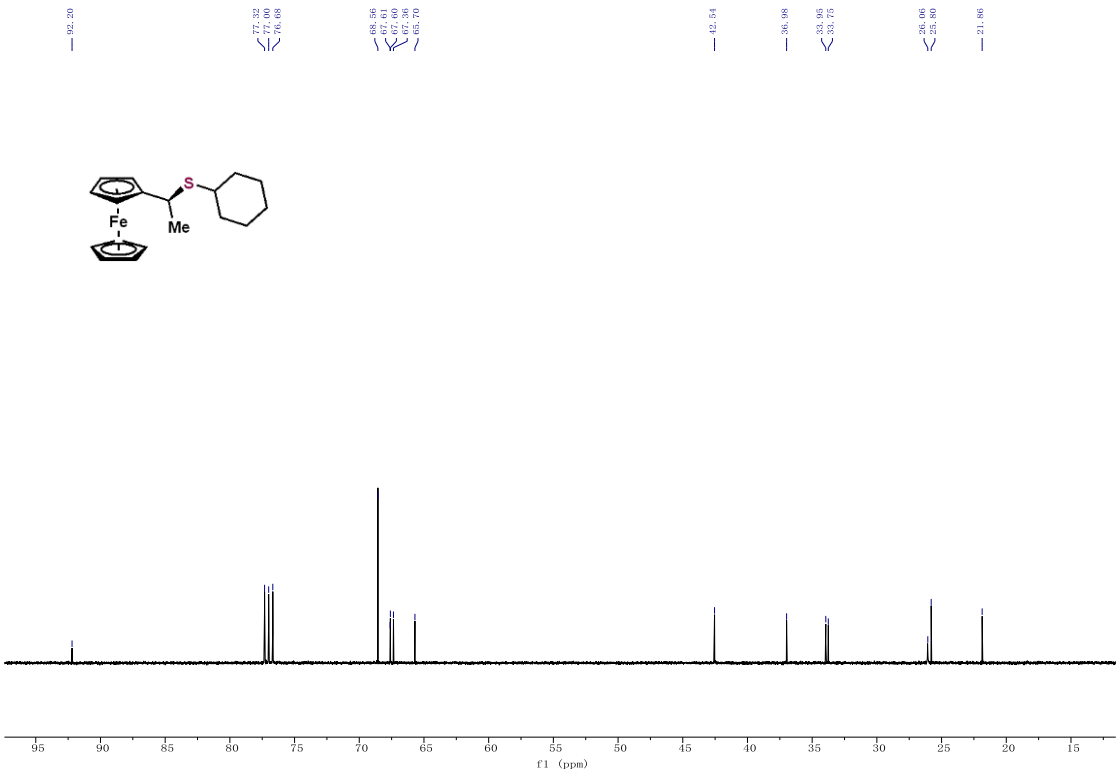
^{13}C NMR (101 MHz, $CDCl_3$)

(S)-1-(cyclohexylthio)ethylferrocene (11)

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

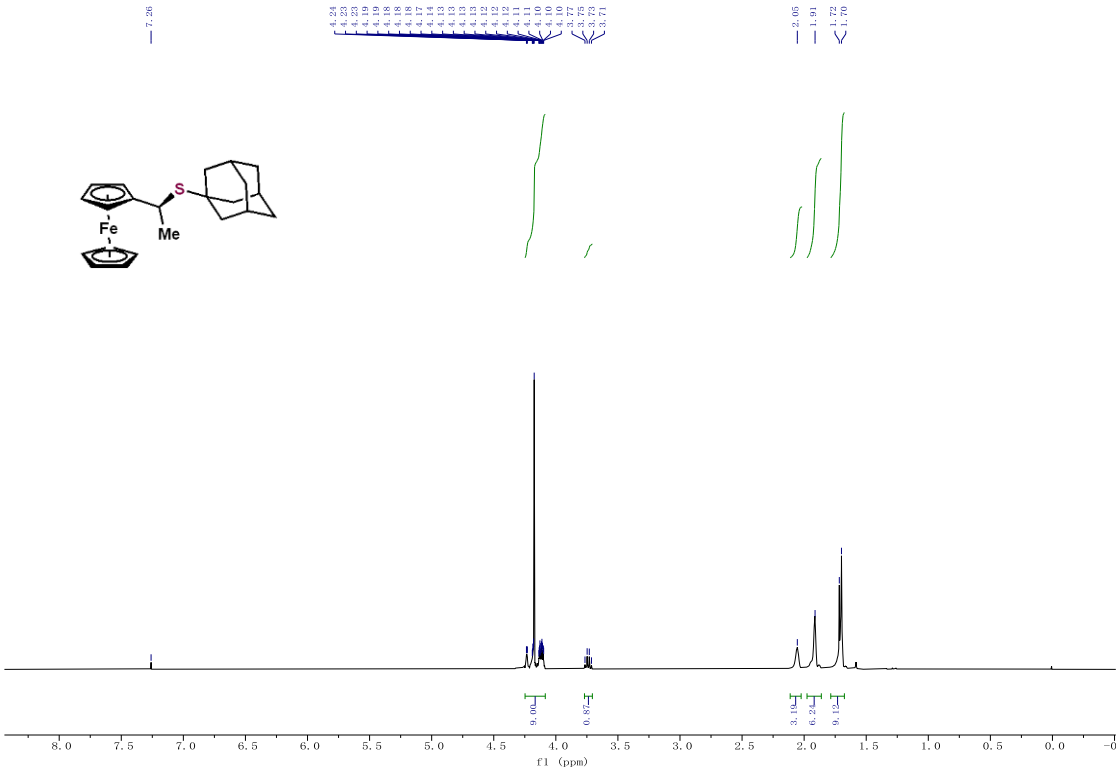


^{13}C NMR (101 MHz, $CDCl_3$)

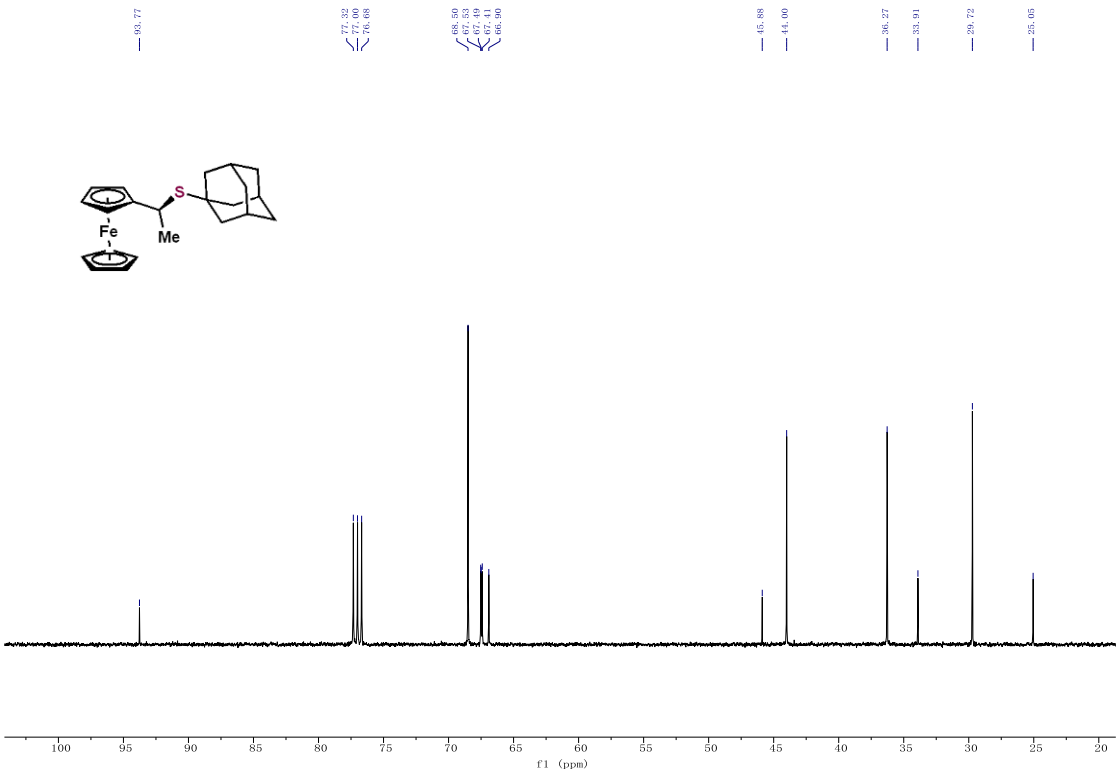


(S)-1-(((3*s*,5*s*,7*s*)-adamantan-1-yl)thio)ethylferrocene (12)

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

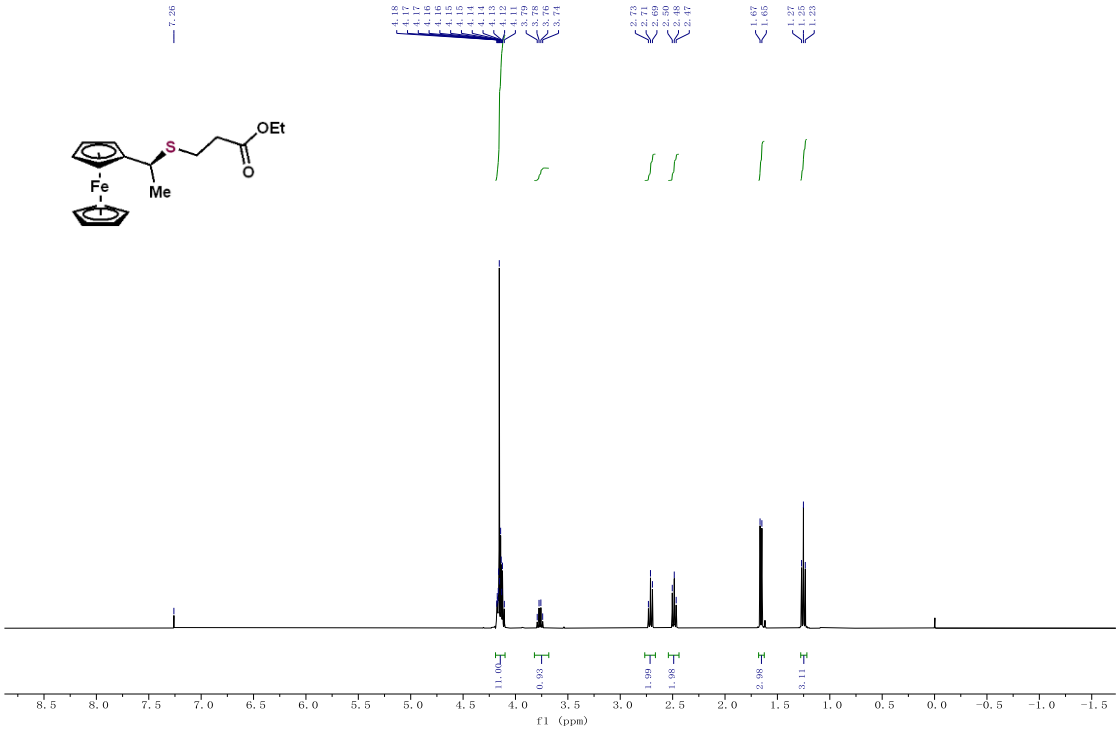


^{13}C NMR (101 MHz, $CDCl_3$)

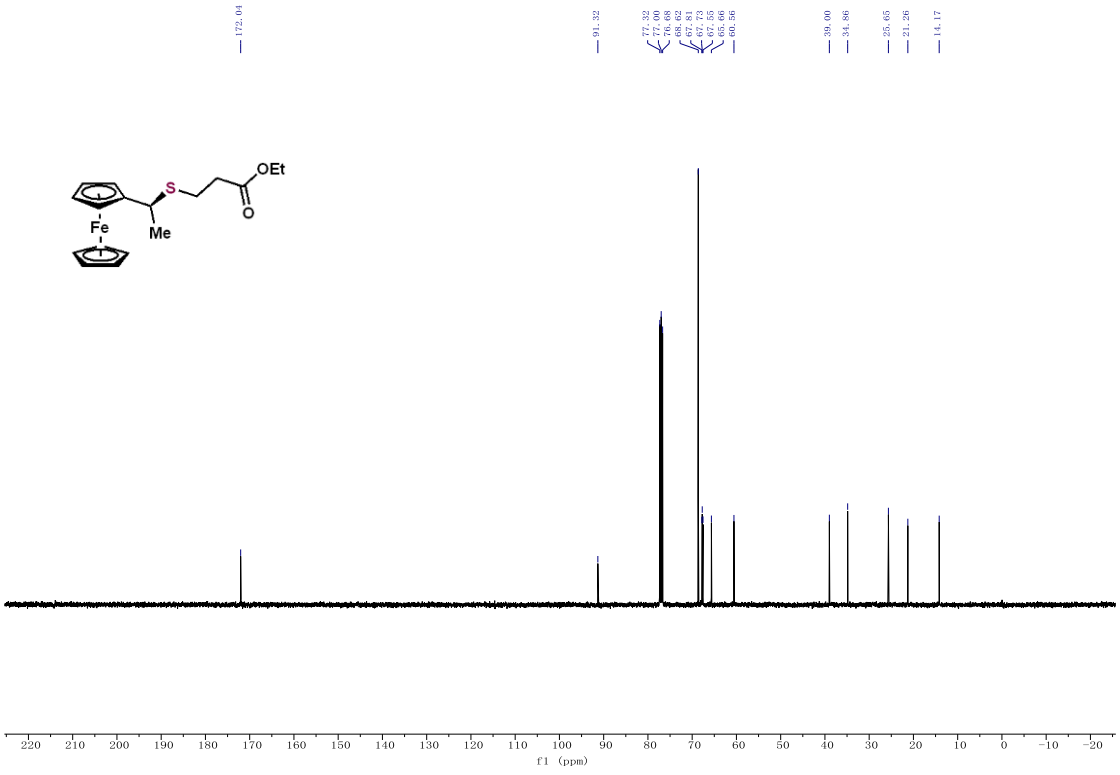


(S)-ethyl 3-((1-(ferrocene-2-yl)ethyl)thio)propanoate (13)

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

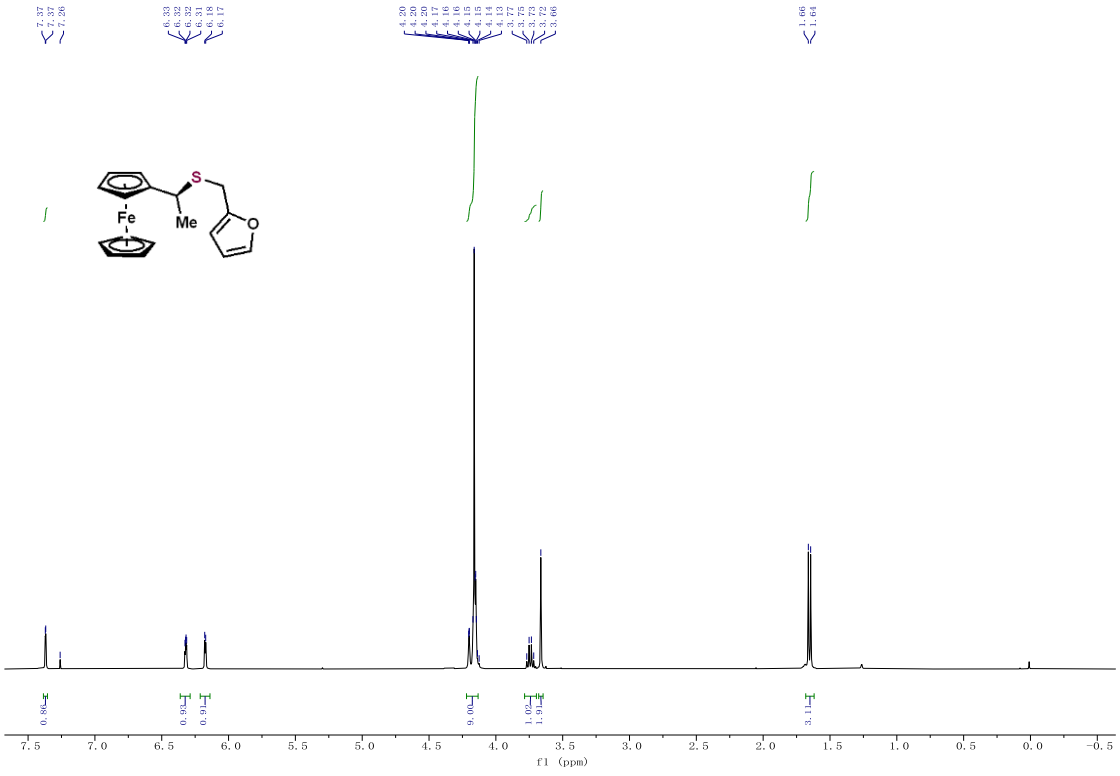


^{13}C NMR (101 MHz, $CDCl_3$)

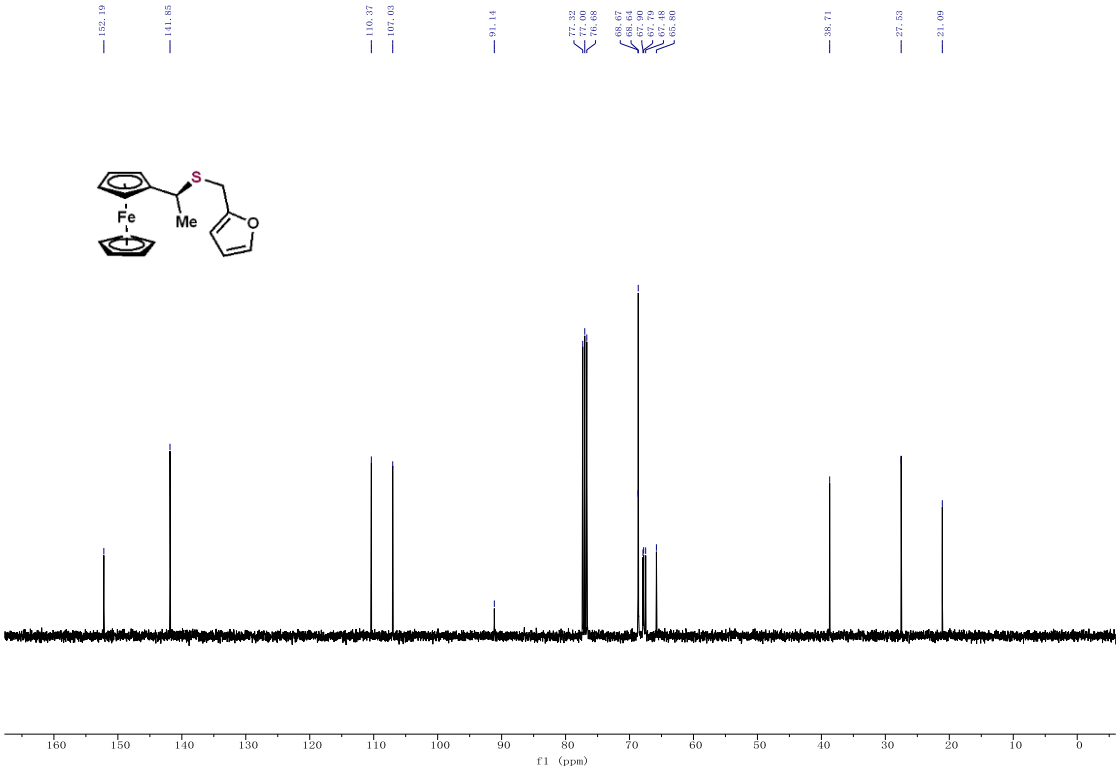


(S)-2-((1-(ferrocene-2-yl)ethyl)thio)methyl)furan (14)

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

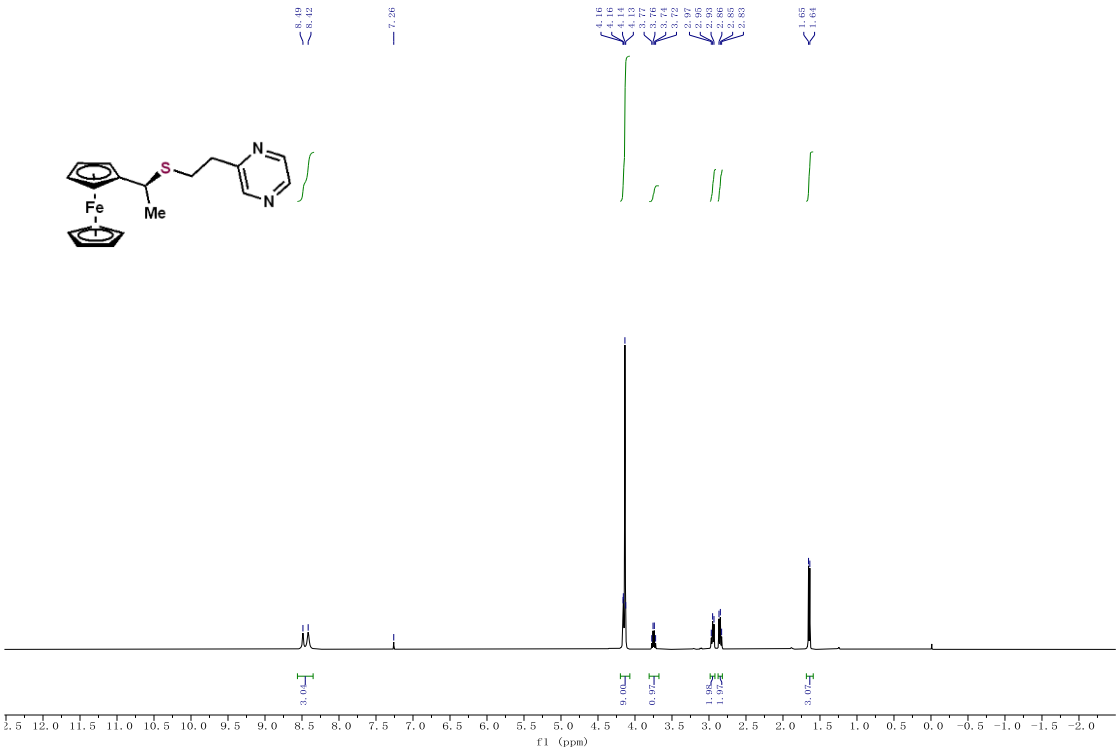


^{13}C NMR (101 MHz, $CDCl_3$)

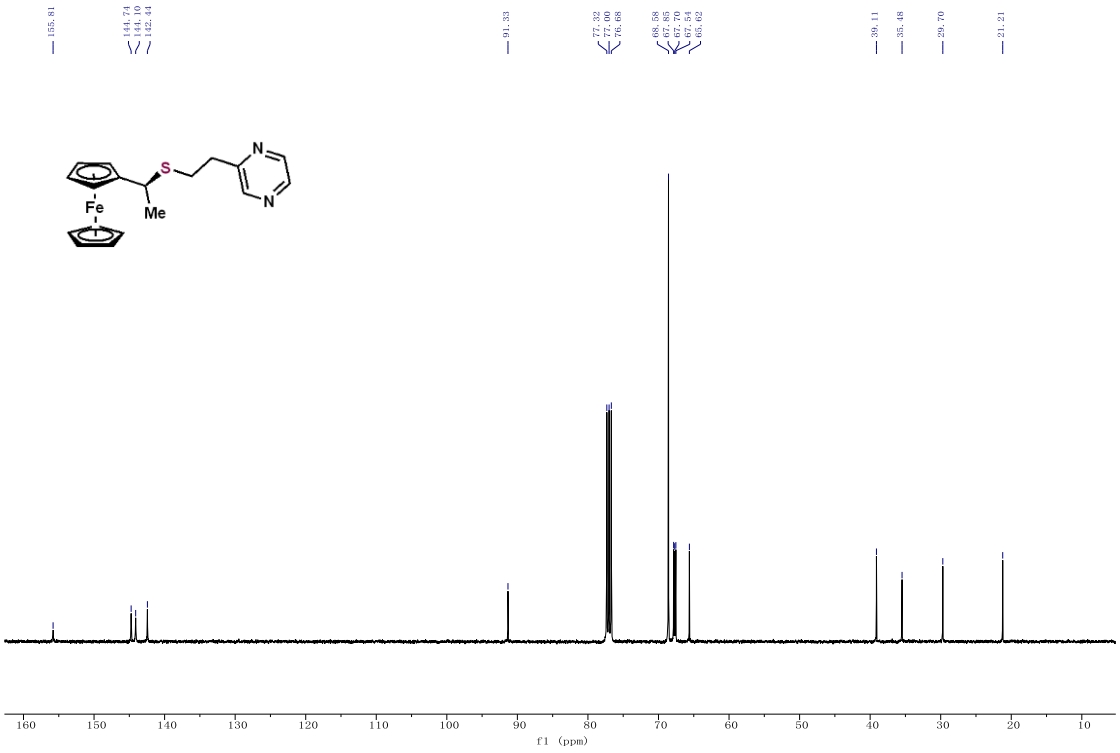


(S)-2-(2-((1-(ferrocene-2-yl)ethyl)thio)ethyl)pyrazine (15)

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

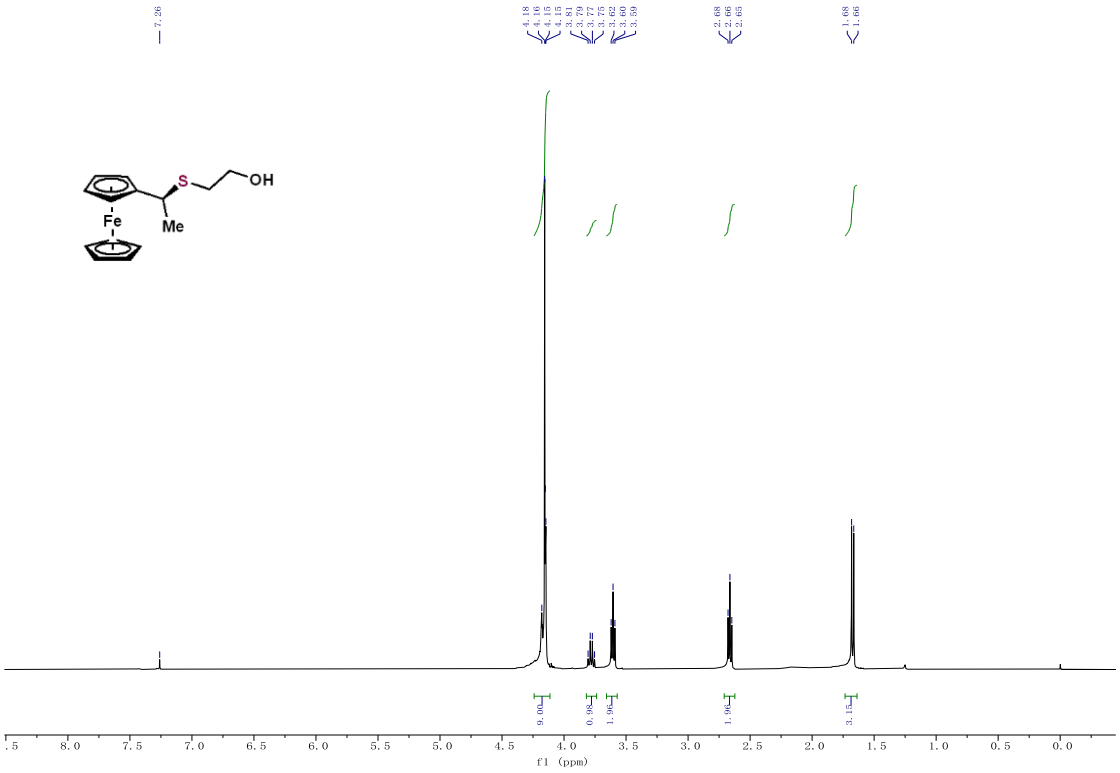


^{13}C NMR (101 MHz, $CDCl_3$)

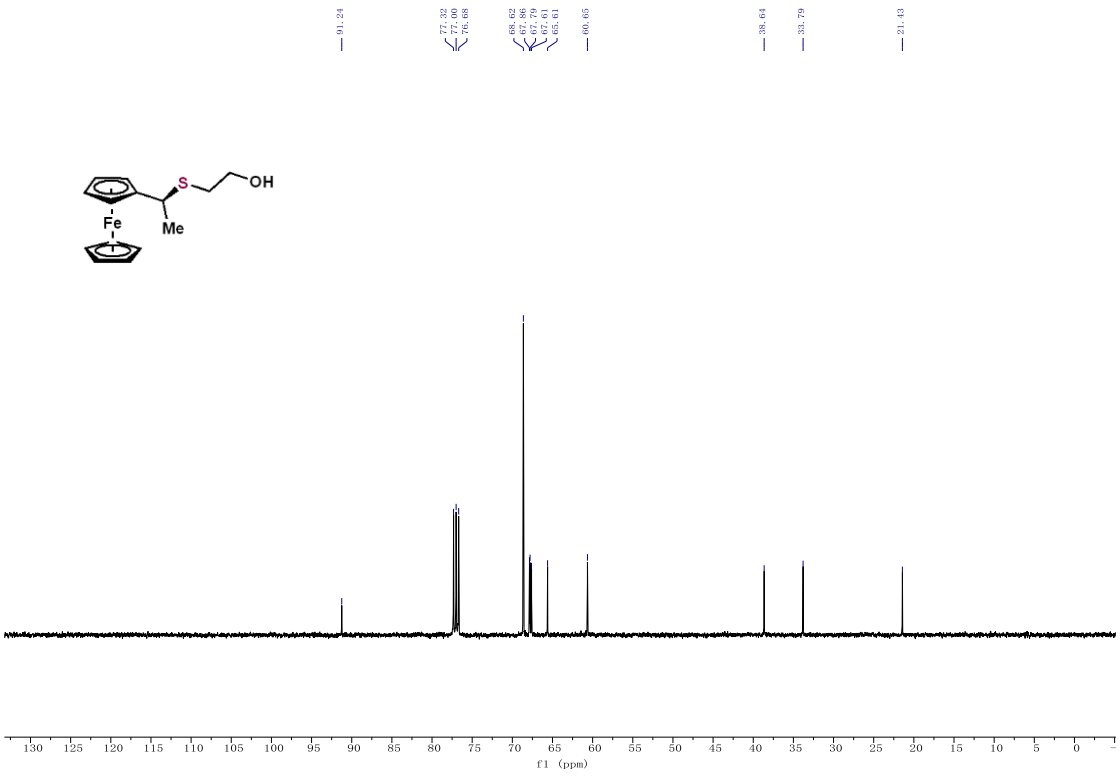


(S)-1-(2-hydroxyethylthio)ethylferrocene (16)

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

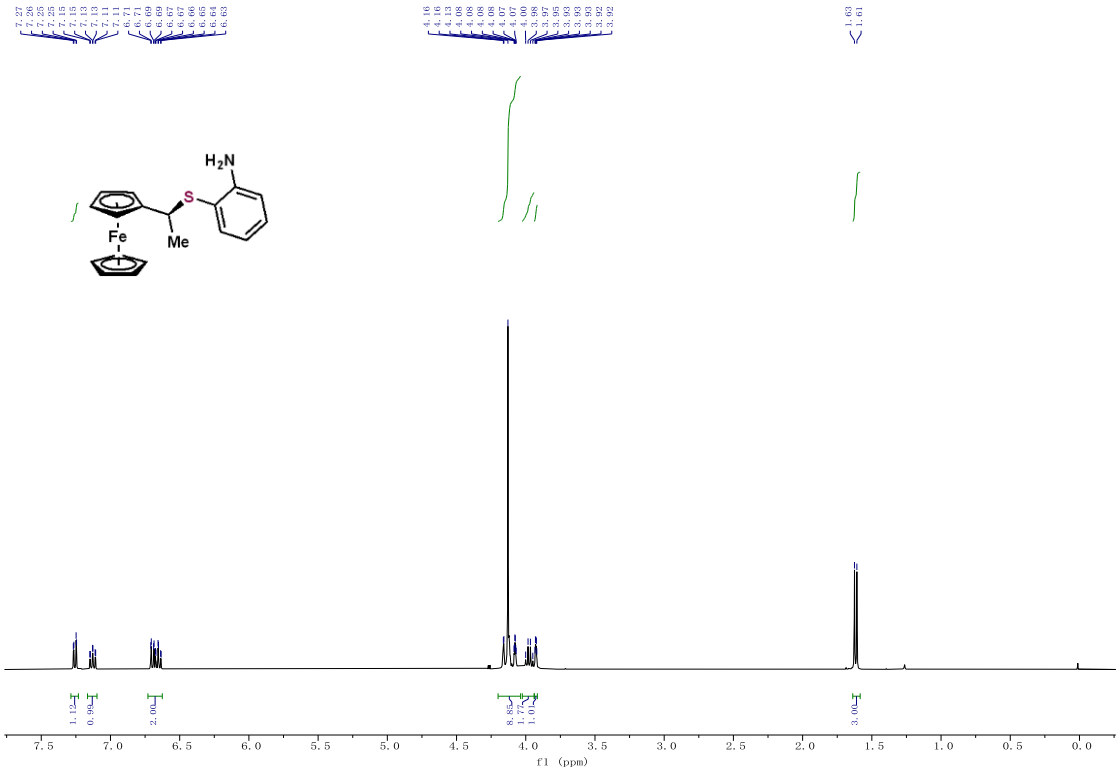


^{13}C NMR (101 MHz, $CDCl_3$)

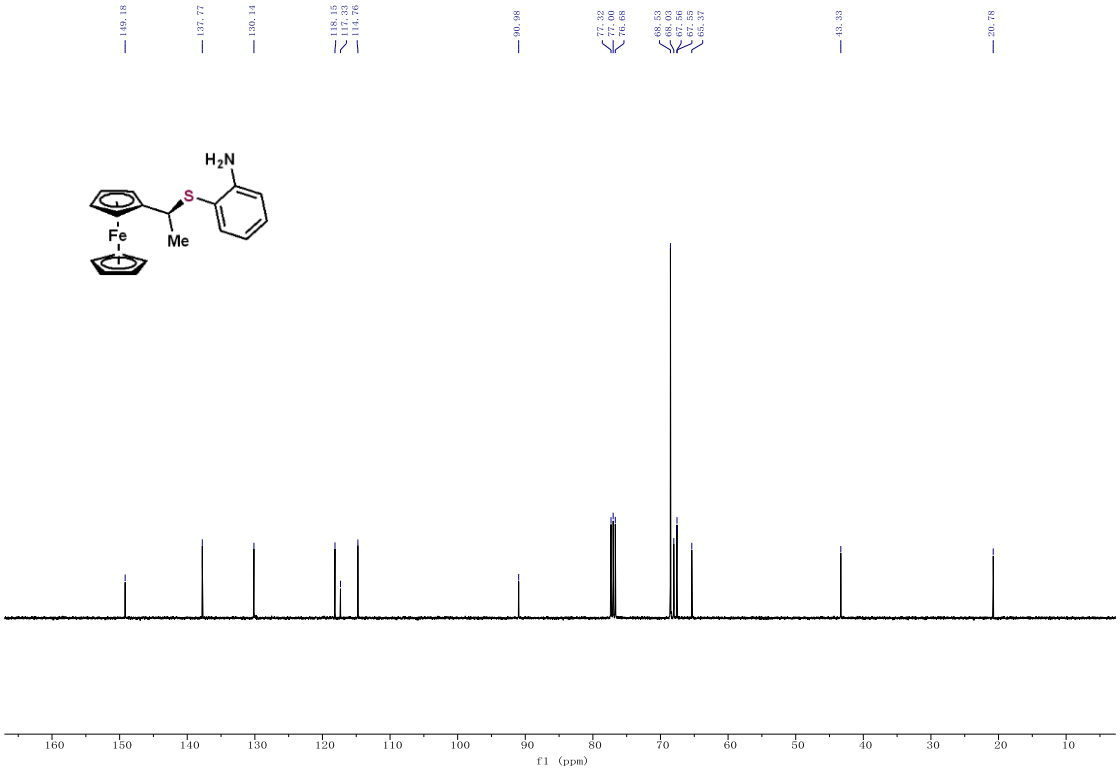


(S)-2-((1-(ferrocene)ethyl)thio)aniline (17)

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

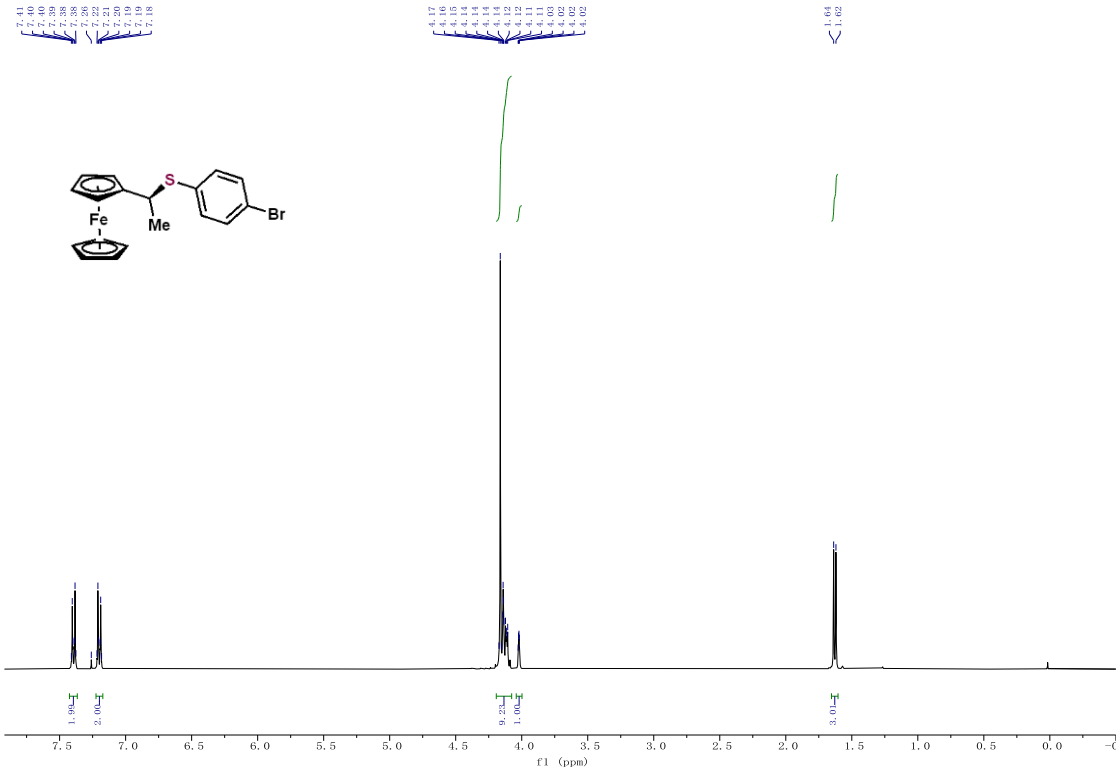


^{13}C NMR (101 MHz, $CDCl_3$)

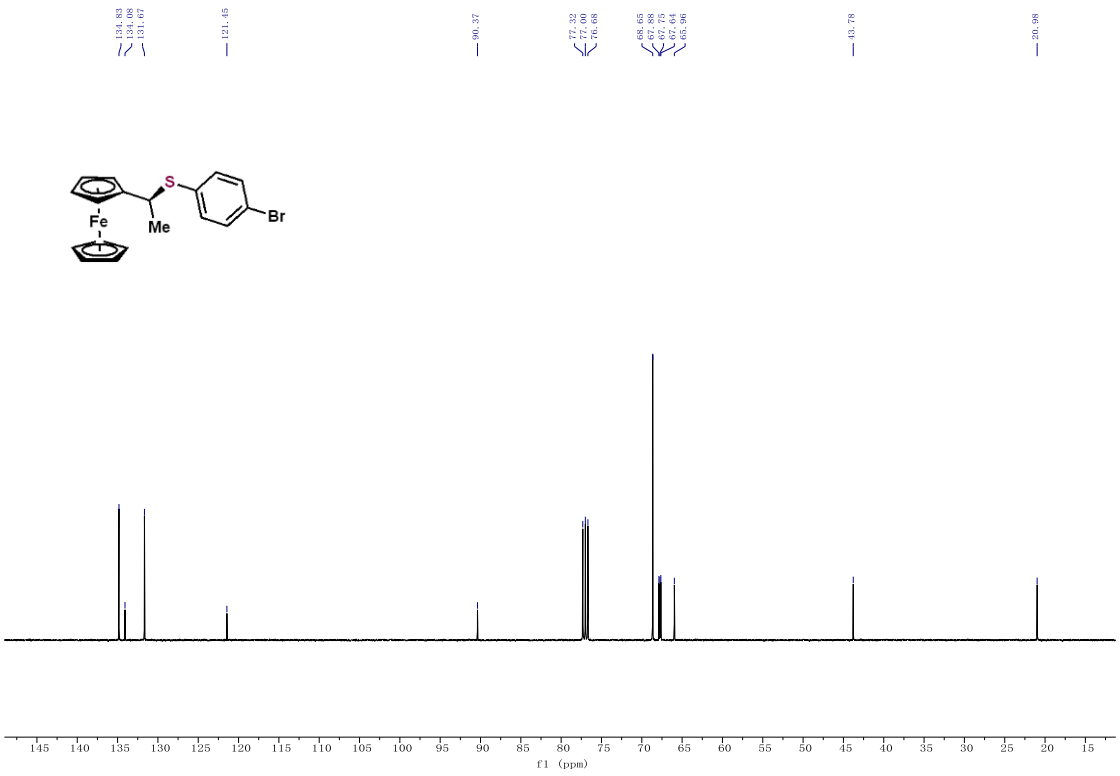


(S)-1-((4-bromophenyl)thio)ethylferrocene (18)

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

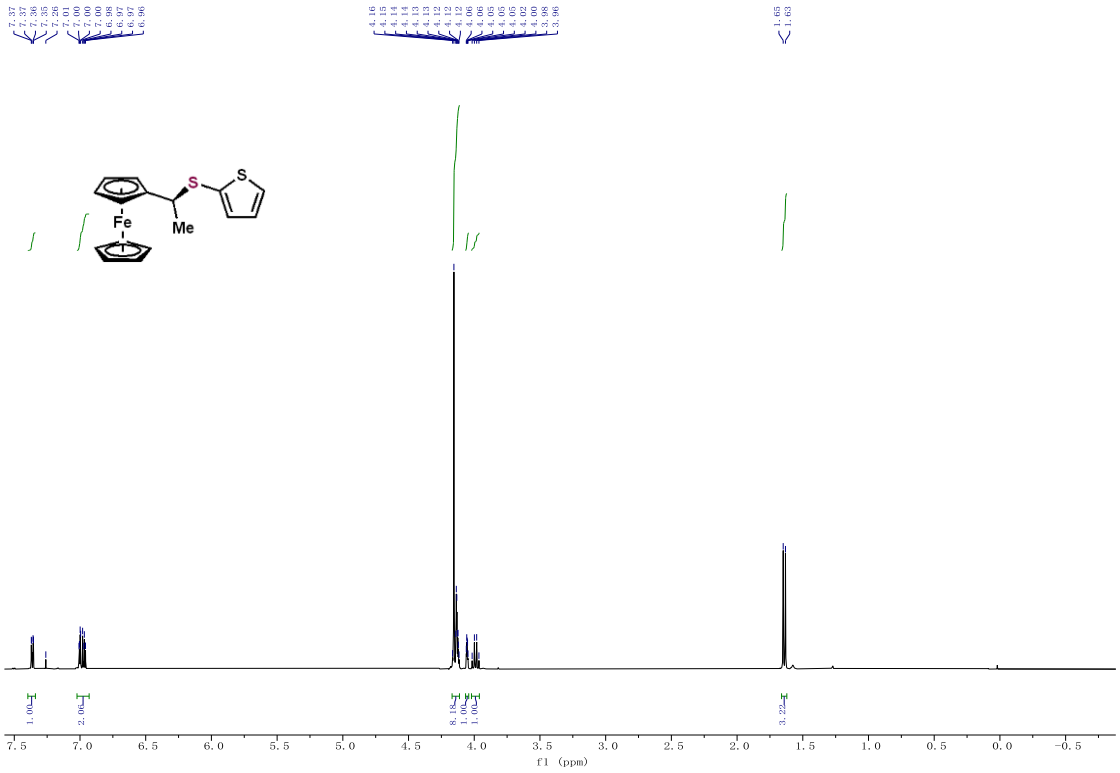


^{13}C NMR (101 MHz, $CDCl_3$)

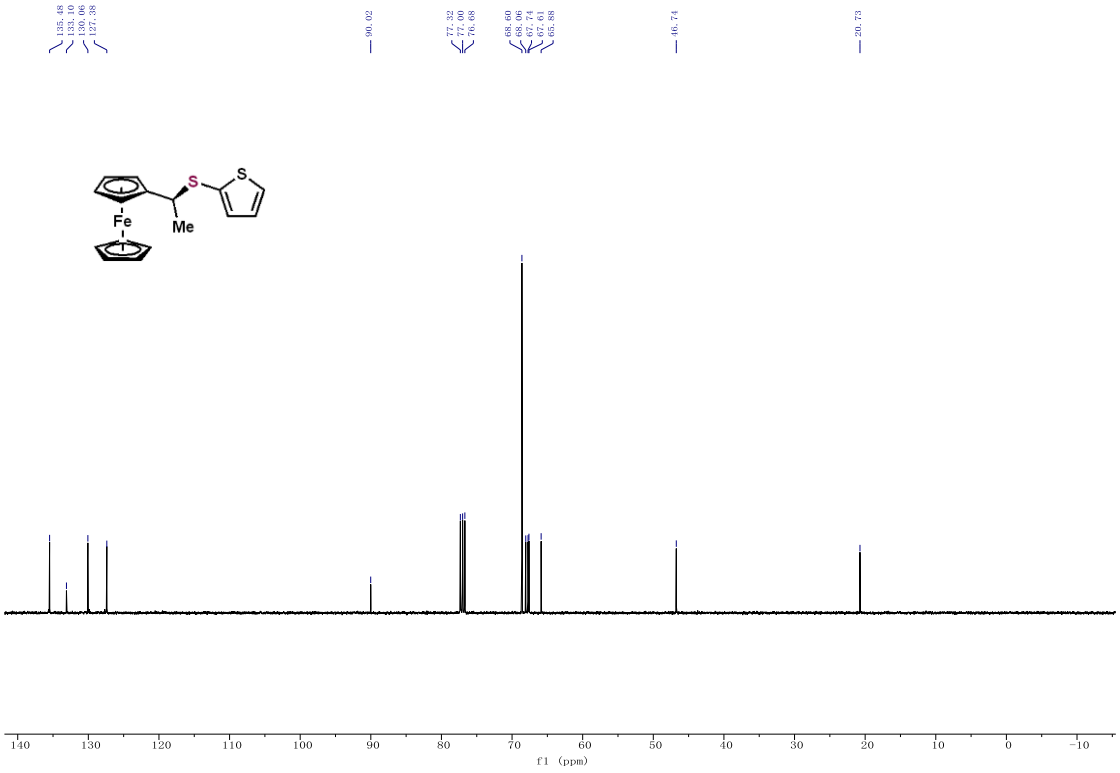


(S)-2-(1-(thiophen-2-ylthio)ethyl)ferrocene (19)

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

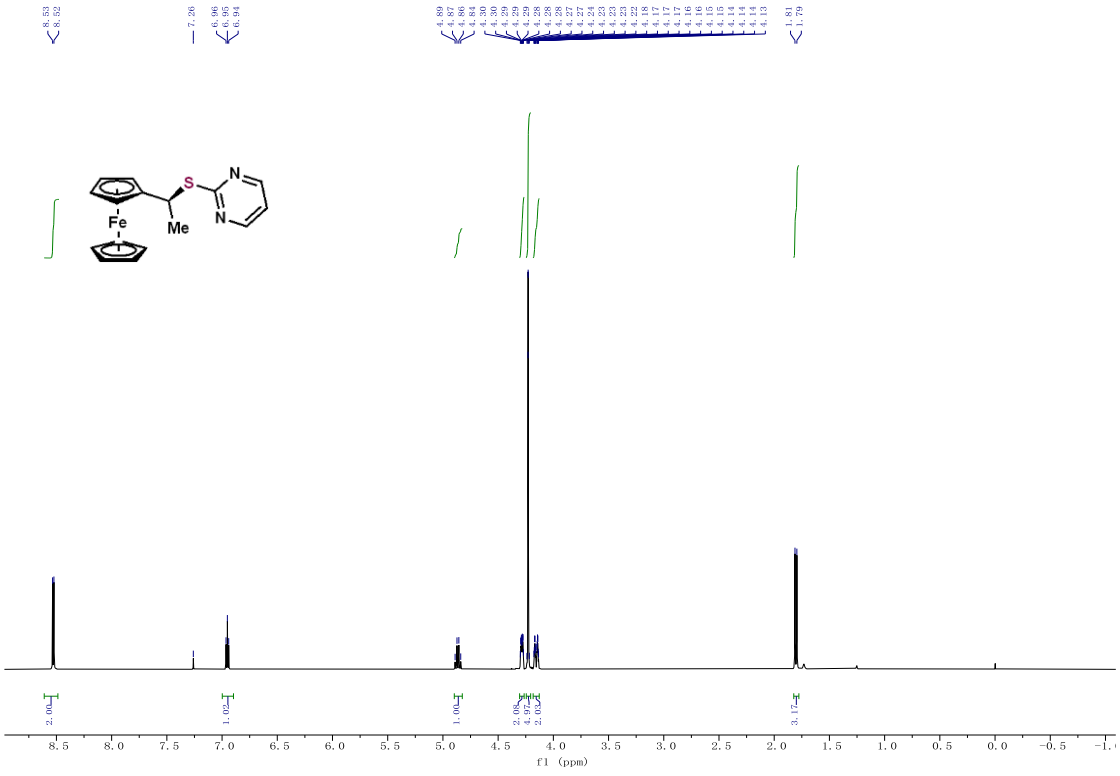


^{13}C NMR (101 MHz, $CDCl_3$)

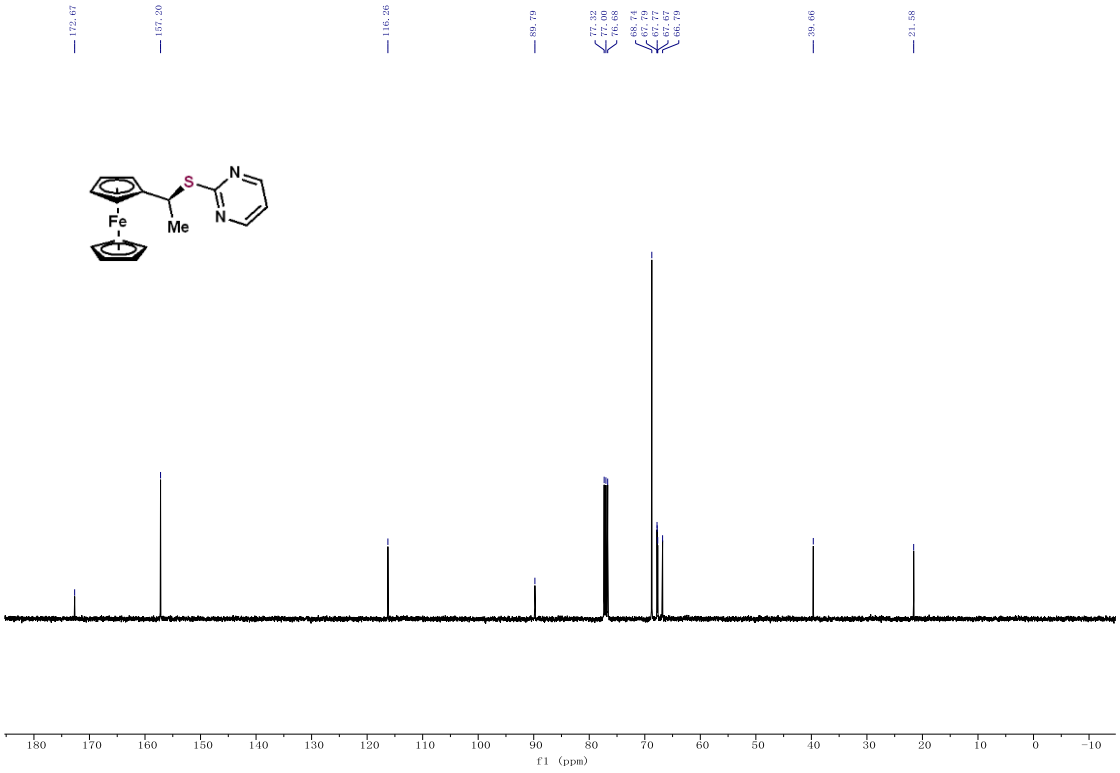


(S)-2-((1-(ferrocene-2-yl)ethyl)thio)pyrimidine (20)

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

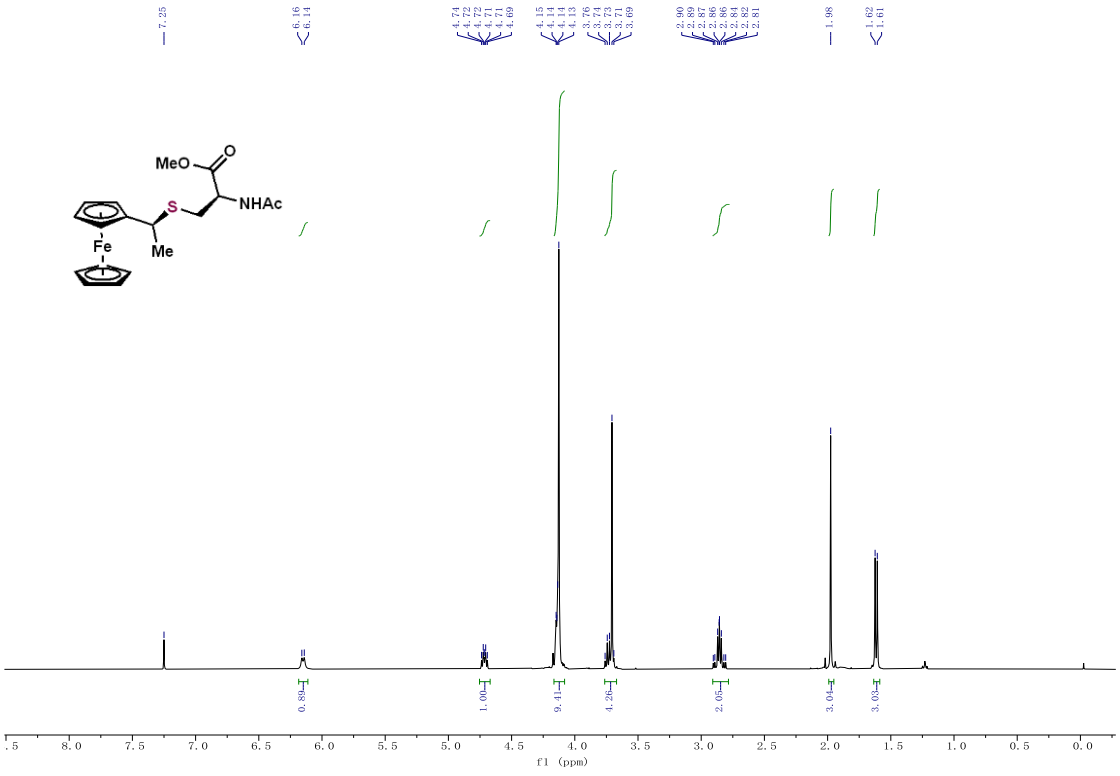


^{13}C NMR (101 MHz, $CDCl_3$)

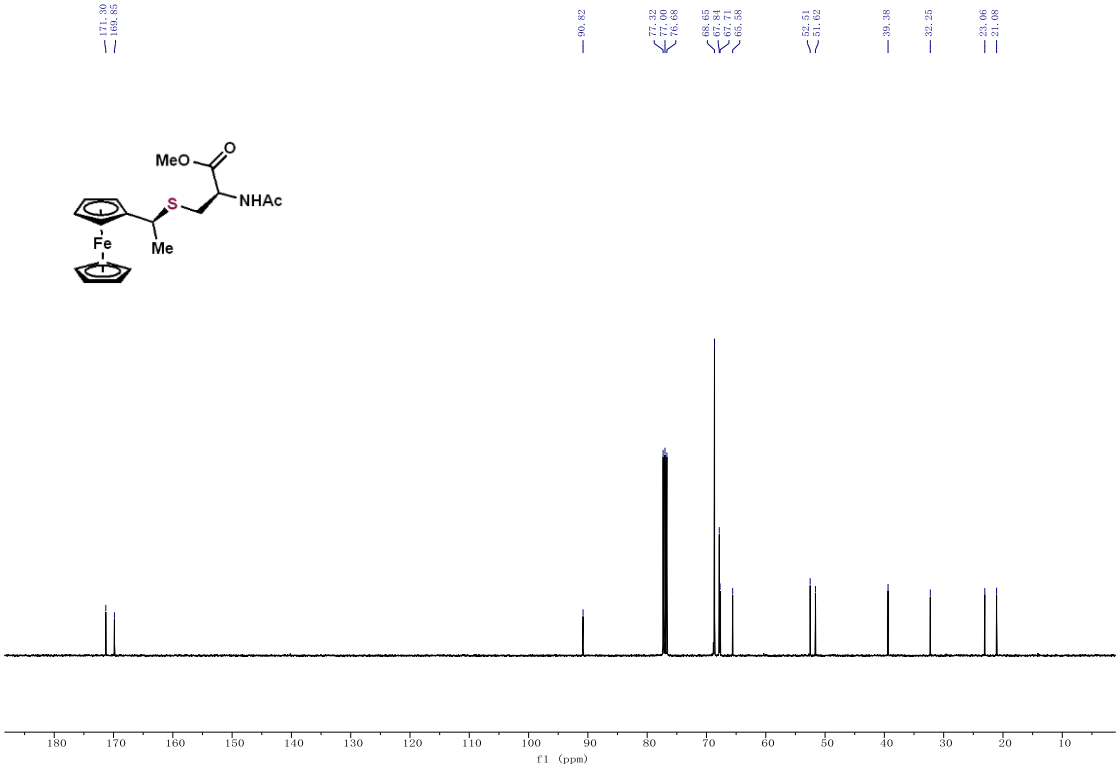


methyl N-acetyl-S-((*S*)-1-(ferrocene-2-yl)ethyl)-L-cysteinate (21)

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

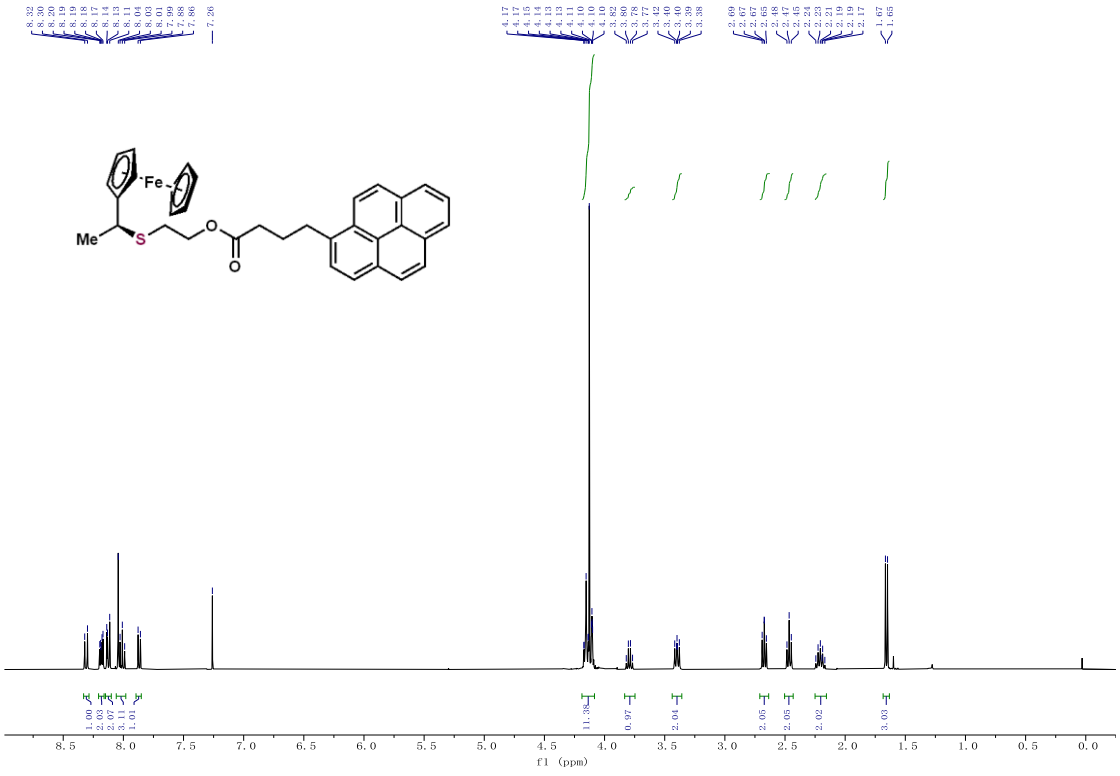


^{13}C NMR (101 MHz, $CDCl_3$)

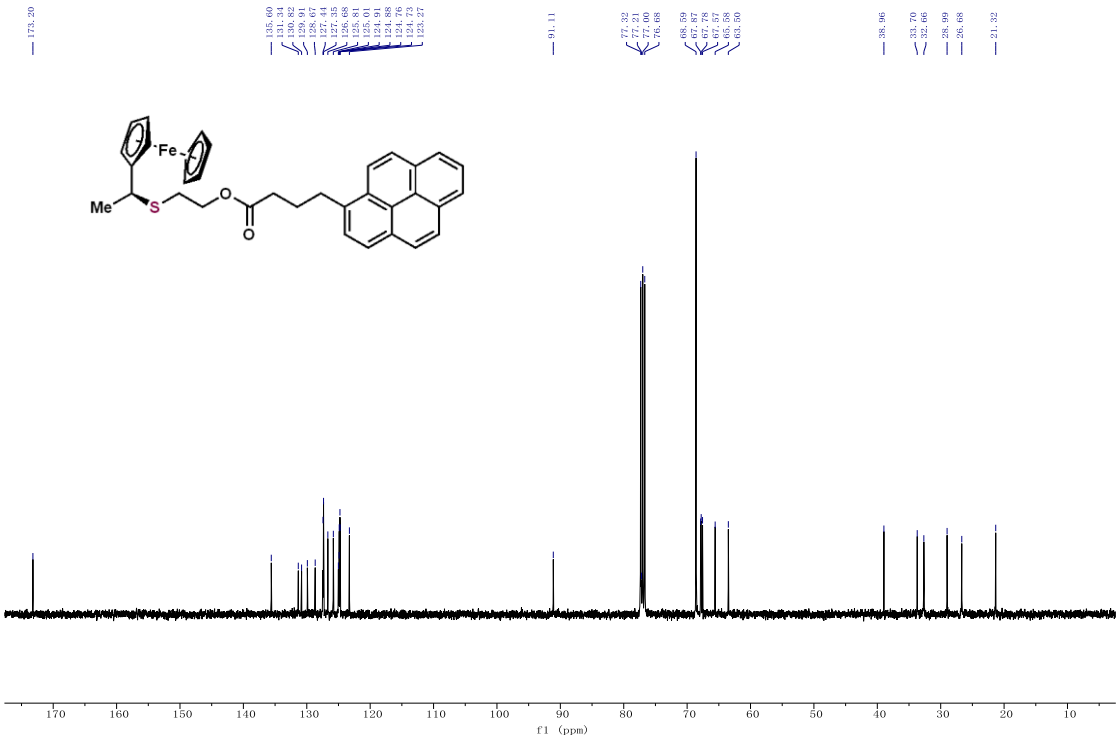


(S)-2-((1-(ferrocene-2-yl)ethyl)thio)ethyl 4-(pyren-1-yl)butanoate (22)

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

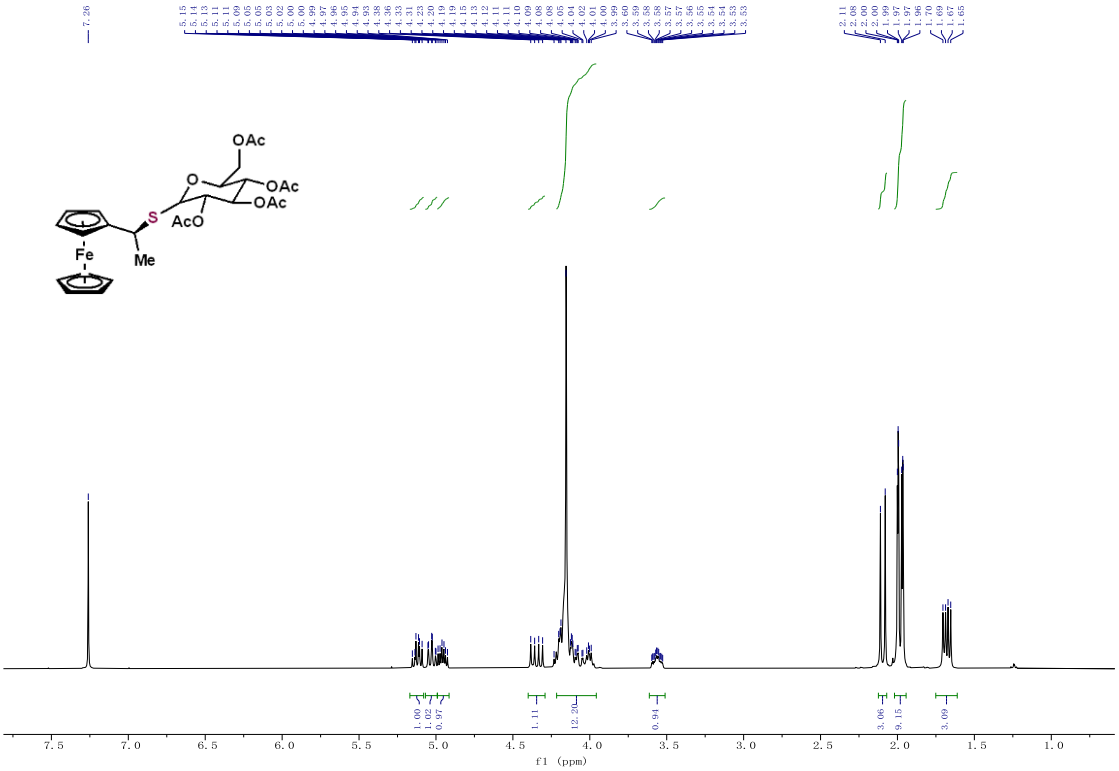


^{13}C NMR (101 MHz, $CDCl_3$)

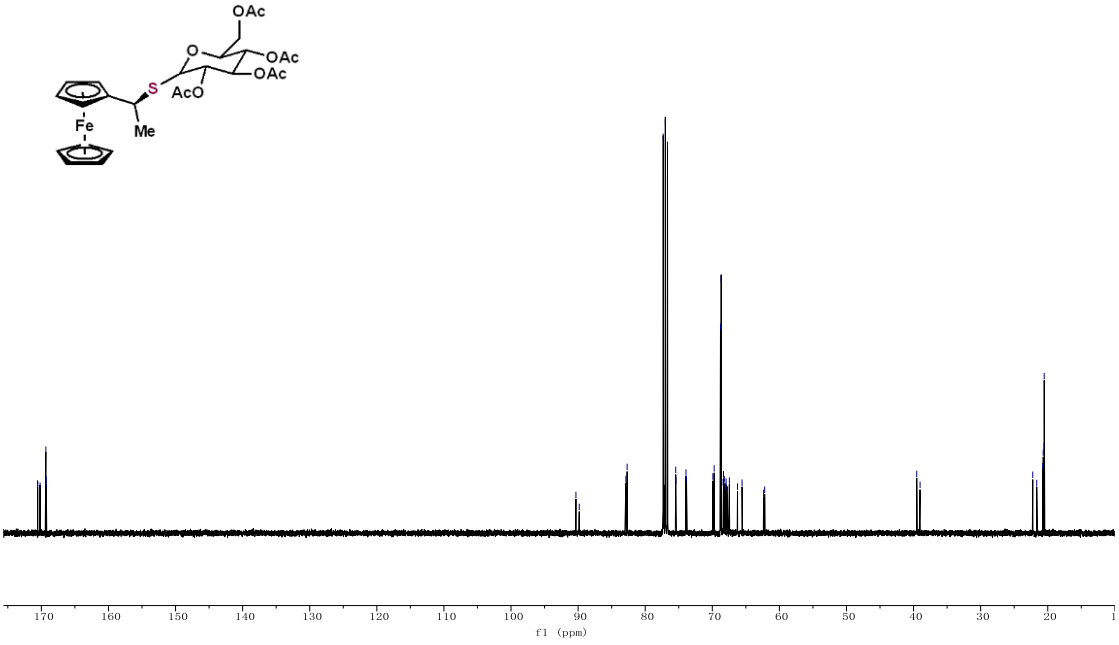


(2S,3S,4R,5S)-2-(acetoxymethyl)-6-(((*S*)-1-((ferrocene-2-yl)ethyl)thio)tetrahydro-2H-pyran-3,4,5-triyl triacetate (23)

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

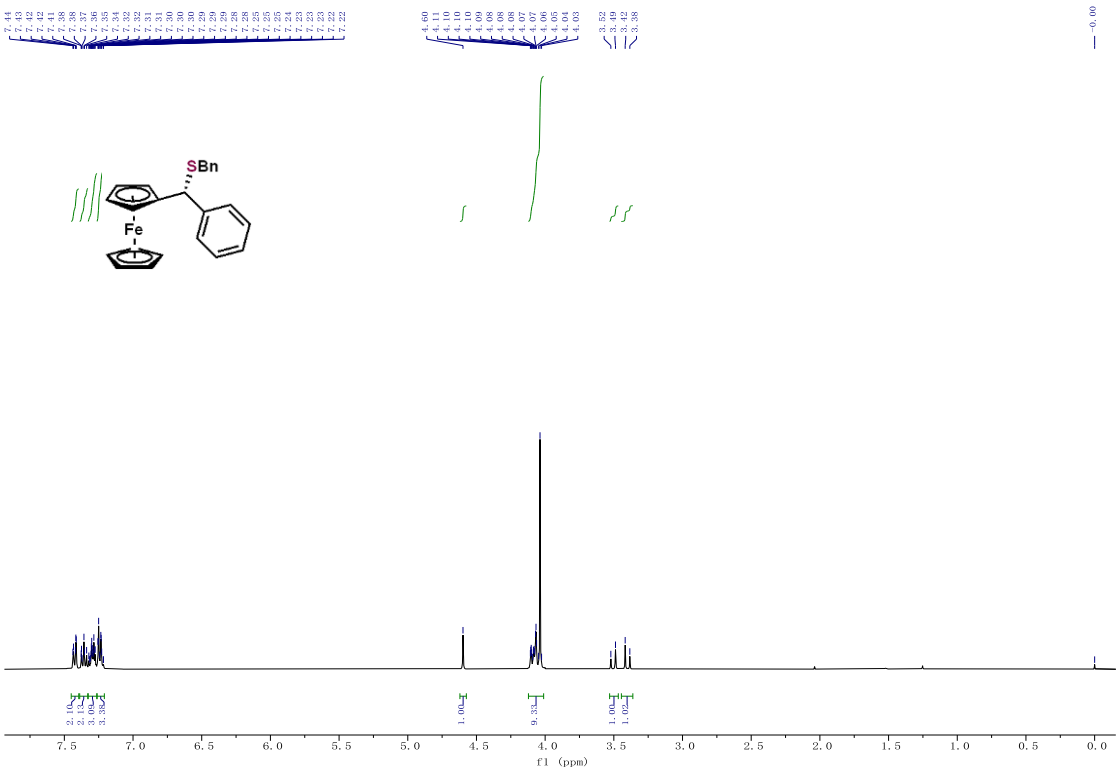


^{13}C NMR (101 MHz, $CDCl_3$)

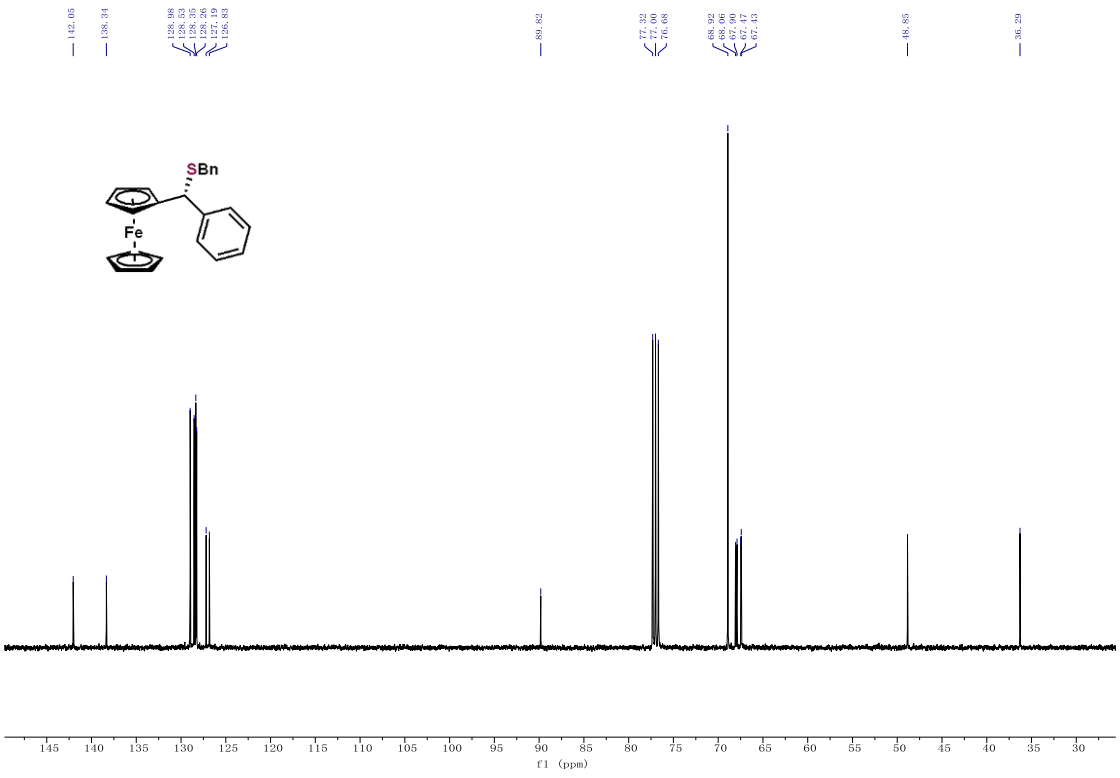


(S)-2-((benzylthio)(phenyl)methyl) ferrocene (24)

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

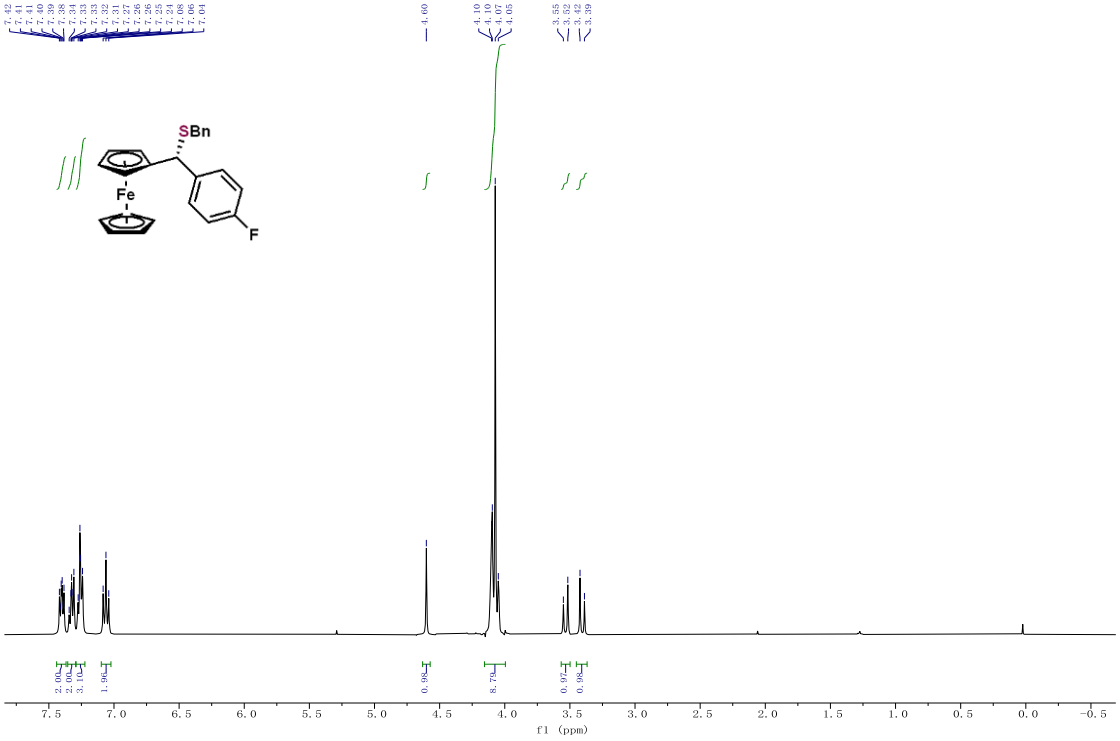


^{13}C NMR (101 MHz, $CDCl_3$)

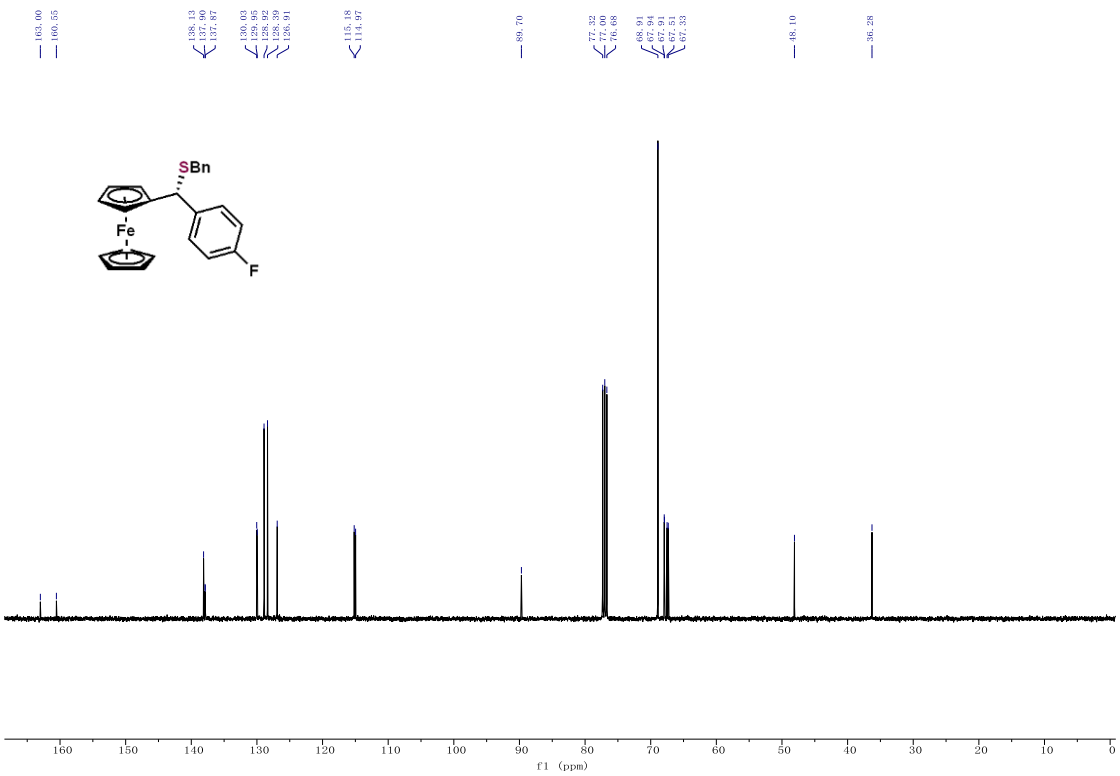


(S)-2-((benzylthio)(4-fluorophenyl)methyl) ferrocene (25)

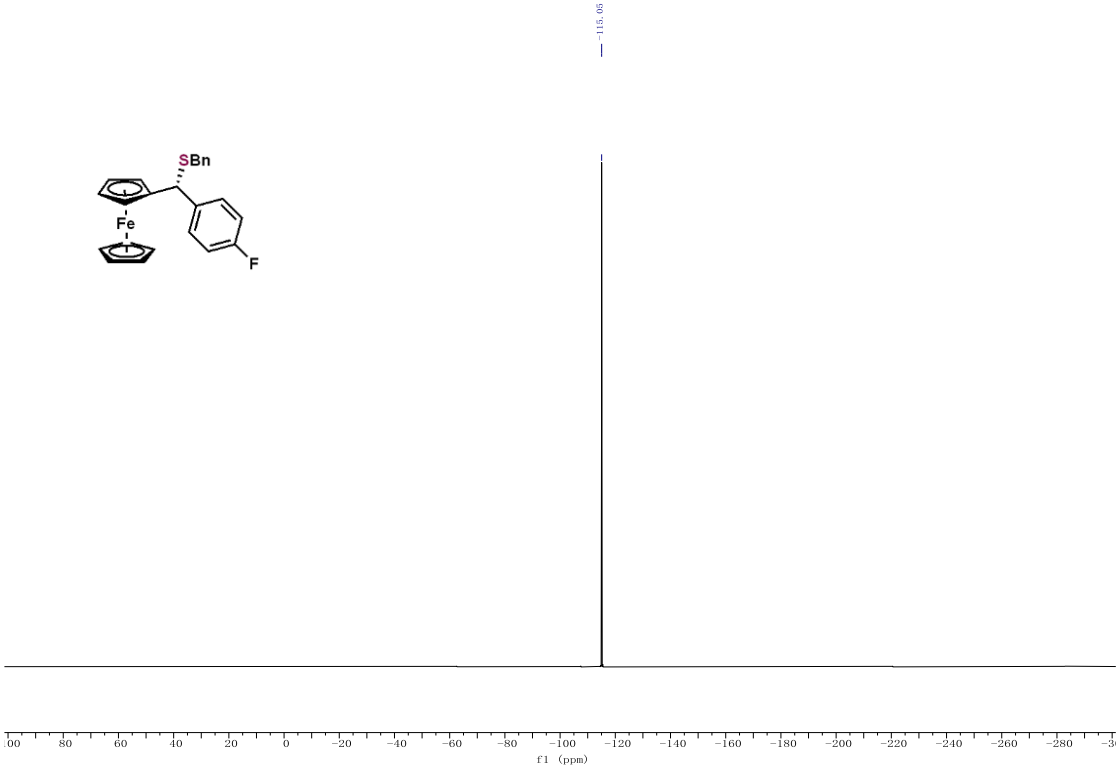
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)

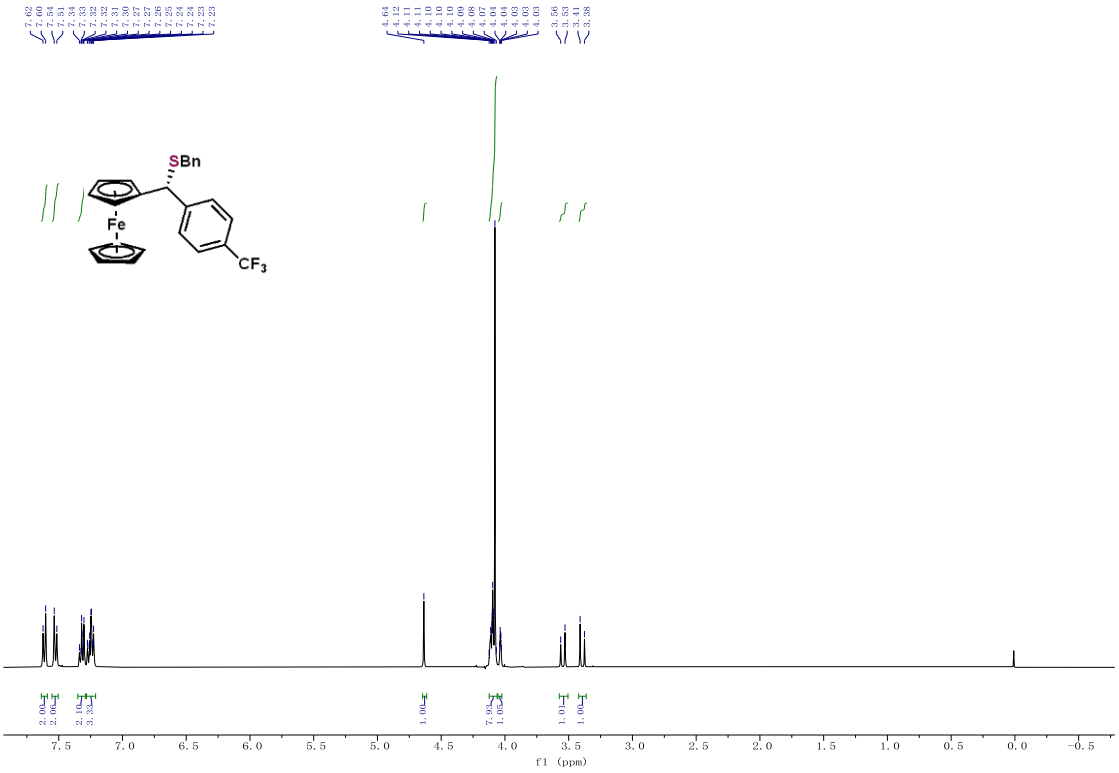


^{19}F NMR (376 MHz, $CDCl_3$)

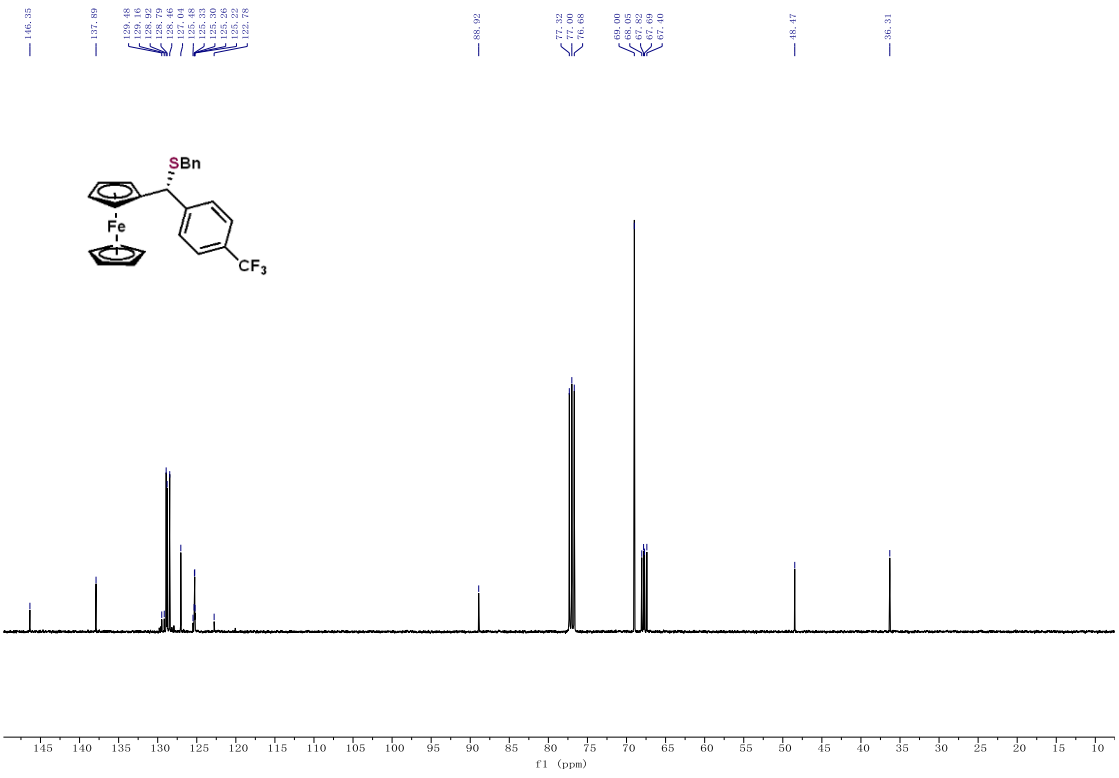


(S)-2-((benzylthio)(4-(trifluoromethyl)phenyl)methyl) ferrocene (26)

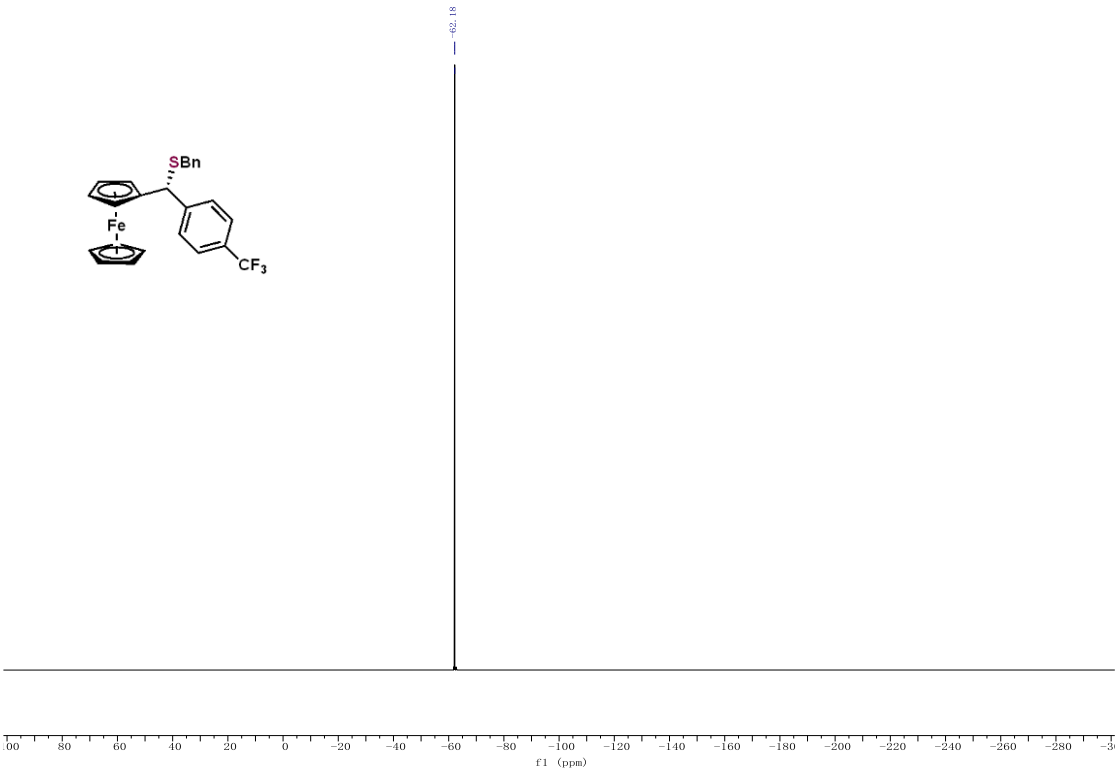
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)

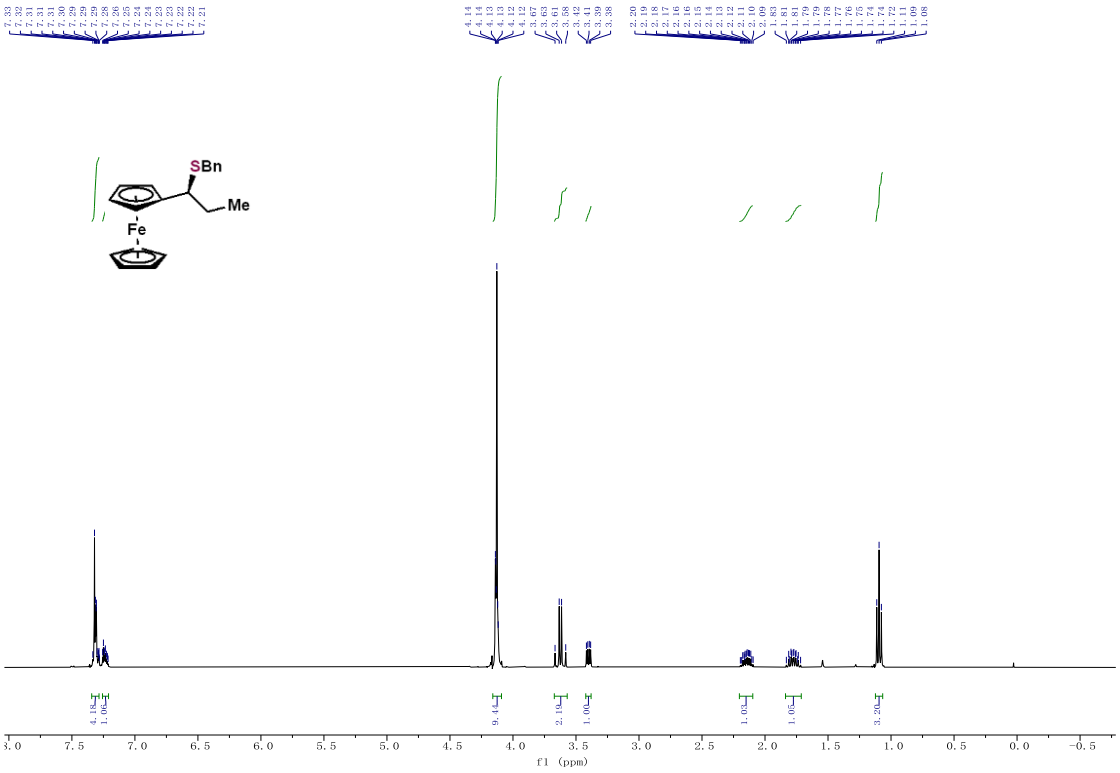


^{19}F NMR (376 MHz, $CDCl_3$)

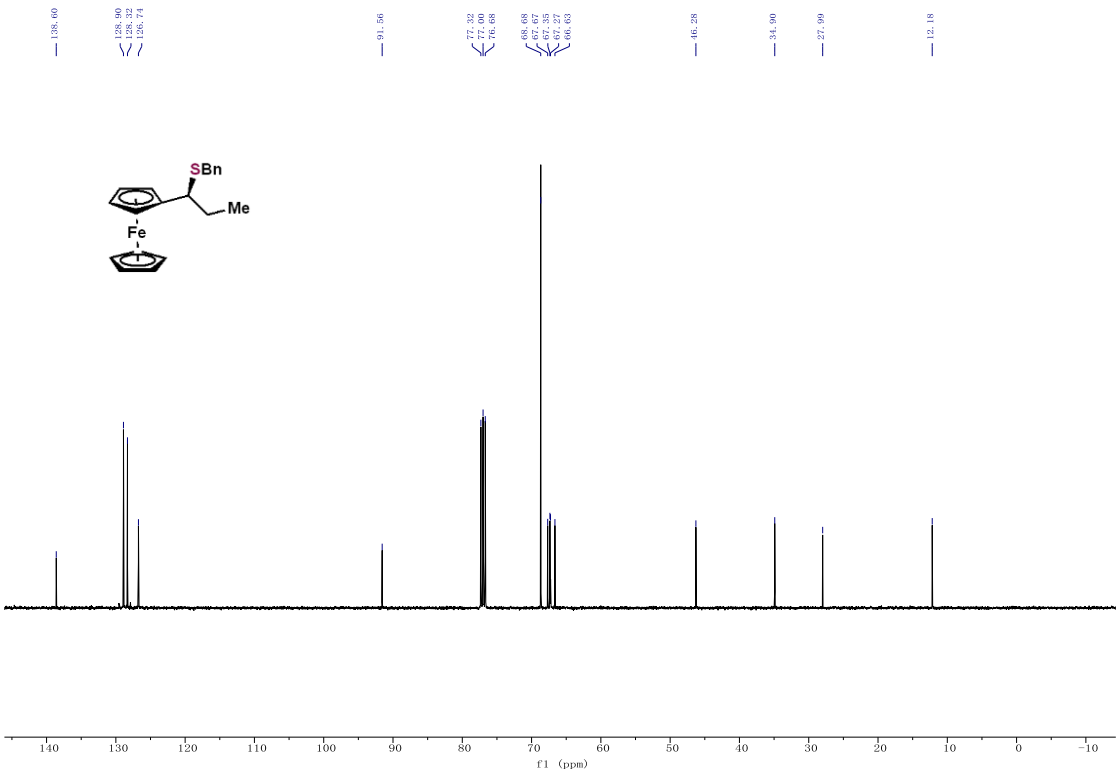


(S)-1-(benzylthio)propylferrocene (27)

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

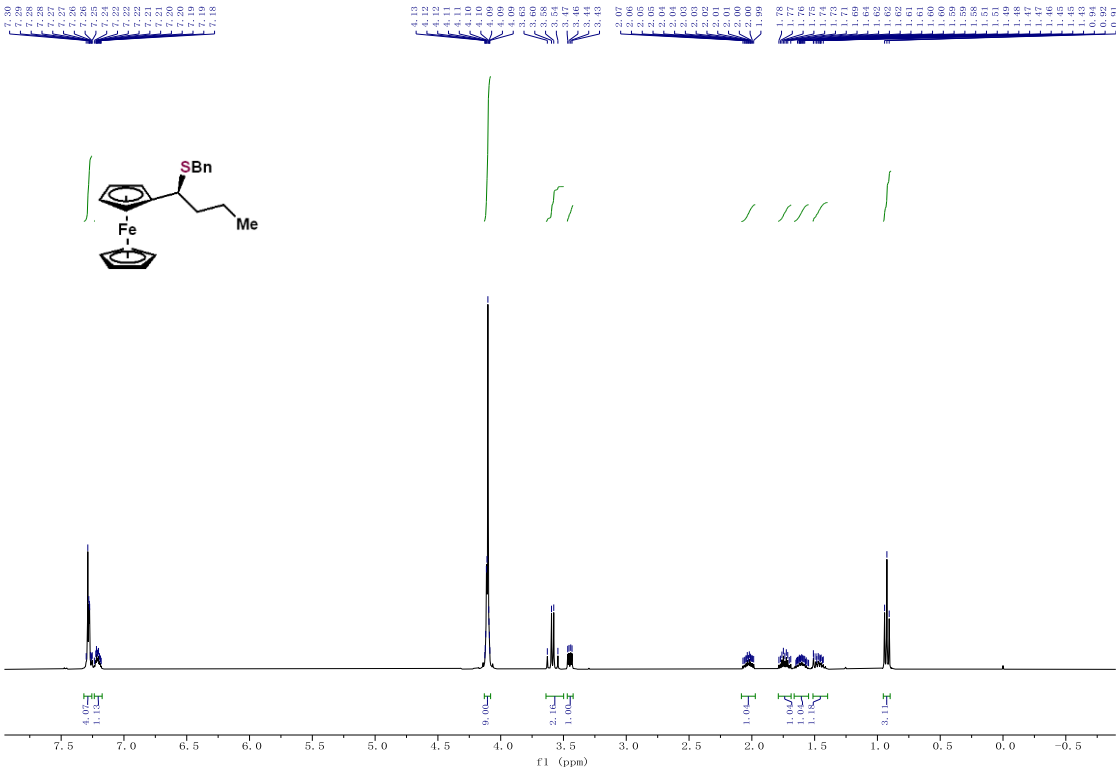


^{13}C NMR (101 MHz, $CDCl_3$)

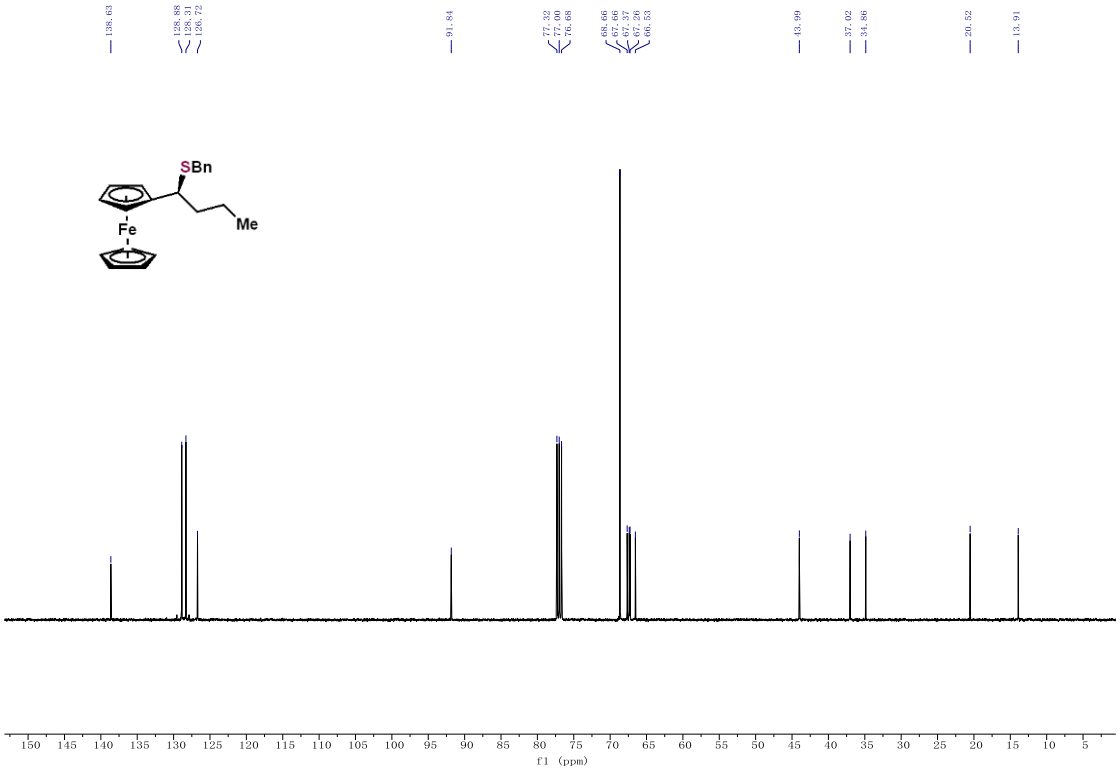


(S)-1-(benzylthio)butylferrocene (28)

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

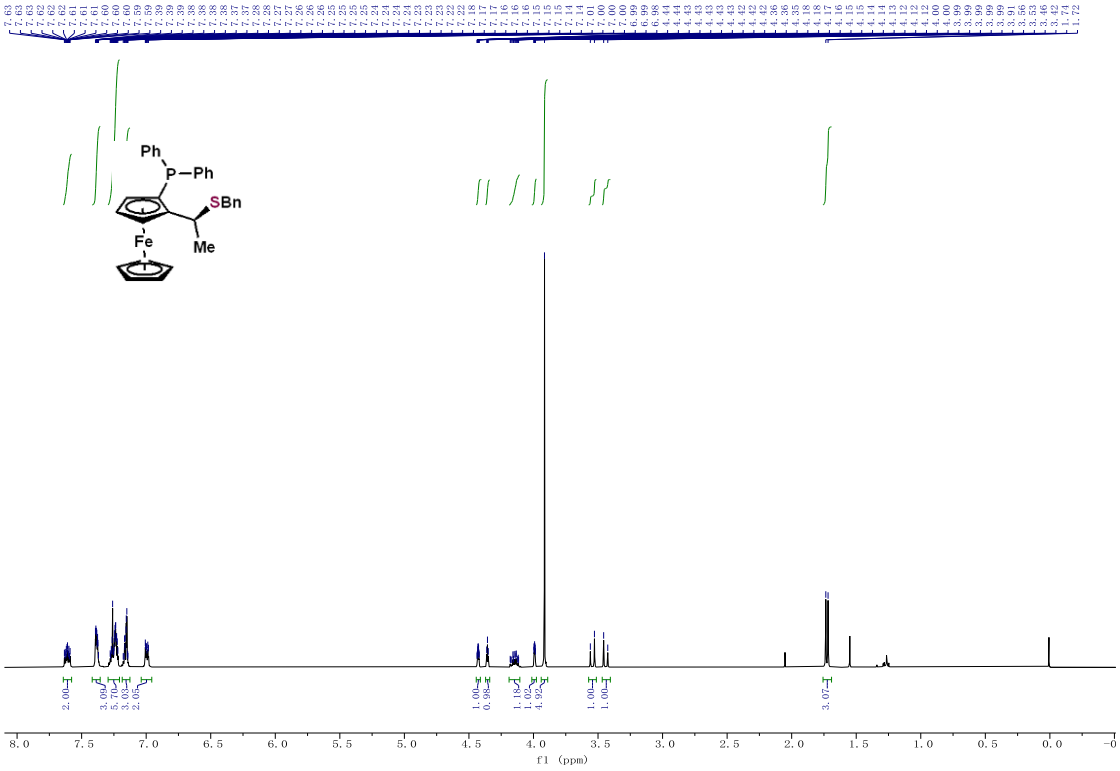


^{13}C NMR (101 MHz, $CDCl_3$)

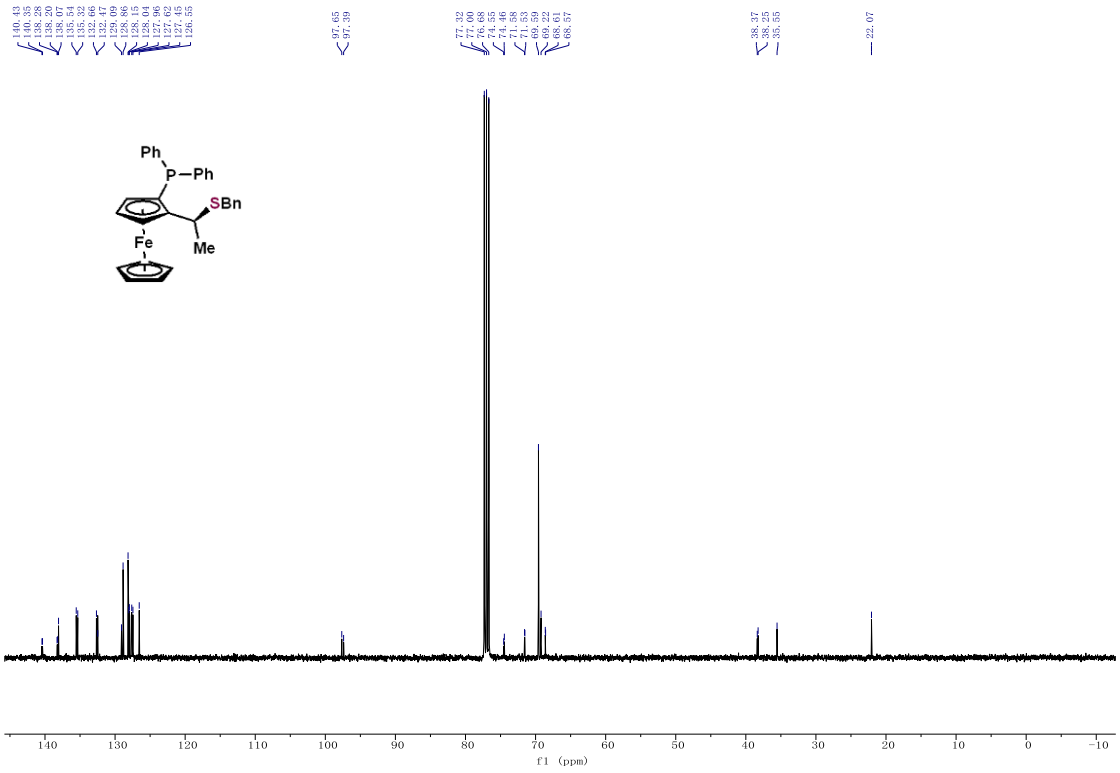


(*S*,$_p$*R*)-2-(1-Benzylthio)-1-diphenylphosphino-ferrocene (29)

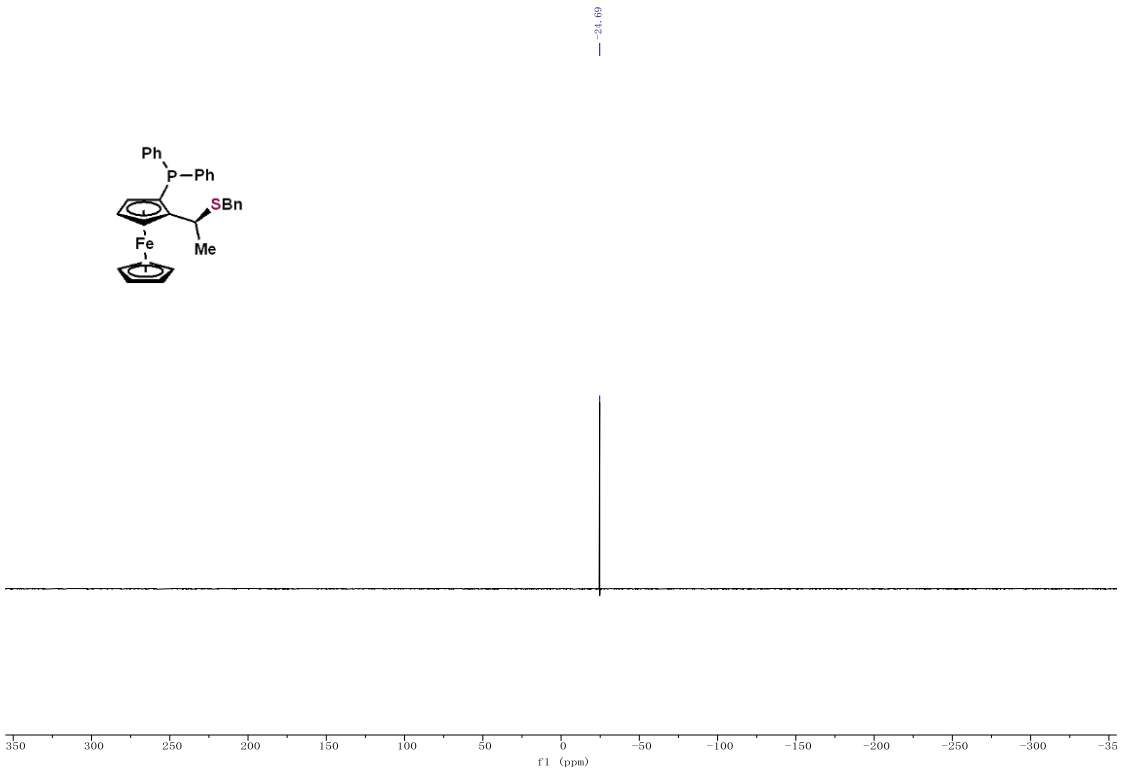
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)

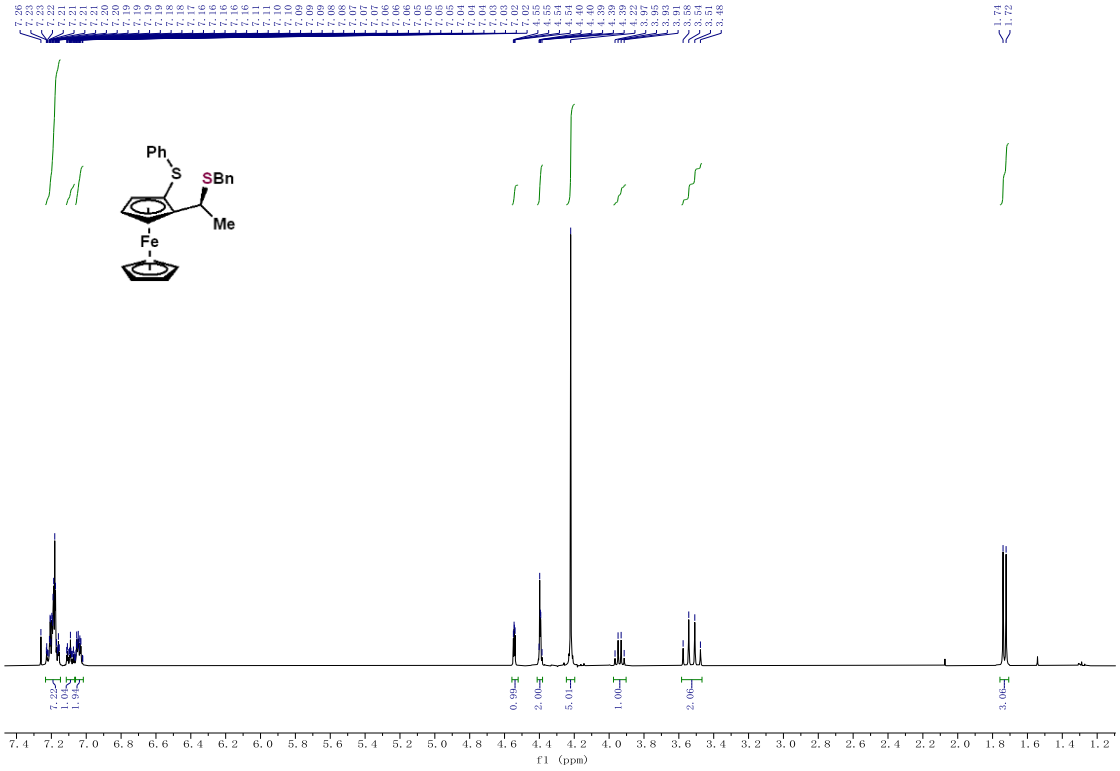


^{31}P NMR (160 MHz, $CDCl_3$)

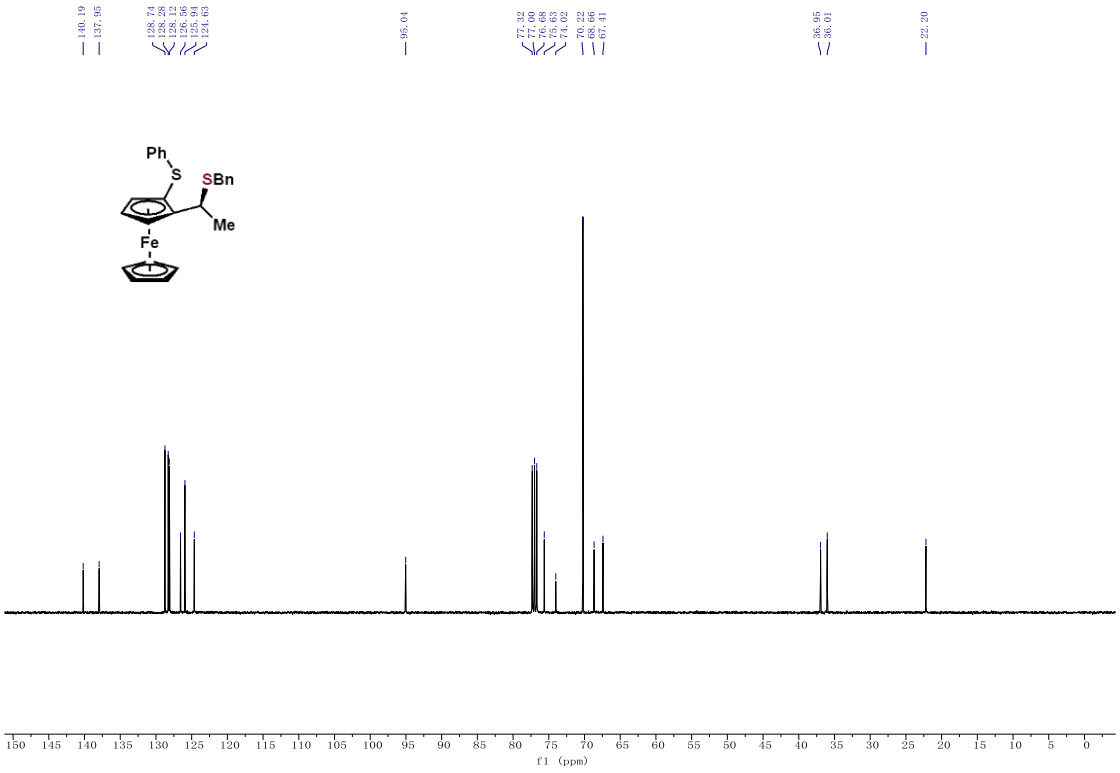


(*S*,$_p$*R*)-2-(1-Benzylthio)-1-phenylthio-ferrocene (30)

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

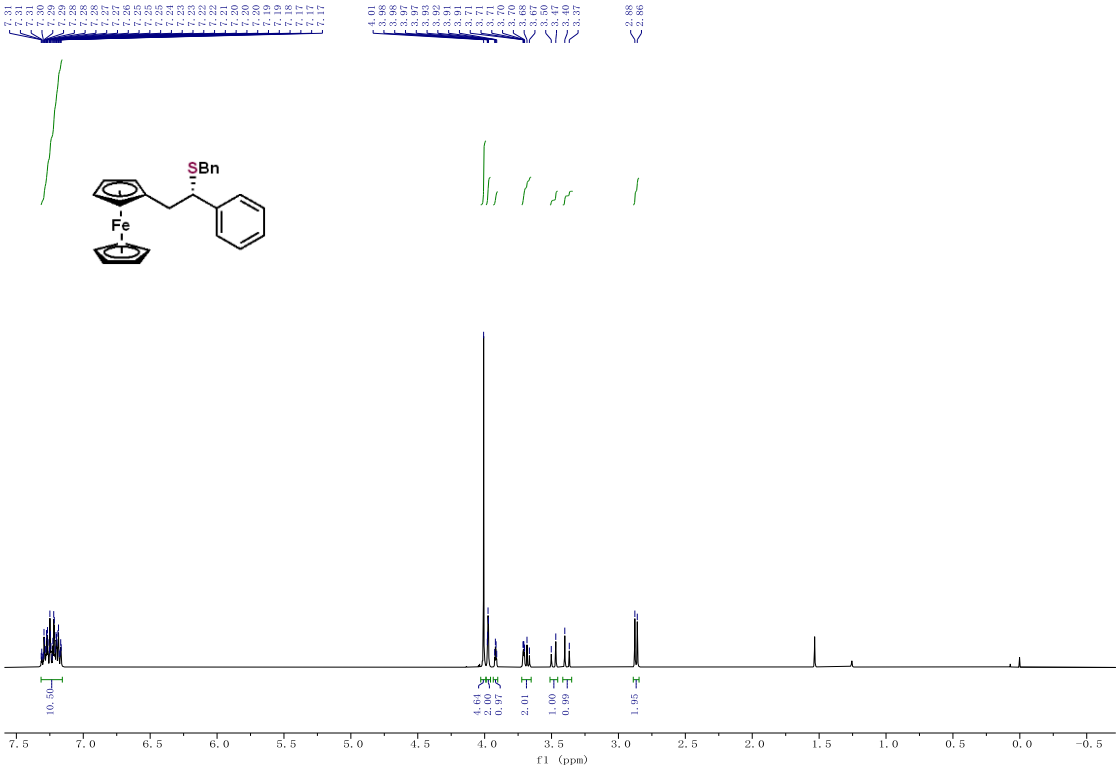


^{13}C NMR (101 MHz, $CDCl_3$)

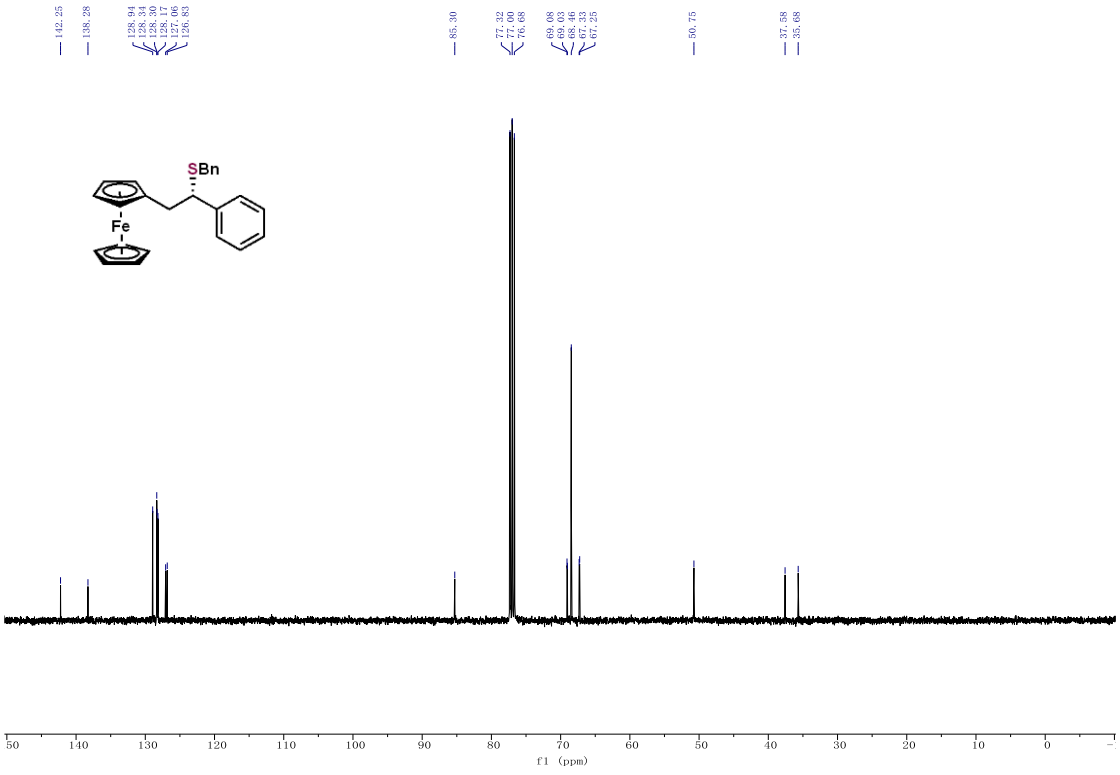


(S)-2-(benzylthio)-2-phenylethylferrocene (31)

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

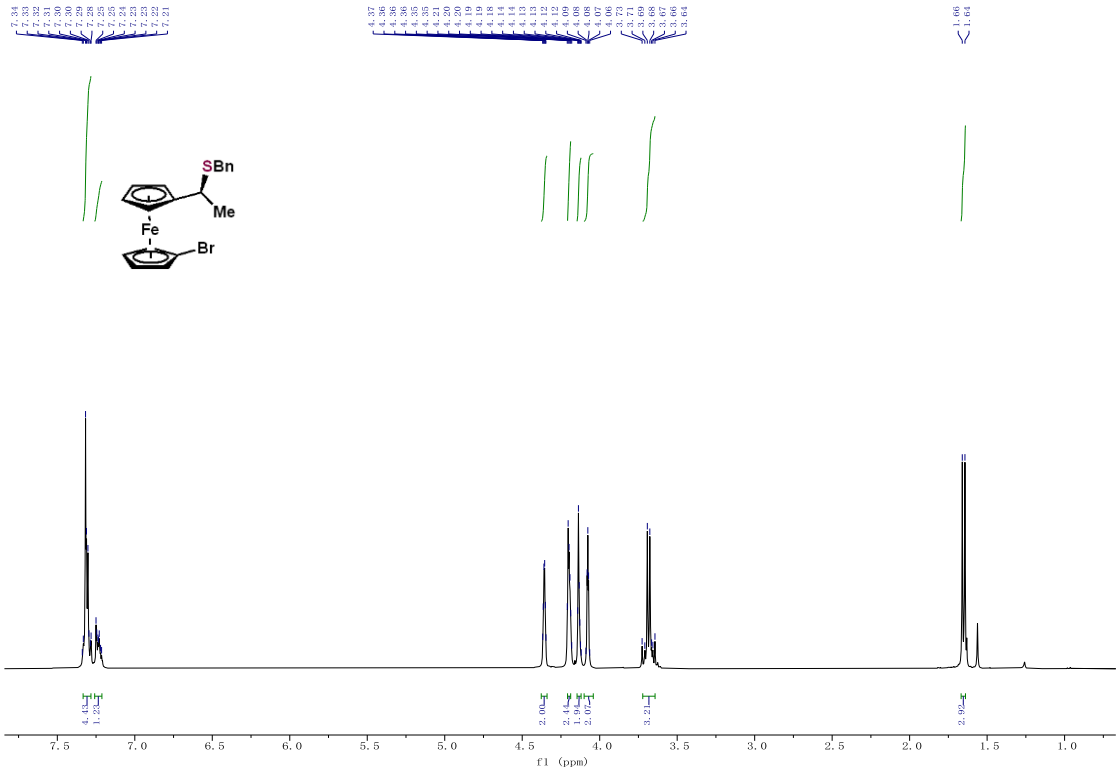


^{13}C NMR (101 MHz, $CDCl_3$)

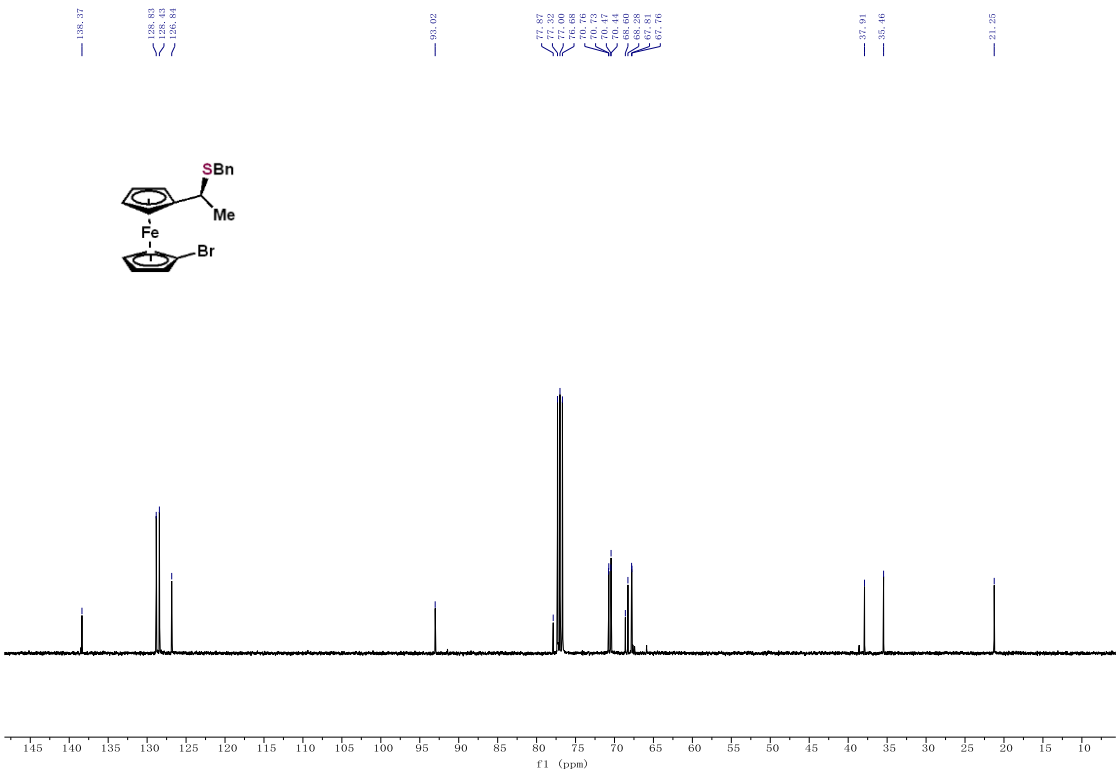


(S)-1-(1-(benzylthio)ethyl)-1'-bromoferrocene (32)

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

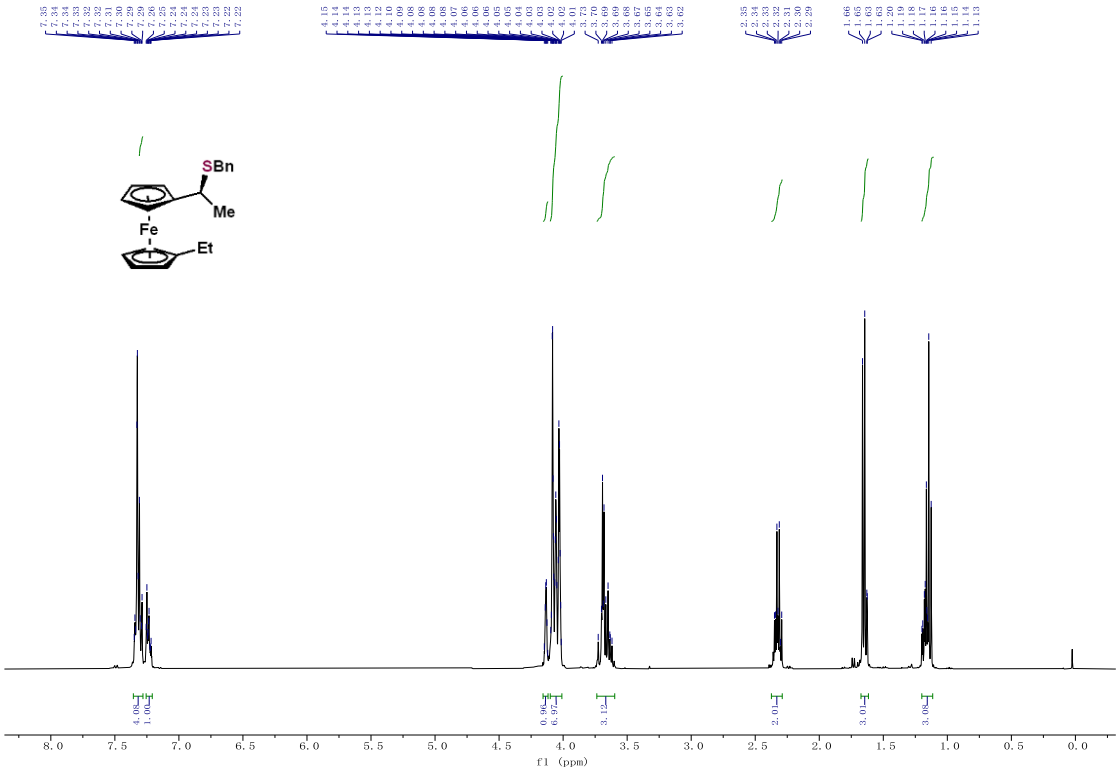


^{13}C NMR (101 MHz, $CDCl_3$)

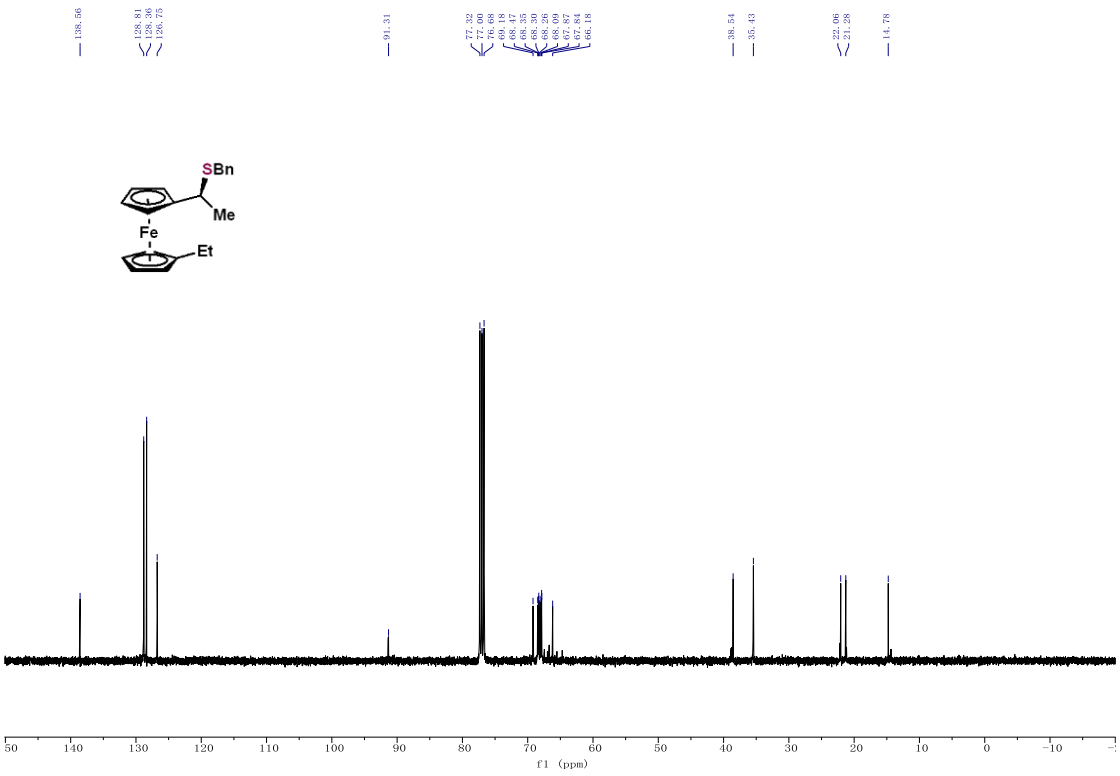


(S)-1-(1-(benzylthio)ethyl)-1'-ethylferrocene (33)

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

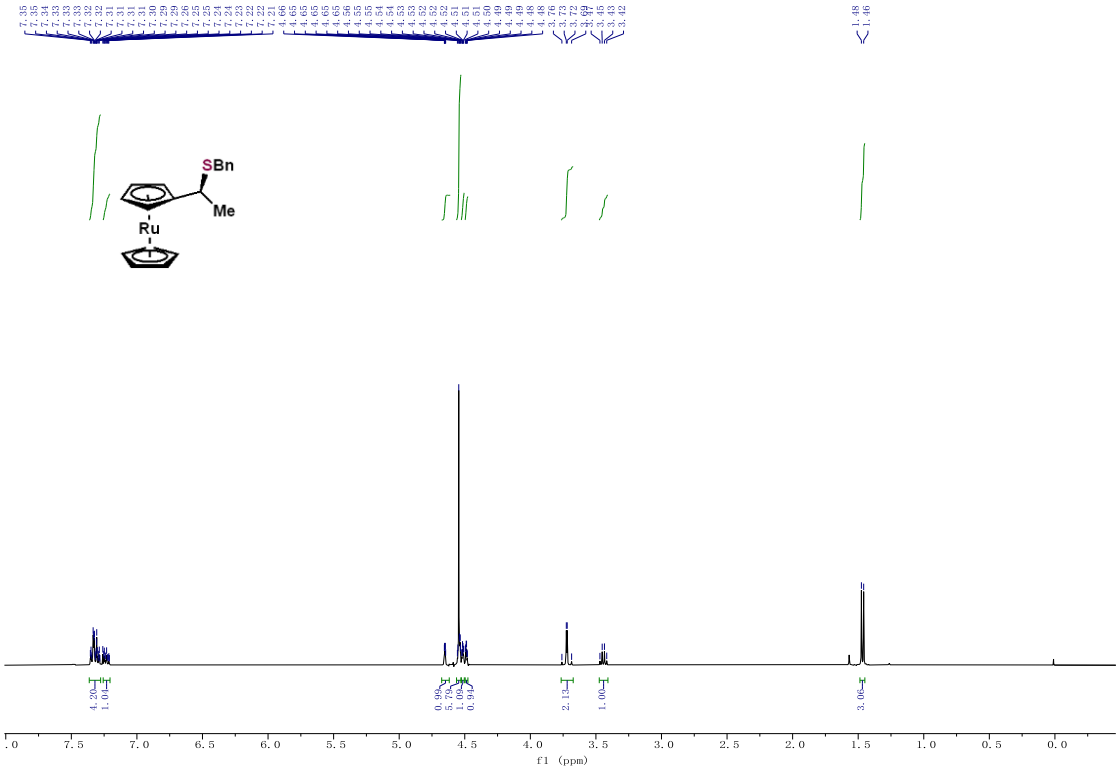


^{13}C NMR (101 MHz, $CDCl_3$)

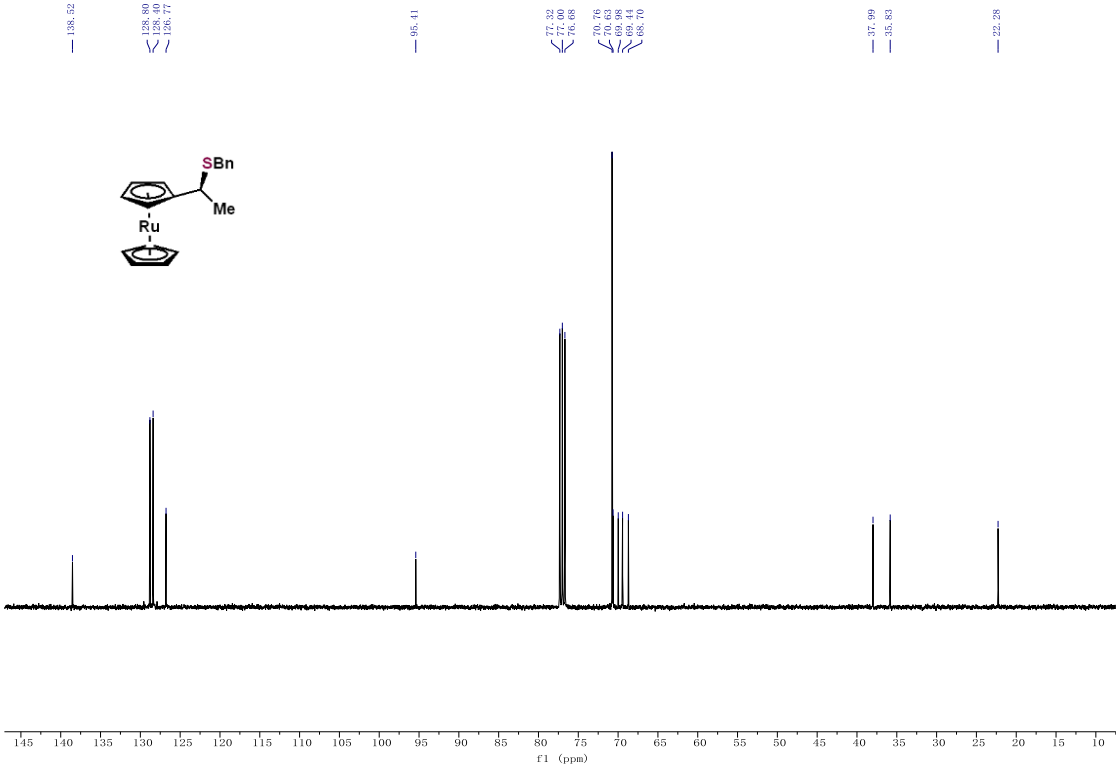


(S)-1-(benzylthio)ethylruthenocene (34)

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

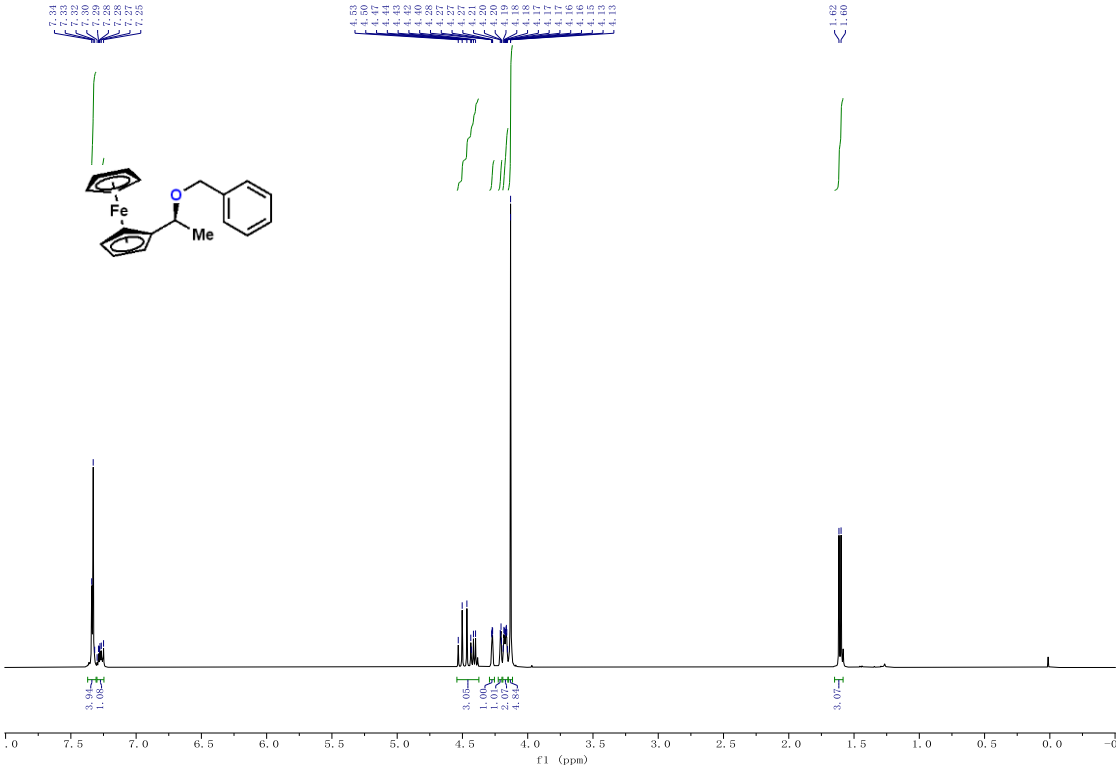


^{13}C NMR (101 MHz, $CDCl_3$)

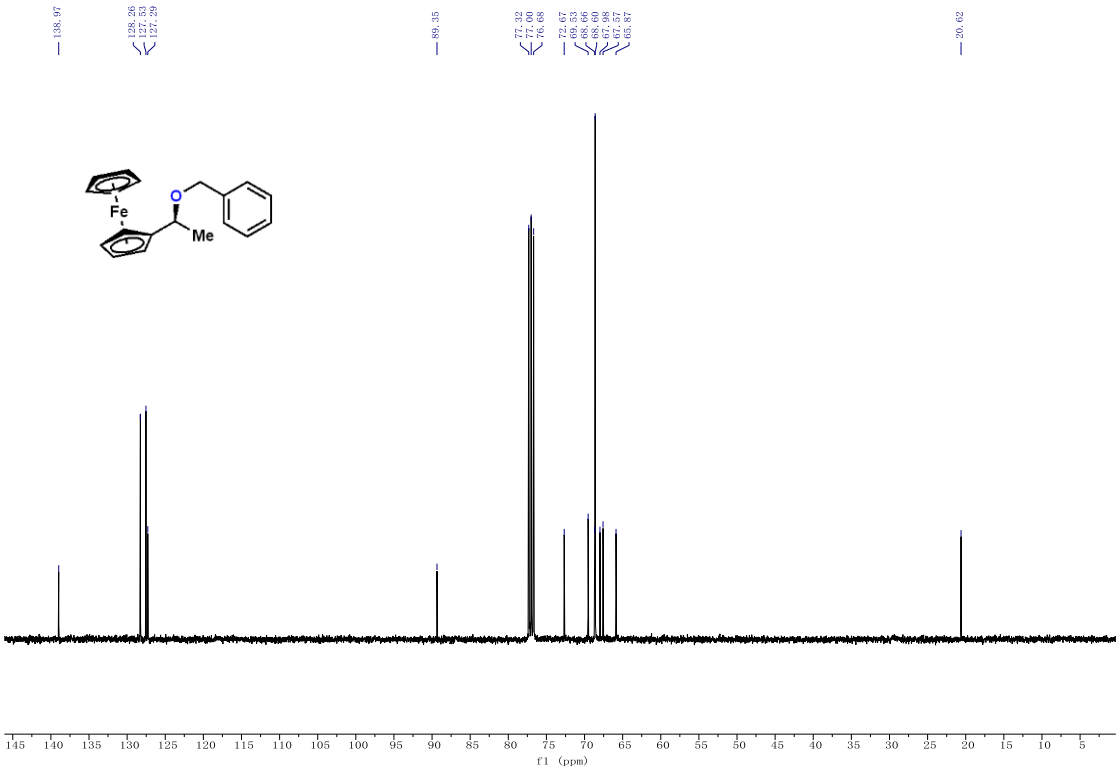


(S)-1-(benzyloxy)ethylferrocene (35)

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

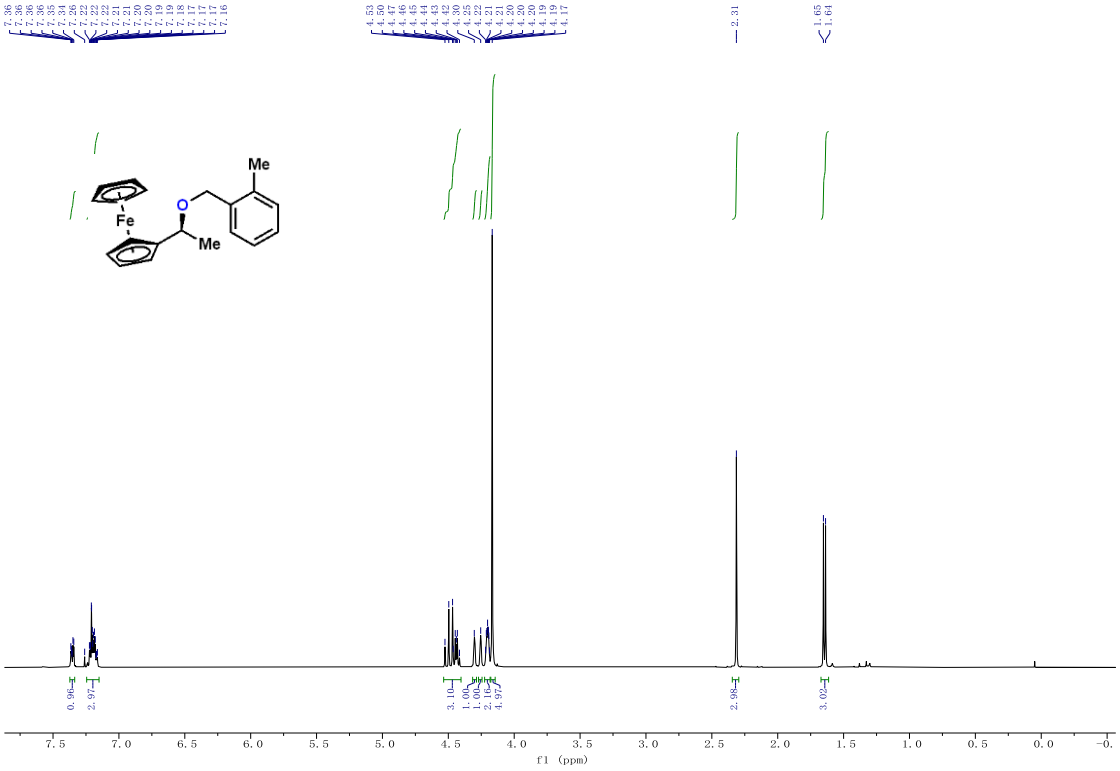


^{13}C NMR (101 MHz, $CDCl_3$)

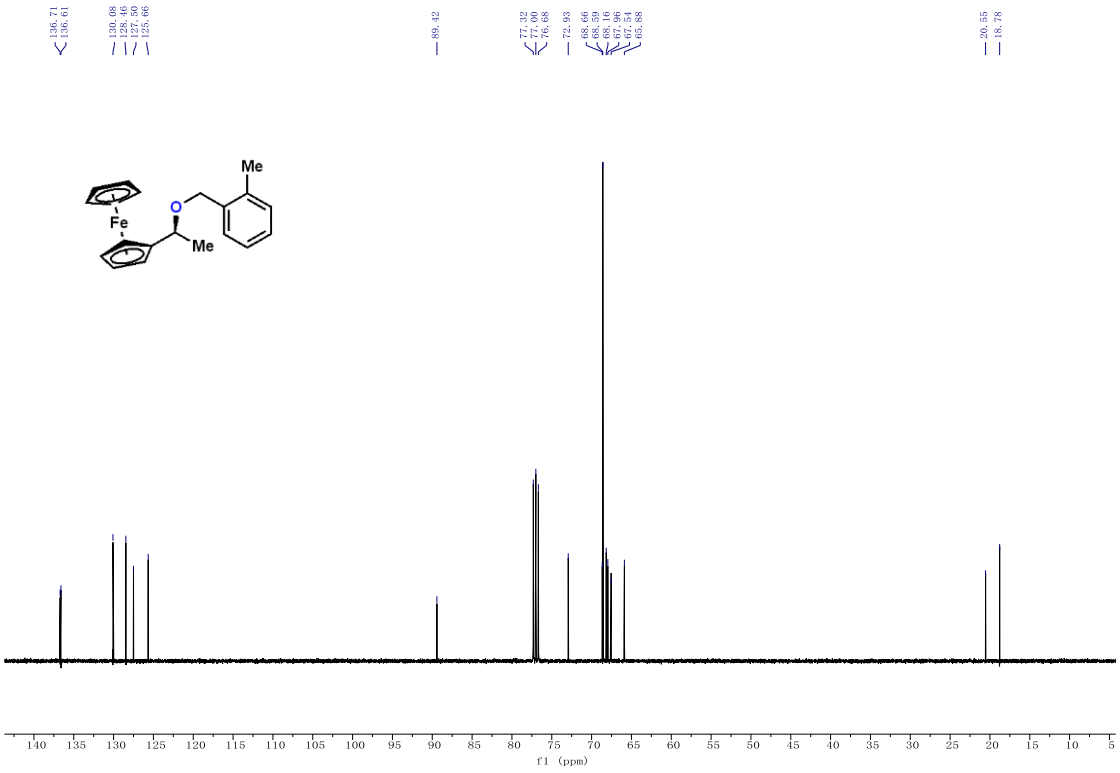


(S)-1-((2-methylbenzyl)oxy)ethylferrocene (36)

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

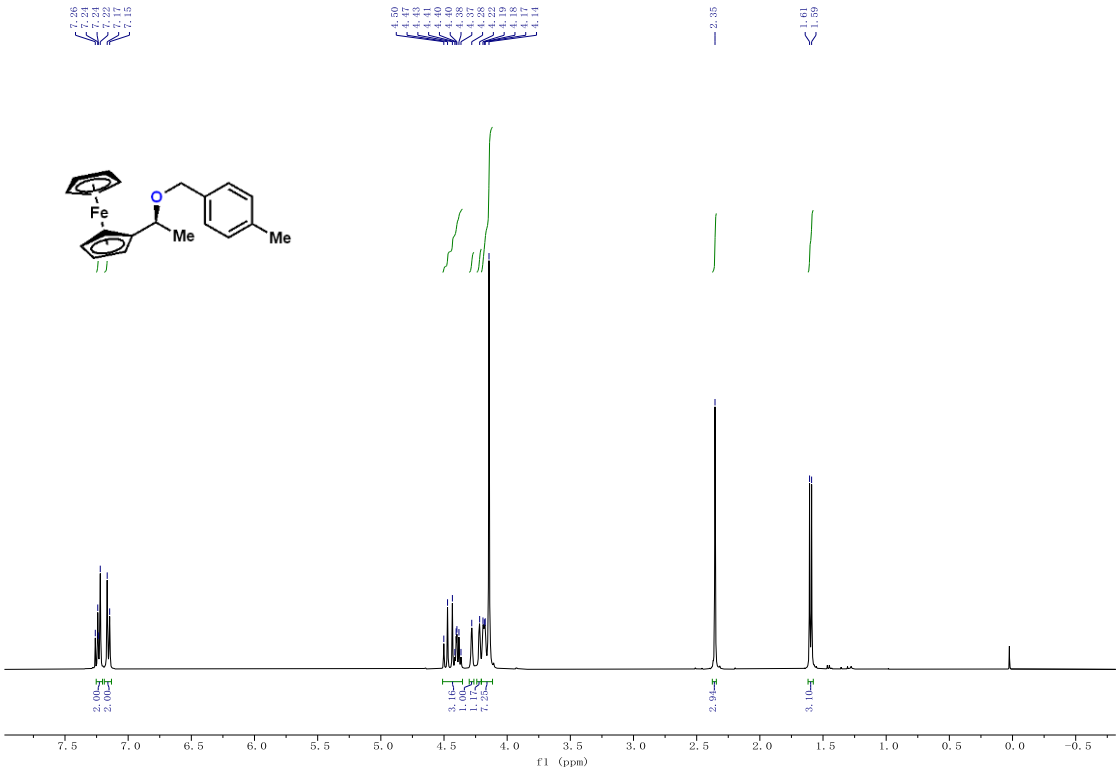


^{13}C NMR (101 MHz, $CDCl_3$)

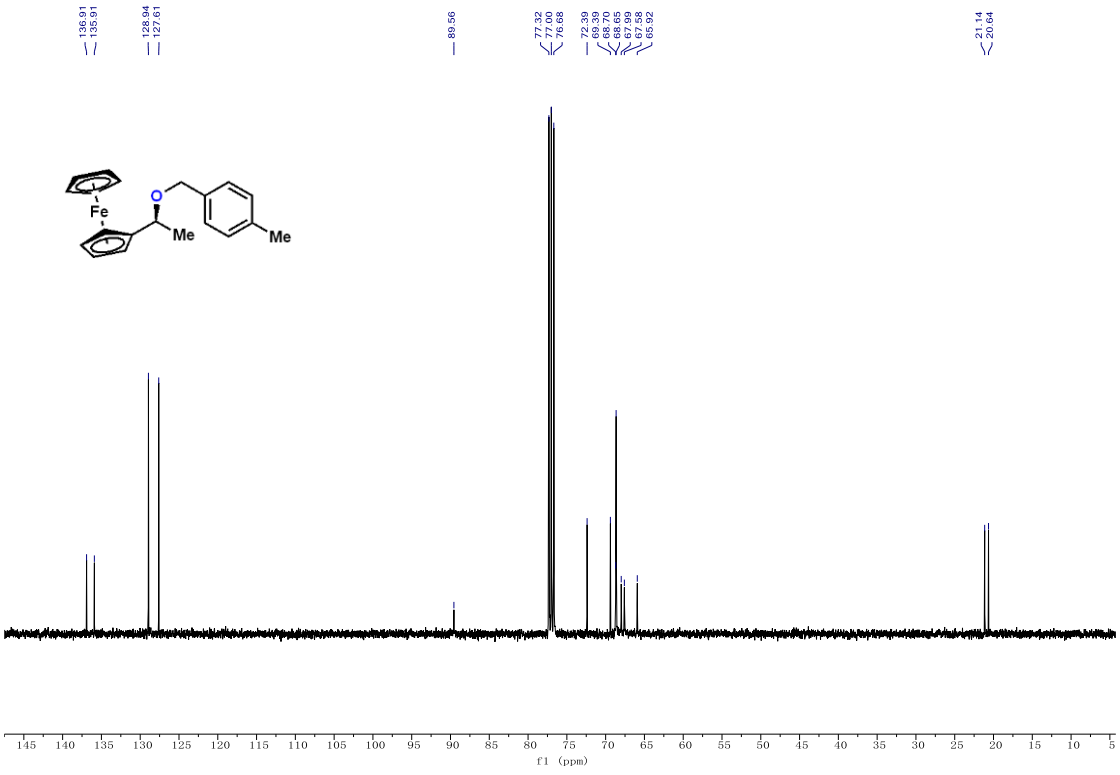


(S)-1-((4-methylbenzyl)oxy)ethylferrocene (37)

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

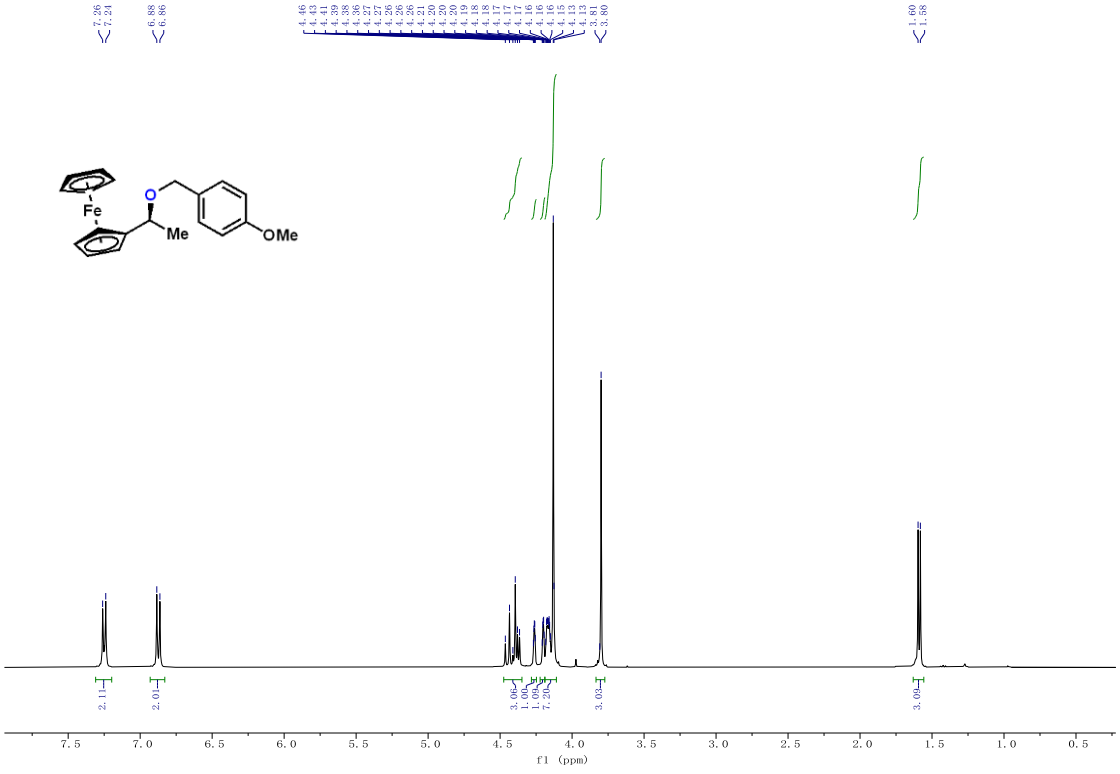


^{13}C NMR (101 MHz, $CDCl_3$)

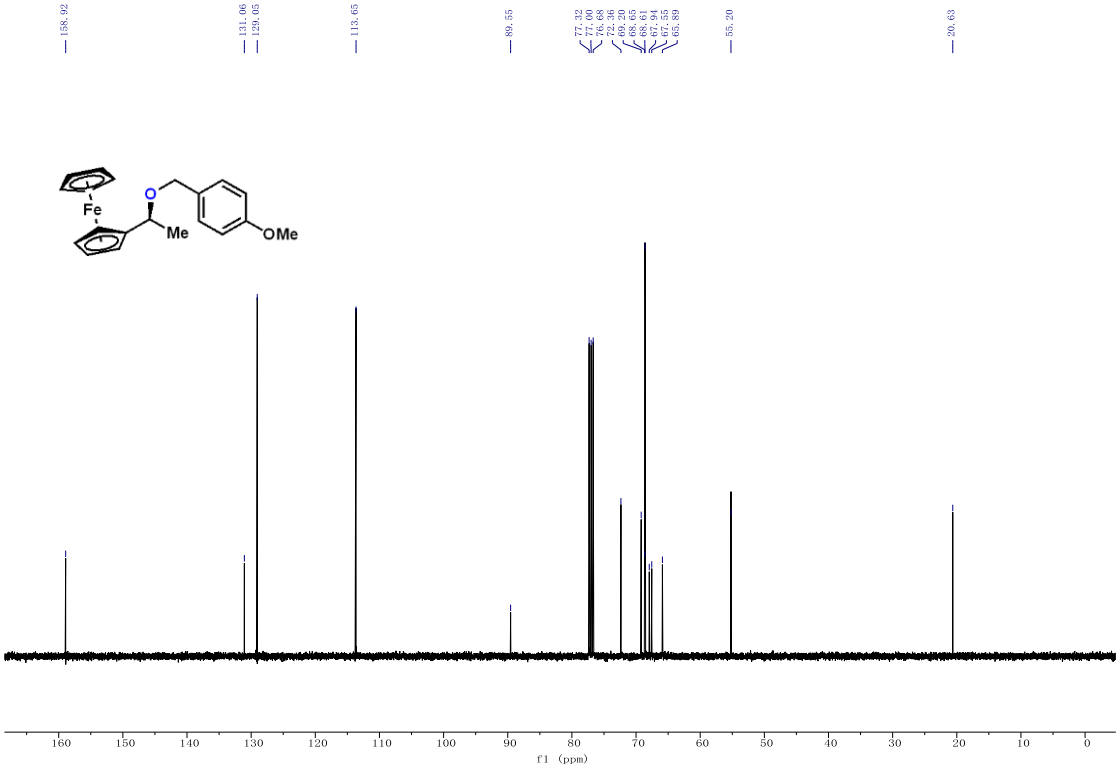


(S)-1-((4-methoxybenzyl)oxy)ethylferrocene (38)

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

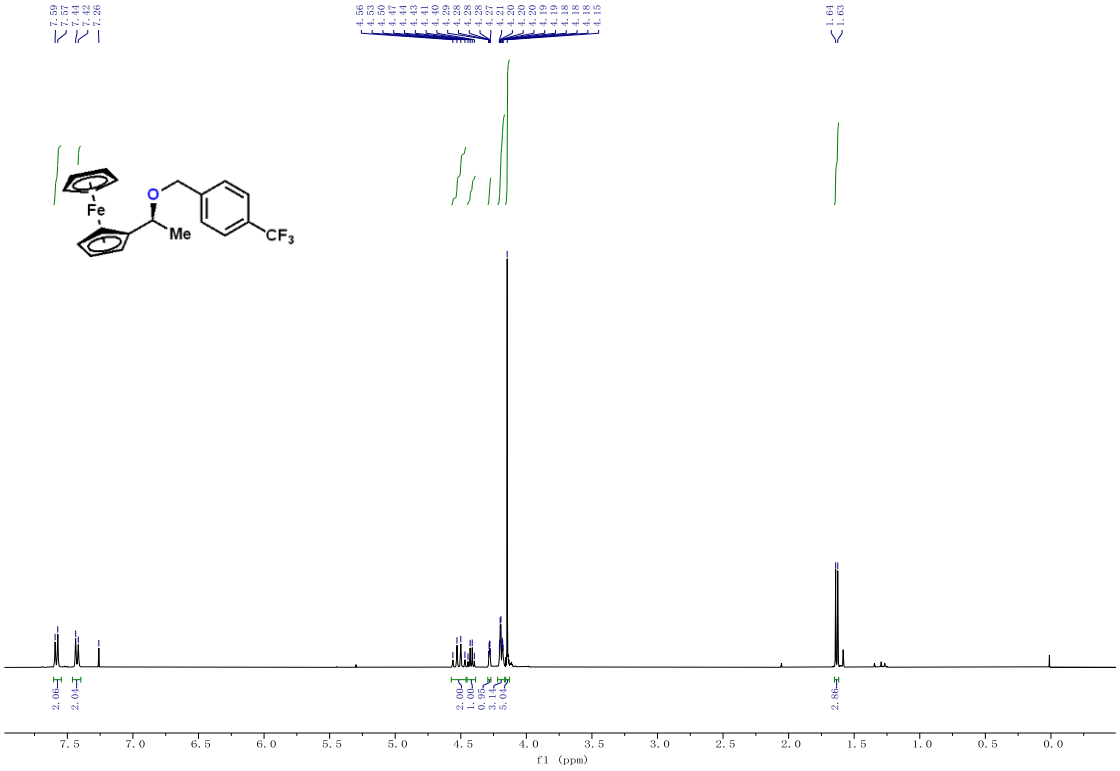


^{13}C NMR (101 MHz, $CDCl_3$)

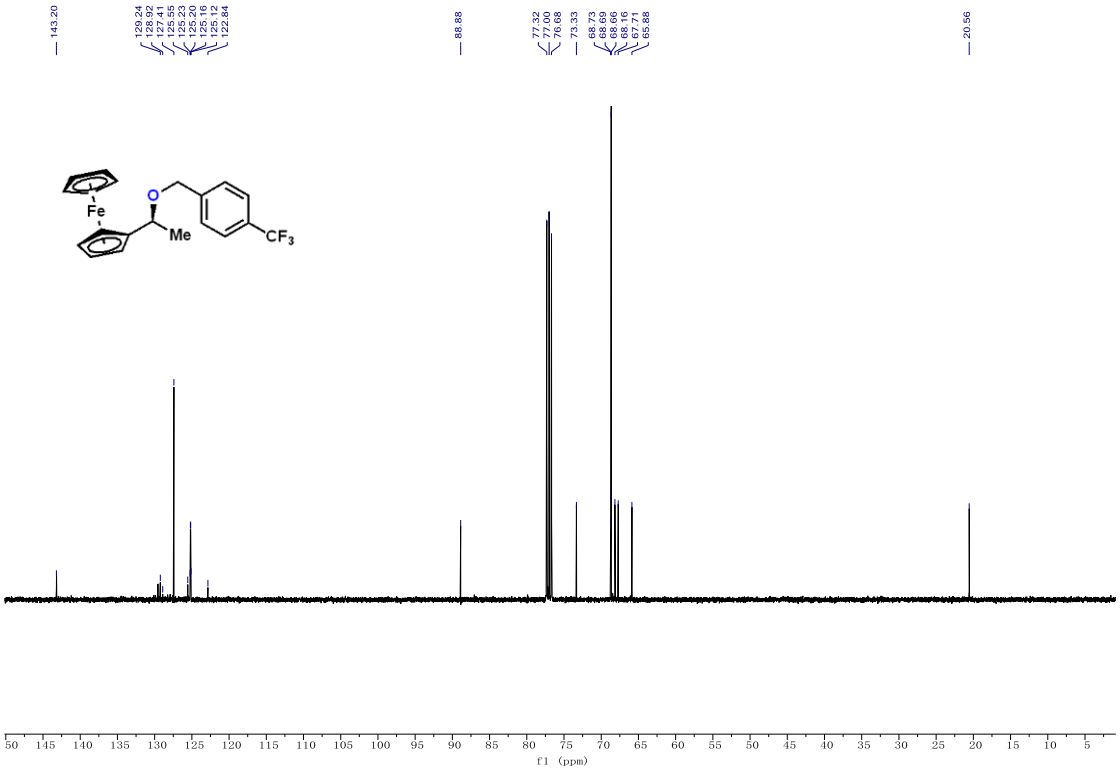


(S)-1-((4-(trifluoromethyl)benzyl)oxy)ethylferrocene (39)

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



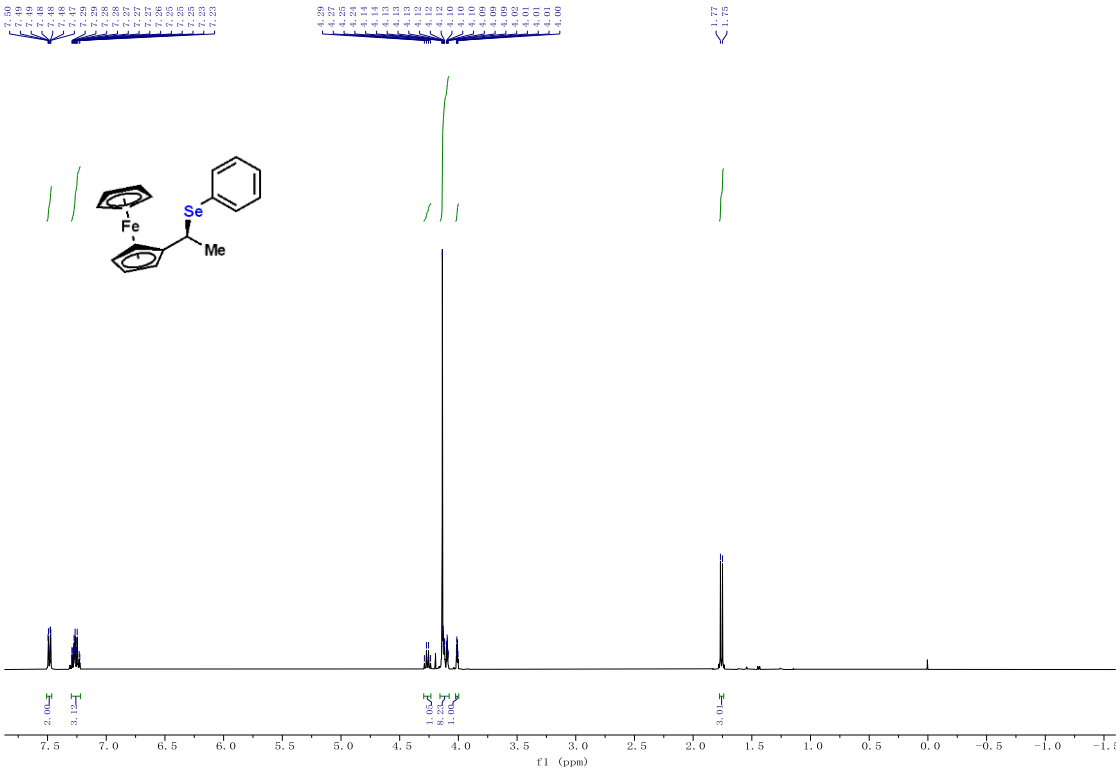
^{13}C NMR (101 MHz, $CDCl_3$)



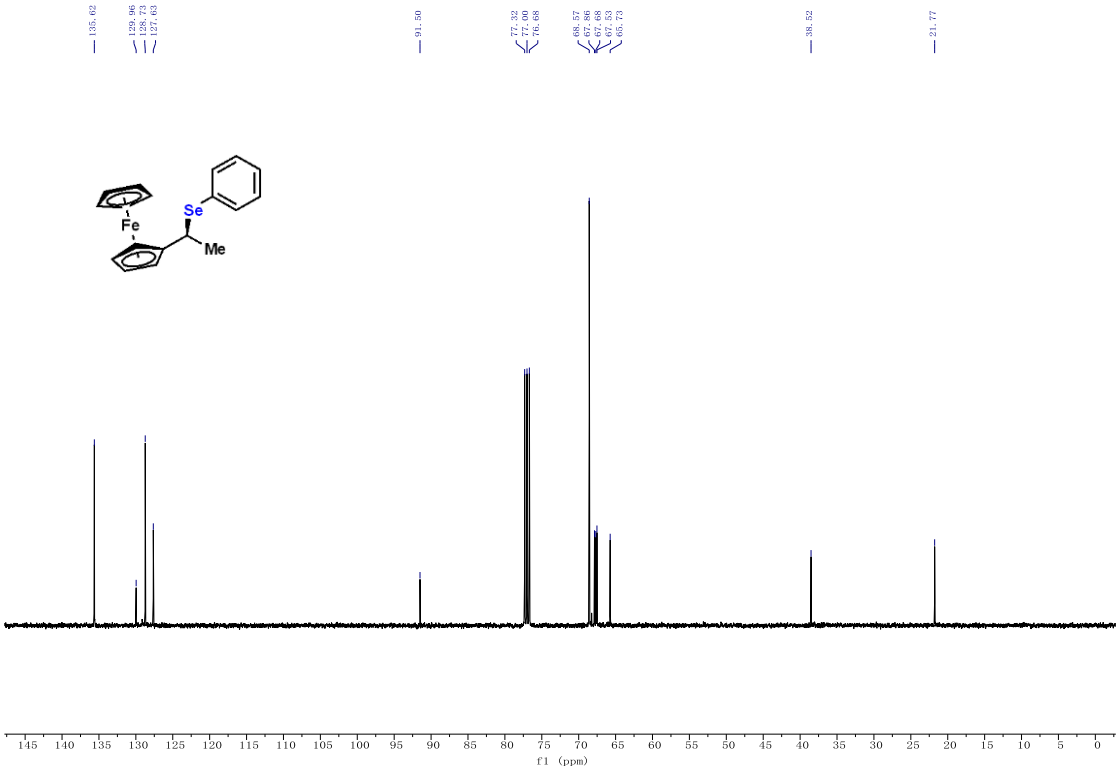
^{19}F NMR (376 MHz, $CDCl_3$)

(S)-1-(phenylselanyl)ethylferrocene (40)

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

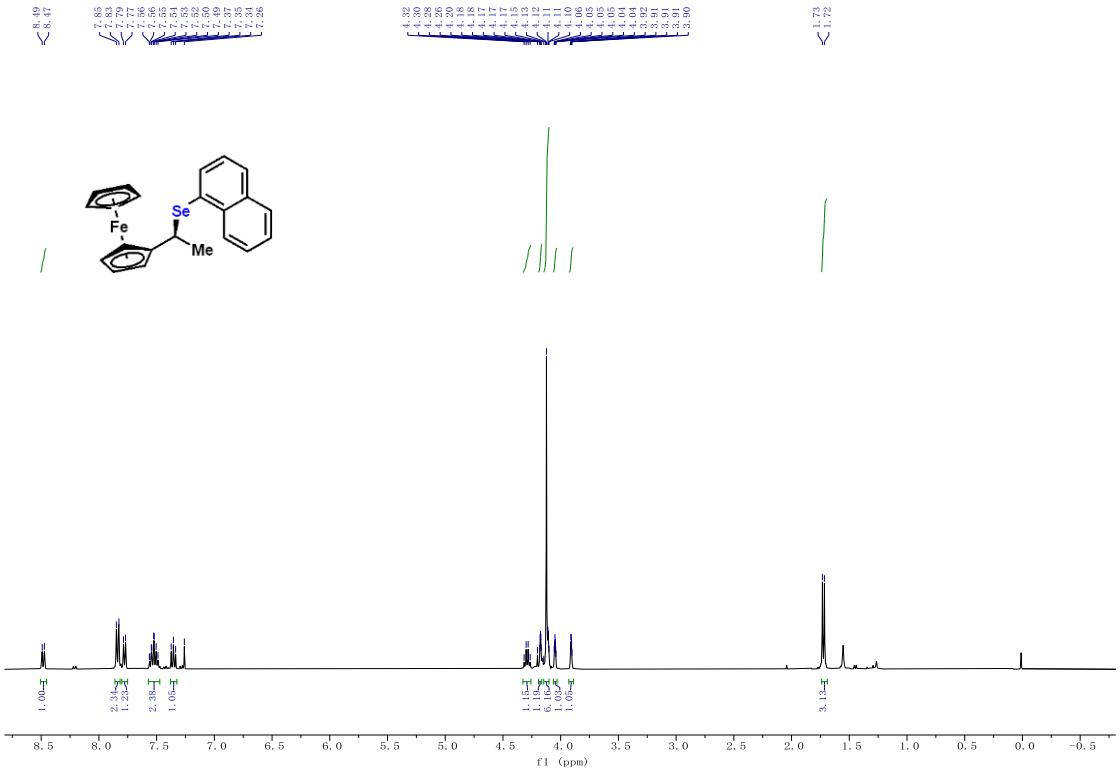


^{13}C NMR (101 MHz, $CDCl_3$)

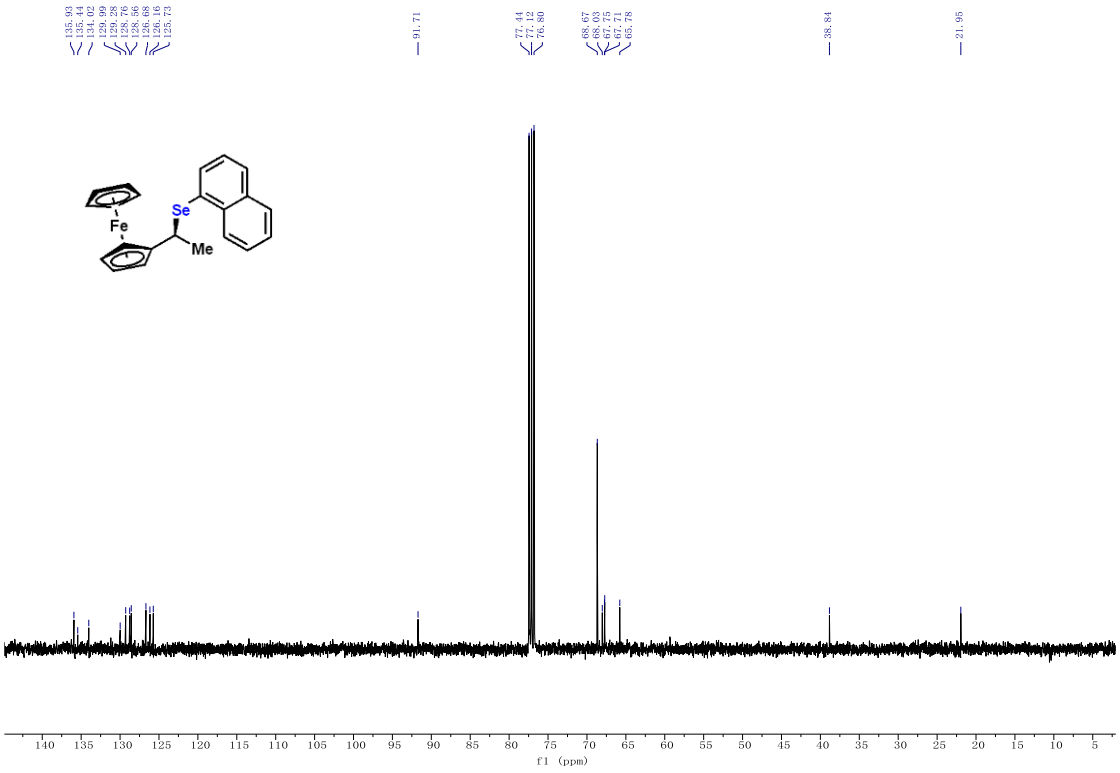


(S)-1-(naphthalen-1-ylselanyl)ethylferrocene (41)

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

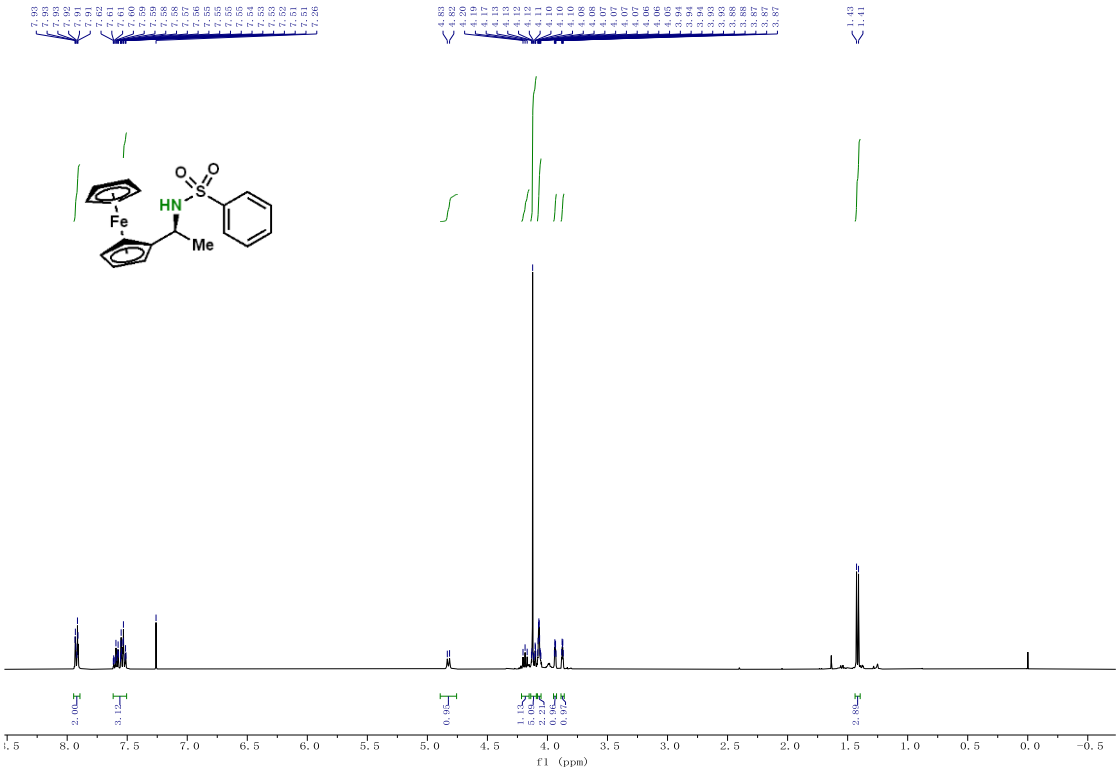


^{13}C NMR (101 MHz, $CDCl_3$)

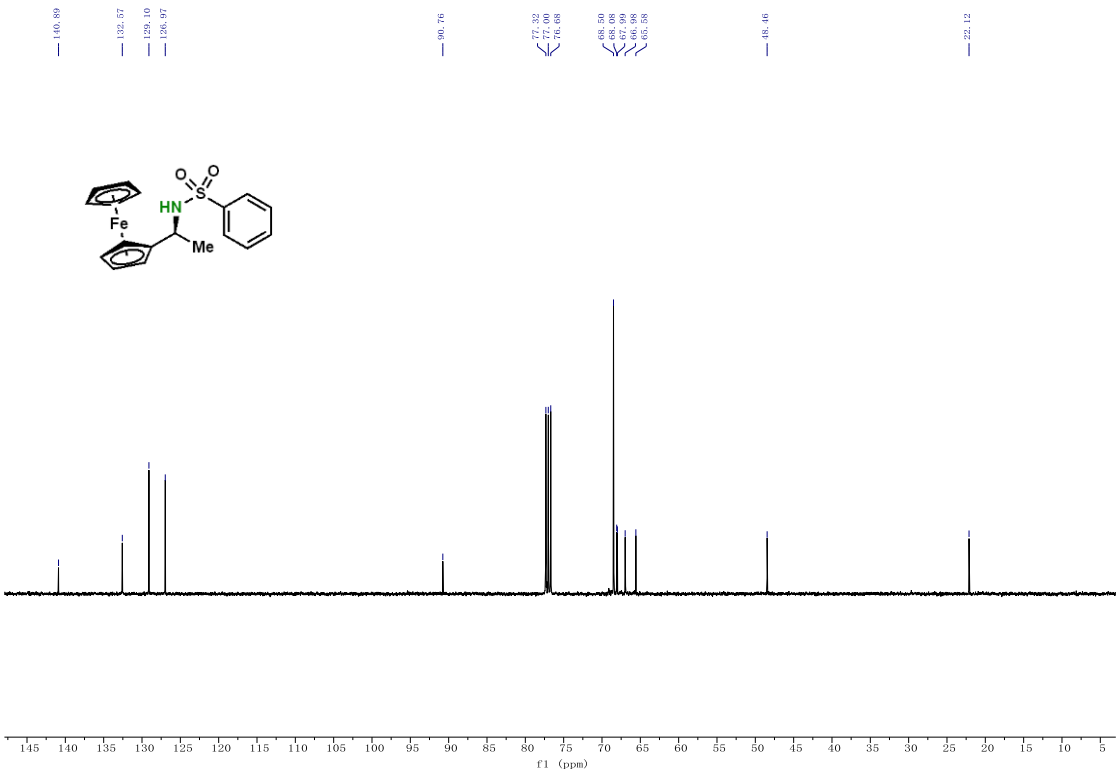


(S)-N-(1-(ferrocene-2-yl)ethyl)benzenesulfonamide (42)

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

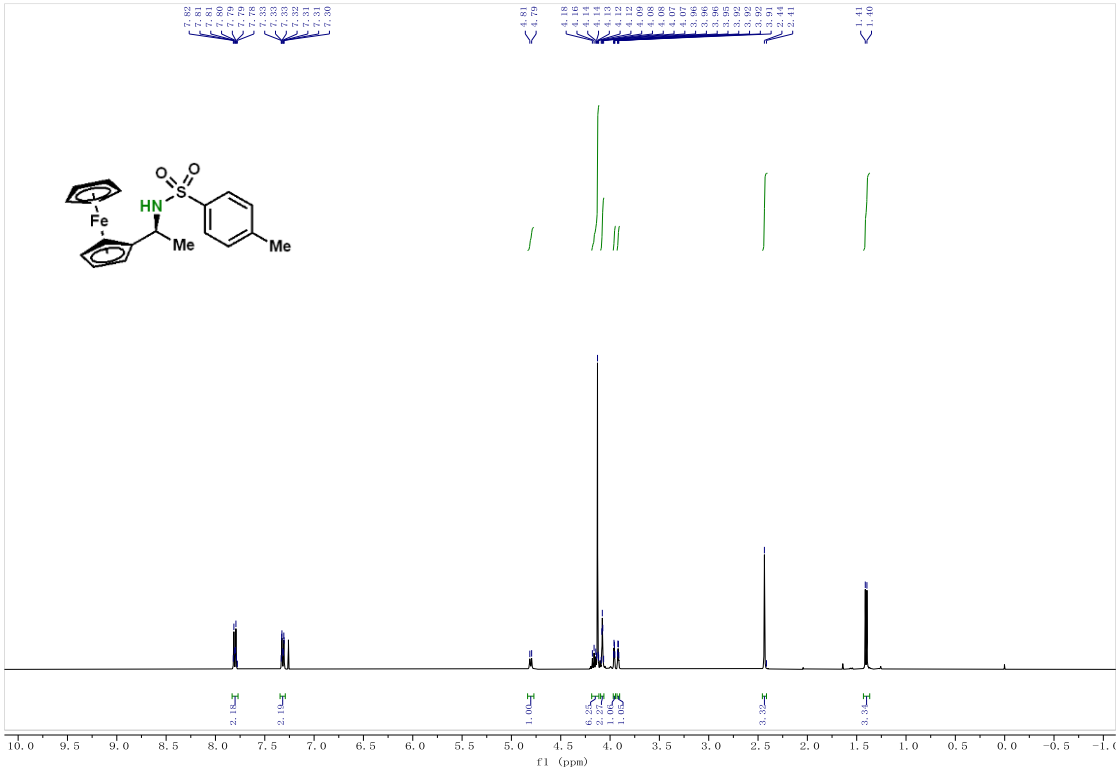


^{13}C NMR (101 MHz, $CDCl_3$)

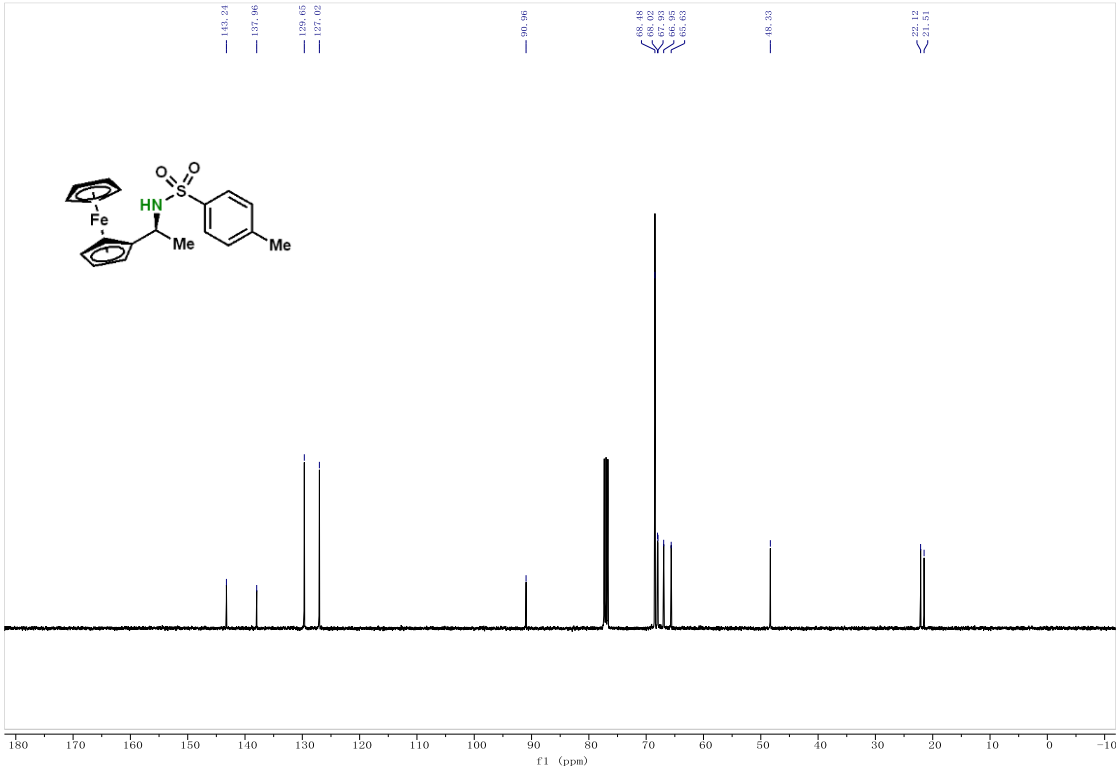


(S)-4-methyl-N-(1-(ferrocene-2-yl)ethyl)benzenesulfonamide (43)

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

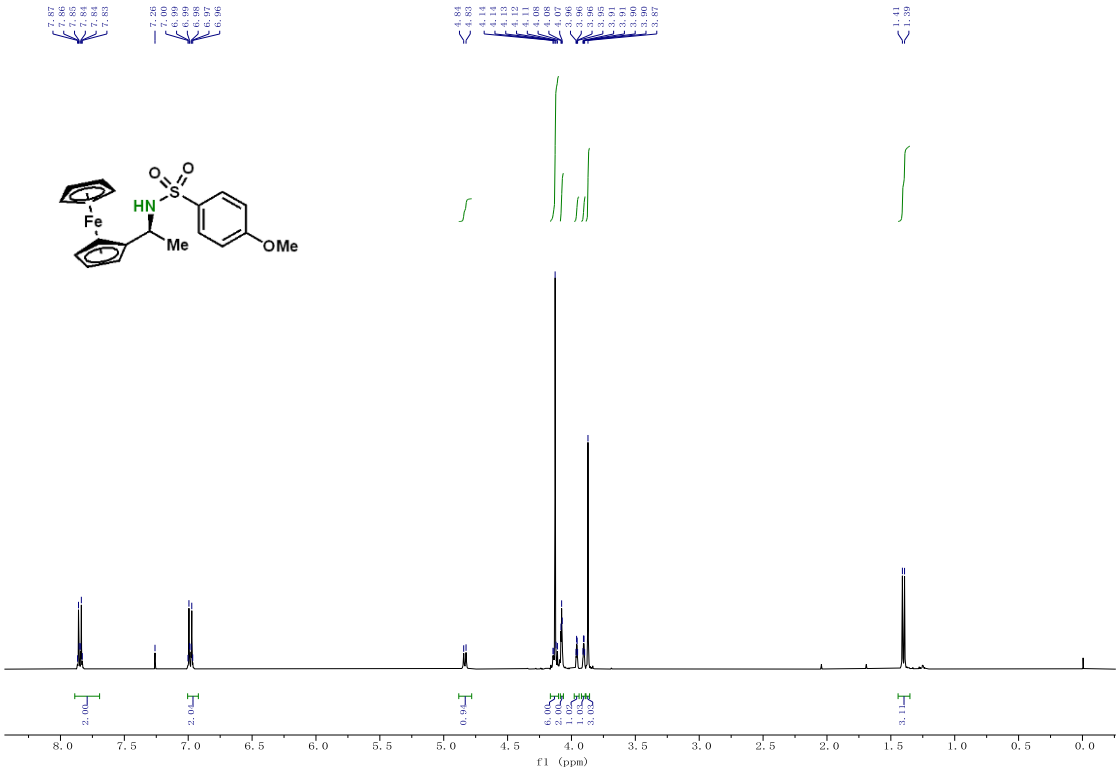


^{13}C NMR (101 MHz, $CDCl_3$)

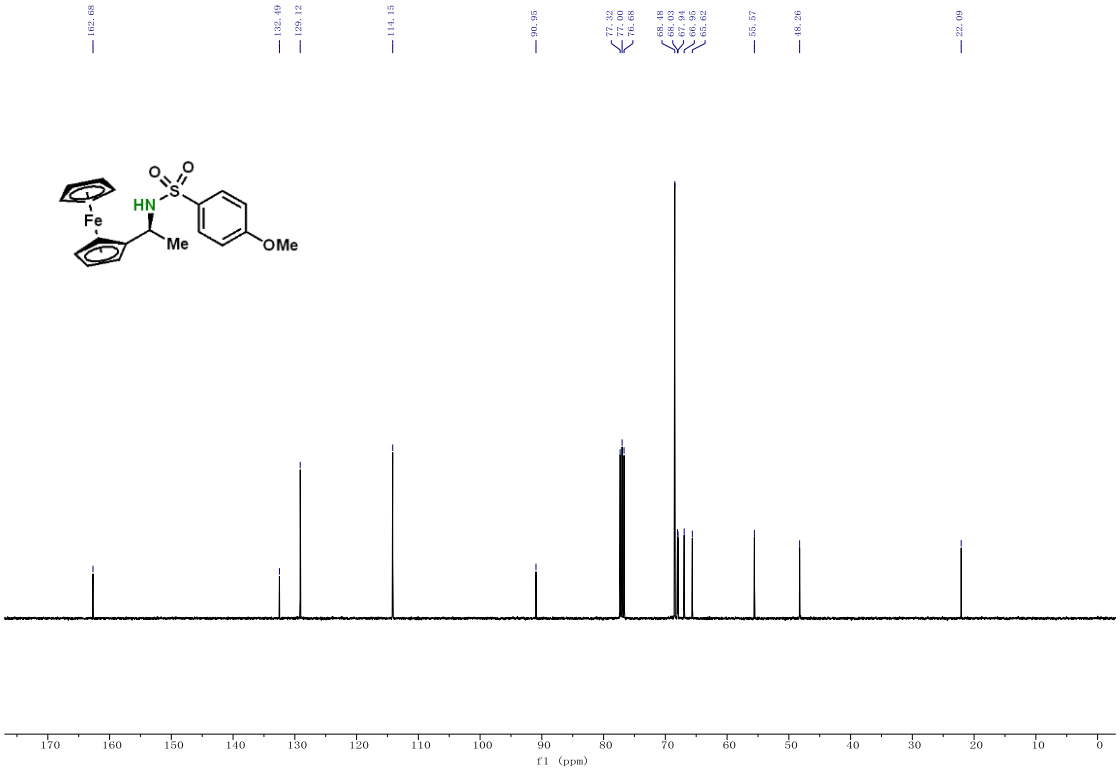


(S)-4-methoxy-N-(1-(ferrocene-2-yl)ethyl)benzenesulfonamide (44)

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

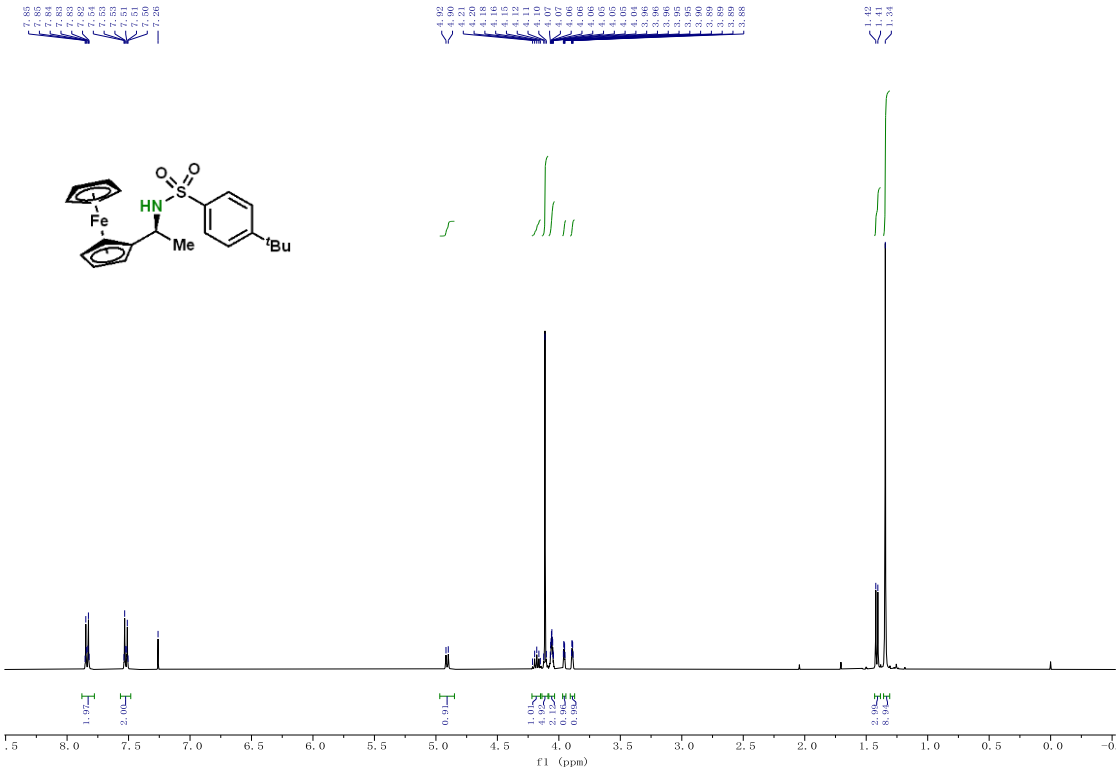


^{13}C NMR (101 MHz, $CDCl_3$)

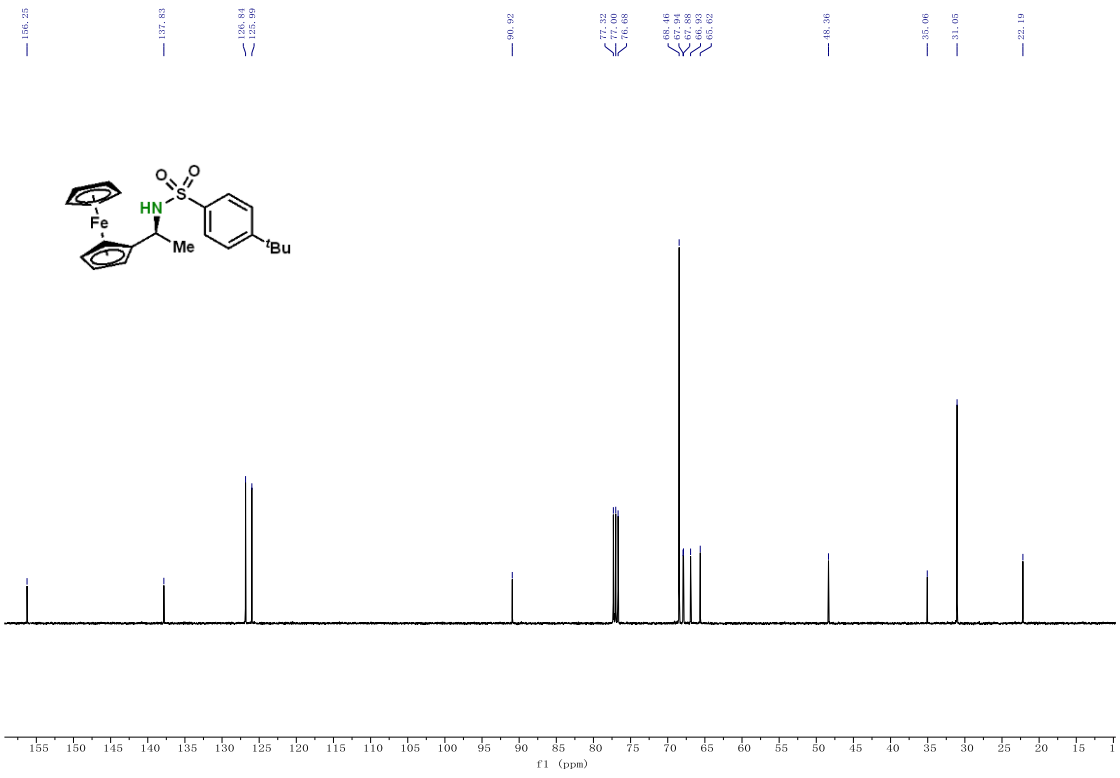


(S)-4-(tert-butyl)-N-(1-(ferrocene-2-yl)ethyl)benzenesulfonamide (45)

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

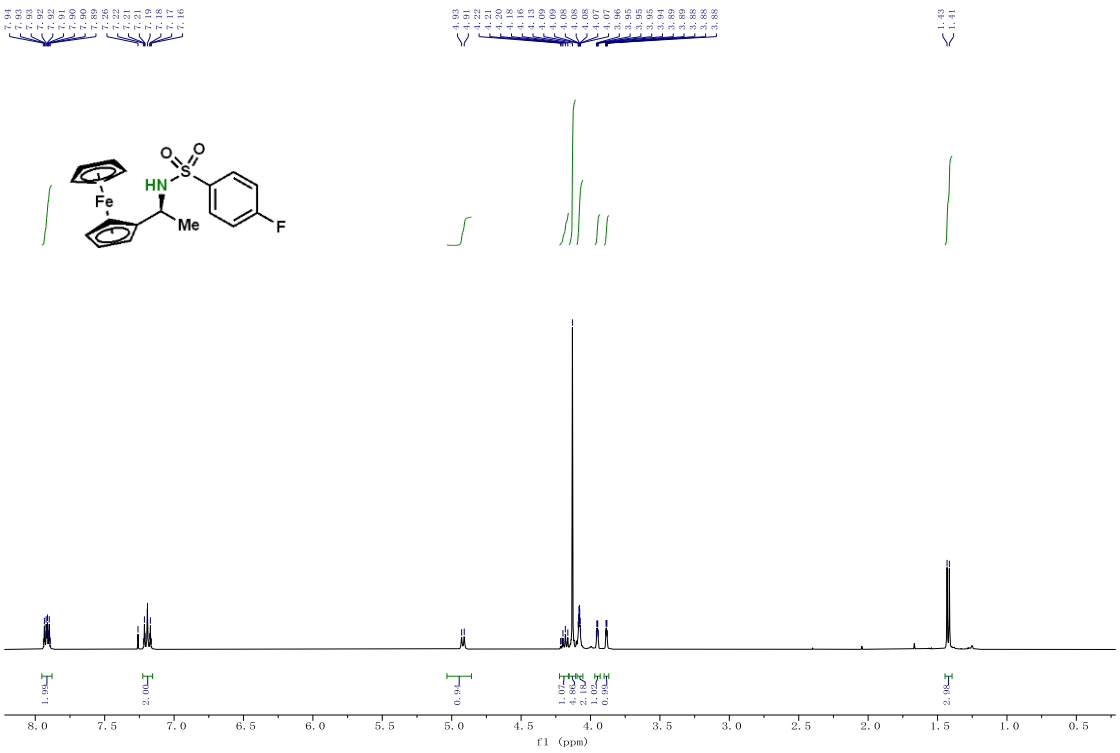


^{13}C NMR (101 MHz, $CDCl_3$)

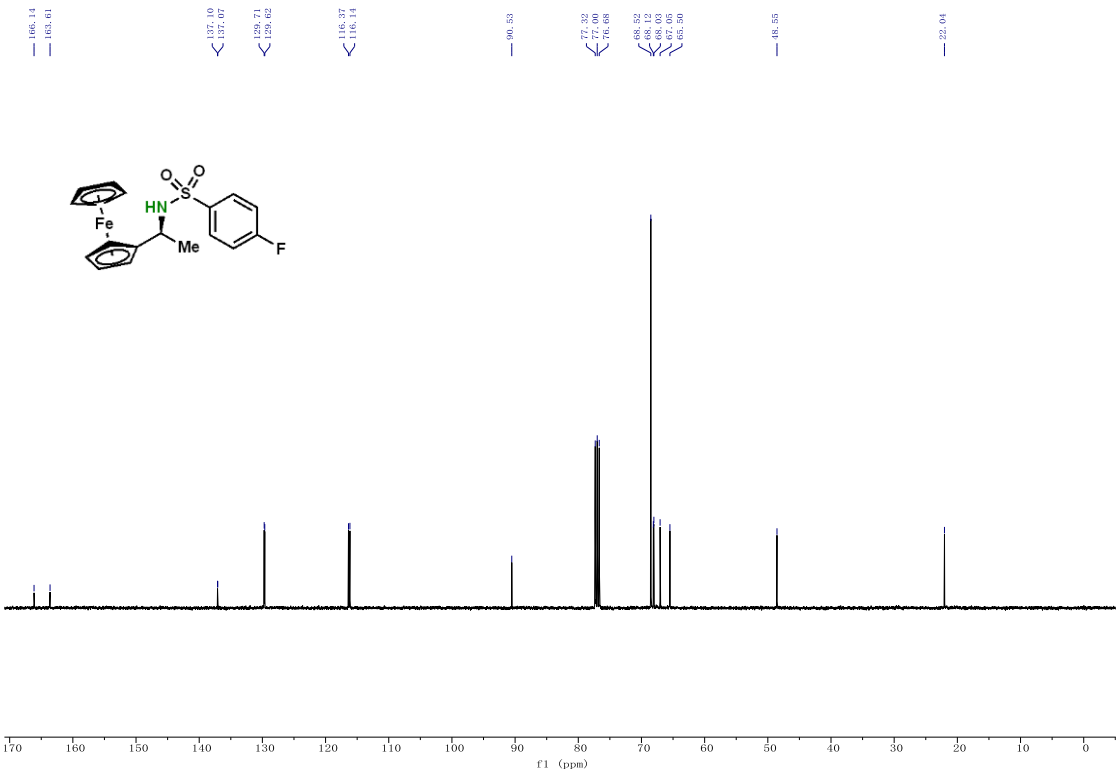


(S)-4-fluoro-N-(1-(ferrocene-2-yl)ethyl)benzenesulfonamide (46)

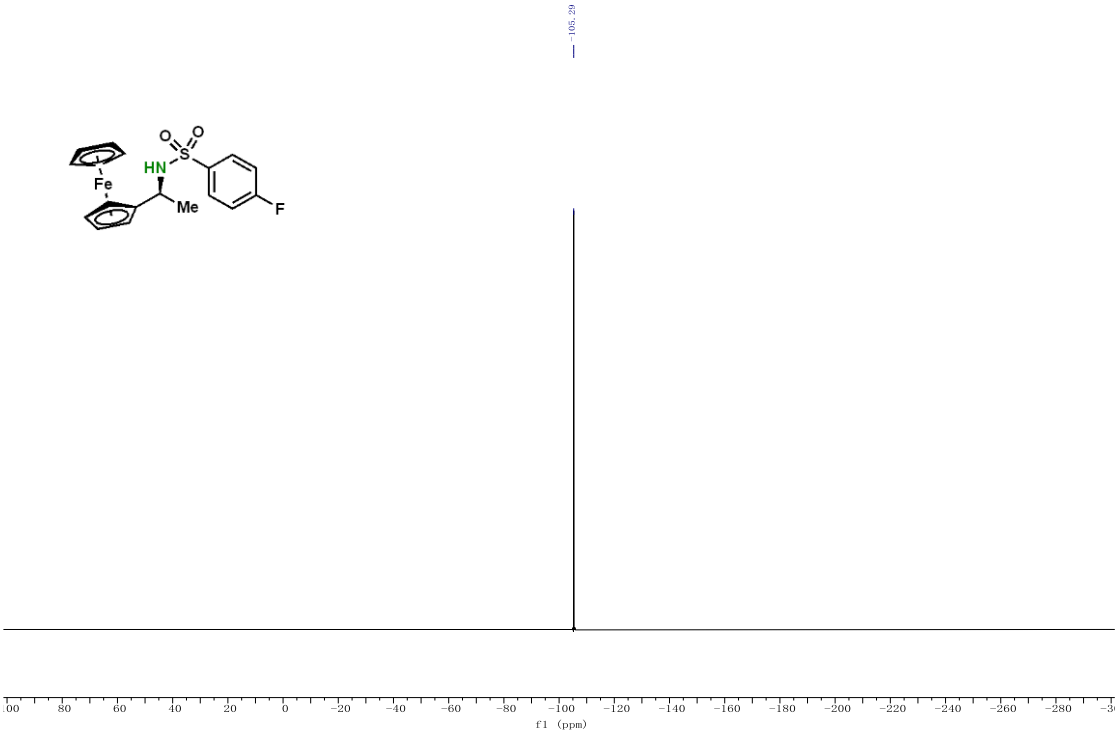
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)

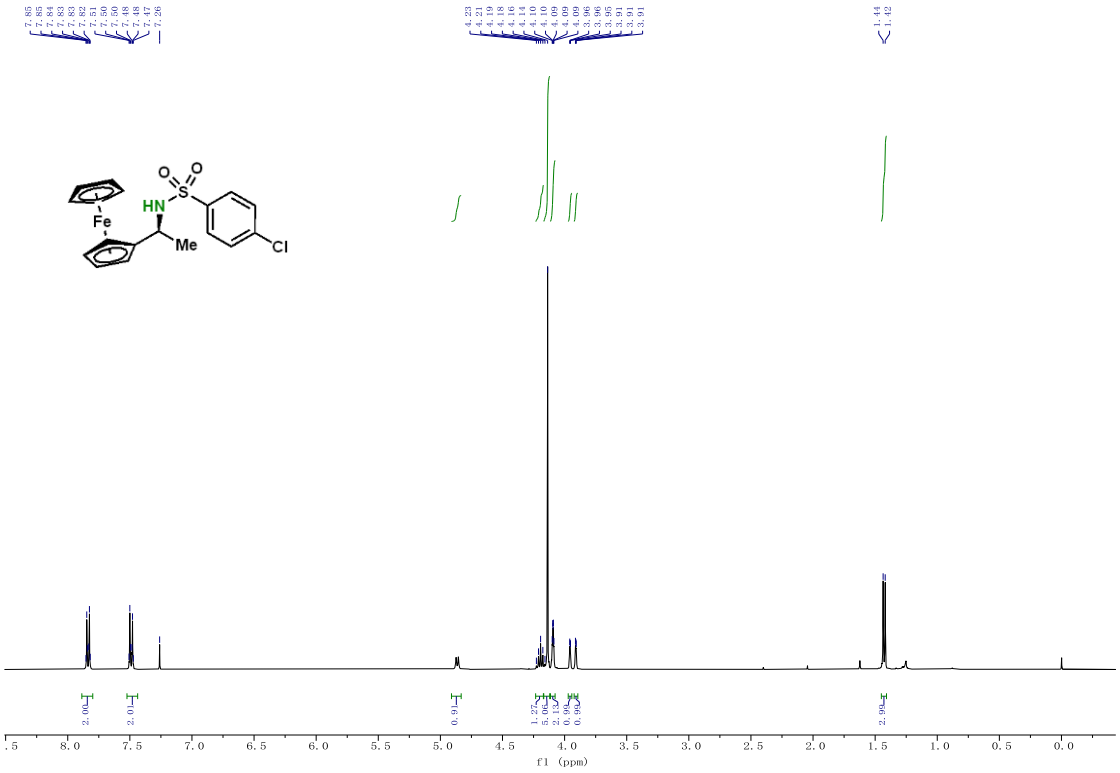


^{19}F NMR (376 MHz, $CDCl_3$)

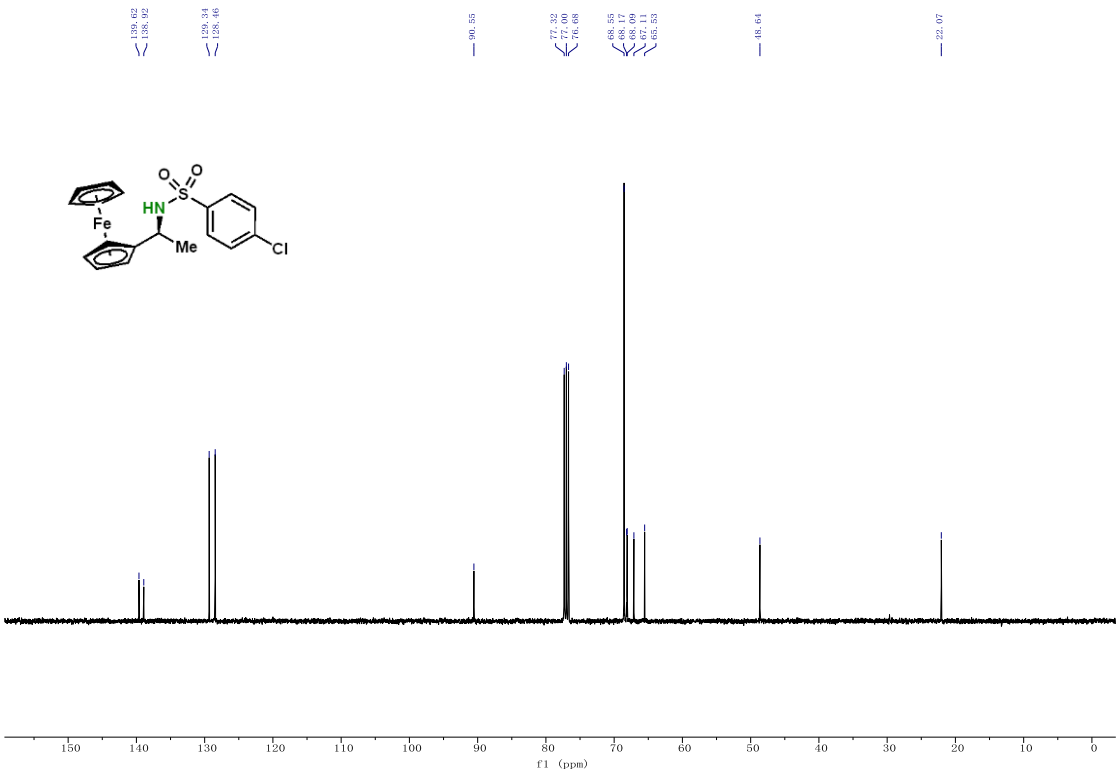


(S)-4-chloro-N-(1-(ferrocene-2-yl)ethyl)benzenesulfonamide (47)

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

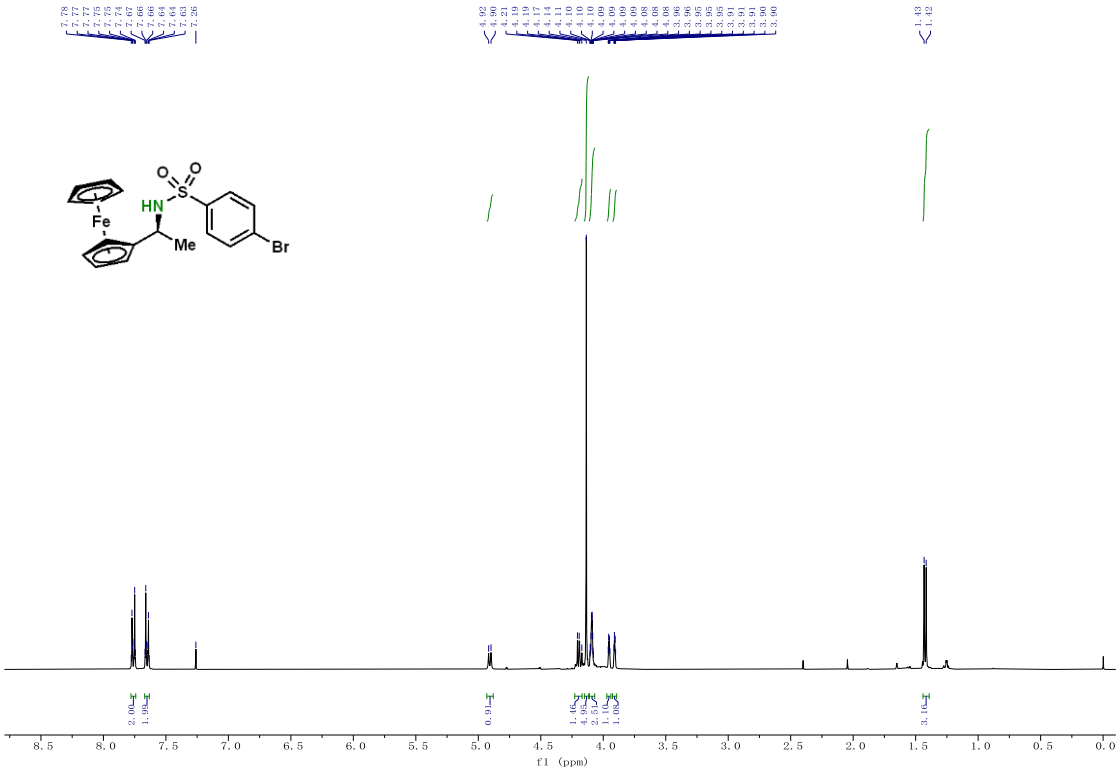


^{13}C NMR (101 MHz, $CDCl_3$)

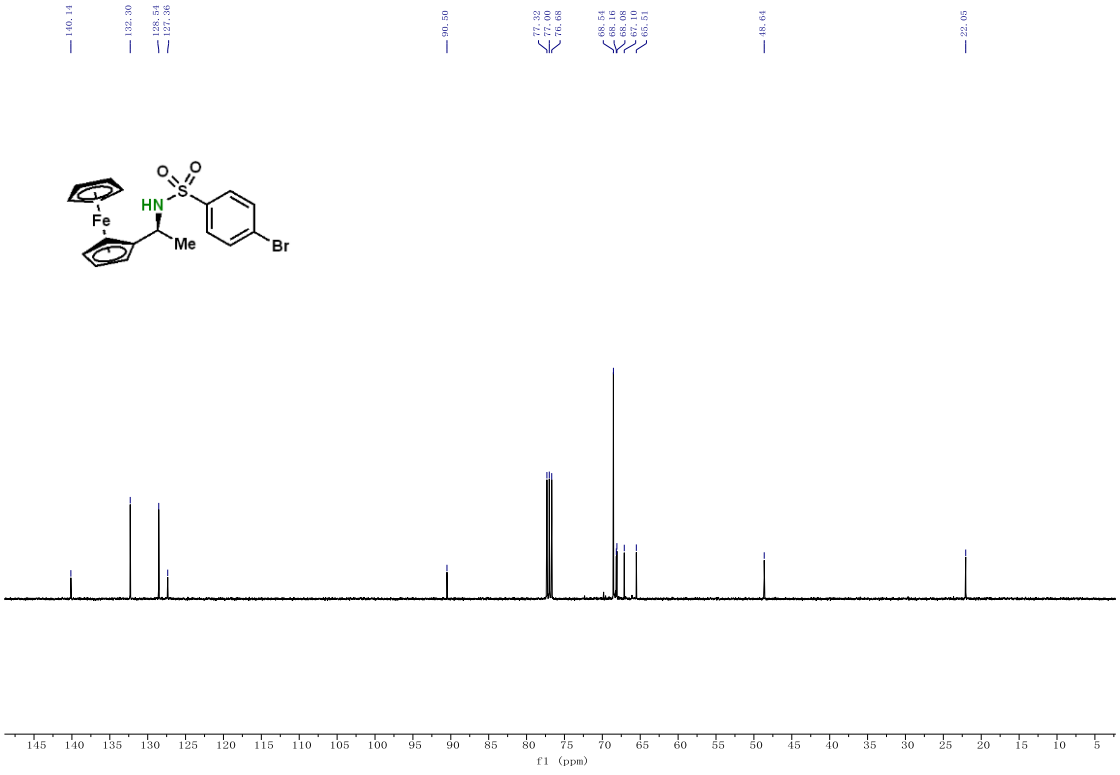


(S)-4-bromo-N-(1-(ferrocene-2-yl)ethyl)benzenesulfonamide (48)

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

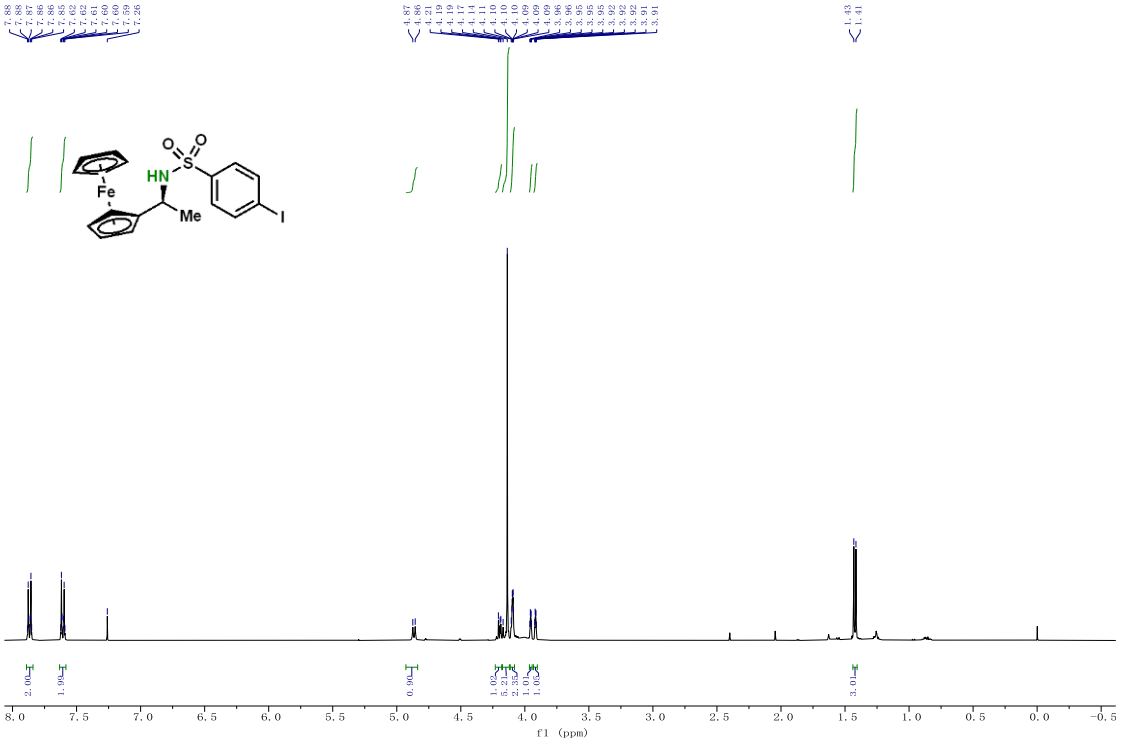


^{13}C NMR (101 MHz, $CDCl_3$)

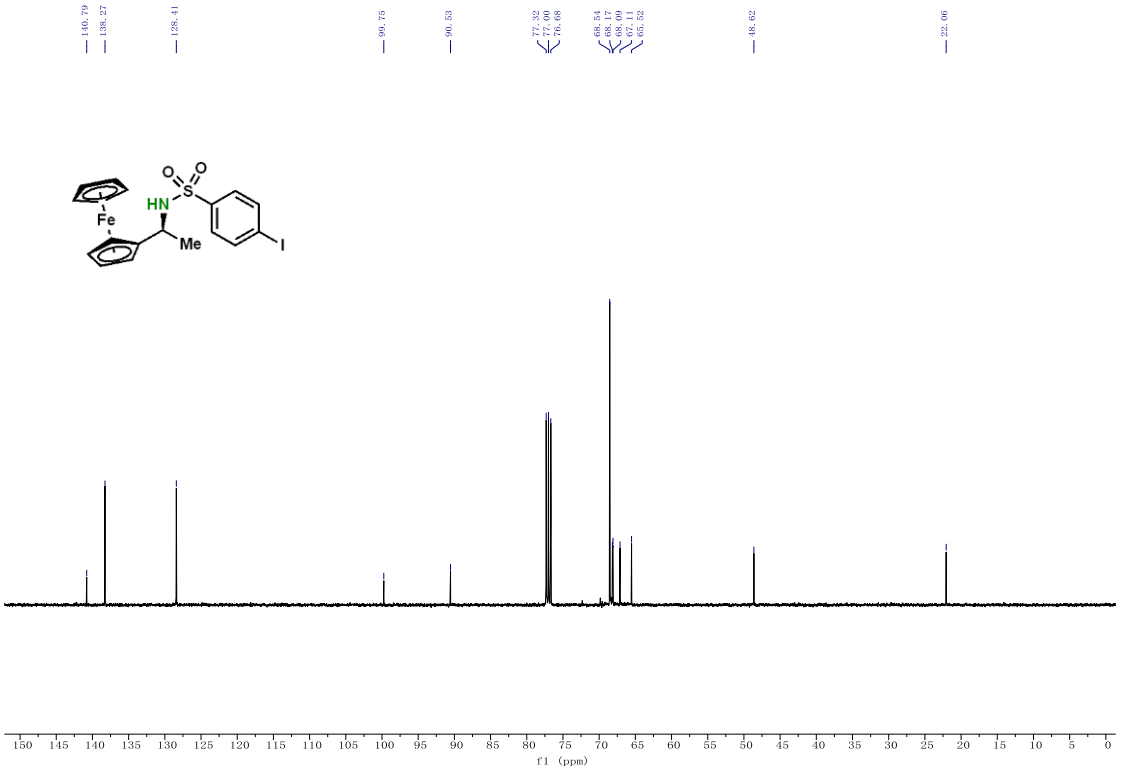


(S)-4-iodo-N-(1-(ferrocene-2-yl)ethyl)benzenesulfonamide (49)

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

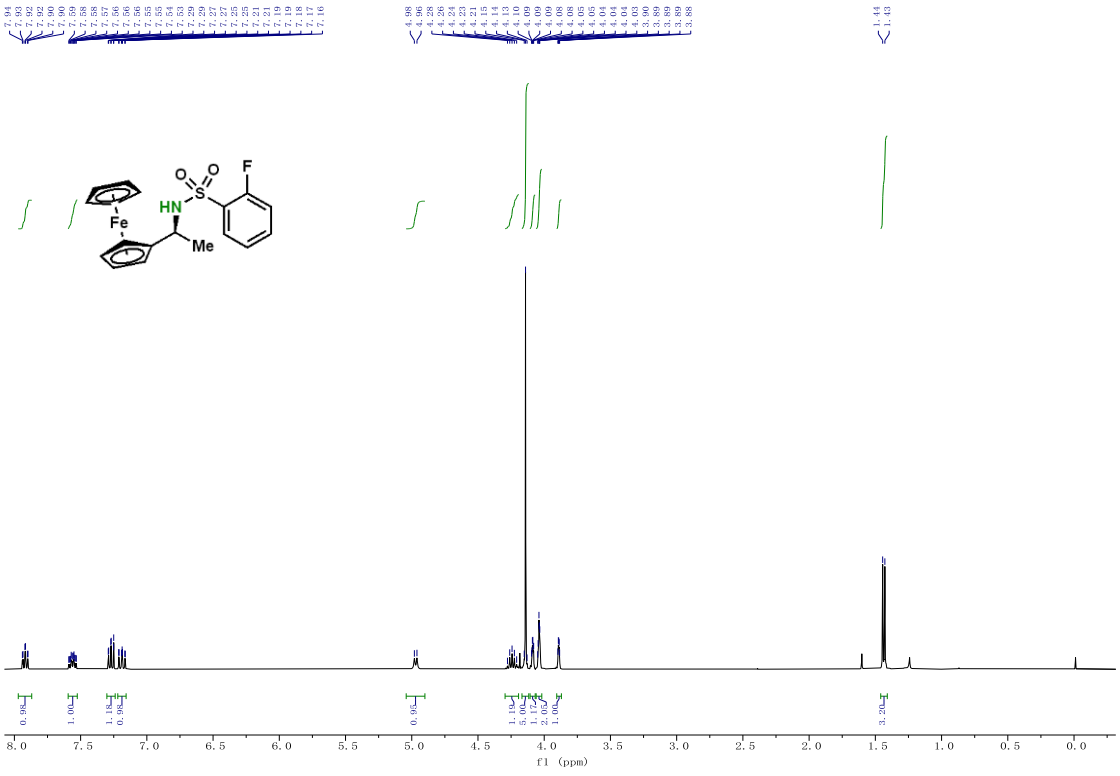


^{13}C NMR (101 MHz, $CDCl_3$)

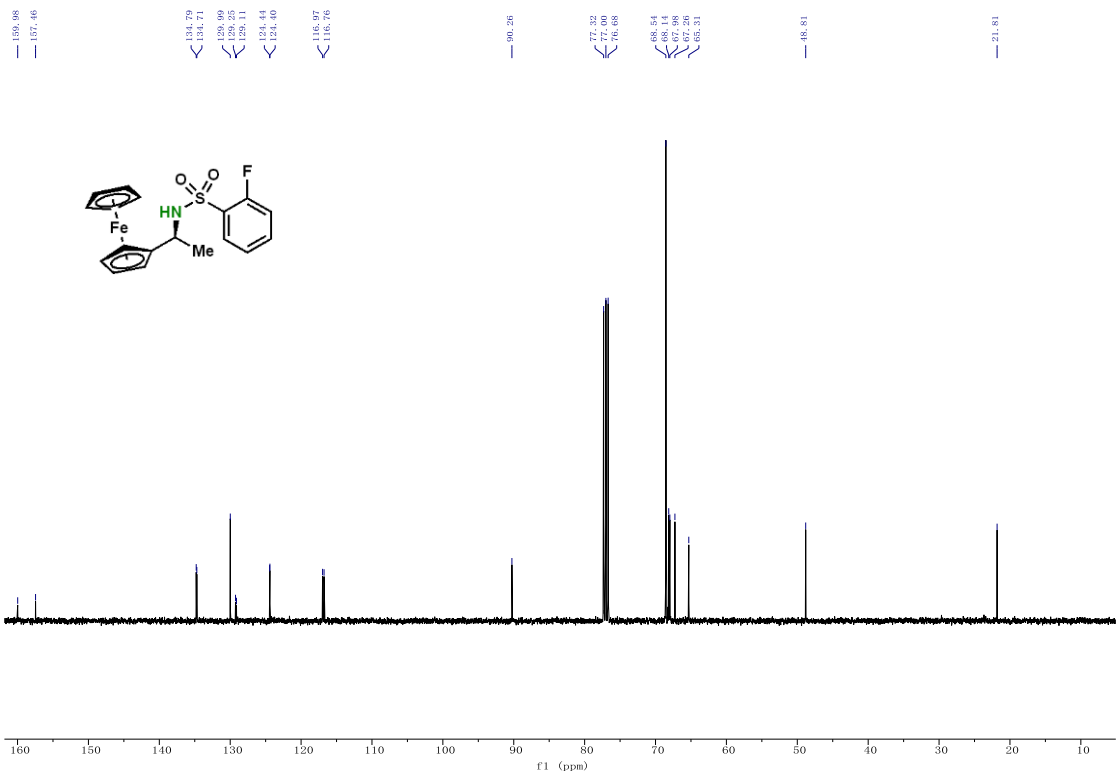


(S)-2-fluoro-N-(1-(ferrocene-2-yl)ethyl)benzenesulfonamide (50)

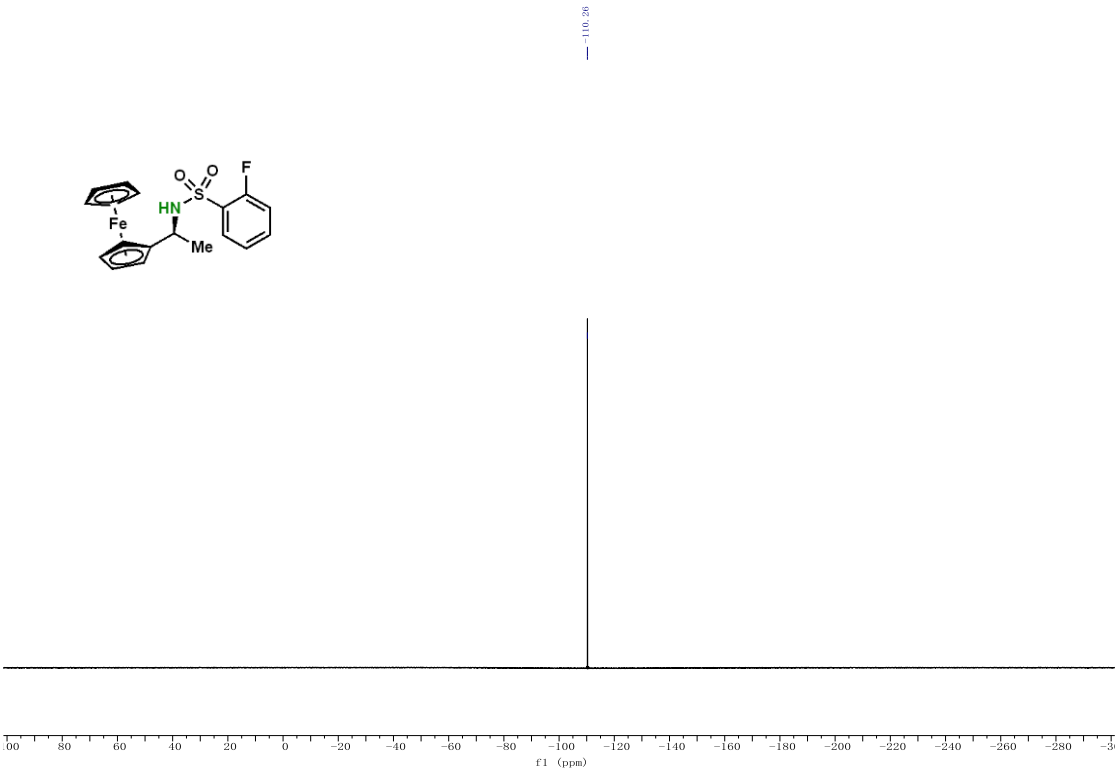
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)

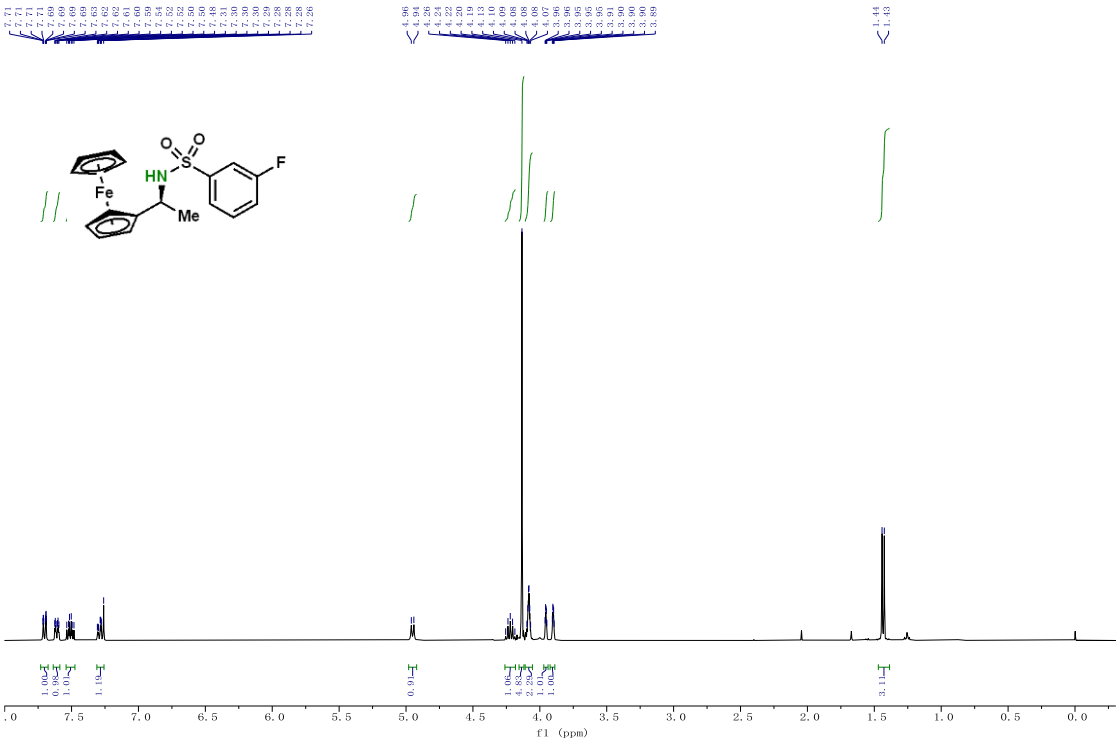


^{19}F NMR (376 MHz, $CDCl_3$)

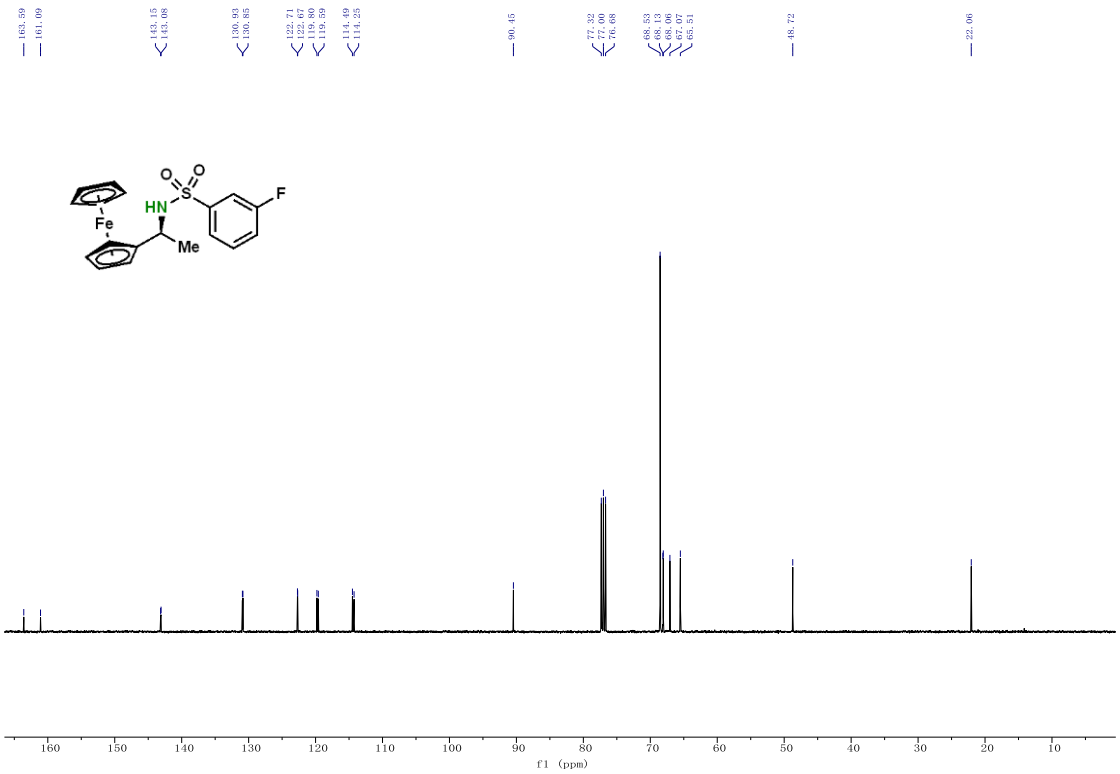


(S)-3-fluoro-N-(1-(ferrocene-2-yl)ethyl)benzenesulfonamide (51)

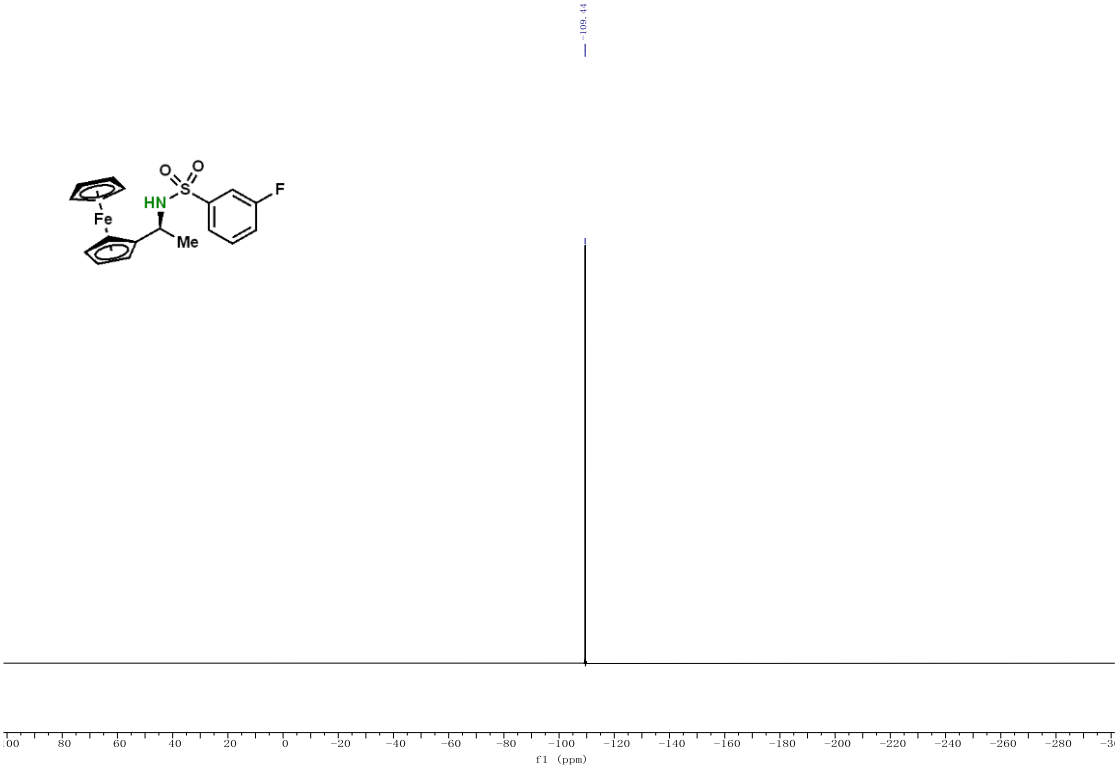
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)

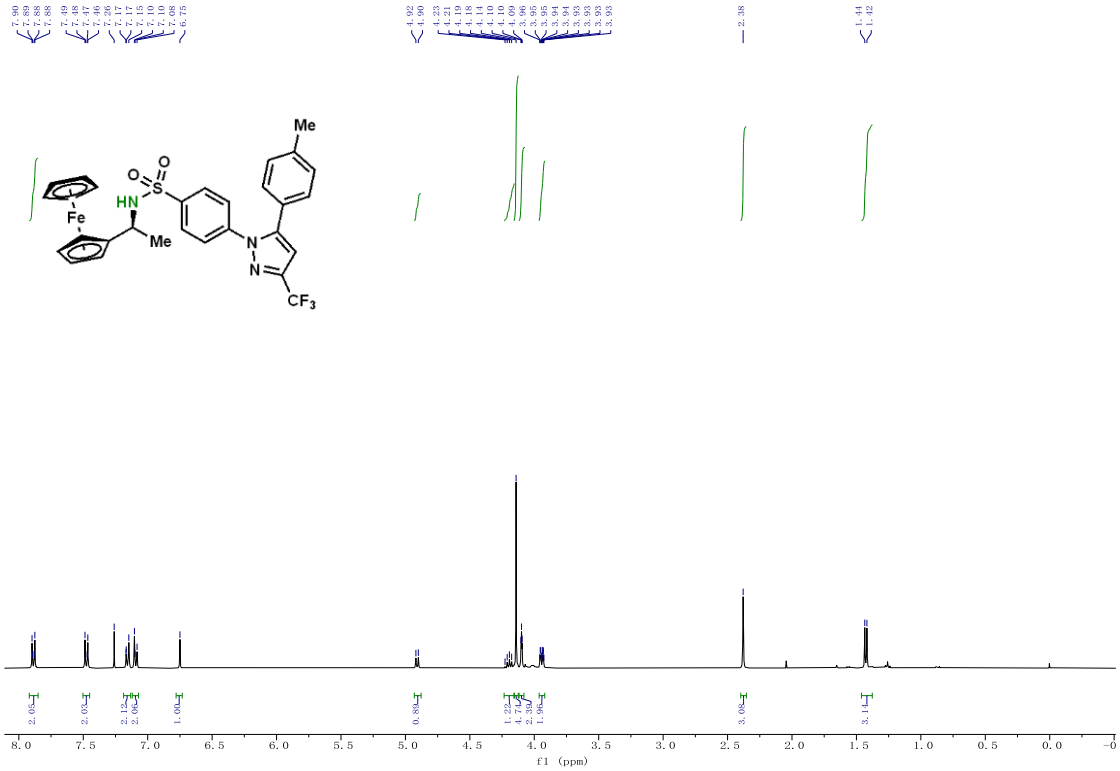


^{19}F NMR (376 MHz, $CDCl_3$)

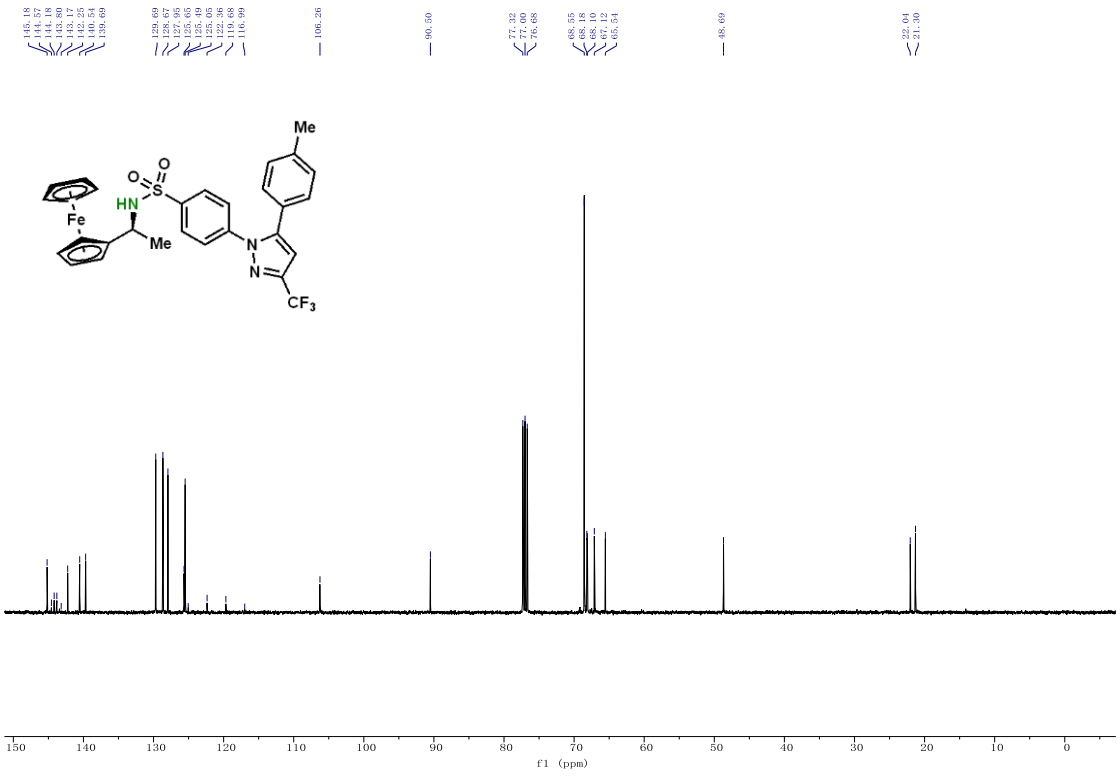


(S)-N-(1-(ferrocene-2-yl)ethyl)-4-(5-(p-tolyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl)benzenesulfonamide (52)

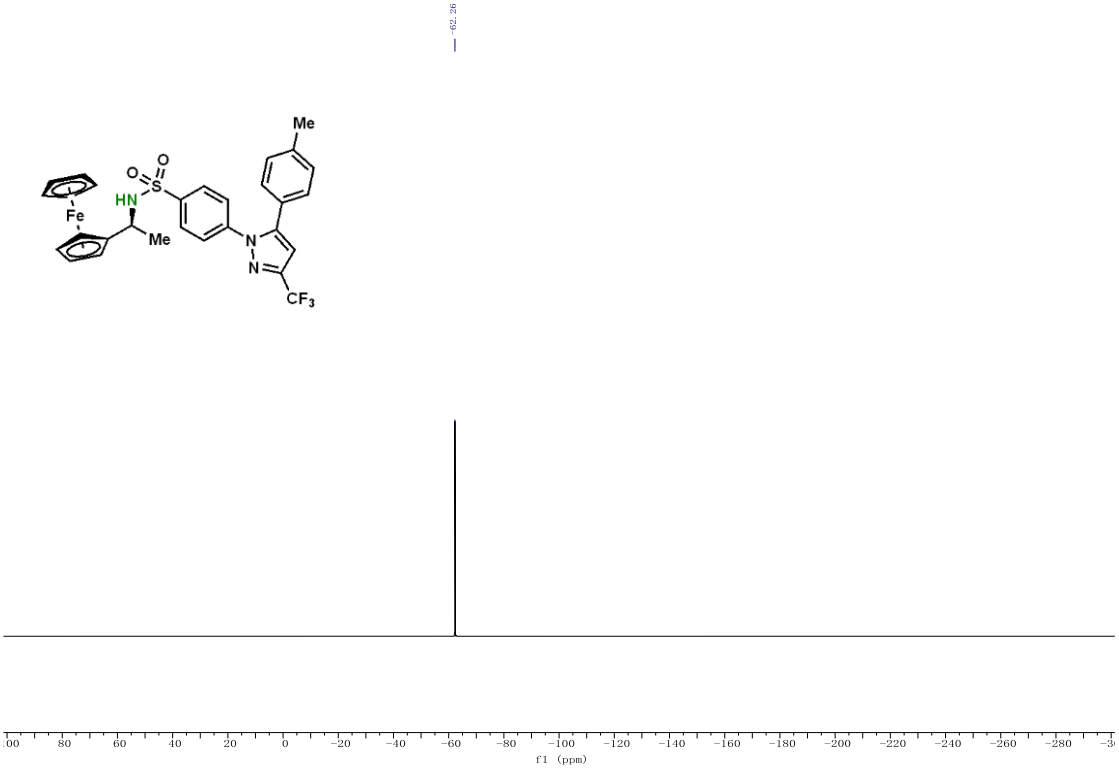
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)

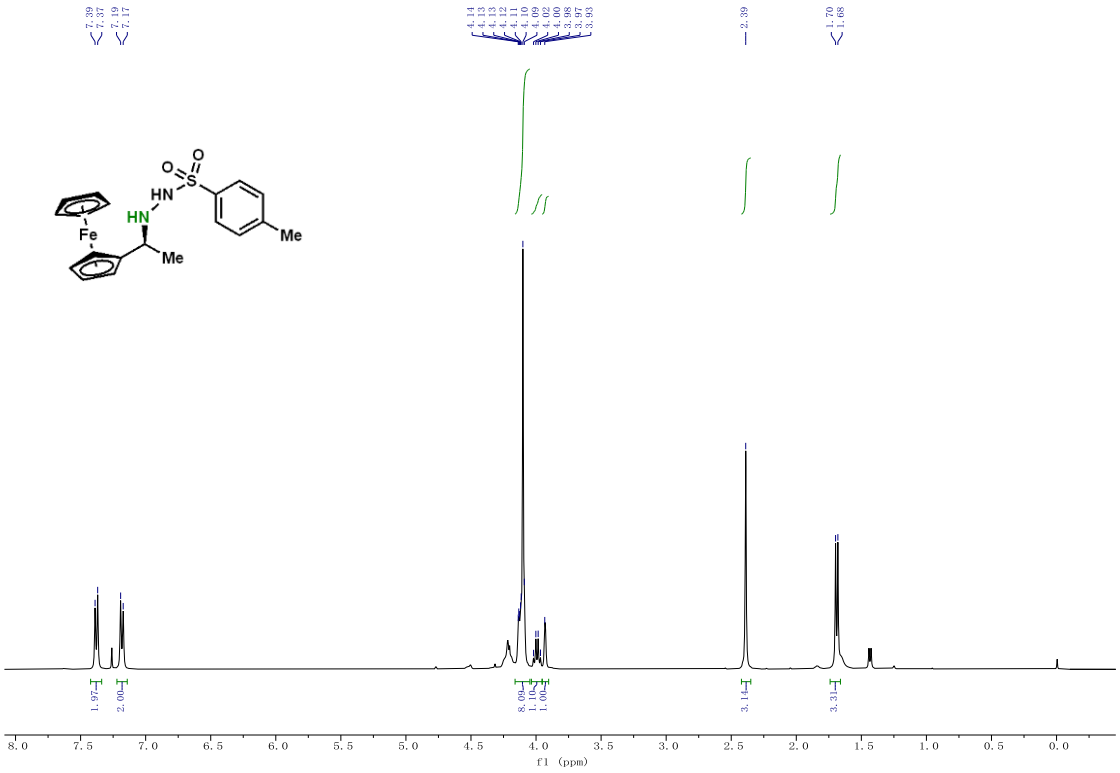


^{19}F NMR (376 MHz, $CDCl_3$)

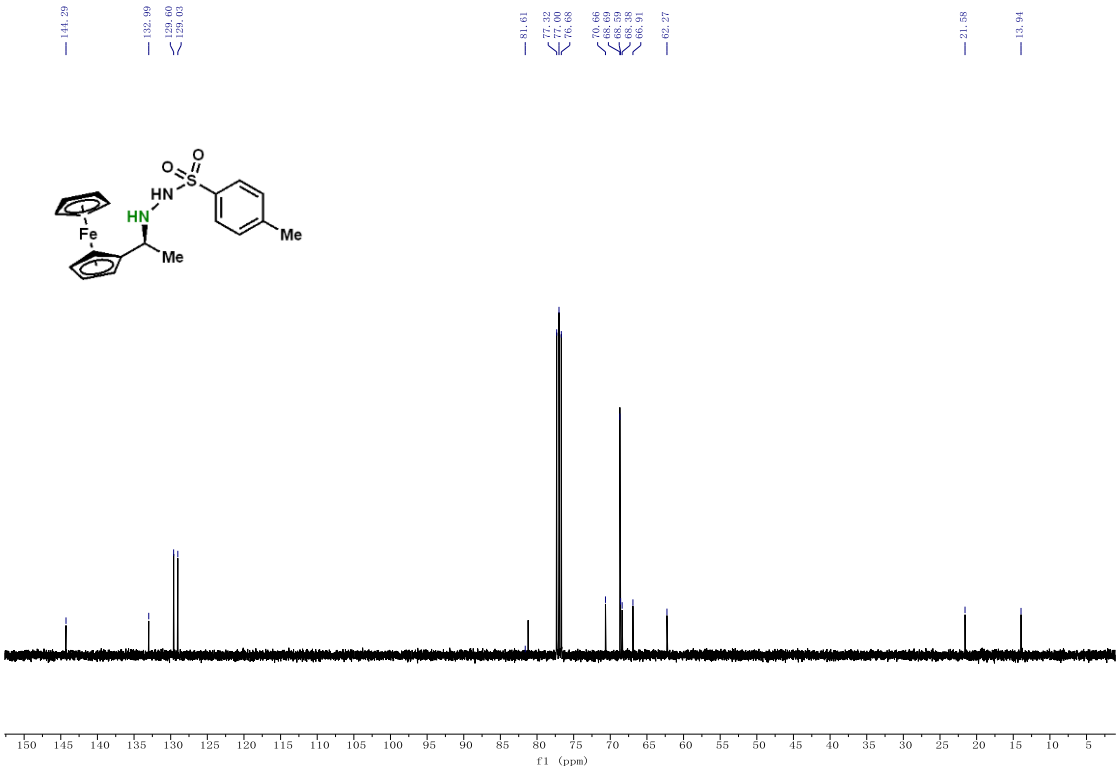


(S)-4-methyl-N'-(1-(ferrocene-2-yl)ethyl)benzenesulfonohydrazide (53)

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

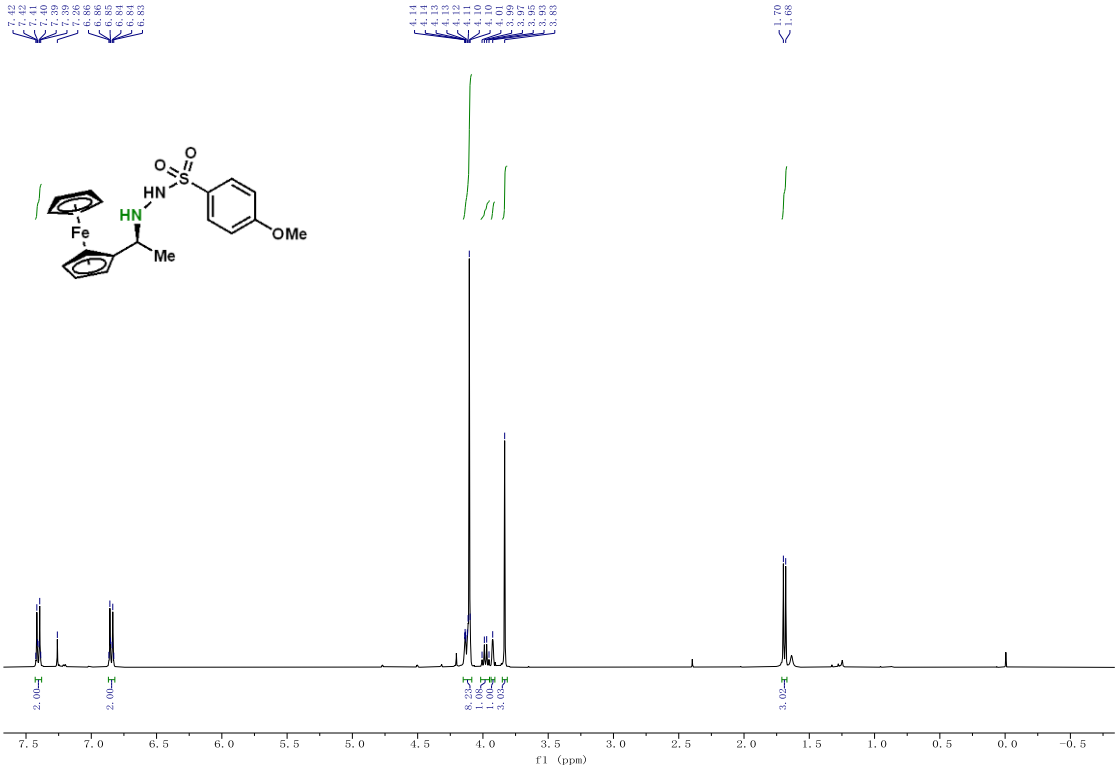


^{13}C NMR (101 MHz, $CDCl_3$)

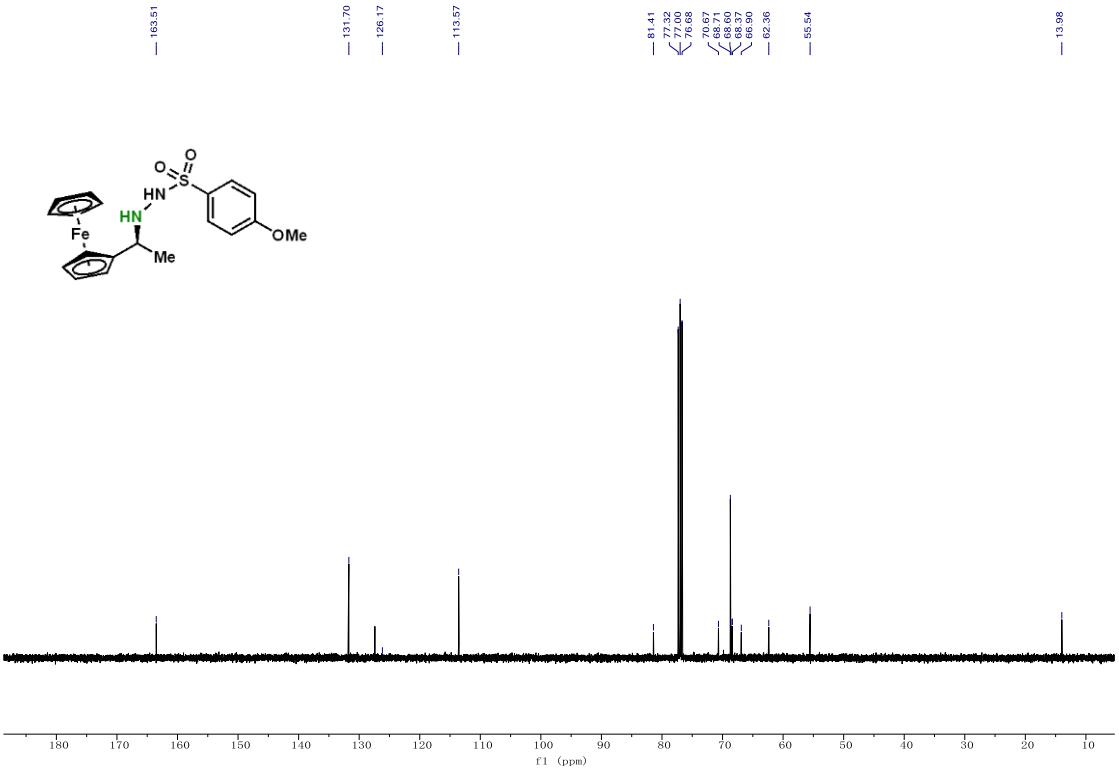


(S)-4-methoxy-N'-(1-(ferrocene-2-yl)ethyl)benzenesulfonohydrazide (54)

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

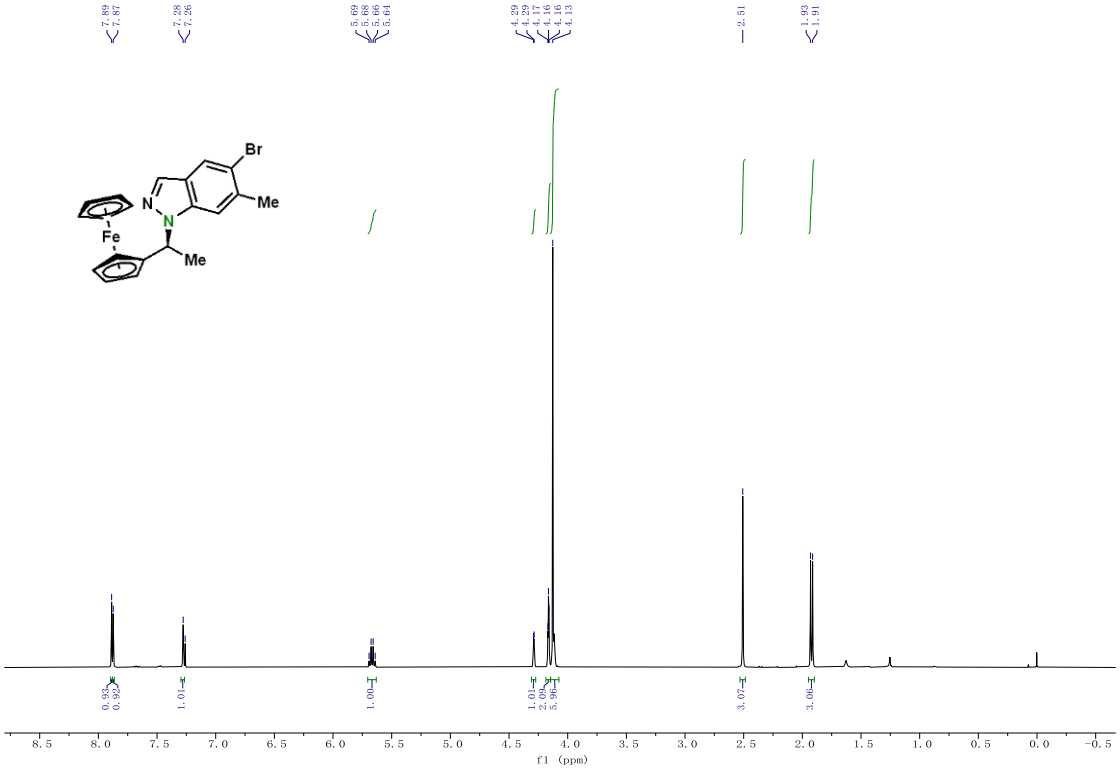


^{13}C NMR (101 MHz, $CDCl_3$)

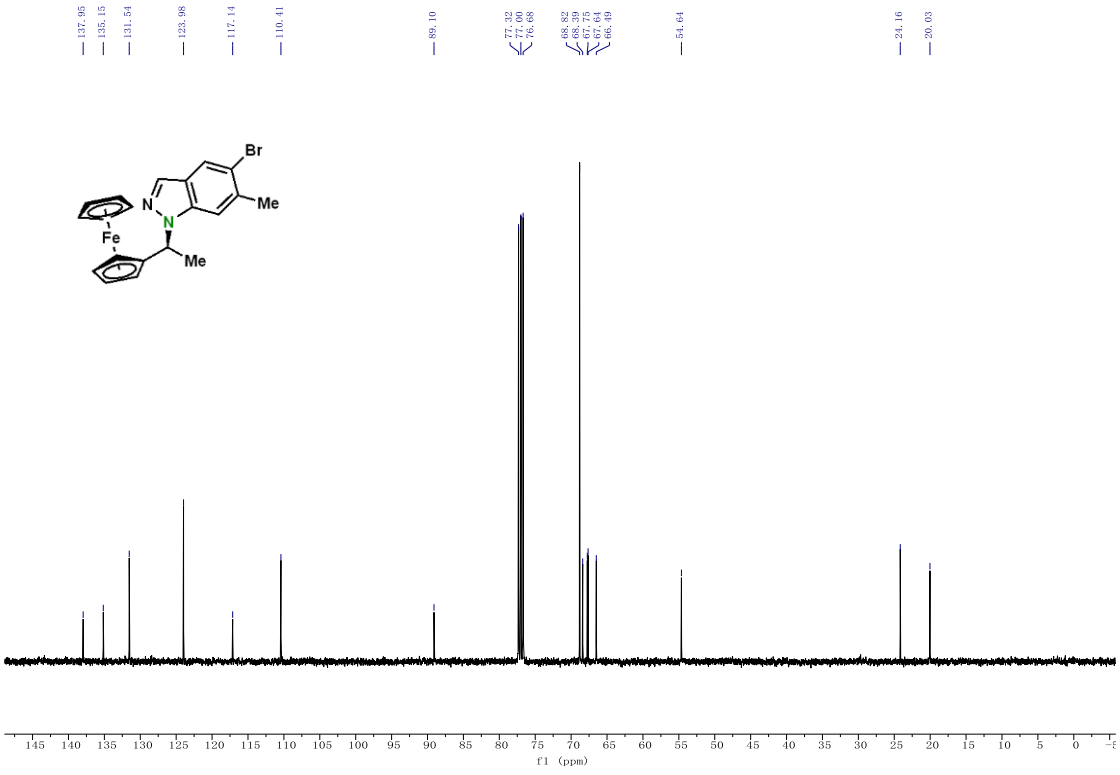


(S)-5-bromo-6-methyl-1-(1-(ferrocene-2-yl)ethyl)-1H-indazole (55)

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

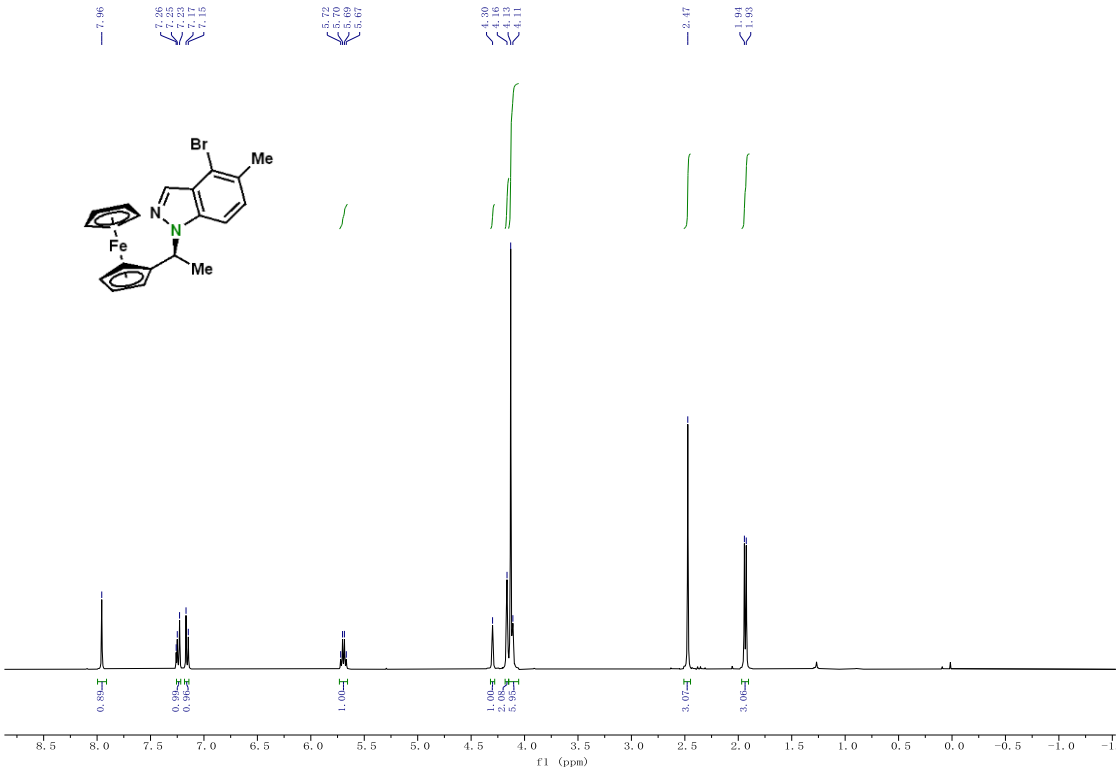


^{13}C NMR (101 MHz, $CDCl_3$)

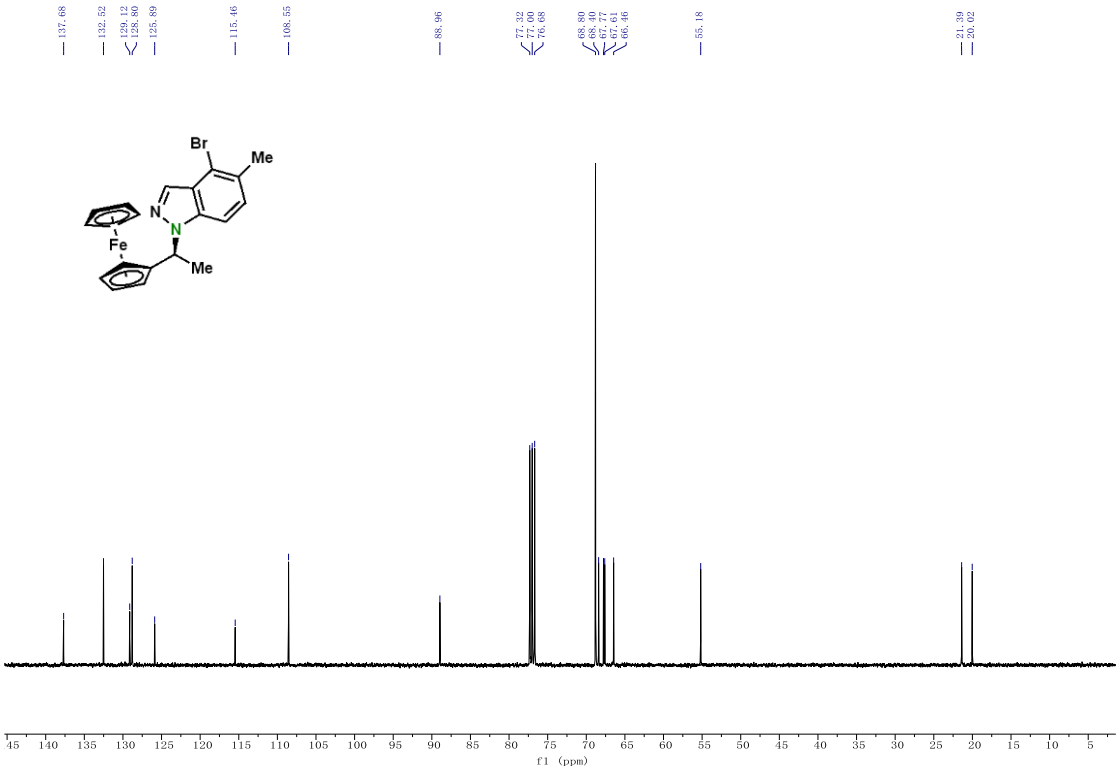


(S)-4-bromo-5-methyl-1-(1-(ferrocene-2-yl)ethyl)-1H-indazole (56)

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

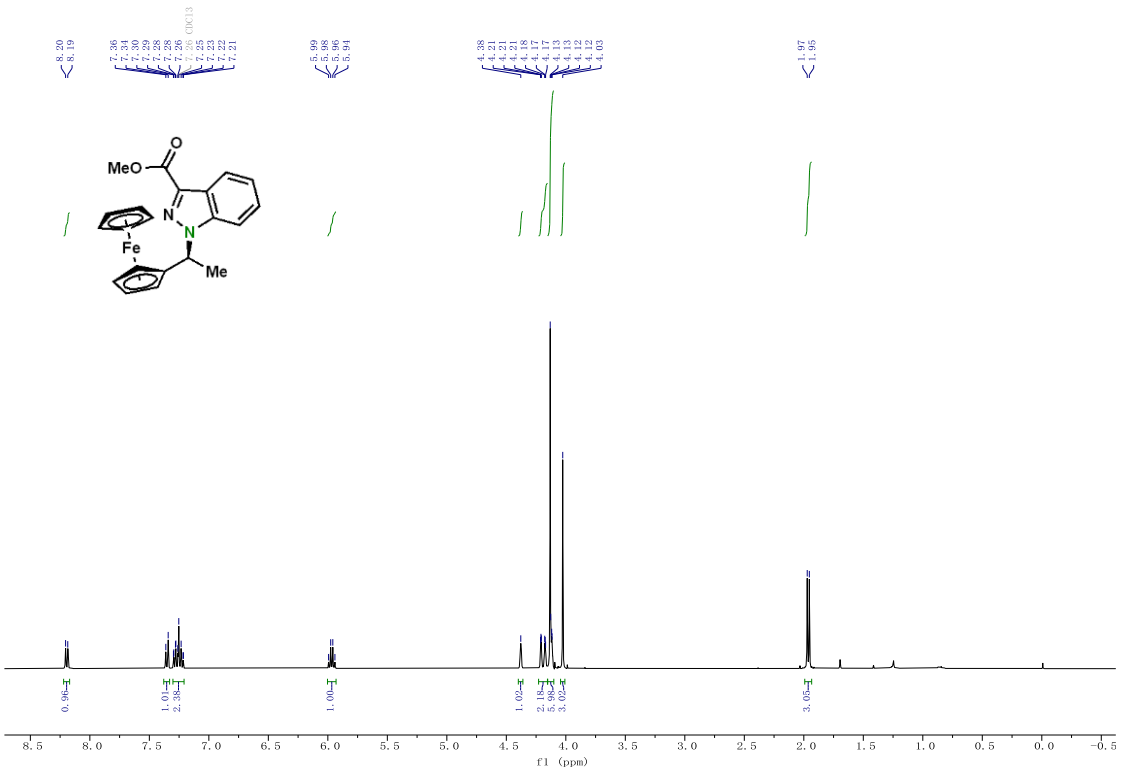


^{13}C NMR (101 MHz, $CDCl_3$)

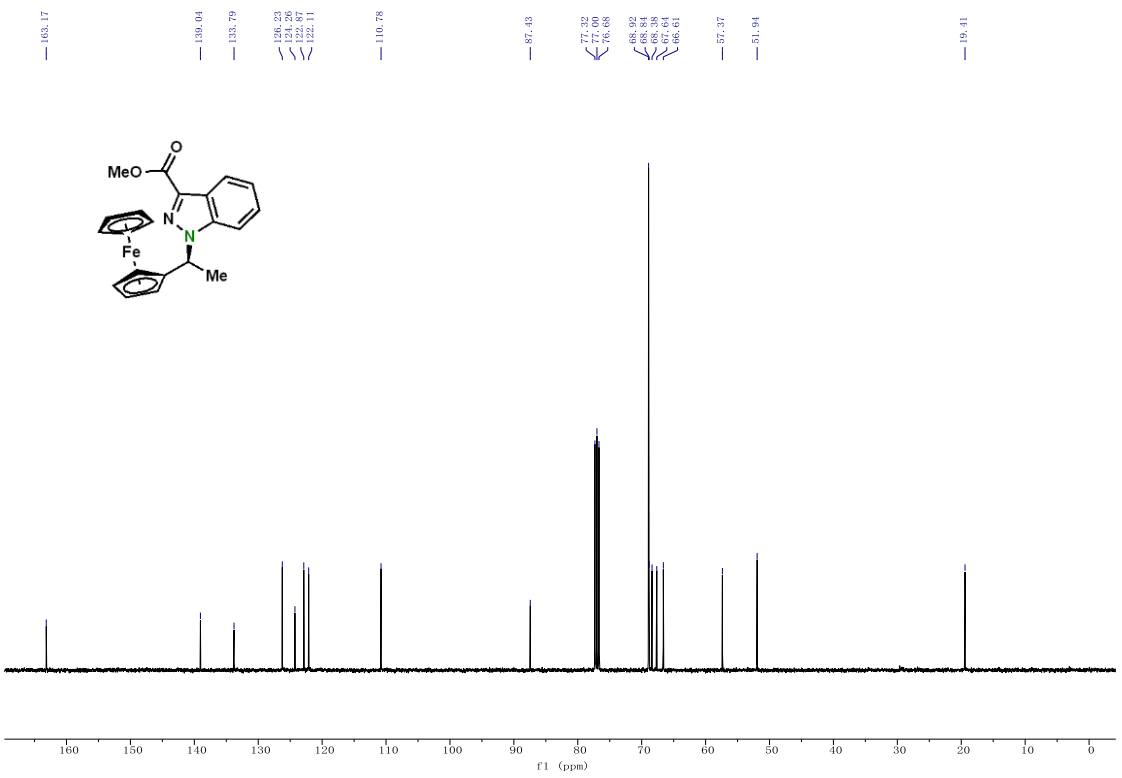


methyl *(S)*-1-(1-(ferrocene-2-yl)ethyl)-1H-indazole-3-carboxylate (57)

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

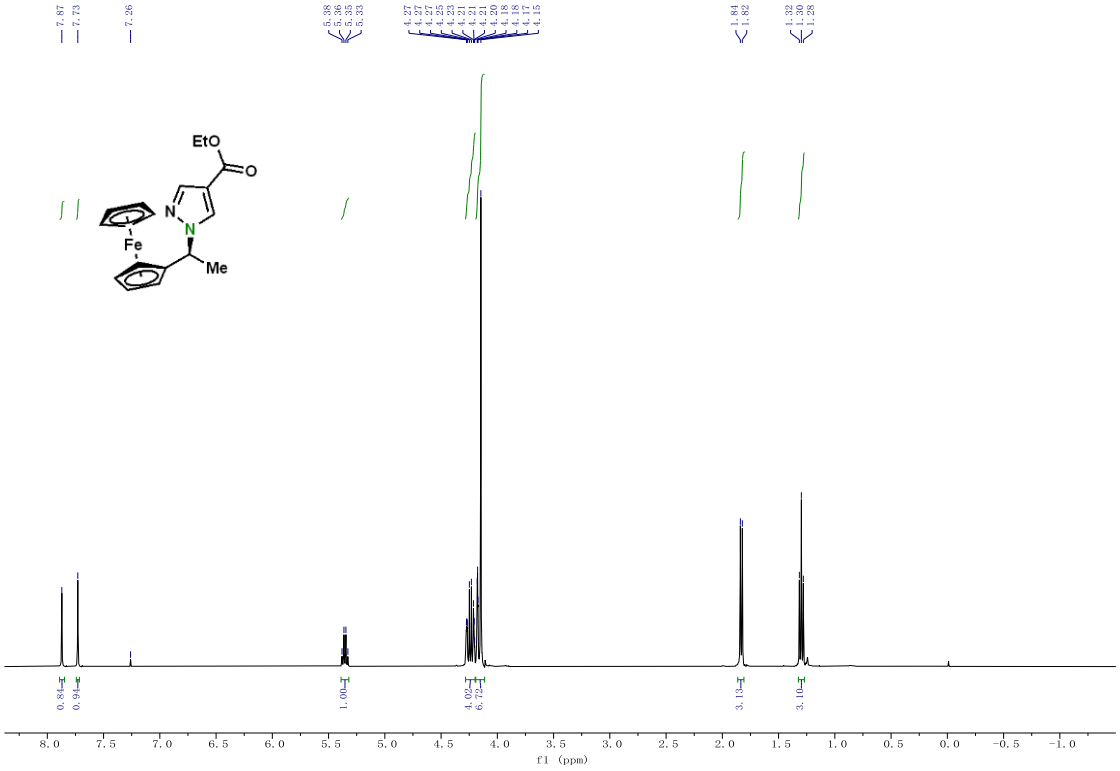


^{13}C NMR (101 MHz, $CDCl_3$)

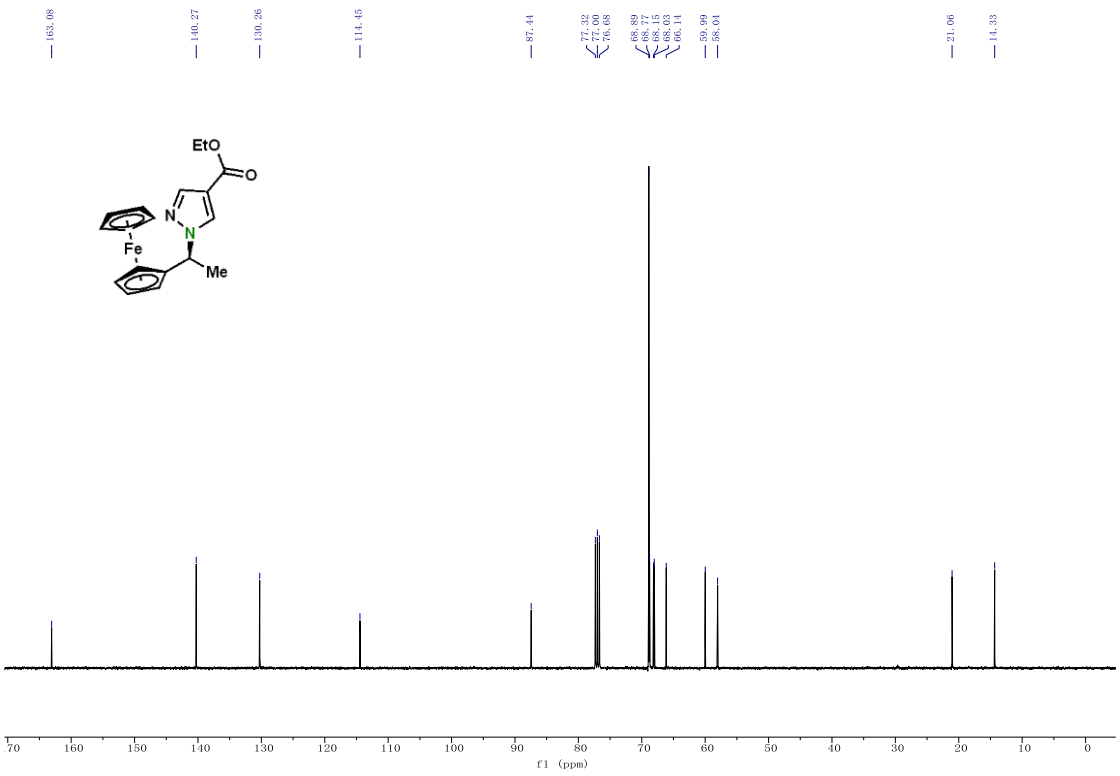


ethyl *(S)*-1-(1-(ferrocene-2-yl)ethyl)-1H-pyrazole-4-carboxylate (58)

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

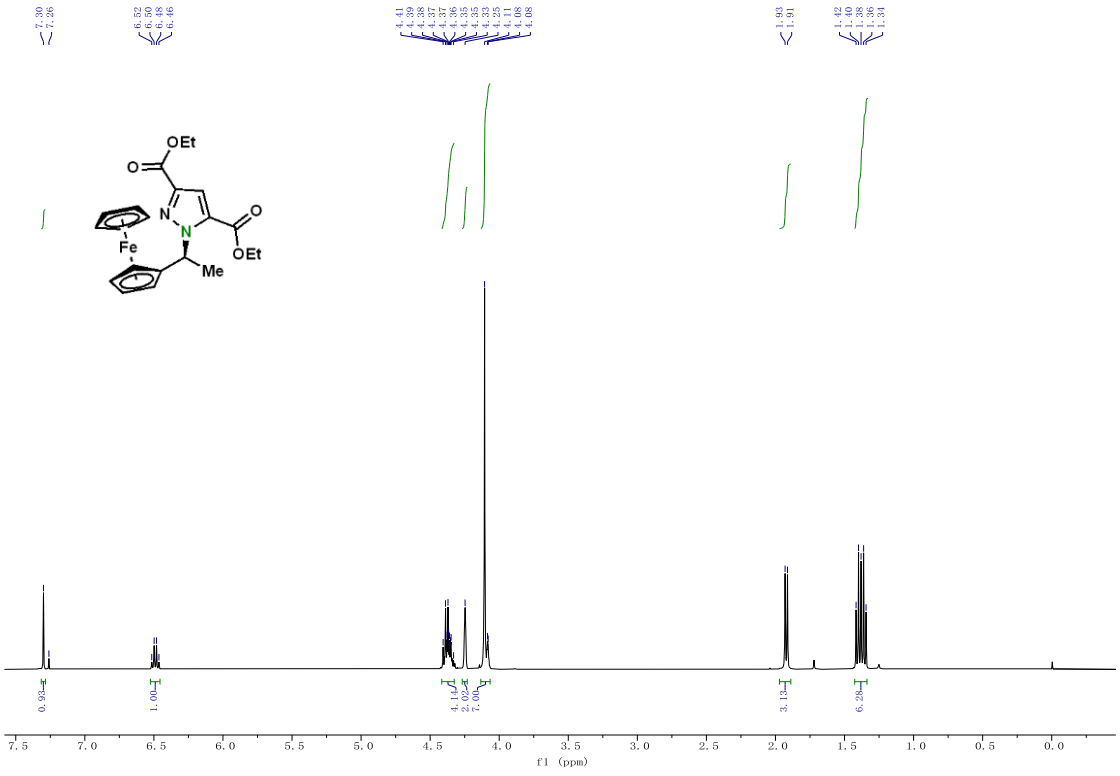


^{13}C NMR (101 MHz, $CDCl_3$)

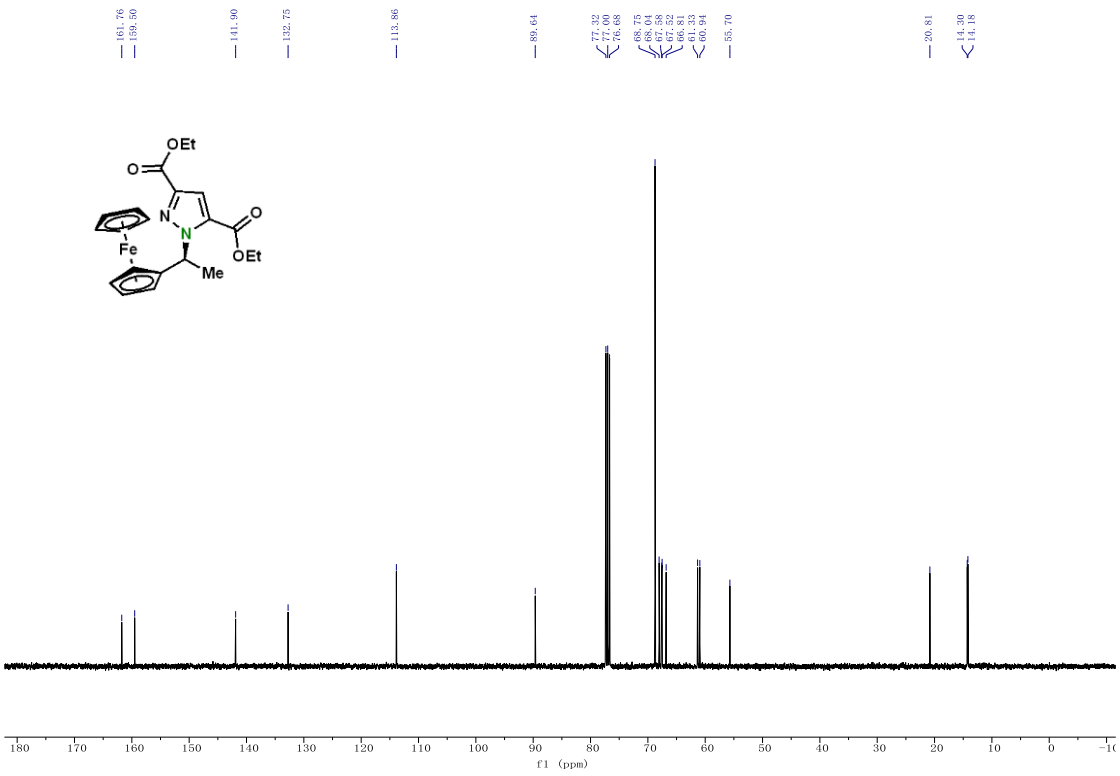


diethyl *(S)*-1-(1-(ferrocene-2-yl)ethyl)-1H-pyrazole-3,5-dicarboxylate (59)

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

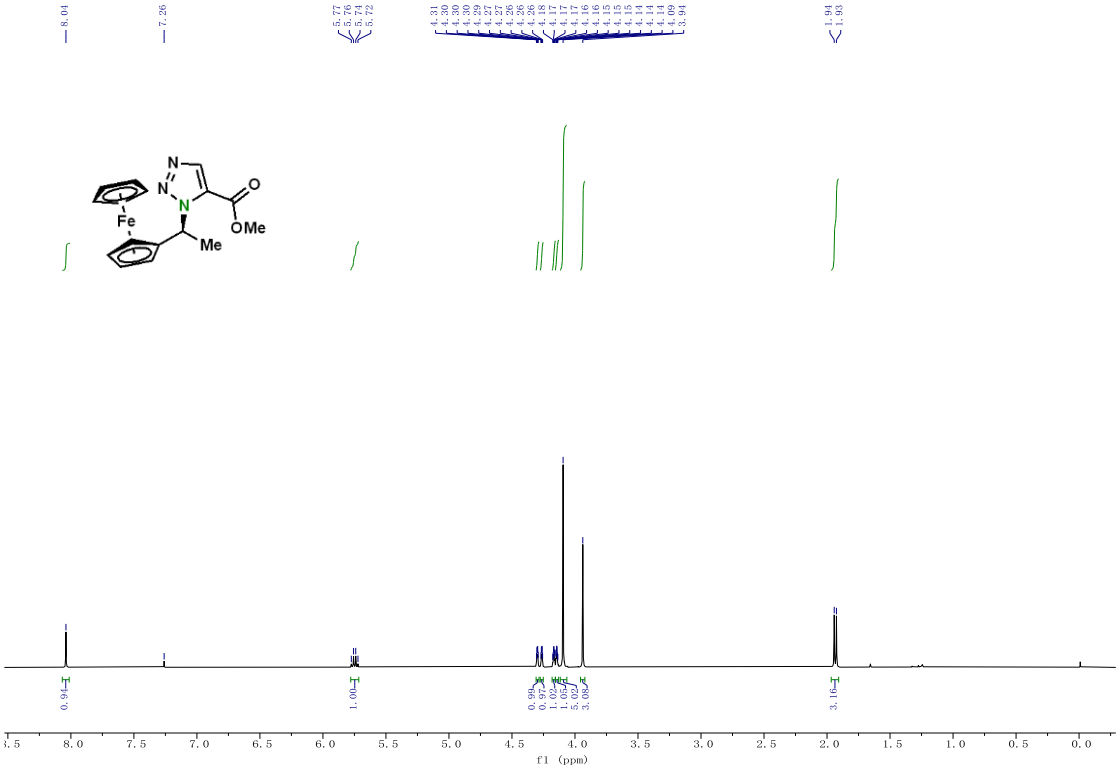


^{13}C NMR (101 MHz, $CDCl_3$)

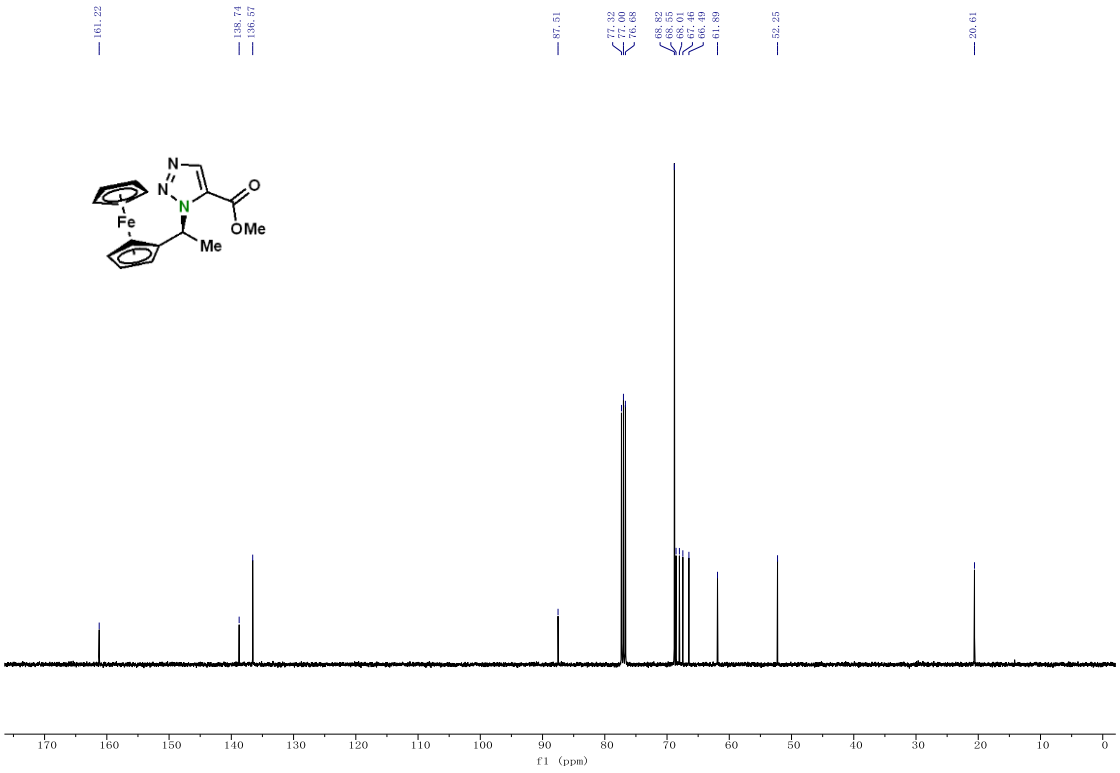


methyl *(S)*-1-(1-(ferrocene-2-yl)ethyl)-1H-1,2,3-triazole-5-carboxylate (60)

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

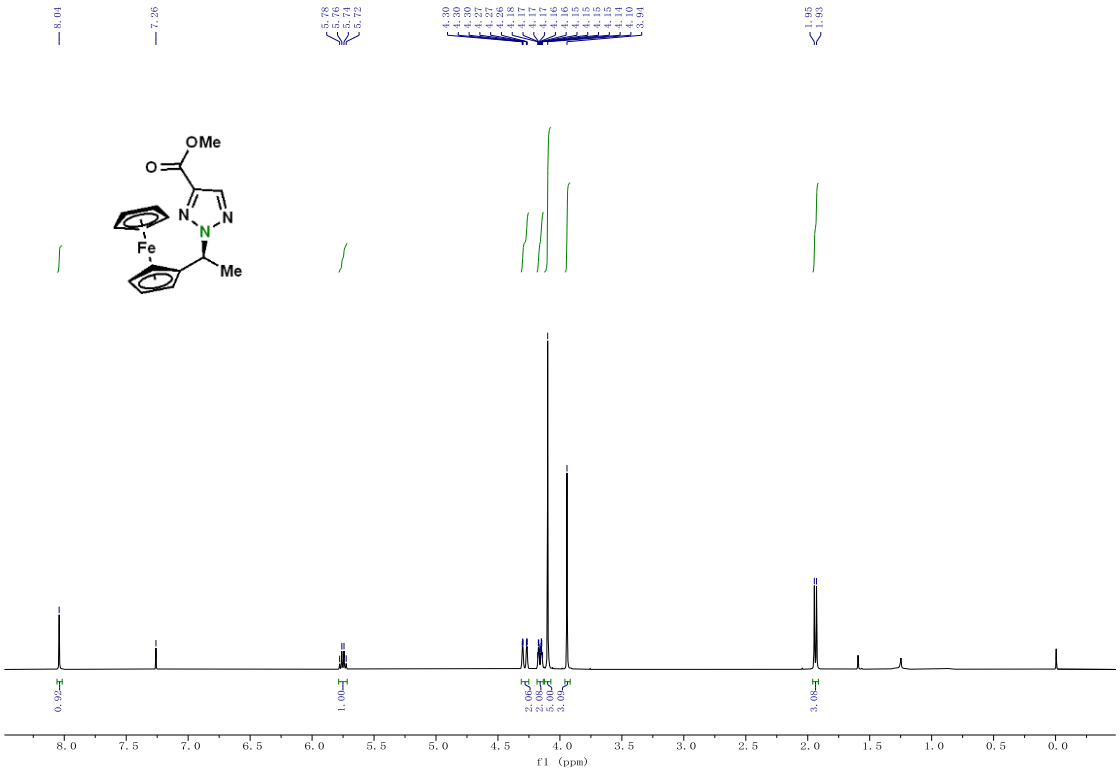


^{13}C NMR (101 MHz, $CDCl_3$)

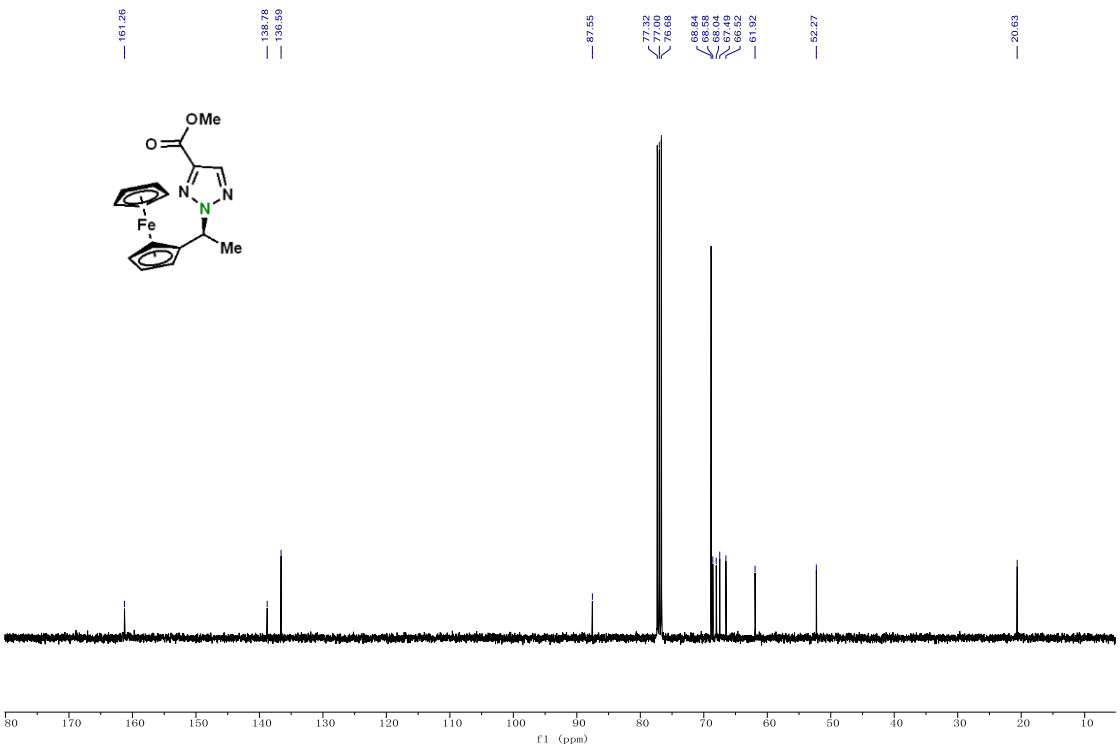


methyl *(S)*-2-(1-(ferrocene-2-yl)ethyl)-2H-1,2,3-triazole-4-carboxylate (61)

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

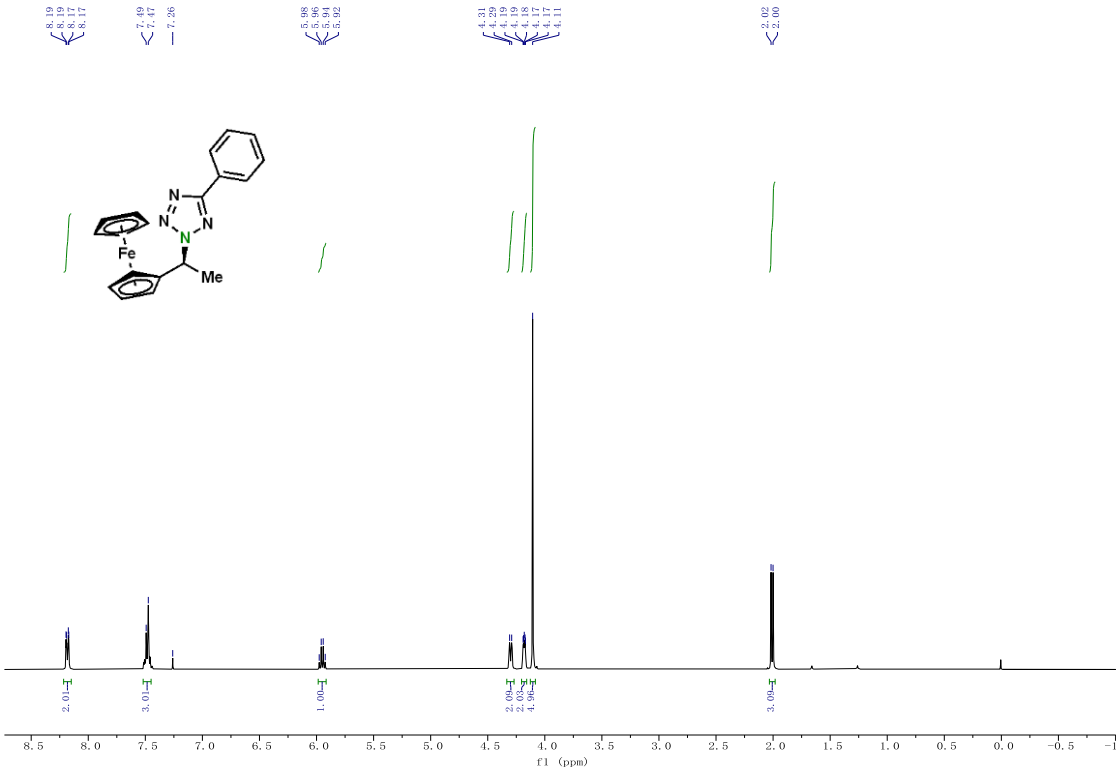


^{13}C NMR (101 MHz, $CDCl_3$)

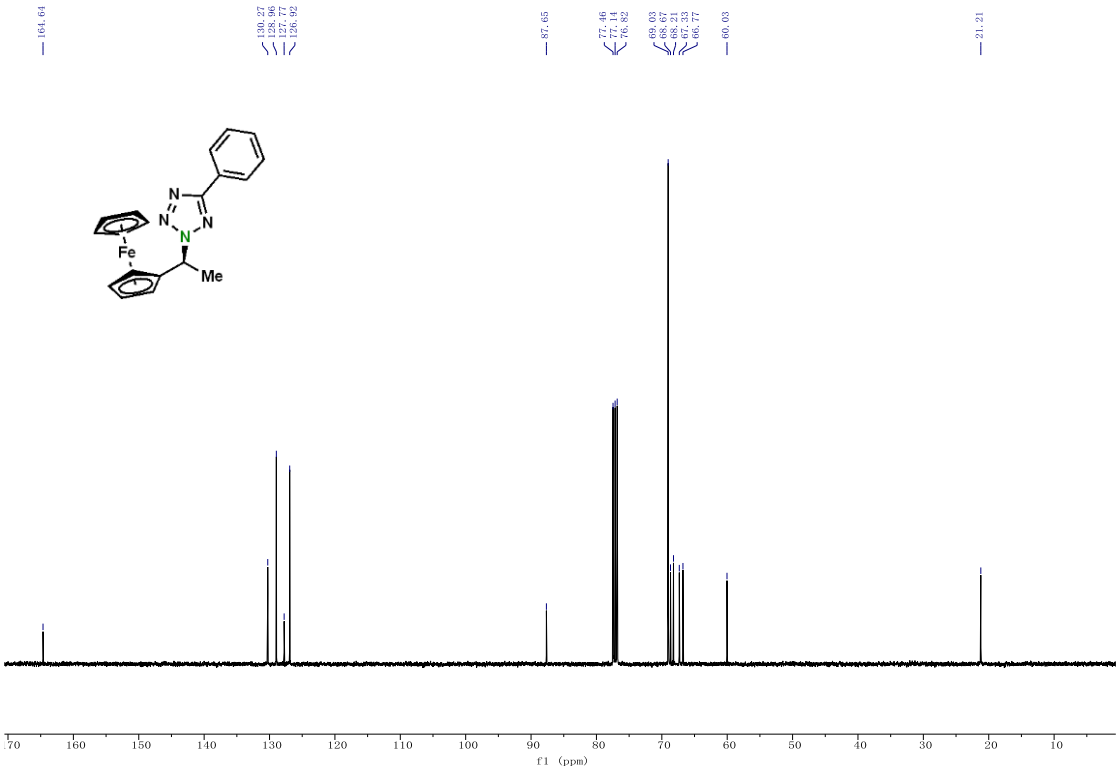


(S)-5-phenyl-2-(1-(ferrocene-2-yl)ethyl)-2H-tetrazole (62)

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

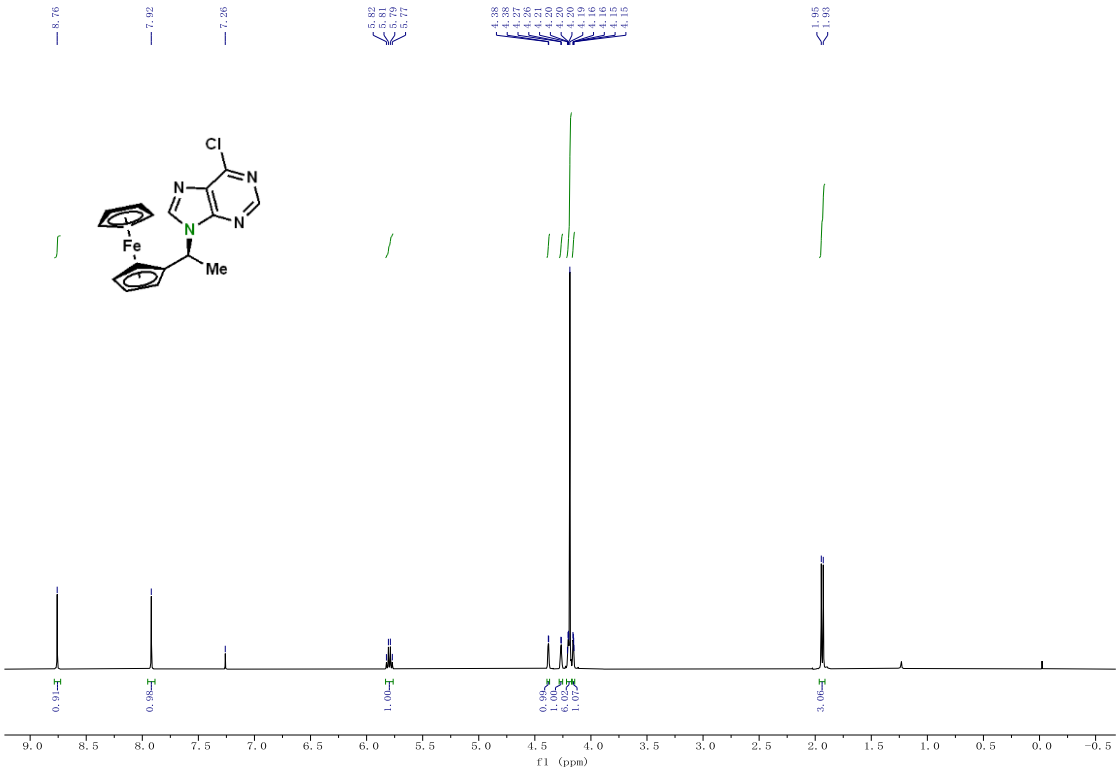


^{13}C NMR (101 MHz, $CDCl_3$)

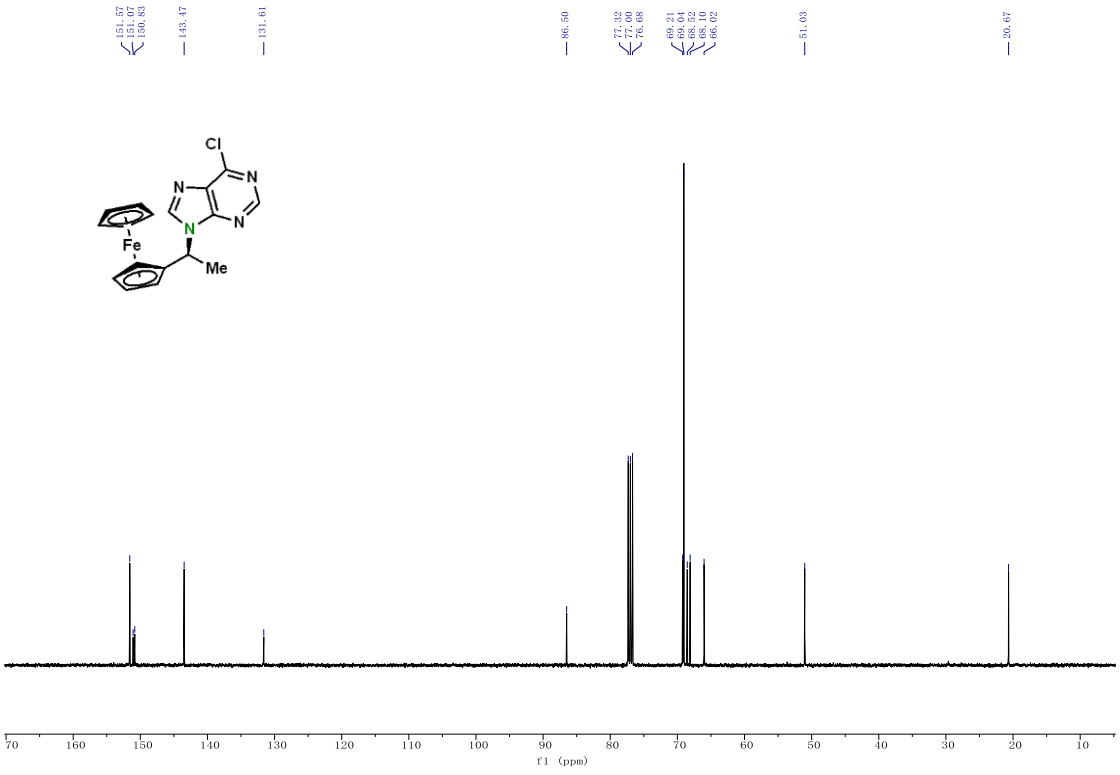


(S)-6-chloro-9-(1-(ferrocene-2-yl)ethyl)-9H-purine (63)

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

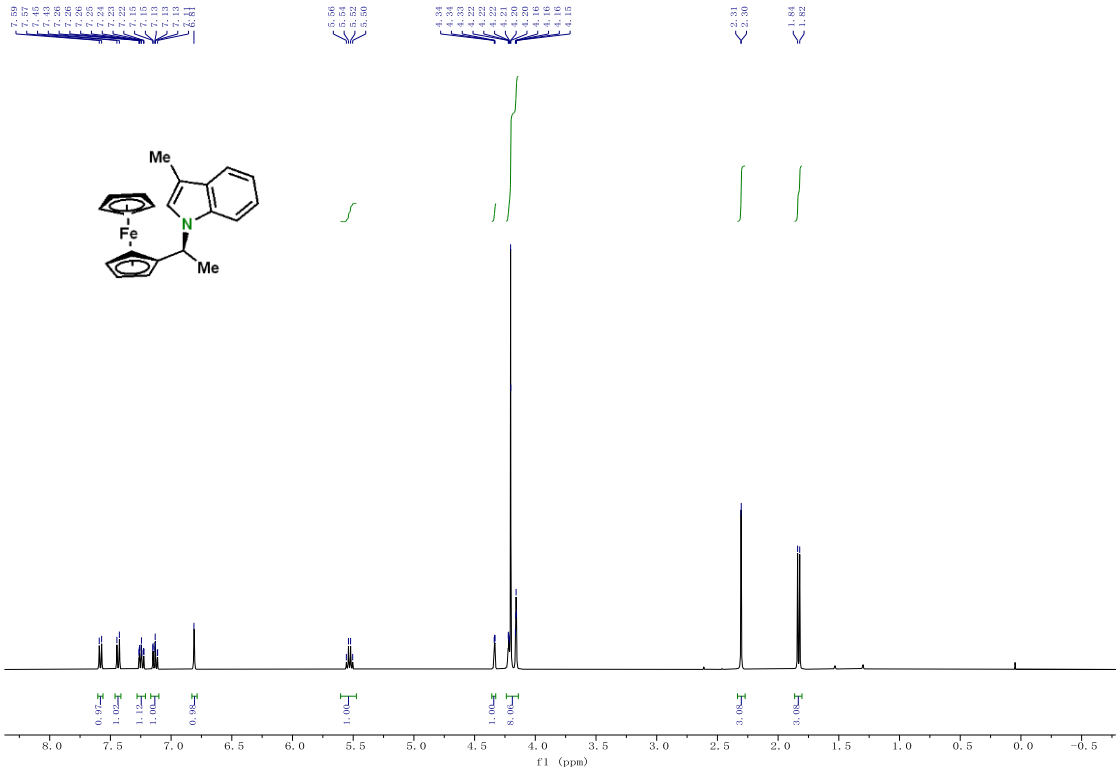


^{13}C NMR (101 MHz, $CDCl_3$)

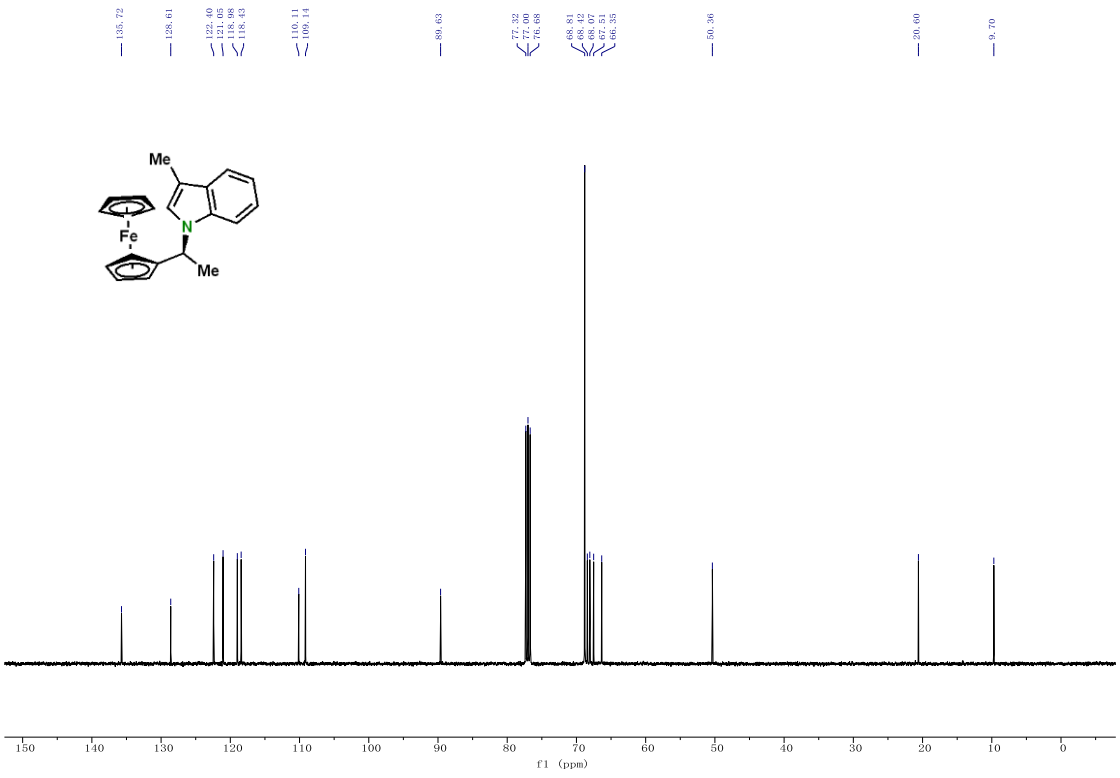


(S)-3-methyl-1-(1-(ferrocene-2-yl)ethyl)-1H-indole (64)

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

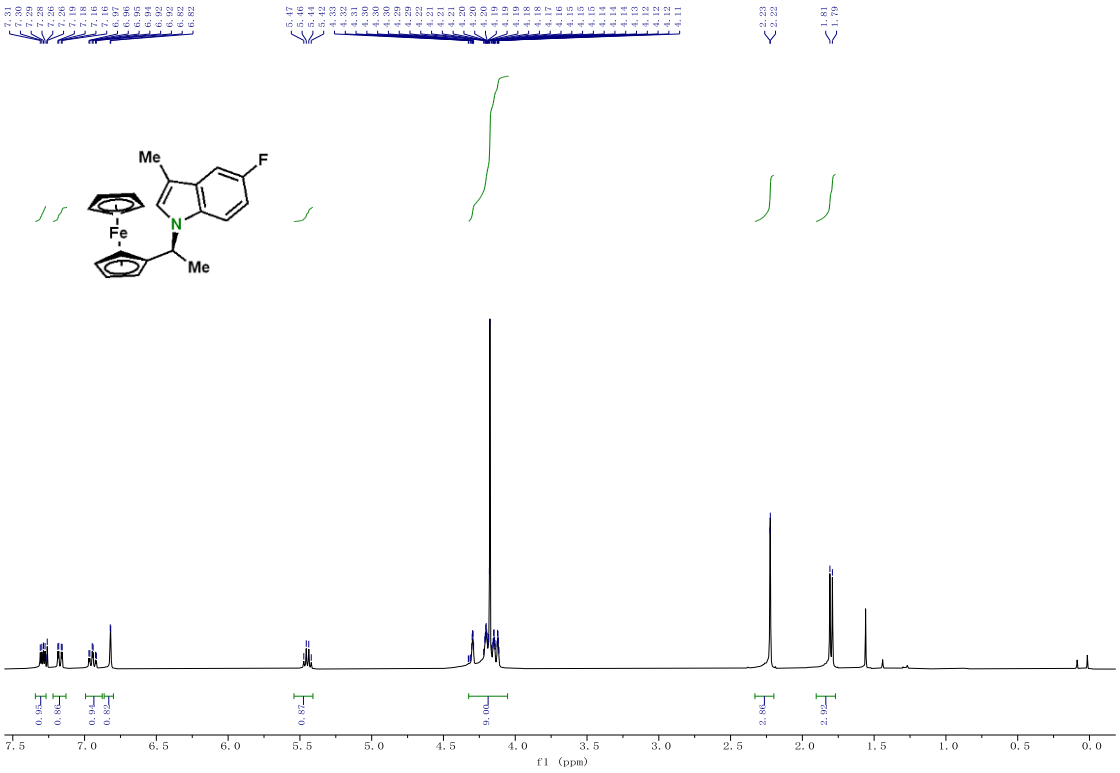


^{13}C NMR (101 MHz, $CDCl_3$)

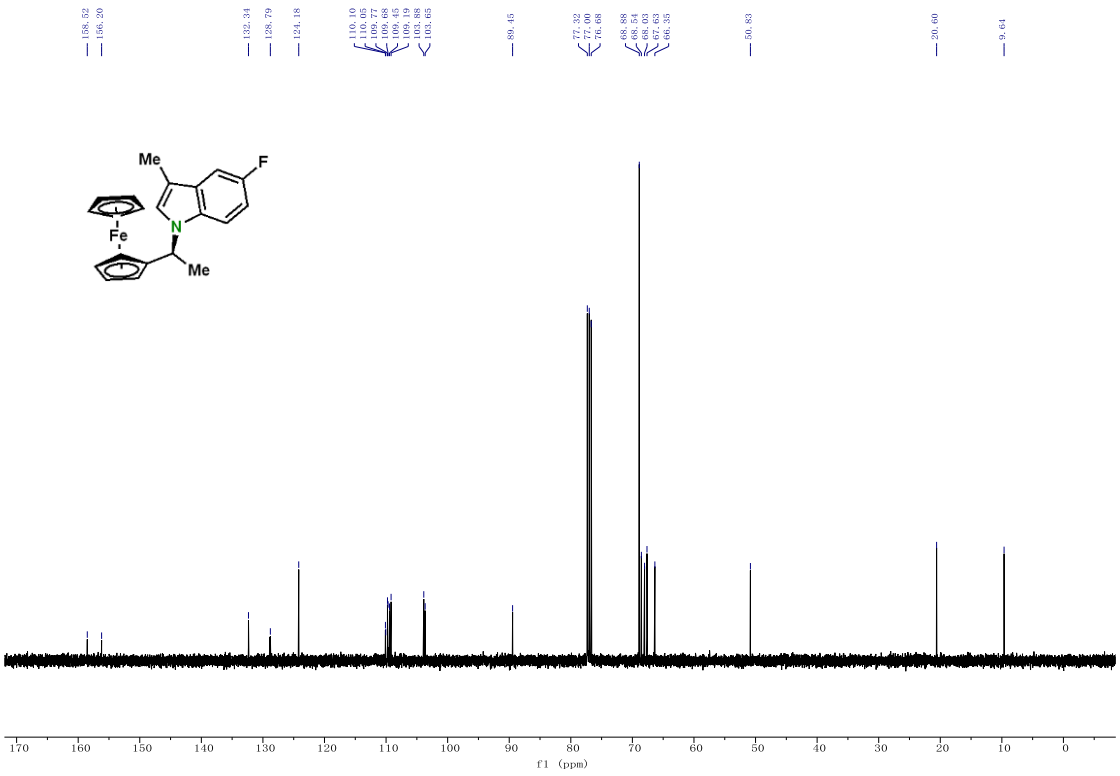


(S)-5-fluoro-3-methyl-1-(1-(ferrocene-2-yl)ethyl)-1H-indole (65)

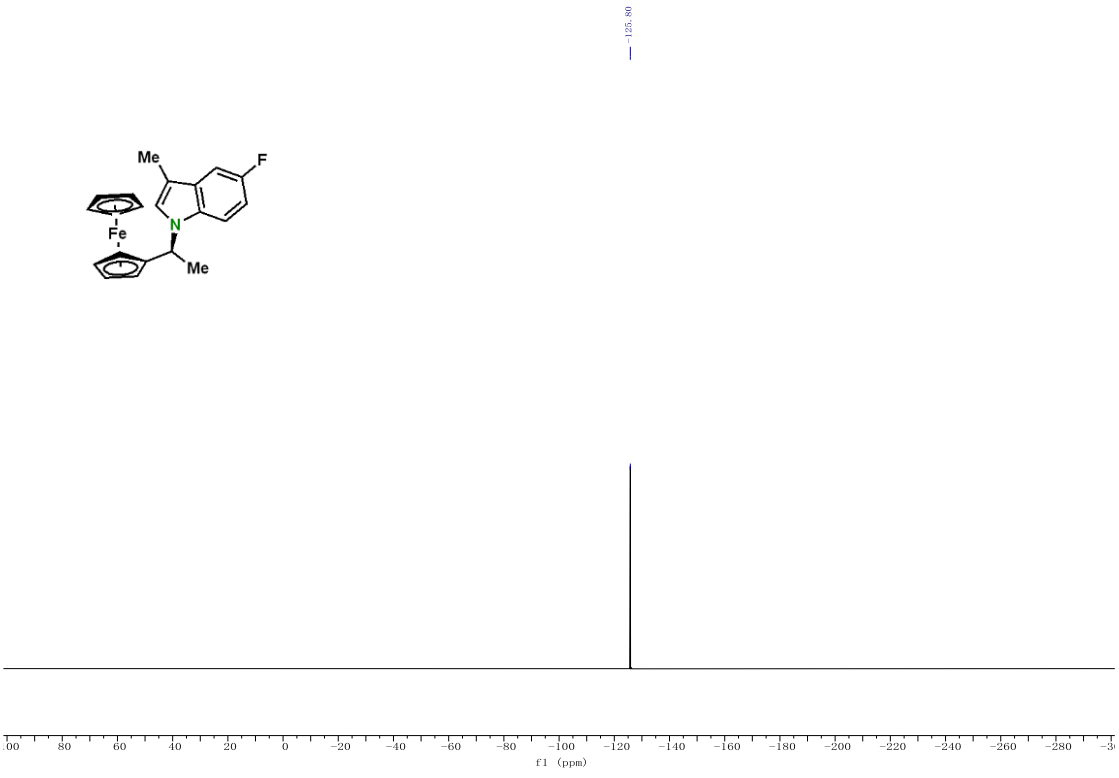
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)

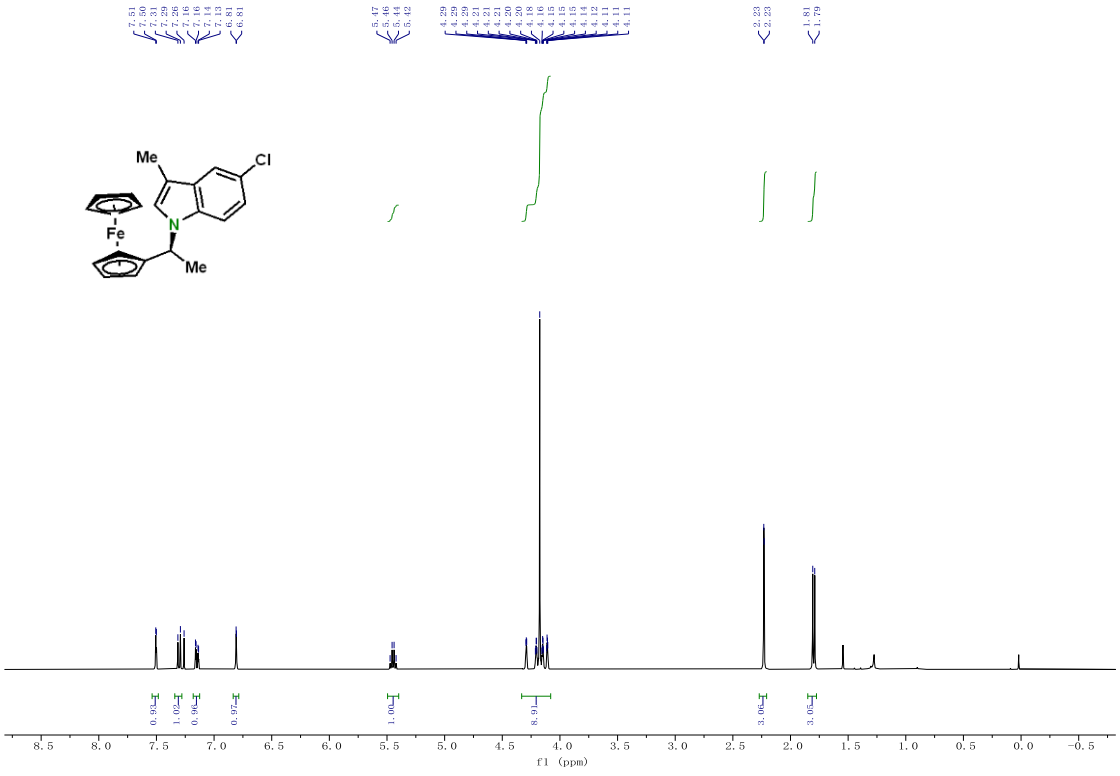


^{19}F NMR (376 MHz, $CDCl_3$)

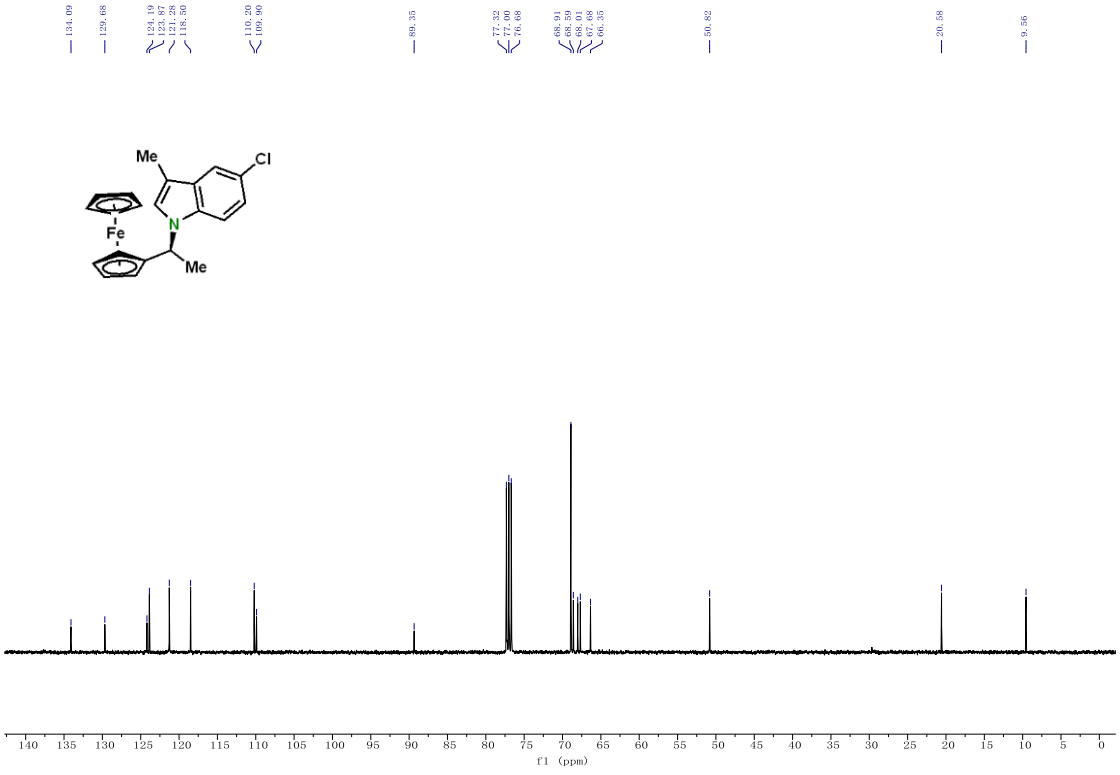


(S)-5-chloro-3-methyl-1-(1-(ferrocene-2-yl)ethyl)-1H-indole (66)

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

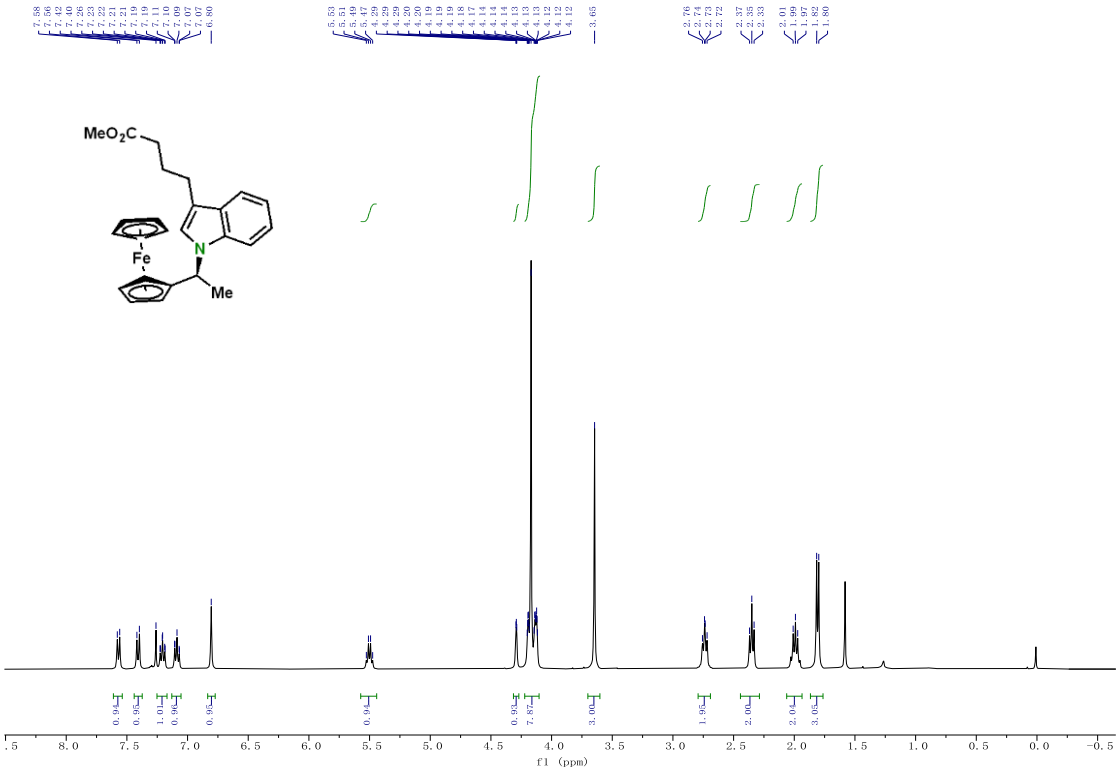


^{13}C NMR (101 MHz, $CDCl_3$)

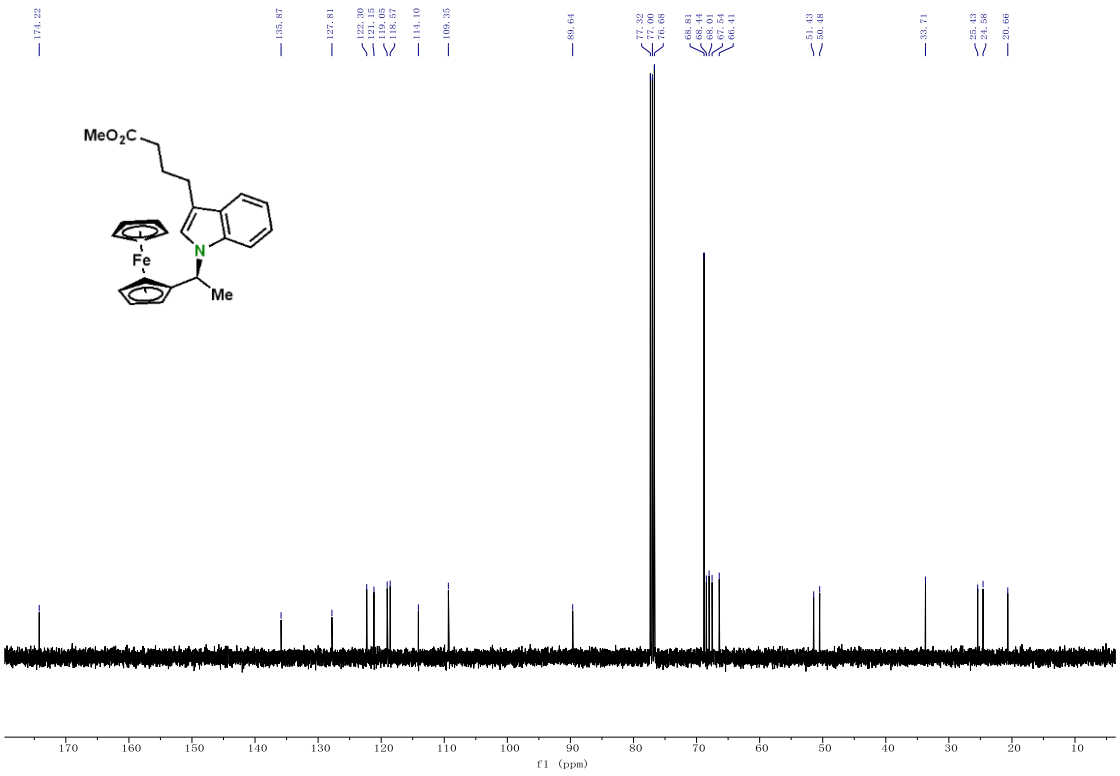


methyl *(S)*-4-(1-(1-(ferrocene-2-yl)ethyl)-1H-indol-3-yl)butanoate (67)

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

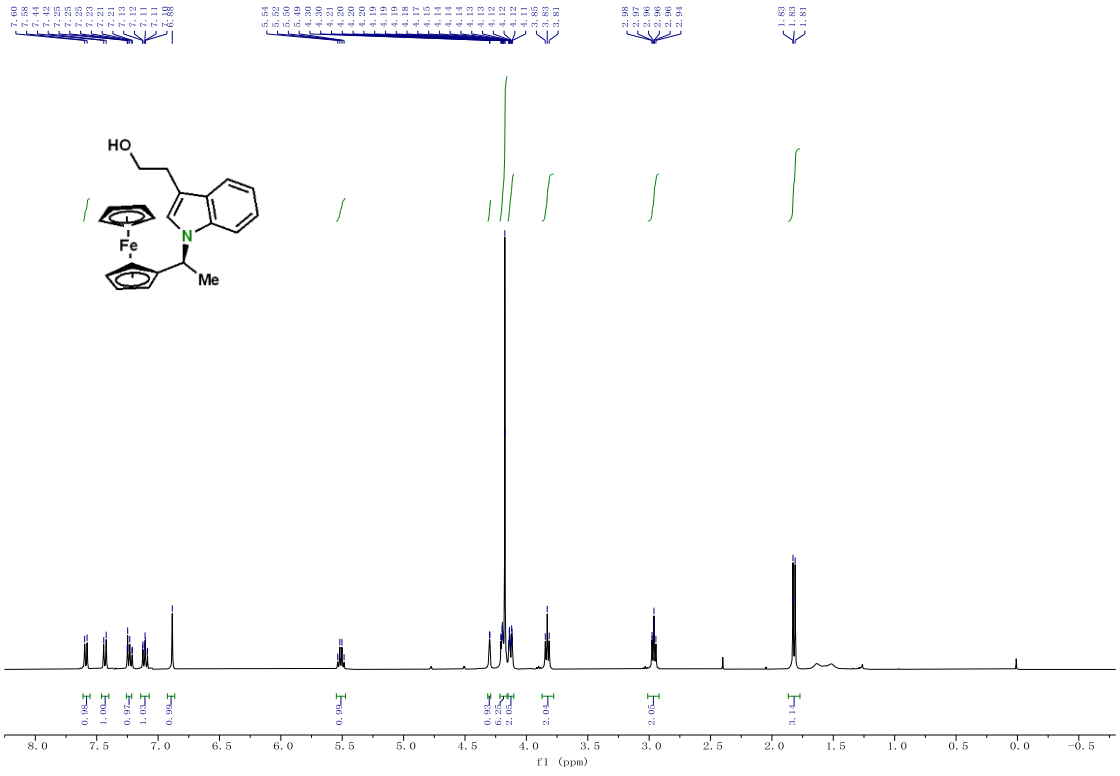


^{13}C NMR (101 MHz, $CDCl_3$)

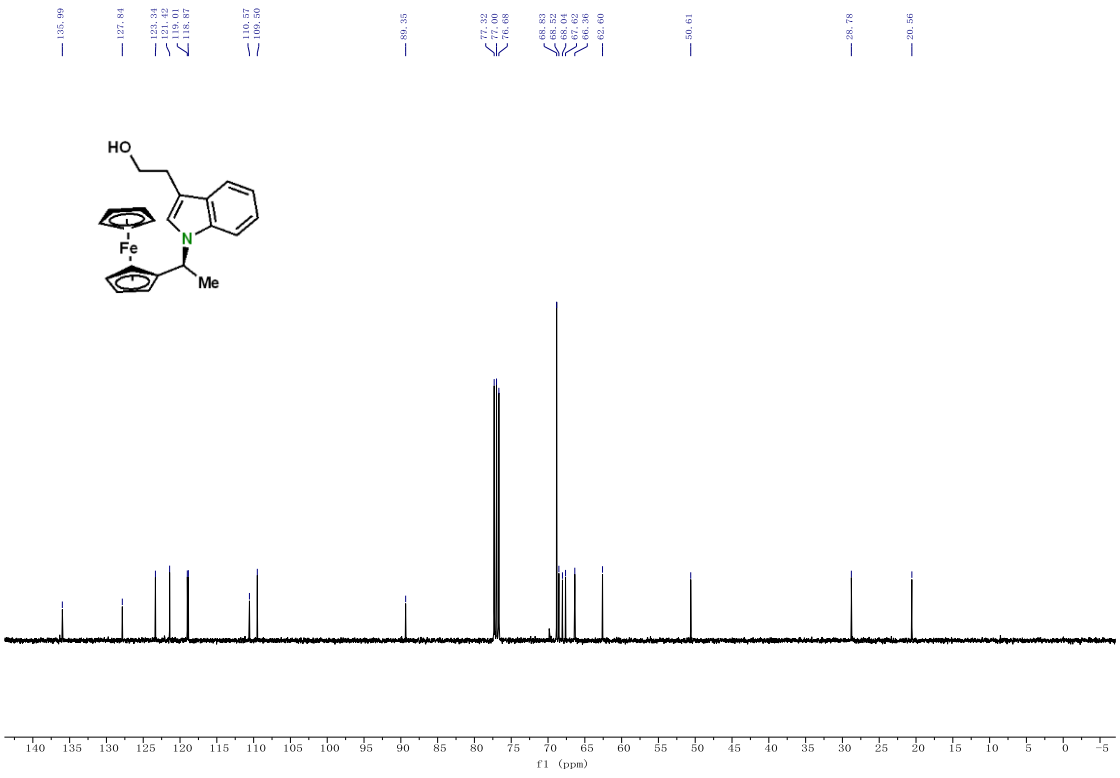


(S)-2-(1-(1-(ferrocene-2-yl)ethyl)-1H-indol-3-yl)ethan-1-ol (68)

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

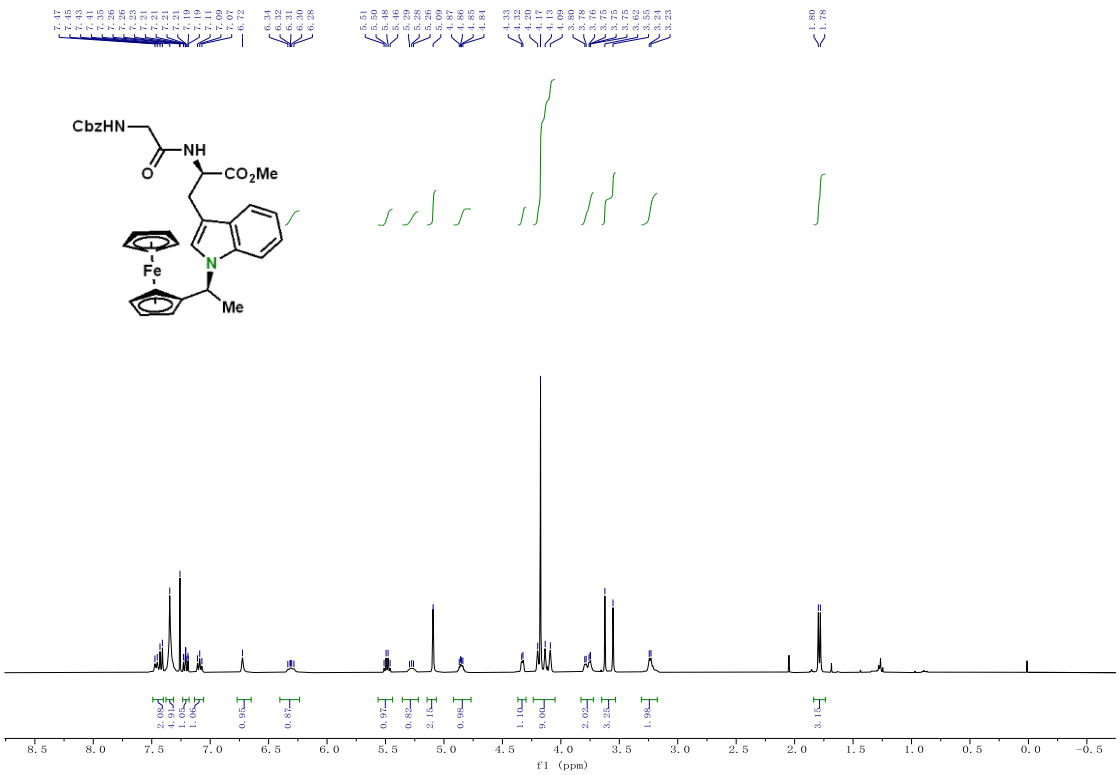


^{13}C NMR (101 MHz, $CDCl_3$)

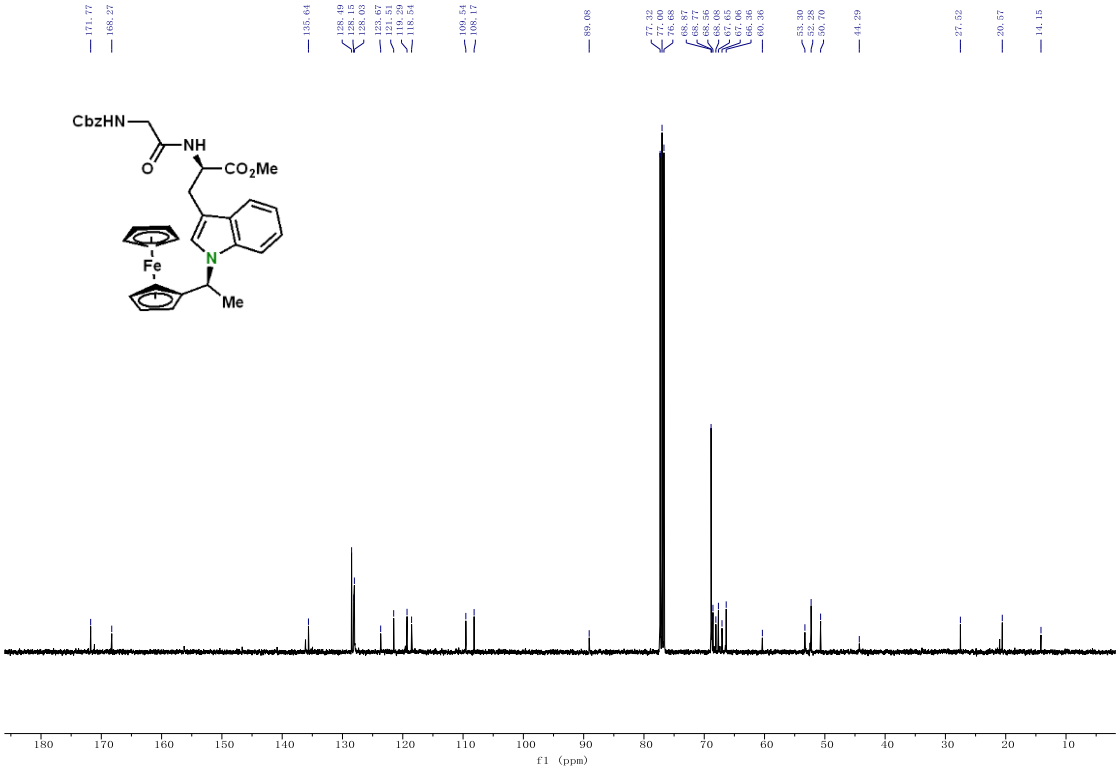


methyl (R)-2-(2-(((benzyloxy)carbonyl)amino)acetamido)-2-(1-((*S*)-1-(ferrocene-2-yl)ethyl)-1H-indol-3-yl)acetate (69)

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

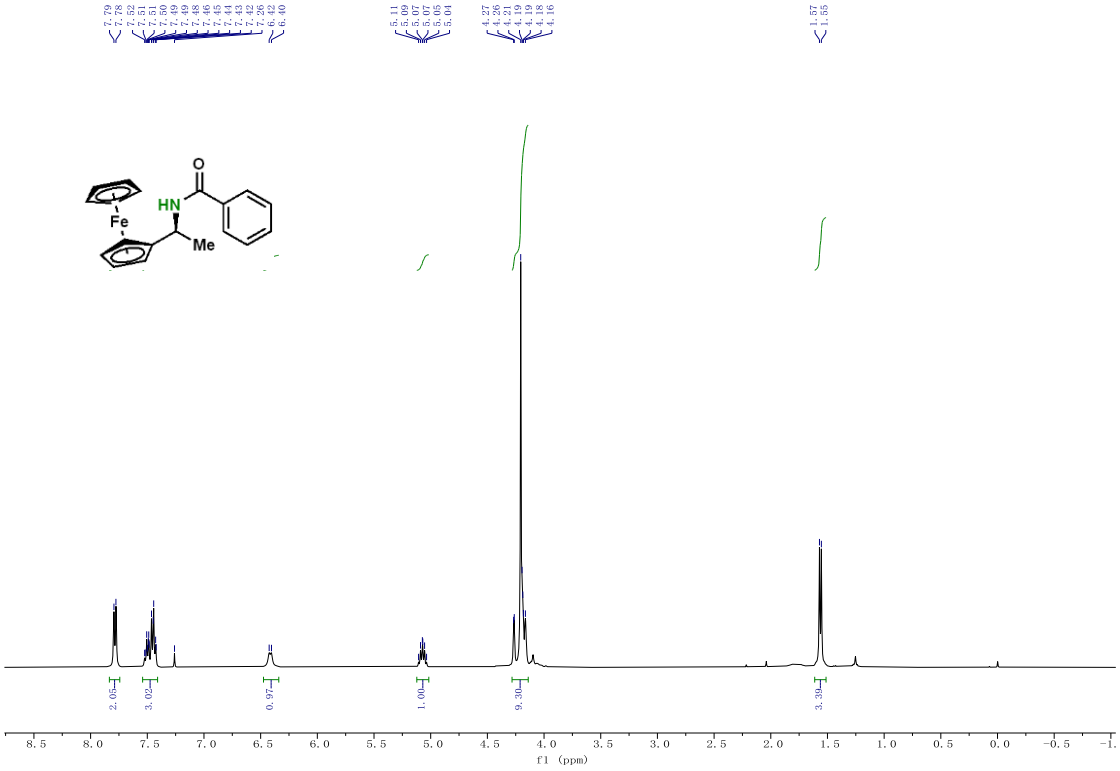


^{13}C NMR (101 MHz, $CDCl_3$)

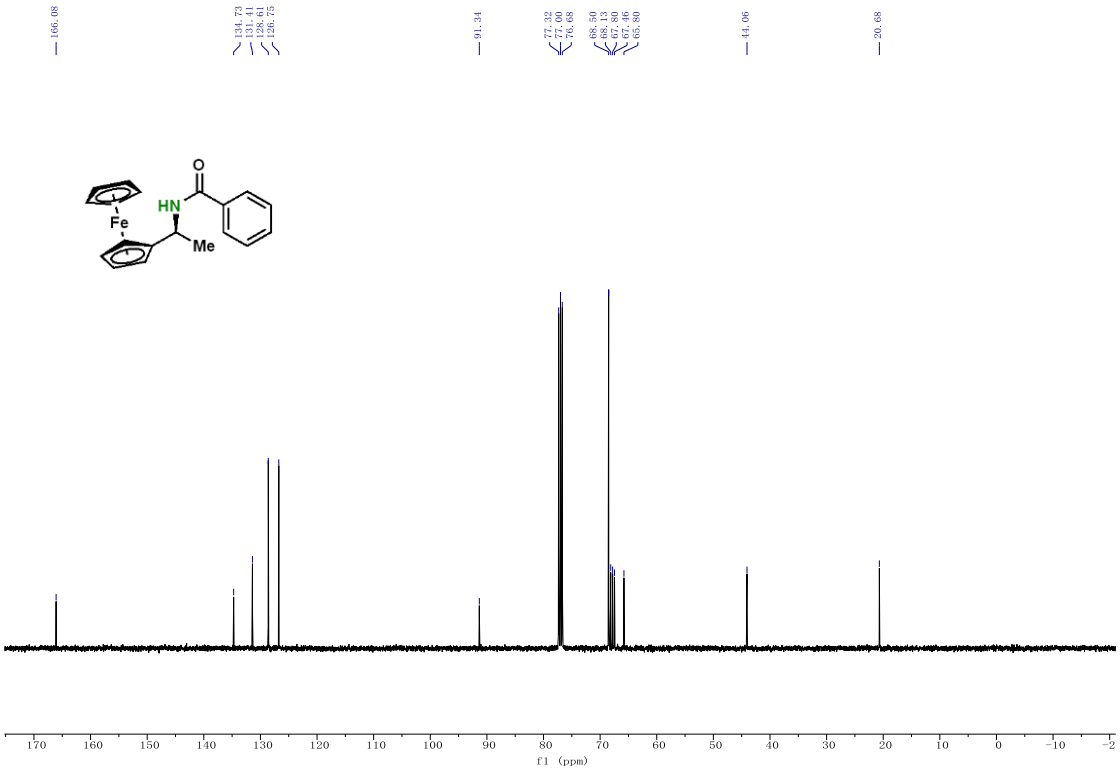


(S)-N-(1-(ferrocene-2-yl)ethyl)benzamide (70)

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

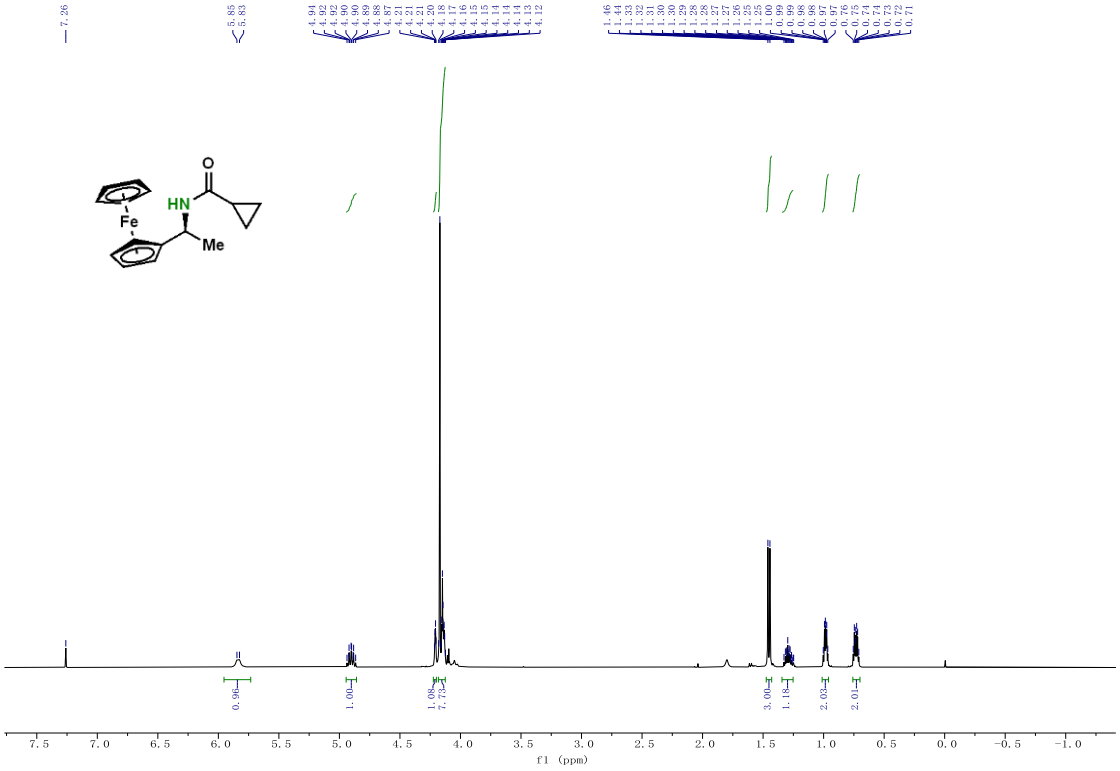


^{13}C NMR (101 MHz, $CDCl_3$)

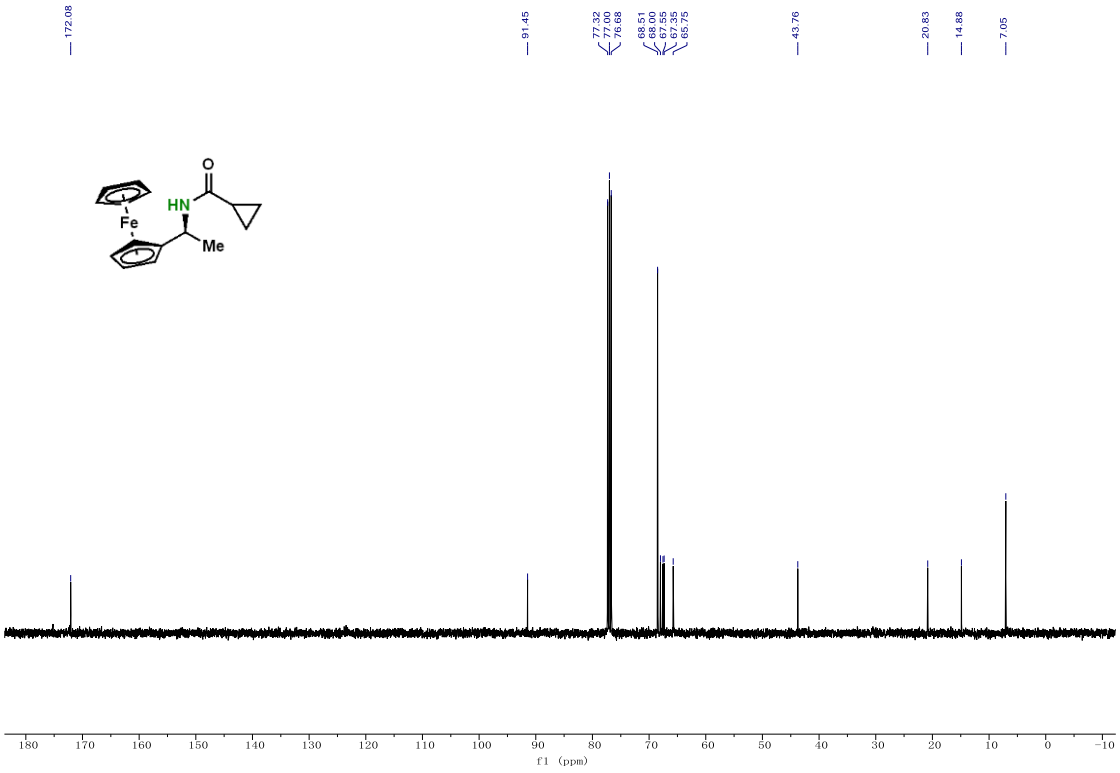


(S)-N-(1-(ferrocene-2-yl)ethyl)cyclopropanecarboxamide (71)

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

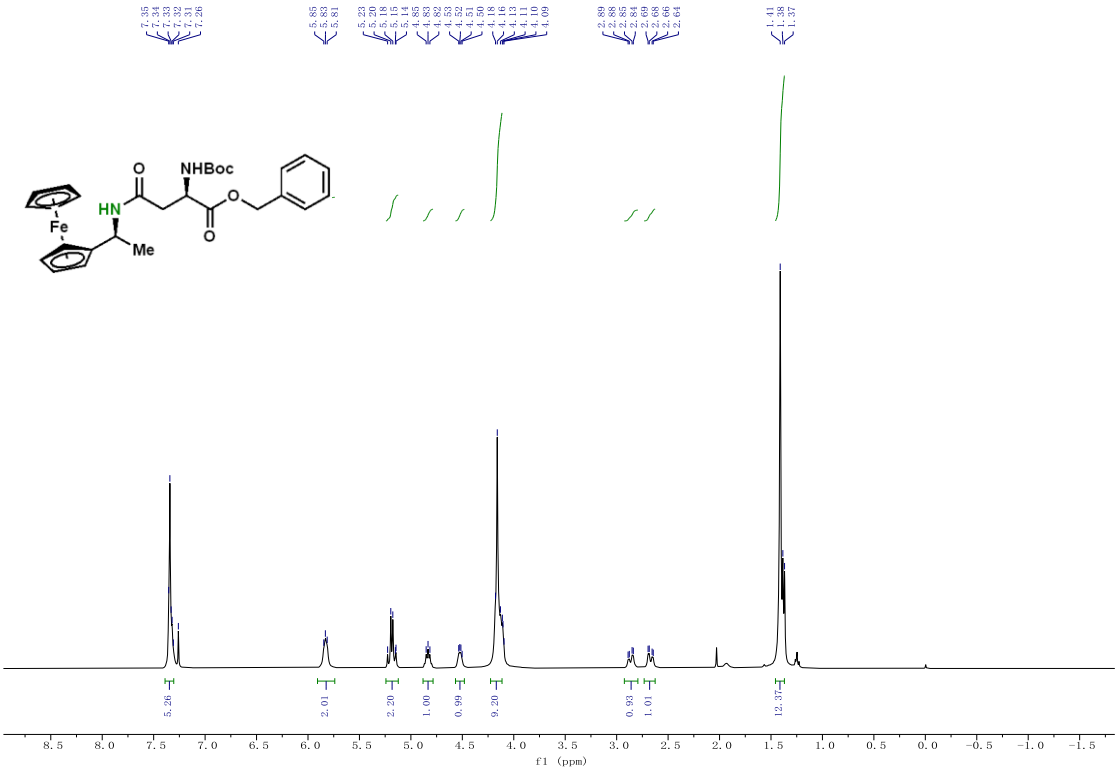


^{13}C NMR (101 MHz, $CDCl_3$)

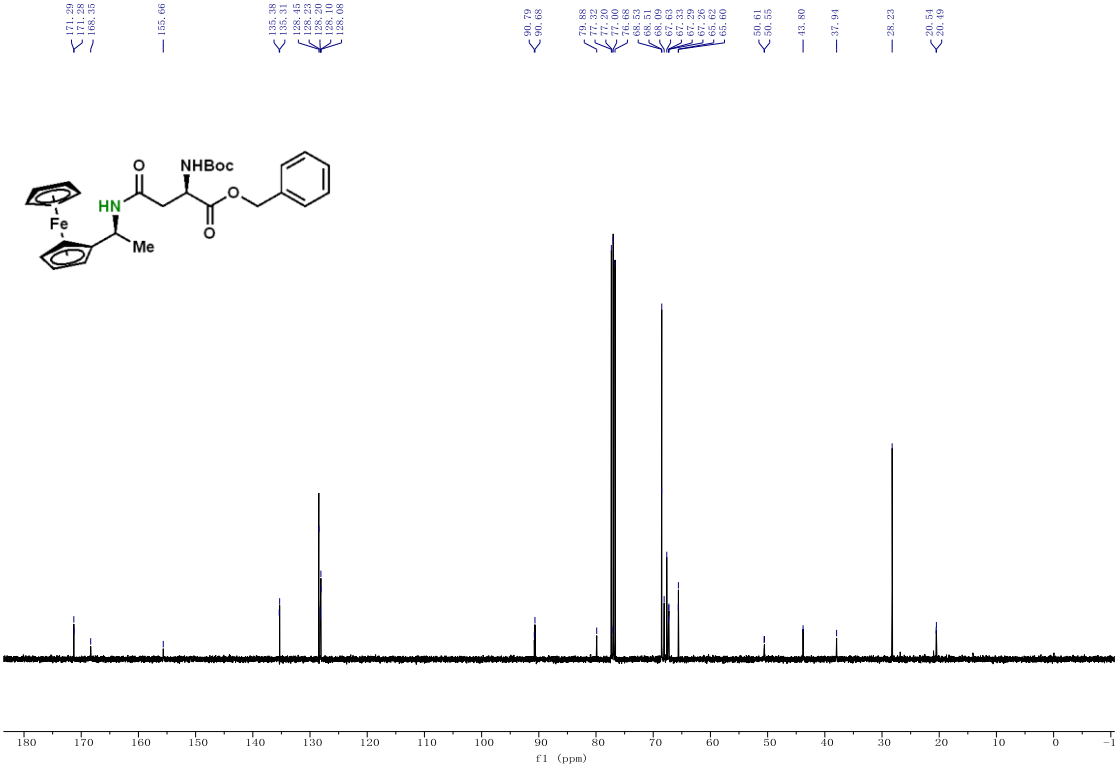


benzyl N2-(tert-butoxycarbonyl)-N4-((*S*)-1-(ferrocene-2-yl)ethyl)-D-asparaginate (72)

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

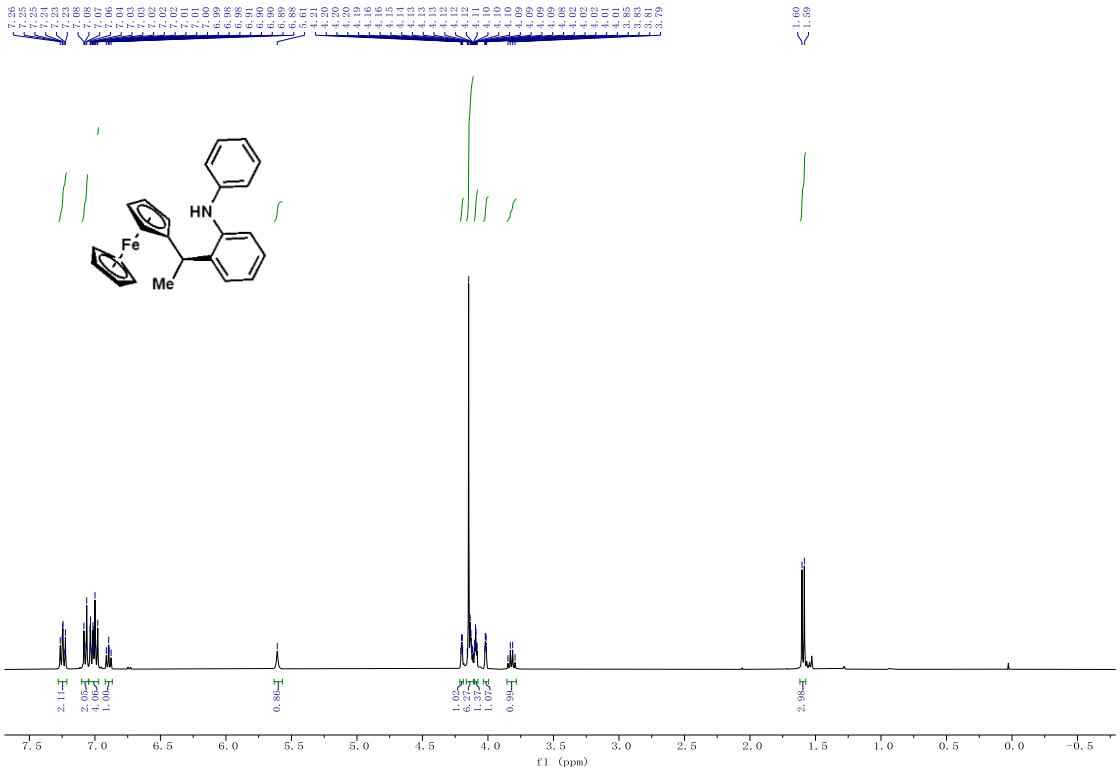


^{13}C NMR (101 MHz, $CDCl_3$)

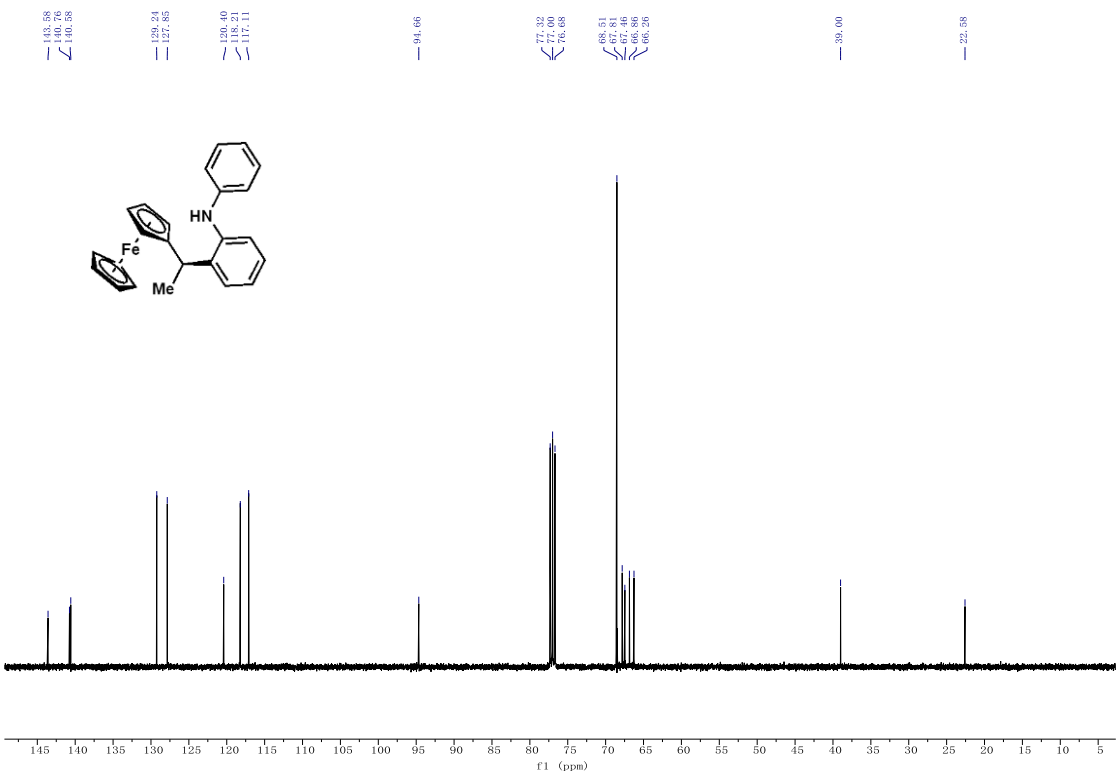


(S)-N-phenyl-2-(1-(ferrocene-2-yl)ethyl)aniline (73)

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

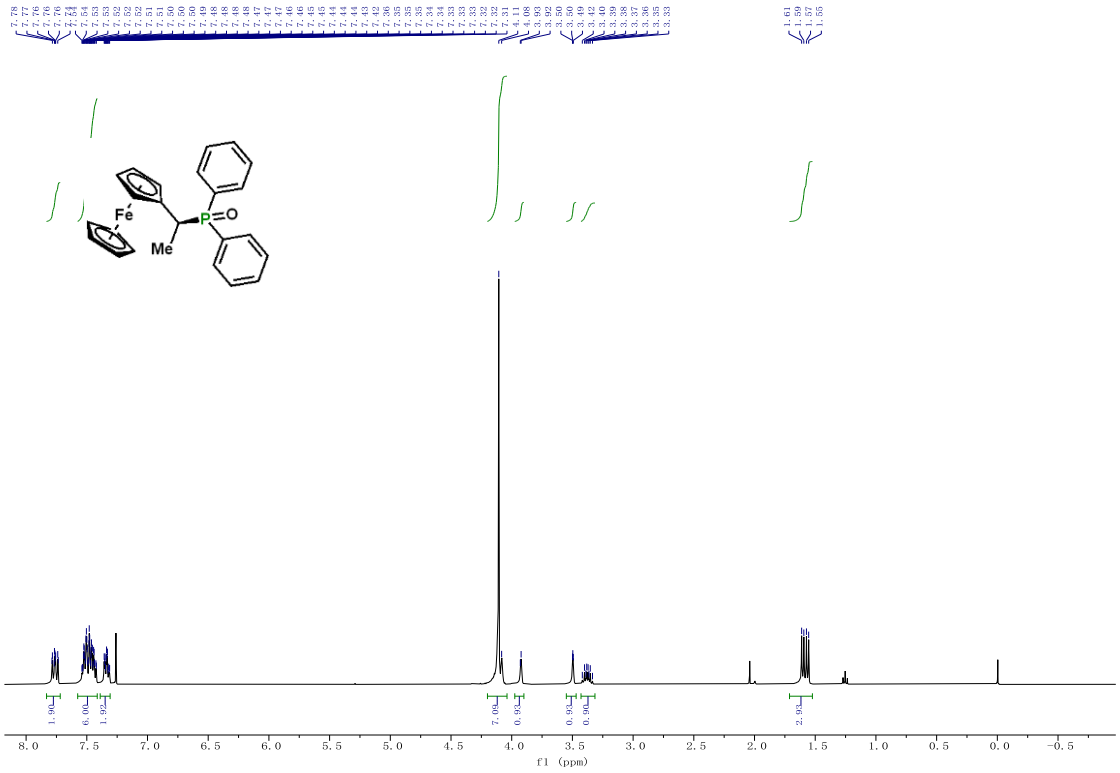


^{13}C NMR (101 MHz, $CDCl_3$)

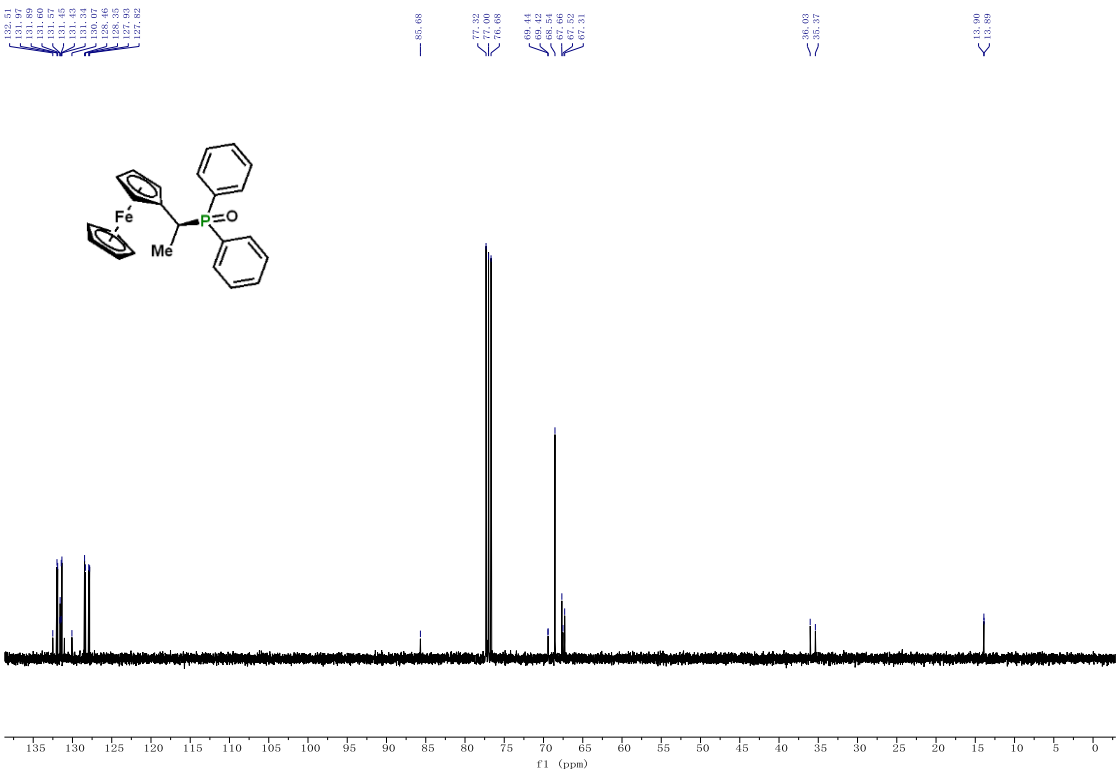


(S)-diphenyl(1-(thiophen-2-yl)ethyl)phosphine oxide (74)

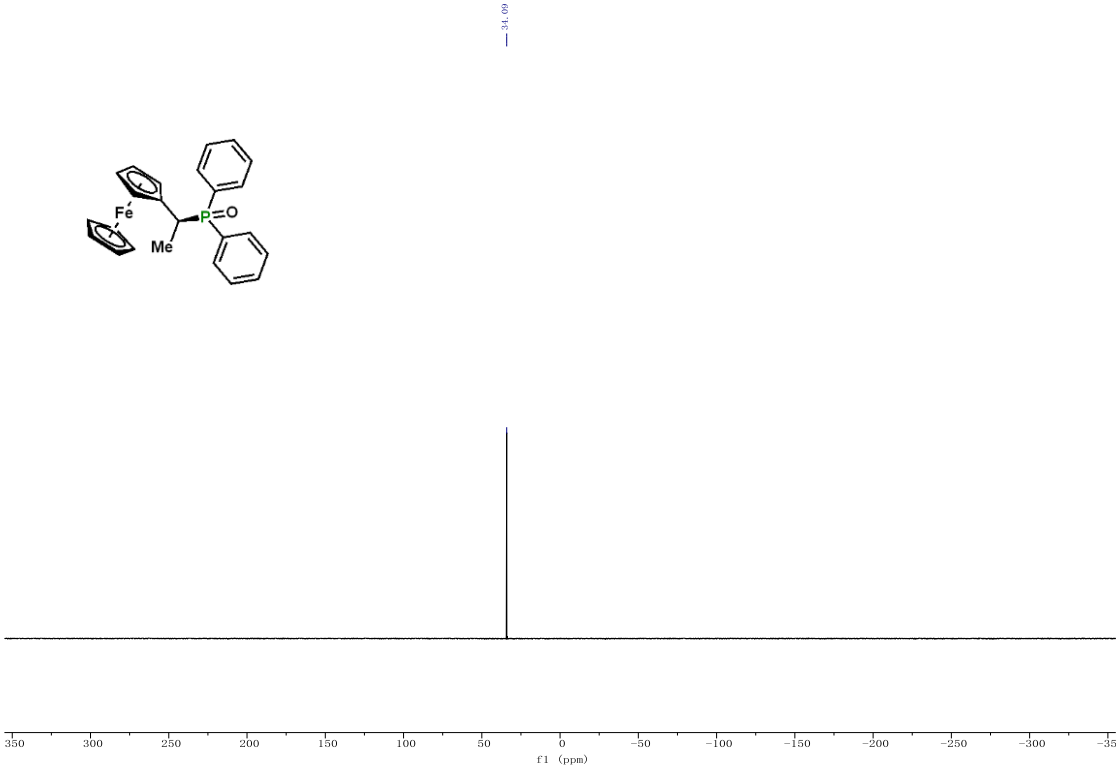
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)

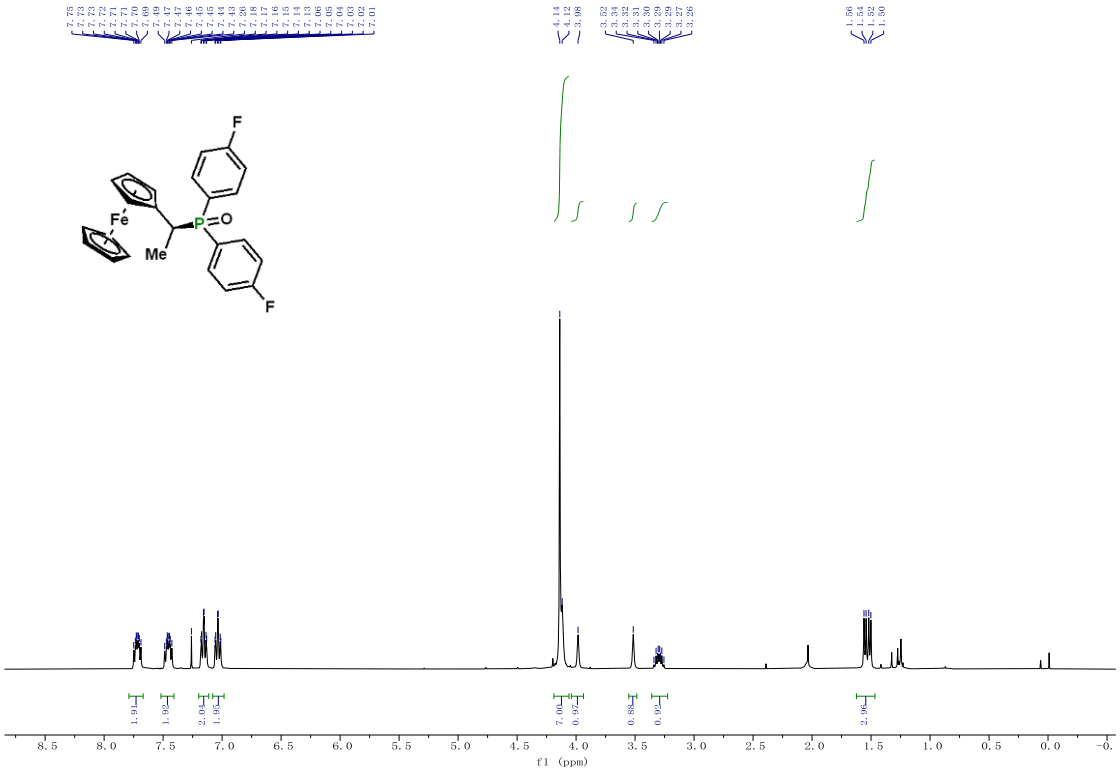


^{31}P NMR (160 MHz, $CDCl_3$)

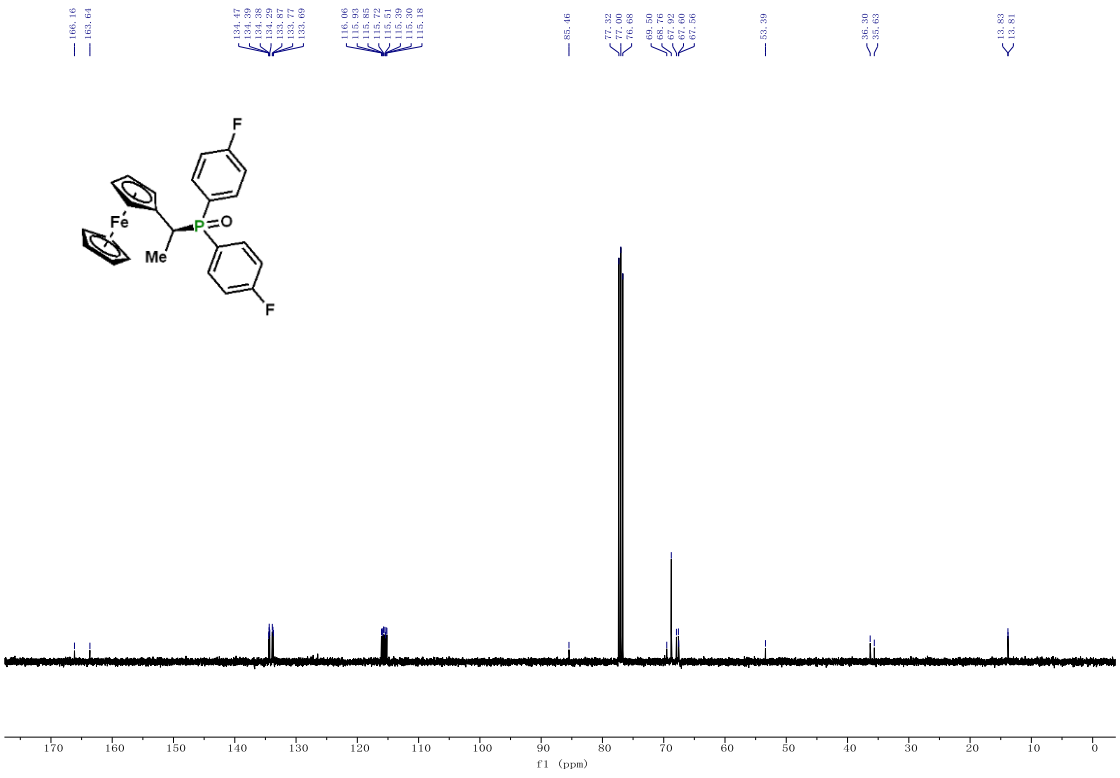


(S)-bis(4-fluorophenyl)(1-(ferrocene-2-yl)ethyl)phosphine oxide (75)

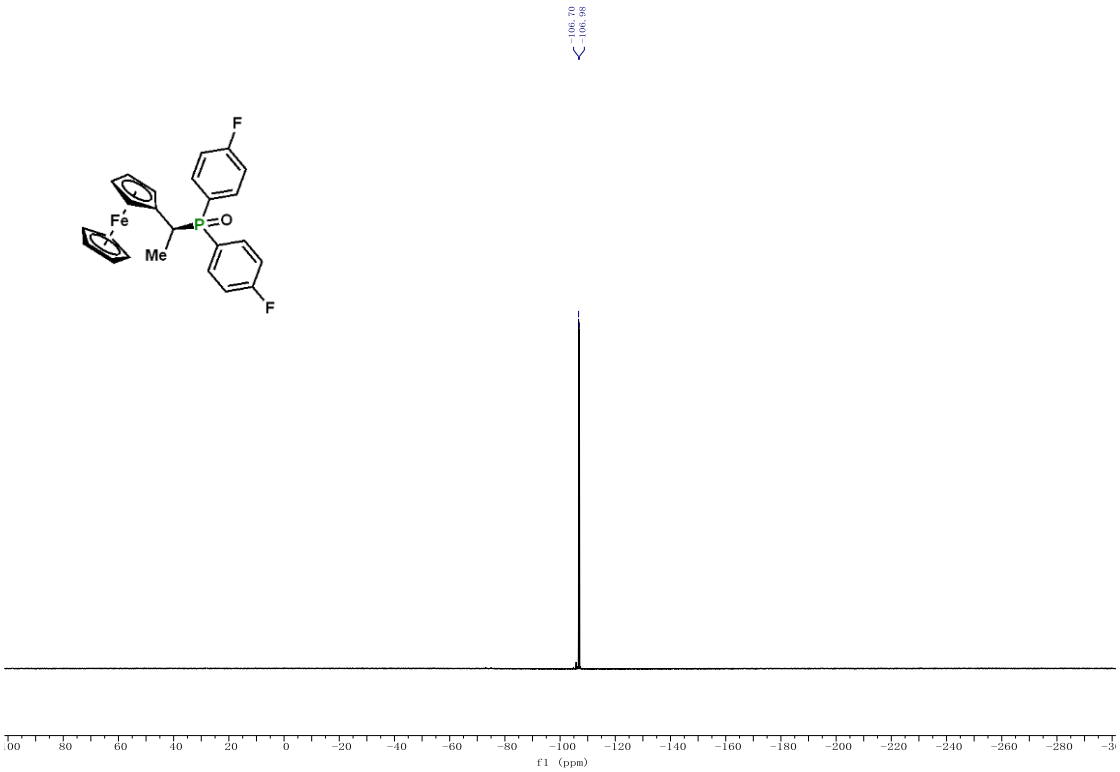
^{1}H NMR (400 MHz, $CDCl_3$)



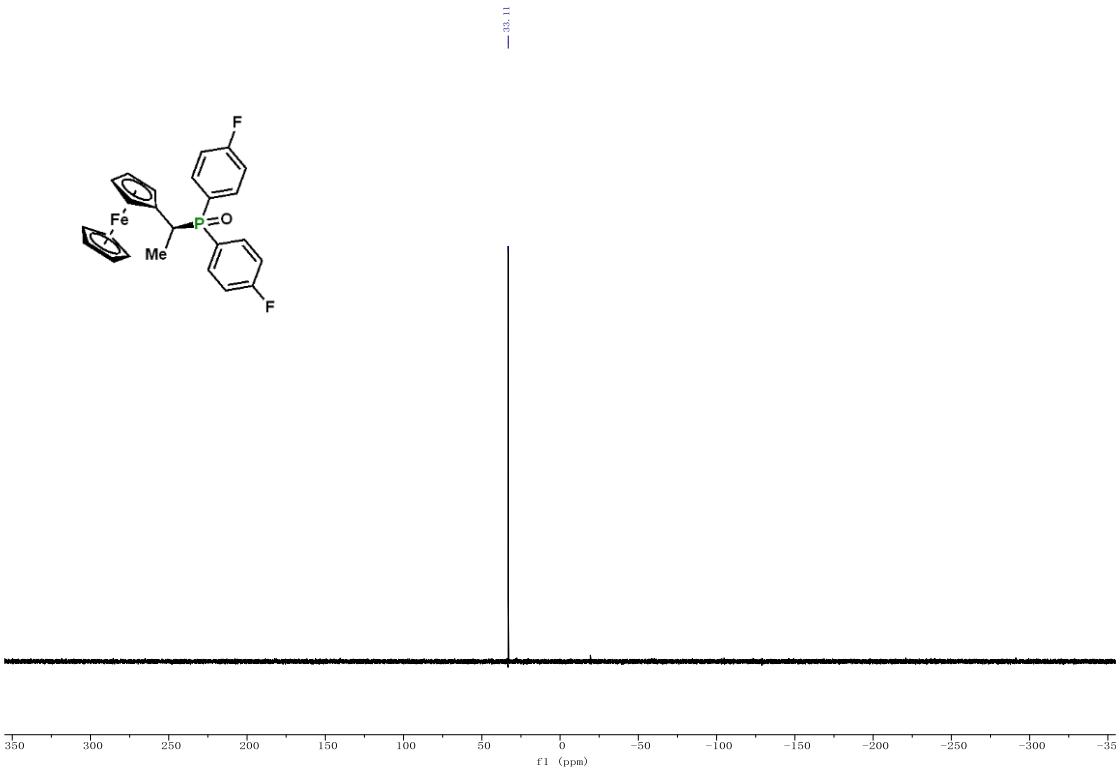
^{13}C NMR (101 MHz, $CDCl_3$)



^{19}F NMR (376 MHz, $CDCl_3$)

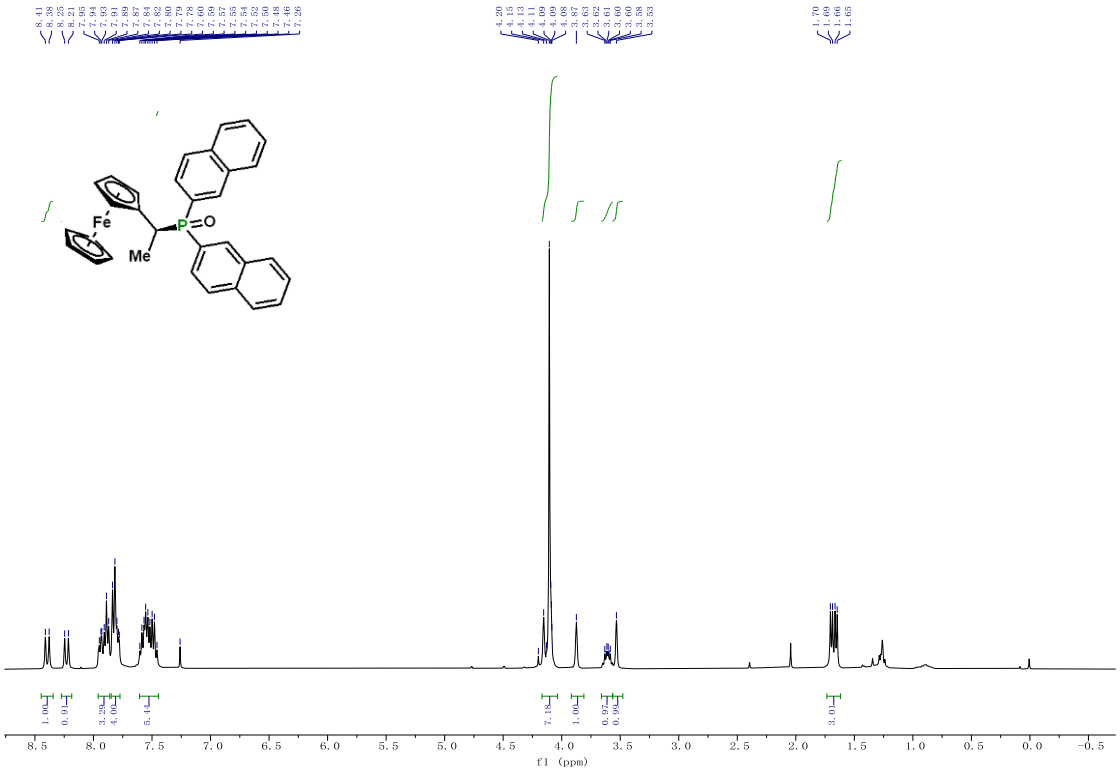


^{31}P NMR (160 MHz, $CDCl_3$)

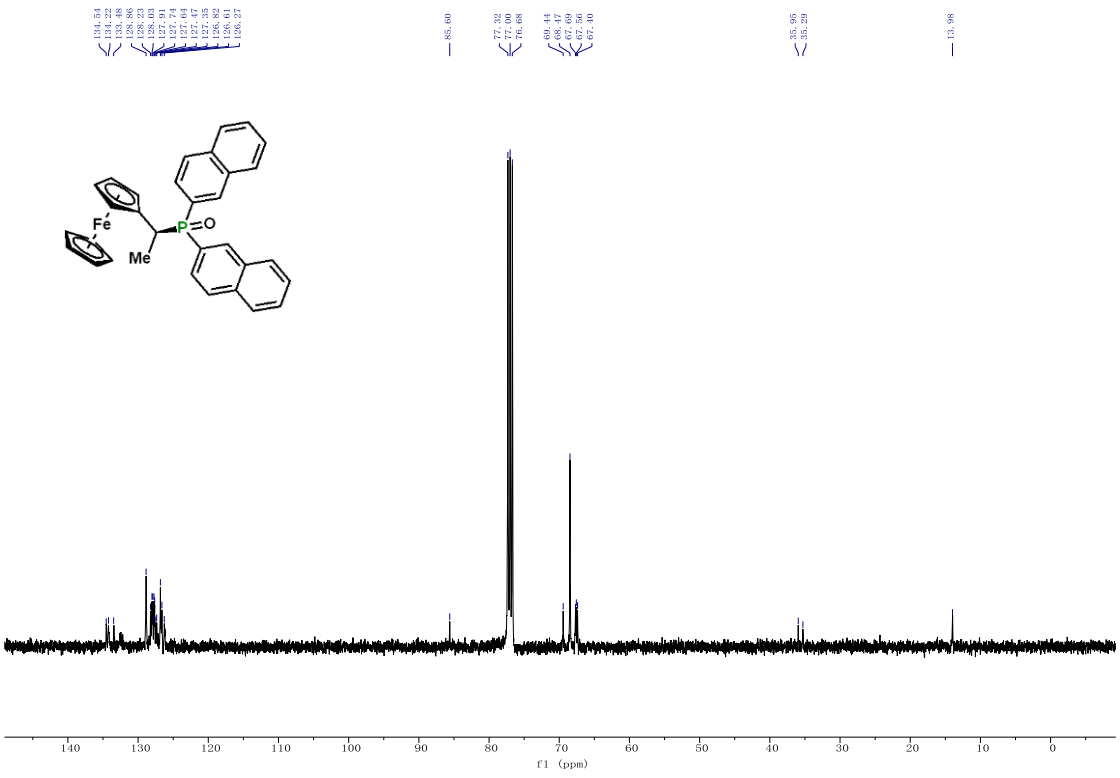


(S)-di(naphthalen-2-yl)(1-(ferrocene-2-yl)ethyl)phosphine oxide (76)

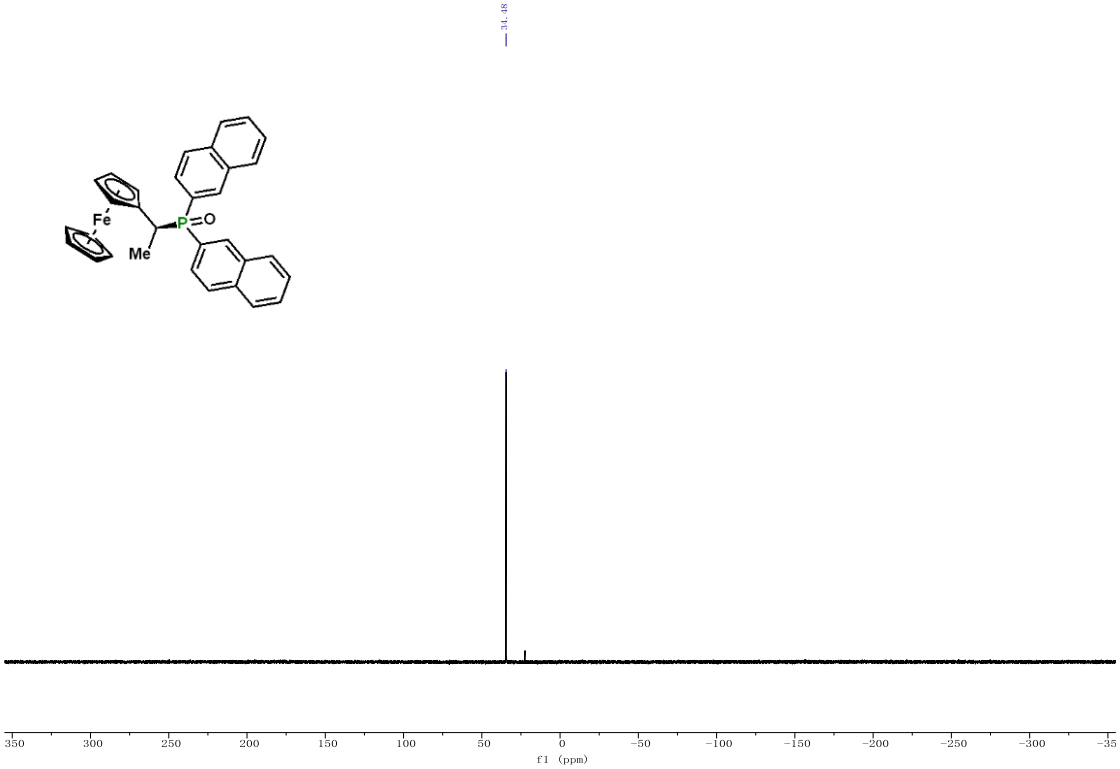
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)



^{31}P NMR (160 MHz, $CDCl_3$)



10. References

(1) B. J. Ueberbacher, H. Griengl, H. Weber, Ortho-lithiation of free ferrocenyl alcohols: a new method for the synthesis of planar chiral ferrocene derivatives. *Chem. Commun.* **28**, 3287–3289 (2008).

(2) Y. Zhu, C. Yang, Q. Lin, J. Li, T.-P. Loh, P. Chen, Z. Jia, Rapid C–S Coupling in Water via Ion-Pair-Catalyzed Dehydration. *Org. Lett.* **27**, 2110–2115 (2025).

(3) S. Zhang, W. Gu, F. Yang, L. Ma, Z. Shi, X. Li, Z. Zhao, A Route to the Mild Synthesis of α-Selenomethylketones via Vinyl Azides. *J. Org. Chem*. **90**, 4897–4908 (2025).

(4) G. L. Tolnai, J. P. Brand, J. Waser, Gold-catalyzed direct alkynylation of tryptophan in peptides using TIPS-EBX. *Beilstein J. Org. Chem.* **12**, 745–749 (2016).

(5) C. Nottingham, R. Benson, H. Müller-Bunz, P. J. Guiry, Synthesis of Ferrocene Oxazoline N,O Ligands and Their Application in Asymmetric Ethyl- and Phenylzinc Additions to Aldehydes. *J. Org. Chem.* **80**, 10163–10176 (2015).

(6) M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, et al. Gaussian 16, Revision A.03, *Gaussian, Inc., Wallingford, CT* (2016**)**.

(7) CYLview20; Legault, C. Y. Université de Sherbrooke, 2020, (http://www.cylview.org).

(8) J. P. Perdew, Y. Wang, Accurate and Simple Analytic Representation of the Electron-Gas Correlation Energy. *Phys. Rev. B: Condens. Matter Mater. Phys.* **45**, 13244–13249 (1992).

(9) J. P. Perdew, J. A. Chevary, S. H. Vosko, K. A. Jackson, M. R. Pederson, D. J. Singh, C. Fiolhais, Atoms, Molecules, Solids, and Surfaces: Applications of The Generalized Gradient Approximation for Exchange and Correlation. *Phys. Rev. B: Condens. Matter Mater. Phys.* **46**, 6671–6687 (1992).

(10) G. A. Petersson, A. Bennett, T. G. Tensfeldt, M. A. Allaham, W. A. Shirley, J. Mantzaris, A Complete Basis Set Model Chemistry. I. The Total Energies of Closed-Shell Atoms and Hydrides of the First-Row Elements. *J. Chem. Phys.* **89**, 2193–2218 (1988).

(11) M. Dolg, U. Wedig, H. Stoll, H. Preuss, Energy-adjusted ab initio pseudopotentials for the first row transition elements. *J. Chem. Phys*. **86**, 866–872 (1987).

(12) J. M. L. Martin, A. Sundermann, Correlation consistent valence basis sets for use with the Stuttgart-Dresden-Bonn relativistic effective core potentials: The atoms Ga-Kr and In-Xe. *J. Chem. Phys*. **114**, 3408–3420 (2001).

(13) S. Grimme, S. Ehrlich, L. Goerigk, Effect of the Damping Function in Dispersion Corrected Density Functional Theory. *J. Comput. Chem.* **32**, 1456–1465 (2011).

(14) A. V. Marenich, C. J. Cramer, D. G. Truhlar, Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the Bulk Dielectric Constant and Atomic Surface Tensions. *J. Phys. Chem. B.* **113**, 6378−6396 (2009).
(15) K. Fukui, The path of chemical reactions - the IRC approach. *Acc. Chem. Res. 14*, 363−368 (1981).
(16) S. Grimme, J. Antony, S. Ehrlich, H. Krieg, A Consistent and Accurate ab Initio Parametrization of Density Functional Dispersion Correction (DFT-D) for the 94 Elements H-Pu. *J. Chem. Phys.* **132**, 154104−154123 (2010).
(17) M. J. Frisch, J. A. Pople, J. S. Binkley, Self-Consistent Molecular Orbital Methods 25. Supplementary Functions for Gaussian Basis Sets. *J. Chem. Phys.* **80**, 3265−3269 (1984).