Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.


# Supplementary Information

## High Regioselectivity Ferrocenyl Cyclohexene/Cyclopentene Isomerization through Benzynes Transfer Coupling

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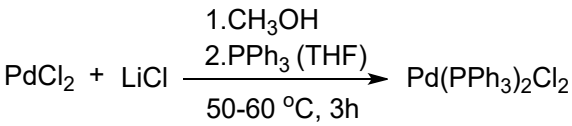
# Contents

## 1. General experimental procedures

The catalytic reactions were performed under an argon atmosphere using the oven-dried Schlenk flask. All reactions without catalyst were carried out under air. The chemicals were purchased from Aladdin and TCI Chemicals. All solvents and materials were pre-dried, redistilled or recrystallized before use. $^{1}H$ NMR (400 MHz) and $^{13}C$ NMR (101 MHz) spectra were recorded on a Bruker Avance 400 spectrometer with $CDCl_3$ as the solvent. Chemical shifts are reported in ppm by assigning TMS resonance in the $^{1}H$ NMR spectra as 0.00 ppm and $CDCl_3$ resonance in the $^{13}C$ spectra as 77.0 ppm. All coupling constants (*J* values) were reported in Hertz (Hz). Column chromatography was performed on silica gel 300–400 mesh. Melting points were determined using a Gallenkamp melting point apparatus and are uncorrected. The FT-IR spectra were recorded from KBr pellets or thin film from $CHCl_3$ on the NaCl window in the 4000-400 $cm^{-1}$ ranges on a Nicolet 5DX spectrometer. High-resolution mass spectra were recorded on a Waters G2-XS Qtof mass spectrometer. X-ray Crystallography diffraction data of **3a, 3b, 3c and 3t** were collected at room temperature with a Bruker SMART Apex CCD diffractometer with Mo-K$\alpha$ radiation ($\lambda$ = 0.71073 Å ) with a graphite monochromator using the $\omega$-scan mode. Data reductions and absorption corrections were performed with SAINT and SADABS software, respectively. The structure was solved by direct methods and refined on $F^2$ by full-matrix least squares using SHELXTL. All non-hydrogen atoms were treated anisotropically. The positions of hydrogen atoms were generated geometrically.

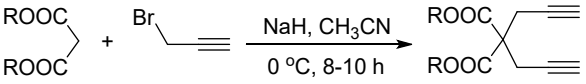
**(1) General procedure for preparation of tetrayne 1:**

Preparation of catalyst $Pd(PPh_3)_2Cl_2$:




3.54 g $PdCl_2$ and 4 g LiCl were mixed in a 500 mL three-necked flask with 150-200 mL methanol as solvent, magnetically stirred and heated in oil bath at 50-60 °C. After the solid was dissolved, 25 mL of THF (removed water with sodium wire) containing 13.1 g $PPh_3$ were added in the above three-necked flask, and the color of the solution changed from brown to yellow, reflux reaction for 3 hours. After reaction solution cooled, filtered and washed with anhydrous ethanol, yellow solid $Pd(PPh_3)_2Cl_2$ catalyst was obtained finally.

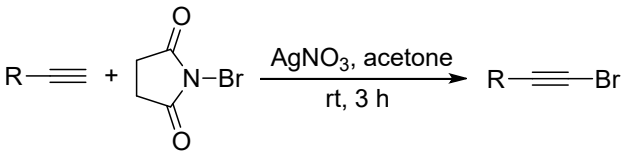
Preparation of diyne substrates:




R = Me, Et, $^{i}$Pr

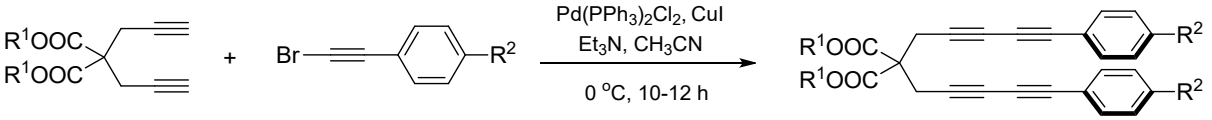
10 g NaH (60%) and 200-300 mL acetonitrile were added in 500 mL three-necked flask with magnetic stirring. 100 mmol malonate and 30 g 3-bromopropyne (98%) were added in the above 500 mL three-necked flask dropwise in turn by separatory funnel, magnetically stirred for 8-10 h under ice-water bath. The organic phase was extracted with ethyl acetate and dried with anhydrous $MgSO_4$. The solvent was evaporated in vacuo and diyne substrates as white solid were obtained finally.

Preparation of brominated alkynes:




21.36 g 1-bromopyrrolidine-2, 5-dione (NBS), 0.85 g $AgNO_3$, and 100 mmol phenylacetylene or substituted phenylacetylene or alkyl alkyne were added in 250 mL three-necked flask in turn, 150 mL acetone as a solvent, magnetically stirred at room temperature for 3 h. The organic phase was extracted with *n*-hexane and dried with anhydrous $MgSO_4$. The solvent was evaporated in vacuo and brominated alkynes compound as brown solid were obtained finally.

Preparation of tetrayne substrate**s:**




$R^1$ = Me, Et, $^i$Pr

$R^2$ = H, *p*-Me, *p*-Et, *p*-$^i$Pr, *p*-Cl, *p*-F, *p*-OMe, *m*-Me, *m*-Cl, *m*-F

0.6 g $Pd(PPh_3)_2Cl_2$, 0.5 g CuI and 40 mmol diyne substrate were added in 500 mL three-necked flask, protected with anhydrous anaerobic conditions under argon. After 0.5 h, 250-300 mL acetonitrile, 16.16 g $Et_3N$ and 100 mmol brominated aryl alkyne were added in turn, magnetically stirred for 10-12 h under ice-water bath. The organic phase was extracted with ethyl acetate and dried with anhydrous $MgSO_4$. It was separated by column chromatography on silica gel to obtain tetrayne substrate as white solid finally.

**(2) General procedure for preparation of functionalized aromatic ferrocene derivative 3:**

Tetraynes (1.0 mmol), cyclohexenyl/cyclopentenyl ferrocene (1.0 equiv) were added to toluene (3 mL), the mixture was stirred at room temperature then heated at 110 °C for 6 hours in air. Then the reaction mixture was cooled to room temperature, quenched with saturated NaCl, and extracted with ethyl acetate (3×10 mL). The combined organic extracts were dried over anhydrous $MgSO_4$, filtered, and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel (petroleum ether /ethyl acetate = 80/1) to afford functionalized aromatic ferrocene derivatives.

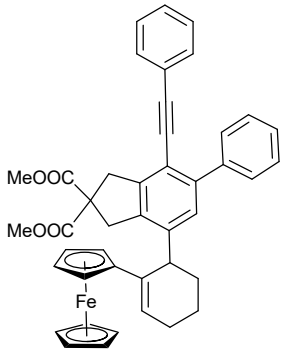
**References:**

1. (*a*) J. Chen, V. Palani and T. R. Hoye, Reactions of HDDA-derived benzynes with sulfides: mechanism, modes, and three-component reactions, *J. Am. Chem. Soc.*, 2016, **138**, 4318–4321; (*b*) N, K. Lee, S. Y. Yun, P. Mamidipalli, R. M. Salzman, D. Lee, T. Zhou and Y. Xia, Hydroarylation of arynes catalyzed by silver for biaryl synthesis, *J. Am. Chem. Soc.*, 2014, **136**, 4363–4368; (*c*) B. Liu, C. Mao, Q. Hu, L. Yao and Y. Hu, Direct methylation and carbonylation of in situ generated arynes via HDDA-Wittig coupling, *Org. Chem. Front.*, 2019, **6**, 2788–2791; (*d*) X. Zheng, B. Liu, F. Yang, Q. Hu, L. Yao, Y. Hu, Access to benzoxazepines and fully substituted indoles via HDDA coupling, *Org. Lett.*, 2020, **22**, 956–959.

2. (*a*) X. Li, C. Han, H. Yao and A. Lin, Organocatalyzed [3 + 2] annulation of cyclopropenones and *β*-ketoesters: an approach to substituted butenolides with a quaternary center, *Org. Lett.*, 2017, **19**, 778–781; (*b*) C. M. Vanos and T. H. Lambert, Development of a catalytic platform for nucleophilic substitution: cyclopropenone-catalyzed chlorodehydration of alcohols, *Angew. Chem. Int. Ed.*, 2011, **50**, 12222–12226.

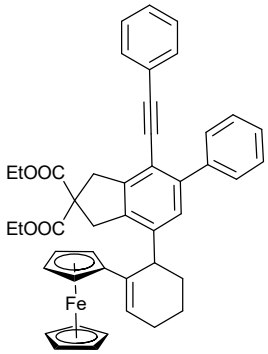
3. (*a*) L. Yao, Q. Hu, Y. Lei, L. Bao and Y. Hu, C–O/C–S difunctionalized benzene derivatives via multicomponent coupling of tetraynes, *Org. Chem. Front*., 2020, **7,** 3633–3637; (*b*) L. Yao, B. Fang, Q. Hu, Y. Lei, L. Bao and Y. Hu, Phenanthrenes/dihydrophenanthrenes: the selectivity controlled by different benzynes and allenes, *Chem. Commun*., 2020, **56**, 15185–15188; (*c*) D. Zhang, M. Li, J. Li, A. Lin and H. Yao, Rhodium-catalyzed intermolecular enantioselective Alder-ene type reaction of cyclopentenes with silylacetylenes, *Nat. Chem.*, 2021, **12**, 6627; (*d*) V. Palani, J. Chen, T. R. Hoye, Reactions of Hexadehydro-Diels-Alder (HDDA)-Derived Benzynes with Thioamides: Synthesis of Dihydrobenzothiazino-Heterocyclics, *Org. Lett.,* 2016, **18**, 6312–6315.

## 2. Characterization Data for the New Compounds



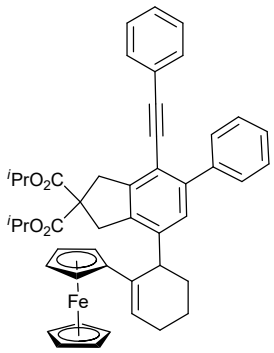

**Dimethyl 7-(2-ferrocenyl-2-en-1-yl)-5-phenyl-4-(phenylethynyl)-1H-indene-2, 2(3H)-dicarboxylate (3a)**

White solid; 559.6 mg (83%); m. p. 194-198 ℃; TLC (petroleum ether/EtOAc = 8:1): $R_f$ = 0.50; **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 7.59-7.27 (m, 2H), 7.42-7.30 (m, 8H), 7.07 (s, 1H), 6.23 (s, 1H), 4.44 (s, 1H), 4.16-3.98 (m, 9H), 3.94-3.92 (m, 2H), 3.87 (d, $J$ = 6.4 Hz, 6H), 3.81-3.71 (m, 2H), 2.30-2.18 (m, 2H), 2.08-2.00 (m, 1H), 1.85-1.81 (m, 1H), 1.60-1.59 (m, 2H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 172.2, 172.1, 143.4, 142.5, 141.8, 140.6, 131.4, 128.3, 128.1, 127.2, 123.8, 123.6, 115.6, 95.5, 87.4, 69.3, 68.3, 68.0, 66.8, 64.6, 60.1, 53.2, 41.3, 40.6, 39.4, 29.4, 25.6, 17.2. **FT-IR** (KBr): $v$ = 3642, 2948, 1736, 1438, 1241, 1070, 818, 752, 702, 487 cm$^{-1}$; **HRMS** (WATERS): *m/z* calcd for $C_{43}H_{38}FeO_4$ $[M+H]^+$ 675.2198, found 675.2195.



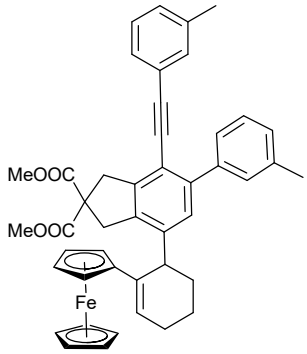

**Diethyl 7-(2-ferrocenyl-2-en-1-yl)-5-phenyl-4-(phenylethynyl)-1H-indene-2, 2(3H)-dicarboxylate (2b)**

White solid; 598 mg (85%); m. p. 157-160 ℃; TLC (petroleum ether/EtOAc = 8:1): $R_f$ = 0.65; **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 7.59-7.57 (d, $J$ = 7.6 Hz, 2H), 7.42-7.31 (m, 8H), 7.08 (s, 1H), 7.10 (d, $J$ = 4.4 Hz, 1H), 6.26 (s, 1H), 4.40 (s, 1H), 4.37-4.30 (m, 4H), 4.12-4.01 (m, 9H), 3.74-3.87 (m, 2H), 3.80 (d, $J$ = 16.4 Hz , 2H), 2.24-2.17 (m, 2H), 2.09-2.03 (m, 1H), 1.85 (d, $J$ = 12.8 Hz, 1H), 1.61 (s, 2H), 1.36 (q, $J$ = 6.8 Hz, 6H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 171.9, 171.8, 171.6, 143.6, 142.5, 141.9, 141.8, 140.7, 140.6, 136.9, 128.6, 127.8, 127.2, 123.7, 115.7, 115.5, 95.6, 95.4, 87.9, 87.5, 86.7, 69.0, 67.8, 67.5, 66.8, 64.4, 62.0, 61.8, 60.0, 59.4, 41.2, 41.0, 40.5, 39.9, 39.3, 32.8, 29.4, 25.7, 23.3, 17.2, 14.2, 14.1. **FT-IR** (KBr): $v$ = 3464, 2940, 1731, 1441, 1237, 1064, 814, 757, 696, 489 cm$^{-1}$; **HRMS** (WATERS): *m/z* calcd for $C_{45}H_{42}FeO_4$ $[M+H]^+$ 703.2511, found 703.2507.



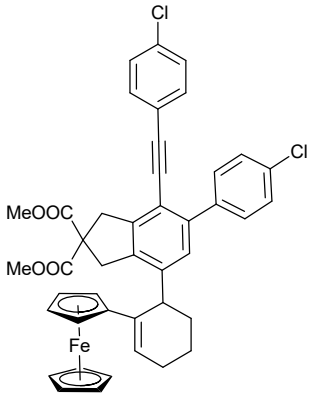

**Diisopropyl 7-(2-ferrocenyl-2-en-1-yl)-5-phenyl-4-(phenylethynyl)-1H-indene-2, 2(3H)-dicarboxylate (3c)**

White solid; 592 mg (81 % yield); m. p. 153-158 ℃; TLC (petroleum ether/EtOAc = 8:1): $R_f$ = 0.84; **$^{1}$H NMR** (400 MHz, $CDCl_3$) $\delta$ 7.59-7.56 (m, 2H), 7.41-7.31 (m, 8H), 7.07 (s, 1H), 6.26 (s, 1H), 5.22-5.12 (m, 2H), 4.40 (t, $J$ = 1.0 Hz, 1H), 4.12-3.96 (m, 9H), 3.92-3.78 (m, 4H), 2.28-2.17 (m, 2H), 2.08-2.03 (m, 1H), 1.87-1.83 (m, 2H), 1.60 (s, 2H), 1.37-1.32 (m, 12H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 171.3, 143.8, 142.4, 140.7, 134.0, 129.5, 128.0, 127.1, 123.8, 123.7, 115.5, 95.4, 87.5, 69.4, 66.9, 64.5, 60.0, 41.1, 40.5, 39.3, 29.4, 26.9, 25.6, 22.7, 21.7, 17.2, 14.2. **FT-IR** (KBr): $v$ = 3449, 2935, 1725, 1460, 1246, 1193, 1105, 816, 758, 695, 488 cm$^{-1}$; **HRMS** (WATERS): *m/z* calcd for $C_{47}H_{40}FeO_4$ $[M+H]^+$ 731.2824, found 731.2826.



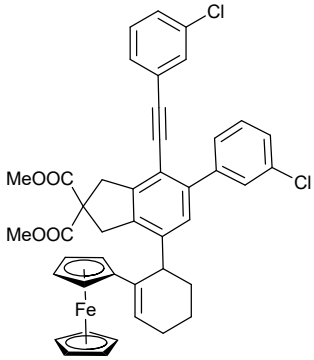

**Dimethyl 7-(2-ferroceneyl-2-en-1-yl)-5-(m-tolyl)-4-(m-tolylethynyl)-1H-indene-2, 2(3H)-dicarboxylate (3d)**

White solid; 563 mg (80 % yield); m. p. 157-159 ℃; TLC (petroleum ether/EtOAc = 8:1): $R_f$ = 0.56; **$^{1}$H NMR** (400 MHz, $CDCl_3$) $\delta$ 7.43 (s, 1H), 7.34-7.28 (m, 2H), 7.21-7.13 (m, 5H), 7.07 (s, 1H), 6.25 (s, 1H), 4.40 (t, $J$ = 1.0 Hz, 1H), 4.12-4.01 (m, 9H), 3.93 (s, 2H), 3.87 (d , $J$ = 7.2 Hz, 6H), 3.78-3.74 (m, 2H), 2.37 (d, $J$ = 21.6 Hz, 6H), 2.28-2.19 (m, 2H), 2.08-2.02 (m, 1H), 1.85-1.81 (m, 1H), 1.60 (s, 2H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 172.2, 172.1, 131.9, 128.9, 128.6, 128.4, 128.3, 128.1, 127.9, 127.7, 126.6, 123.8, 123.5, 115.6, 95.7, 87.3, 69.4, 60.0, 53.2, 41.3, 40.7, 39.9, 39.2, 29.6, 23.4, 21.2, 17.2. **FT-IR** (KBr): $v$ = 3470, 2929, 1746, 1437, 1242, 1067, 883, 820, 785, 697, 489 cm$^{-1}$; **HRMS** (WATERS): *m/z* calcd for $C_{45}H_{42}FeO_4$ $[M+H]^+$ 703.2505, found 703.2507.




**Dimethyl 5-(4-chlorophenyl)-4-((4-chlorophenyl)ethynyl)-7-(2-ferroenceyl-2-en-1-yl)-1H-indene-2, 2(3H)-dicarboxylate (3e)**

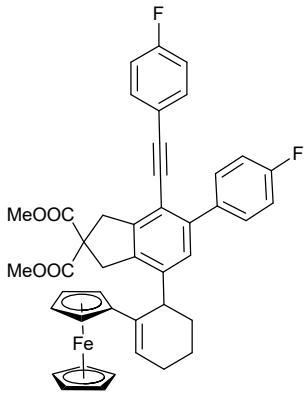
White solid; 632 mg (85 % yield); m. p. 135-137 ℃; TLC (petroleum ether/EtOAc = 8:1): $R_f$ = 0.57; **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 7.48 (d, $J$ = 8.0 Hz, 2H), 7.36 (d, $J$ = 8.4 Hz, 2H), 7.33-7.30 (m, 4H), 7.00 (s, 1H), 6.20 (s, 1H), 4.51 (s, 1H), 4.21-4.10 (m, 8H), 3.93-3.90 (m, 4H), 3.86 (d, $J$ = 4.4 Hz, 6H), 3.76-3.72 (m, 1H), 2.29 (s, 2H), 2.07-2.00 (m, 1H), 1.82-1.79 (m, 1H), 1.58-1.53 (m, 2H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 172.1, 141.2, 137.3, 134.2, 133.8, 133.4, 132.5, 130.7, 128.7, 128.2, 128.0, 123.9, 121.8, 115.2, 94.7, 88.1, 69.2, 68.2, 66.7, 64.5, 60.1, 53.2, 41.2, 40.5, 39.3, 29.4, 25.6, 17.3. **FT-IR** (KBr): $v$ = 3434, 2936, 1731, 1576, 1437, 1243, 1067, 868, 786, 490 cm$^{-1}$; **HRMS** (WATERS): *m/z* calcd for $C_{43}H_{36}Cl_2FeO_4$ $[M+H]^+$ 743.1418, found 743.1409.




**Dimethyl 5-(3-chlorophenyl)-4-((3-chlorophenyl)ethynyl)-7-(2-ferroceneyl-2-en-1-yl)-1H-indene-2, 2(3H)-dicarboxylate (3f)**

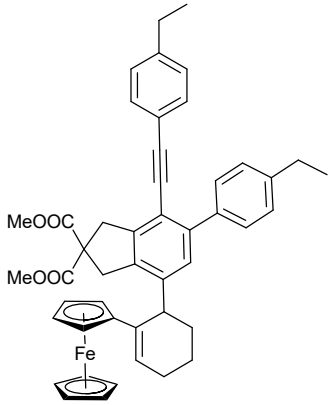
White solid; 661 mg (89 % yield); m. p. 187-189 ℃; TLC (petroleum ether/EtOAc = 8:1): $R_f$ = 0.54; **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 7.64 (s, 1H), 7.40-7.33 (m, 4H), 7.29-7.25 (m, 3H), 6.24 (s, 1H), 4.48 (s, 1H), 4.18-4.14 (m, 7H), 4.07 (s, 1H), 3.96 (s, 1H), 3.90 (s, 2H), 3.87 (d, $J$ = 6.0 Hz, 6H), 3.80-3.72 (m, 2H), 2.33-2.22 (m, 2H), 2.07-2.02 (m, 1H), 1.82 (d, $J$ = 12.0 Hz, 1H), 1.60-1.58 (m, 2H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 172.0, 143.7, 142.5, 142.4, 142.1, 137.5, 134.2, 129.2, 128.1, 127.4, 124.0, 115.1, 94.6, 88.1, 69.3, 68.3, 68.2, 66.7, 64.6, 59.9, 53.3, 41.2, 40.5, 39.4, 29.4, 25.6, 17.2. **FT-IR** (KBr): $v$ = 3462, 2936,

1735, 1589, 1440, 1249, 1075, 881, 783, 491 $cm^{-1}$; **HRMS** (WATERS): *m/z* calcd for $C_{43}H_{36}Cl_2FeO_4$ $[M+H]^+$ 743.1418, found 743.1413.




**Dimethyl 5-(4-fluorophenyl)-4-((4-fluorophenyl)ethynyl)-7-(2-ferroceneyl-2-en-1-yl)-1H-indene-2, 2(3H)-dicarboxylate (3g)**

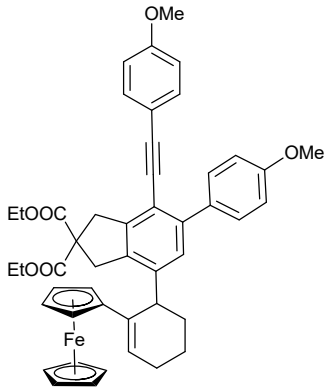
White solid; 589 mg (83 % yield); m. p. 175-176 ℃; TLC (petroleum ether/EtOAc = 8:1): $R_f$ = 0.50; $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.52 (t, $J$ = 13.6 Hz, 2H), 7.36-7.33 (m, 2H), 7.11-7.01 (m, 5H), 6.26 (s, 1H), 4.43 (s, 1H), 4.14-4.11 (m, 6H), 4.02 (d, $J$ = 11.2 Hz, 2H), 3.91-3.86 (m, 9H), 3.79-3.75 (m, 2H), 2.29-2.19 (m, 2H), 2.10-2.03 (m, 1H), 1.83 (d, $J$ = 12.0 Hz, 1H), 1.60 (s, 2H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 172.2, 172.1, 172.0, 171.9, 163.7, 163.6, 161.2, 162.1, 143.6, 142.0, 141.4, 136.5 (d, $J_{C-F}$ = 4.0 Hz), 133.2 (d, $J_{C-F}$ = 8.1 Hz), 131.0, 128.2, 123.8, 119.6 (d, $J_{C-F}$ = 3.0 Hz), 115.5, 115.4, 114.8, 114.6, 94.7, 87.0, 86.7, 69.0, 67.6 (d, $J_{C-F}$ = 16.2 Hz), 67.5, 66.7, 64.5, 59.2, 53.1, 53.0, 41.1, 39.9, 32.7, 29.5, 23.3 (d, $J_{C-F}$ = 4.0 Hz), 17.2. **FT-IR** (KBr): $v$ = 3445, 2932, 1746, 1599, 1507, 1439, 1228, 1061, 834, 490 $cm^{-1}$; **HRMS** (WATERS): *m/z* calcd for $C_{43}H_{36}F_2FeO_4$ $[M+H]^+$ 711.2009, found 711.2004.




**Dimethyl 5-(4-ethylphenyl)-4-((4-ethylphenyl)ethynyl)-7-(2-ferroceneyl-2-en-1-yl)-1H-indene-2, 2(3H)-dicarboxylate (3h)**

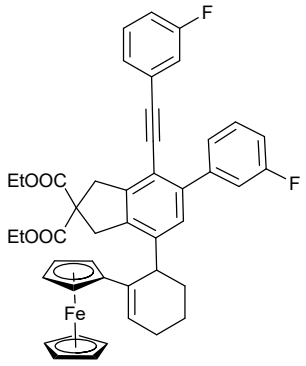
White solid; 585 mg (80 % yield); m. p. 151-153 ℃; TLC (petroleum ether/EtOAc = 8:1): $R_f$ = 0.56; **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 7.52 (d, $J$ = 8.0 Hz, 2H), 7.33 (d, $J$ = 8.0 Hz, 2H), 7.24 (d, $J$ = 8.0 Hz, 2H), 7.17 (d, $J$ = 7.6 Hz, 2H), 7.08 (s, 1H), 6.25 (s, 1H), 4.44 (s, 1H), 4.38-4.30 (m, 4H), 4.14-4.03 (m, 9H), 3.95-3.88 (m, 2H), 3.82-3.78 (m, 2H), 2.75-2.65 (m, 4H), 2.30-2.20 (m, 2H), 2.08-2.03 (m, 1H), 1.87 (d, $J$ = 12.8 Hz, 1H), 1.62 (s, 2H), 1.32-1.25 (m, 6H), 1.30-1.23 (m, 6H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$

172.3, 172.2, 172.1, 143.3, 143.1, 142.9, 142.3, 141.7, 141.5, 136.5, 129.3, 137.8, 127.3, 120.9, 115.8, 115.7, 95.8, 95.7, 88.0, 87.1, 86.9, 86.7, 68.9, 67.8, 67.5, 66.8, 64.4, 59.2, 53.1, 53.0, 41.2, 40.5, 40.0, 39.4, 32.8, 28.7, 25.7, 23.3, 17.2, 15.7, 15.6, 15.4. **FT-IR** (KBr): $\nu$ = 3463, 2929, 1736, 1510, 1437, 1244, 1162, 1060, 831, 487 $cm^{-1}$; **HRMS** (WATERS): *m/z* calcd for $C_{47}H_{46}FeO_4$ $[M+H]^+$ 731.2824, found 731.2827.




**Diethyl 5-(4-ferroceneyl)-4-((4-methoxyphenyl)ethynyl)-7-(2-methylcyclohex-2-en-1-yl)-1H-indene-2, 2(3H)-dicarboxylate (3i)**

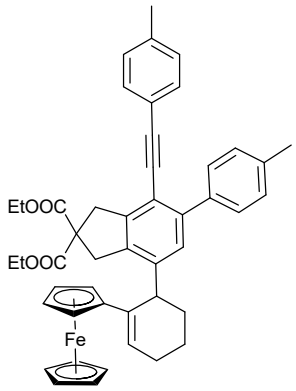
White solid; 625 mg (82 % yield); m. p. 83-85 ℃; TLC (petroleum ether/EtOAc = 8:1): $R_f$ = 0.33; **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 7.53-7.51 (m,2H), 7.34-7.31 (m, 2H), 7.03 (s, 1H), 6.93 (d, $J$ = 8.8 Hz, 2H), 6.85 (d , $J$ = 8.8 Hz, 2H), 6.25 (s, 1H), 4.38-4.39 (m, 1H), 4.34-4.30 (m, 4H), 4.12-3.99 (m, 9H), 3.89 (d, $J$ = 4.8 Hz, 2H), 3.79-3.77 (m, 2H), 2.26-2.15 (m, 2H), 2.07-2.05 (m, 1H), 1.85-1.81 (m, 1H), 1.60 (s, 2H), 1.38-1.28 (m, 6H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 147.6, 144.7, 143.8, 138.8, 137.3, 133.6, 129.8, 127.4, 124.9, 117.4, 98.7, 87.3, 77.2, 75.9, 53.6, 52.3, 33.8, 30.8, 30.1, 23.2, 21.9, 21.5, 19.3, 17.5, 13.9, 13.6. **FT-IR** (KBr): $\nu$ = 3462, 2928, 1732, 1606, 1511, 1462, 1245, 1026, 826, 483 $cm^{-1}$; **HRMS** (WATERS): *m/z* calcd for $C_{47}H_{46}FeO_6$ $[M+H]^+$ 763.7169, found 763.7161.




**Diethyl 5-(3-fluorophenyl)-4-((3-fluorophenyl)ethynyl)-7-(2-ferroenceyl-2-en-1-yl)-1H-indene-2, 2(3H)-dicarboxylate (3j)**

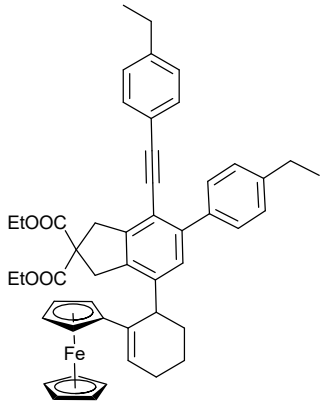
White solid; 642 mg (87 % yield); m. p. 176-178 ℃; TLC (petroleum ether/EtOAc = 8:1): $R_f$ = 0.61; **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 7.42-7.40 (m, 1H), 7.32-7.29 (m, 3H), 7.19-7.16 (m, 1H), 7.08–7.03 (m, 4H), 6.24 (s, 1H), 4.50 (s, 1H), 4.33 (t, $J$ = 7.2 Hz, 1H), 4.22-4.09 (m, 9H), 3.90 (d, $J$ = 7.6 Hz, 2H), 3.85-3.81

(m, 2H), 2.30 (s, 2H), 2.08-2.03 (m, 1H), 1.83 (d, $J$ = 10.0 Hz, 1H), 1.60 (s, 2H), 1.39-1.34 (m, 6H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 171.8, 171.6, 717.5, 163.6, 161.1, 143.9 (d, $J_{C\text{-}F}$ = 10.0 Hz), 137.5, 131.0, 130.0, 129.9 (d, $J_{C\text{-}F}$ = 9.1 Hz), 129.4, 128.6, 127.3, 124.0, 116.5, 115.4, 115.0 (d, $J_{C\text{-}F}$ = 10.1 Hz), 114.3 (d, $J_{C\text{-}F}$ = 7.1 Hz), 114.0 (d, $J_{C\text{-}F}$ = 7.1 Hz), 94.6, 87.9, 69.6, 66.9, 64.7, 62.1, 61.9, 59.9, 59.3, 41.1, 39.9, 39.3, 29.3, 23.3, 17.2, 14.1. **FT-IR** (KBr): $v$ = 3439, 2929, 1736, 1491, 1436, 1246, 1162, 1086, 825, 486 cm$^{-1}$; **HRMS** (WATERS): *m/z* calcd for $C_{45}H_{40}F_2FeO_4$ $[M+H]^+$ 739.2322, found 739.2318.



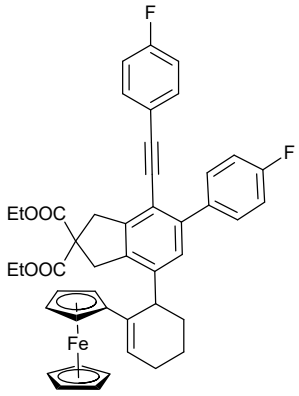

**Diethyl 7-(2-ferroceneyl-2-en-1-yl)-5-(p-tolyl)-4-(m-tolylethynyl)-1H-indene-2, 2(3H)-dicarboxylate (3k)**

White solid; 592 mg (81 % yield); m. p. 166-168 ℃; TLC (petroleum ether/EtOAc = 8:1): $R_f$ = 0.68; **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 7.50 (d, $J$ = 8.0 Hz, 2H), 7.33-7.28 (m, 2H), 7.21 (d, $J$ = 8.0 Hz, 2H), 7.14 (d, $J$ = 8.0 Hz, 2H), 7.07 (s, 1H), 6.26 (s, 1H), 4.40 (s, 1H), 4.12-3.98 (m, 4H), 3.94-3.91 (m, 2H), 3.81-3.77 (m, 2H), 2.39 (d, $J$ = 10.0 Hz, 6H), 2.28-2.18 (m, 2H), 2.12-2.02 (m, 1H), 1.86 (d, $J$ = 13.2 Hz, 1H), 1.61-1.60 (m, 2H), 1.37 (q, $J$ = 7.2 Hz, 6H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 171.9, 171.8, 171.6, 143.6, 143.5, 142.8, 142.2, 141.7, 141.5, 138.1, 134.1, 129.3, 128.3, 120.7, 115.7, 115.6, 95.7, 95.6, 87.9, 87.1, 86.9, 86.7, 69.0, 66.8, 64.4, 61.9, 61.7, 60.0, 59.3, 41.2, 41.1, 40.5, 39.9, 39.3, 32.8, 29.4, 23.0, 21.4, 17.2, 14.3. **FT-IR** (KBr): $v$ = 3414, 2927, 1511, 1460, 1243, 1180, 1103, 1067, 895, 816, 489 cm$^{-1}$; **HRMS** (WATERS): *m/z* calcd for $C_{47}H_{46}FeO_4$ $[M+H]^+$ 731.2824, found 731.2826.



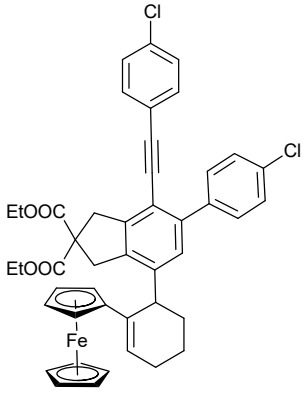

**Diethyl 5-(4-ethylphenyl)-4-((4-ethylphenyl)ethynyl)-7-(2-ferroceneyl-2-en-1-yl)-1H-indene-2, 2(3H)-dicarboxylate (3l)**

White solid; 599 mg (79 % yield); m. p. 150-154 ℃; TLC (petroleum ether/EtOAc = 8:1): $R_f$ = 0.73; **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 7.51 (d, $J$ = 8.0 Hz, 2H), 7.31 (d, $J$ = 8.0 Hz, 2H), 7.22 (d, $J$ = 8.0 Hz, 2H), 7.15 (d, $J$ = 8.0 Hz, 2H), 7.05 (s, 1H), 6.23 (s, 1H), 4.43 (s, 1H), 4.14-3.97 (m, 9H), 3.92-3.90 (m, 2H), 3.85-3.80 (m, 2H), 2.73-2.64 (m, 4H), 2.29-2.16 (m, 2H), 2.09-2.09 (m, 1H), 1.84 (d, $J$ = 11.6 Hz, 1H), 1.58 (s, 2H), 1.38-1.35 (m, 6H), 1.31-1.23 (m, 6H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 172.0, 144.4, 143.5, 143.1, 142.3, 141.5, 136.6, 131.4, 128.2, 127.2, 121.0, 115.7, 95.6, 88.1, 87.1, 69.1, 68.9, 68.1, 67.8, 66.8, 64.4, 61.9, 60.0, 41.2, 40.5, 39.3, 28.9, 28.6, 25.7, 22.7, 17.2, 15.6, 15.4, 14.1, 11.5. **FT-IR** (KBr): $v$ = 3464, 2929, 1730, 1511, 1461, 1242, 1187, 1068, 828, 489 cm$^{-1}$; **HRMS** (WATERS): *m/z* calcd for $C_{49}H_{50}FeO_4$ $[M+H]^+$ 759.3137, found 759.3131.



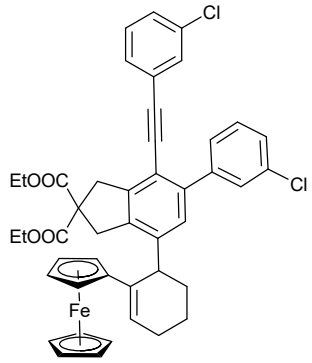

**Diethyl 5-(4-fluorophenyl)-4-((4-fluorophenyl) ethynyl)-7-(2-ferroceneyl-2-en-1-yl)-1H-indene-2, 2(3H)-dicarboxylate (3m)**

White solid; 620 mg (84 % yield); m. p. 147-149 ℃; TLC (petroleum ether/EtOAc = 8:1): $R_f$ = 0.61; **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 7.54-7.51 (m, 2H), 7.36-7.33 (m, 2H), 7.09 (t, $J$ = 8.6 Hz, 2H), 7.05-6.98 (m, 3H), 6.17 (s, 1H), 4.56 (s, 1H), 4.35-4.20 (m, 9H), 3.99 (d, $J$ = 7.6 Hz, 4H), 3.89 (d, $J$ = 11.2 Hz, 2H), 3.81-3.74 (m, 2H), 2.23 (s, 2H), 2.05-2.00 (m, 1H), 1.81 (d, $J$ = 12.4 Hz, 1H), 1.58 (s, 2H), 1.38-1.33 (m, 6H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 171.6, 163.6, 163.5, 161.2 (d, $J_{C-F}$ = 16.2 Hz), 143.6, 141.9, 141.4, 133.8, 133.2 (d, $J_{C-F}$ = 14.1 Hz), 131.0 (d, $J_{C-F}$ = 8.1 Hz), 128.1, 124.2, 119.6, 115.8, 115.3, 114, 94.4, 86.9, 70.0, 67.1, 64.7, 62.1, 59.9, 41.1, 40.4, 39.2, 31.7, 29.3, 25.5, 22.7, 17.1, 14.1. **FT-IR** (KBr): $v$ = 3426, 2928, 1732, 1601, 1509, 1463, 1230, 1070, 836, 488 cm$^{-1}$; **HRMS** (WATERS): *m/z* calcd for $C_{45}H_{40}F_2FeO_4$ $[M+H]^+$ 739.2322, found 739.2317.



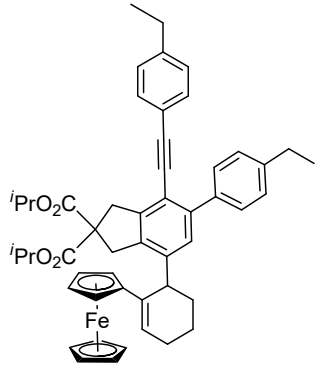
**Diethyl 5-(4-chlorophenyl)-4-((4-chlorophenyl) ethynyl)-7-(2-ferroceneyl-2-en-1-yl)-1H-indene-2, 2(3H)-dicarboxylate (3n)**

White solid; 639 mg (83 % yield); m. p. 165-167 ℃; TLC (petroleum ether/EtOAc = 8:1): $R_f$ = 0.67; **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 7.3 (s, 1H), 7.40-7.31 (m, 5H), 7.27-7.23 (m, 2H),7.04 (s, 1H), 6.28 (s, 1H), 4.41 (s, 1H), 4.36-4.30 (m, 4H), 4.13-4.01 (m, 9H), 3.91-3.86 (m, 2H), 3.81-3.74 (m, 2H), 2.29-2.18 (m, 2H), 2.11-2.03 (m, 1H), 1.85-1.82 (m, 1H), 1.60 (s, 2H),1.36 (q, $J$ = 7.2 Hz, 6H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 171.8, 171.6, 171.4, 143.8, 141.7, 141.2, 139.0, 138.9, 137.5, 137.3, 132.5, 128.7, 127.9, 121.9, 115.2, 115.1, 94.7, 94.6, 88.1, 69.2, 67.8, 67.6, 66.7, 64.5, 62.0, 61.8, 59.9, 59.3, 41.4, 41.0, 40.5, 39.8, 39.3, 32.7, 29.3, 23.3, 17.2, 14.2, 14.1. **FT-IR** (KBr): $v$ = 3435, 2929, 1736, 1247, 1189, 1070, 873, 787, 683, 488 cm$^{-1}$; **HRMS** (WATERS): *m/z* calcd for $C_{45}H_{40}Cl_2FeO_4$ $[M+H]^+$ 771.1731, found 771.1725.



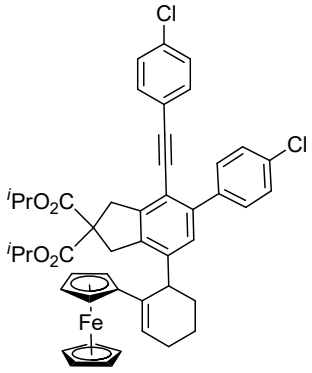

**Diethyl 5-(3-chlorophenyl)-4-((3-chlorophenyl) ethynyl)-7-(2-ferroceneyl-2-en-1-yl)-1H-indene-2, 2(3H)-dicarboxylate (3o)**

White solid; 655 mg (85 % yield); m. p. 160-165 ℃; TLC (petroleum ether/EtOAc = 8:1): $R_f$ = 0.67; **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 7.72 (s, 1H), 7.40-7.32 (m, 5H), 7.27-7.25 (m, 2H), 7.03 (s, 1H), 6.27 (s, 1H), 4.40 (t, $J$ = 1.2 Hz, 1H), 4.37-4.31 (m, 4H), 4.13-4.00 (m, 9H), 3.88 (d, $J$ = 7.6 Hz, 2H), 3.84-3.73 (m, 2H), 2.29-2.17 (m, 2H), 2.10-2.02 (m, 1H), 1.59 (s, 2H), 1.36 (q, $J$ = 7.2 Hz, 6H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 171.7, 171.6, 171.4, 142.4, 142.3, 142.1, 141.6, 141.1, 137.6, 134.2, 129.5, 128.0, 127.4, 123.8, 115.0, 94.5, 88.2, 87.7, 86.7, 69.0, 67.8, 67.5, 66.7, 64.5, 62.0, 61.8, 59.9, 59.3, 41.4, 40.9, 40.5, 39.8, 39.3, 32.7, 29.4, 25.6, 23.3, 17.2, 14.2, 14.1. **FT-IR** (KBr): $v$ = 3437, 2929, 1736, 1469, 1246, 1189, 1070, 872, 786, 488 cm$^{-1}$; **HRMS** (WATERS): *m/z* calcd for $C_{45}H_{40}Cl_2FeO_4$ $[M+H]^+$ 771.1731, found 771.1739.



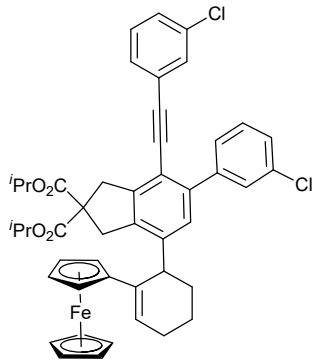
**Diisopropyl 5-(4-ethylphenyl)-4-((4-ethylphenyl) ethynyl)-7-(2-ferroceneyl-2-en-1-yl)-1H-indene-2, 2(3H)-dicarboxylate (3p)**

White solid; 629 mg (80 % yield); m. p. 171-173 ℃; TLC (petroleum ether/EtOAc = 8:1): $R_f$ = 0.80; **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 7.50 (d, $J$ = 8.0 Hz, 2H), 7.30 (d, $J$ = 8.0 Hz, 2H), 7.22 (d, $J$ = 8.0 Hz, 2H), 7.15 (d, $J$ = 8.0 Hz, 2H), 7.05 (s, 1H), 6.24 (s, 1H), 5.22-5.12 (m, 2H), 4.40 (t, $J$ = 1.2 Hz, 1H), 4.11-3.95 (m, 9H), 3.90-3.77 (m, 4H), 2.72-2.63 (m, 4H), 2.27-2.16 (m, 2H), 2.09-2.00 (m, 1H), 1.87-1.83 (m, 1H), 1.60 (s, 2H), 1.36-1.32 (m, 12H), 1.30-1.23 (m, 6H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 171.5, 171.3, 171.1, 143.2, 143.1, 142.9, 142.2, 141.6, 141.4, 138.0, 129.4, 128.1, 127.1, 121.1, 115.8, 115.6, 95.7, 95.5, 87.2, 87.0, 86.8, 69.1, 68.2, 67.9, 67.5, 64.4, 59.9, 59.4, 41.1, 41.0, 40.5, 39.8, 39.3, 32.9, 28.7, 21.7, 21.5, 15.7, 15.6, 15.4. **FT-IR** (KBr): $v$ = 3459, 2970, 2930, 1726, 1511, 1460, 1192, 1104, 827, 489 cm$^{-1}$; **HRMS** (WATERS): *m/z* calcd for $C_{51}H_{54}FeO_4$ $[M+H]^+$ 787.3450, found 787.3442.



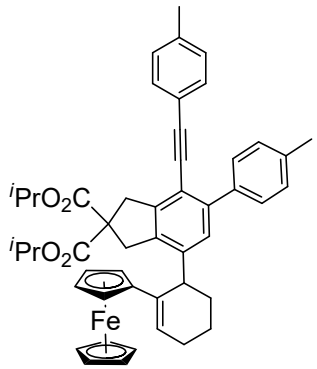

**Diisopropyl 5-(4-chlorophenyl)-4-((4-chlorophenyl) ethynyl)-7-(2-ferroceneyl-2-en-1-yl)-1H-indene-2, 2(3H)-dicarboxylate (3q)**

White solid; 679 mg (85 % yield); m. p. 181-183 ℃; TLC (petroleum ether/EtOAc = 8:1): $R_f$ = 0.77; **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 7.62 (s, 1H), 7.39-7.31 (m, 5H), 7.27-7.25 (m, 2H), 7.03 (s, 1H), 6.28 (s, 1H), 5.22-5.12 (m, 2H), 4.41 (t, $J$ = 1.2 Hz, 1H), 4.13-3.99 (m, 9H), 3.93-3.89 (m, 1H), 3.83-3.81 (m, 2H), 3.73 (t, $J$ = 1.2Hz, 1H), 2.29-2.18 (m, 2H), 2.11-2.02 (m, 1H), 1.85-1.82 (m, 1H), 1.61 (s, 2H), 1.37-1.33 (m, 12H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 171.3, 171.2, 171.1, 171.0, 144.0, 141.7, 141.1, 139.1, 139.0, 137.5, 137.3, 133.3, 130.7, 128.7, 122.0, 115.2, 94.6, 94.5, 88.3, 88.1, 69.2, 69.0, 68.0, 67.5, 64.5, 60.4, 59.9, 59.3, 40.9, 40.4, 39.8, 39.3, 32.7, 29.5, 29.3, 25.6, 21.6, 17.1, 14.2, 14.1. **FT-IR** (KBr): $v$ = 3461, 2981, 2929, 1492, 1378, 1247, 1192, 1098, 824, 428 cm$^{-1}$; **HRMS** (WATERS): *m/z* calcd for $C_{47}H_{44}Cl_2FeO_4$ $[M+H]^+$ 799.2044, found 799.2047.



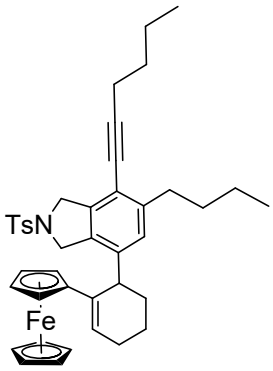

**Diisopropyl 5-(3-chlorophenyl)-4-((3-chlorophenyl) ethynyl)-7-(2-ferroceneyl-2-en-1-yl)-1H-indene-2, 2(3H)-dicarboxylate (3r)**

White solid; 686 mg (86 % yield); m. p. 147-148 ℃; TLC (petroleum ether/EtOAc = 8:1): $R_f$ = 0.71; **$^{1}$H NMR** (400 MHz, $CDCl_3$) $\delta$ 7.47 (d, $J$ = 8.4 Hz, 2H), 7.35 (d, $J$ = 8.4 Hz, 2H), 7.30-7.29 (m, 4H), 7.01 (s, 1H), 6.26 (s, 1H), 5.21-5.12 (m, 2H), 4.40 (t, $J$ = 1.2 Hz, 1H), 4.12-3.99 (m, 9H), 3.92-3.88 (m, 1H), 3.82-3.81 (m, 2H), 3.78-3.74 (m, 1H), 2.26-2.17 (m, 2H), 2.07-2.02 (m, 1H), 1.84-1.81 (m, 1H), 1.61 (s, 2H), 1.36-1.32 (m, 12H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 171.2, 171.1, 144.1, 142.4, 142.3, 142.2, 141.6, 141.1, 137.6, 133.5, 130.7, 128.4, 127.4, 123.8, 115.0, 94.4, 88.2, 87.7, 86.7, 69.5, 68.9, 67.9, 67.4, 64.4, 59.9, 59.4, 41.0, 40.8, 40.5, 39.8, 39.2, 31.8, 29.5, 29.3, 23.3, 21.7, 17.2, 14.2. **FT-IR** (KBr): $v$ = 3456, 2979, 2932, 1725, 1589, 1462, 1275, 1102, 818, 488 cm$^{-1}$; **HRMS** (WATERS): *m/z* calcd for $C_{47}H_{44}Cl_2FeO_4$ $[M+H]^+$ 799.2044, found 799.2037.



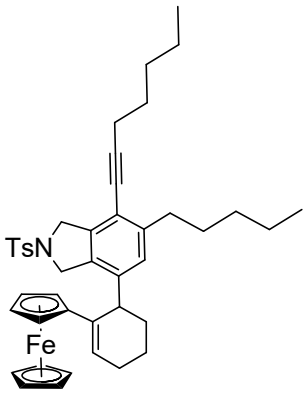

**Diisopropyl 7-(2-ferroceneyl-2-en-1-yl)-5-(m-tolyl)-4-(m-tolylethynyl)-1H-indene-2, 2(3H)-dicarboxylate (3s)**

White solid; 622 mg (82 % yield); m. p. 130-132 ℃; TLC (petroleum ether/EtOAc = 8:1): $R_f$ = 0.72; **$^{1}$H NMR** (400 MHz, $CDCl_3$) $\delta$ 7.45 (s, 1H), 7.36-7.30 (m, 2H), 7.23-7.19 (m, 3H), 7.17-7.12 (m, 2H), 7.06 (s, 1H), 6.26 (s, 1H), 5.23-5.13 (m, 2H), 4.43 (s, 1H), 4.14-3.99 (m, 9H), 3.93-3.82 (m, 4H), 2.46-2.36 (m, 6H), 2.30-2.20 (m, 2H), 2.11-2.02 (m, 1H), 1.86 (d, $J$ = 13.2 Hz, 1H), 6.01 (s, 2H), 1.38-1.33 (m, 12H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 171.3, 137.1, 136.7, 134.0, 132.0, 130.2, 128.9, 128.4, 128.2, 127.9, 127.7, 126.7, 123.6, 115.6, 95.7, 87.4, 69.4, 69.1, 69.0, 68.2, 67.9, 66.9, 64.4, 41.1, 40.5, 39.3, 29.5, 25.6, 21.3, 17.2. **FT-IR** (KBr): $v$ = 3459, 2930, 1727, 1458, 1377, 1343, 1187, 1104, 1104, 787, 490 cm$^{-1}$; **HRMS** (WATERS): *m/z* calcd for $C_{49}H_{50}FeO_4$ $[M+H]^+$ 759.3137, found 759.3134.



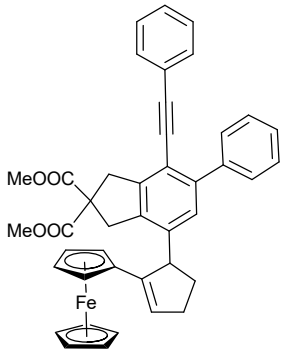

**5-butyl-4-(hex-1-yn-1-yl)-7-(2-ferroceneyl-2-en-1-yl)-2-tosylisoindoline (3t)**

White solid; 532 mg (79 % yield); m. p. 143-145 ℃; TLC (petroleum ether/EtOAc = 8:1): $R_f$ = 0.58; **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 7.84 (d, $J$ = 8.0 Hz, 2H), 7.36 (d, $J$ = 8.0 Hz, 2H), 6.88-6.82 (m, 1H), 6.24 (s, 1H), 4.84-4.64 (m, 4H), 4.38 (s, 1H), 4.12-4.05 (m, 6H), 3.96 (s, 1H), 3.67 (s, 1H), 3.57 (s, 1H), 2.74-2.67 (m, 1H), 2.62-2.54 (m, 1H), 2.49-2.46 (m, 4H), 2.27-2.22 (m, 2H), 1.20-1.92 (m, 1H), 1.77-1.76 (m, 1H), 1.63-1.59 (m, 3H), 1.54-1.48 (m, 6H), 1.29-1.24 (m, 2H), 1.00-0.97 (m, 3H), 0.87 (t, $J$ = 7.2 Hz, 3H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 144.6, 144.3, 143.6, 143.1, 139.1, 139.0, 129.8, 127.6, 123.9, 116.0, 98.1, 69.2, 68.9, 68.0, 67.9, 66.7, 64.4, 54.6, 53.4, 40.6, 30.9, 29.7, 29.5, 22.4, 21.6, 17.2, 14.0, 13.9, 13.6. **FT-IR** (KBr): $v$ = 2930, 2863, 1460, 1350, 1161, 1097, 1042, 815, 674 cm$^{-1}$; **HRMS** (WATERS): *m/z* calcd for $C_{41}H_{47}FeNO_2S$ $[M+H]^+$ 674.2755, found 674.2762.



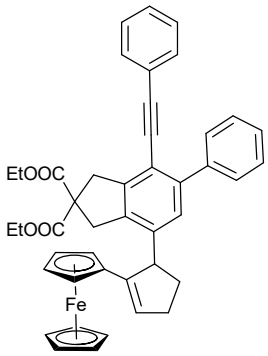

**4-(hept-1-yn-1-yl)-7-(2-ferroceneyl-2-en-1-yl)-5-pentyl-2-tosylisoindoline (3u)**

White solid; 540 mg (77 % yield); m. p. 108-112 ℃; TLC (petroleum ether/EtOAc = 8:1): $R_f$ = 0.55; **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 7.84 (d, $J$ = 7.6 Hz, 2H), 7.36 (d, $J$ = 8.0 Hz, 2H), 6.83 (s, 1H), 6.23 (s, 1H), 4.85-4.64 (m, 4H), 4.39 (s, 1H), 4.13-4.08 (m, 6H), 3.97 (s, 1H), 3.67 (s, 1H), 3.58 (s, 1H), 2.74-2.67 (m, 1H), 2.62-2.55 (m, 1H), 2.49-2.46 (m, 4H), 2.28-2.17 (m, 2H), 1.97-1.92 (m, 1H), 1.66-1.60 (m, 3H), 1.56-1.48 (m, 6H), 1.44-1.35 (m, 3H), 1.32-1.21 (m, 4H), 0.97 (t, $J$ = 7.2 Hz, 3H), 0.85 (t, $J$ = 7.0 Hz, 3H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 144.3, 143.6, 139.1, 133.8, 129.9, 127.6, 123.9, 116.0, 98.1, 69.3, 68.1, 68.0, 66.7, 64.5, 54.6, 53.4, 40.6, 31.1, 30.3, 29.7, 28.6, 25.6, 22.5, 17.2, 14.0. **FT-IR** (KBr): $v$ = 3094, 2960, 2925, 2855, 1450, 1349, 1261, 1163, 1024, 809 cm$^{-1}$; **HRMS** (WATERS): *m/z* calcd for $C_{43}H_{61}FeNO_2S$ $[M+H]^+$ 702.3068, found 702.3063.



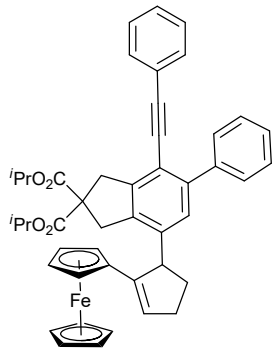

**2-ethyl 2-methyl 7-(2-ferroceneyl-2-en-1-yl)-5-phenyl-4-(phenylethynyl)-1H-indene-2, 2(3H)-dicarboxylate (3v)**

White solid; 541 mg (82 % yield); m. p. 179-183 ℃; TLC (petroleum ether/EtOAc = 8:1): $R_f$ = 0.49; **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 7.63-7.62 (m, 2H), 7.43-7.40 (m, 5H), 7.33 (s, 3H), 7.09 (s, 1H), 6.08 (s, 1H), 4.45 (s, 1H), 4.28 (s, 1H), 4.17 (m, 2H), 4.10-4.07 (m, 6H), 3.95 (s, 2H), 3.89 (s, 3H), 3.83 (s, 3H), 2.59-2.47 (m, 3H), 1.94 (s, 1H), 1.40-1.31 (m, 2H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 172.2, 172.1, 143.5, 143.2, 142.1, 136.8, 131.4, 127.3, 125.1, 123.6, 115.6, 95.5, 87.6, 81.5, 69.1, 67.6, 66.0, 53.2, 50.5, 41.2, 39.7, 31.8, 31.5, 30.3, 21.1, 14.3. **FT-IR** (KBr): $v$ = 3641, 2944, 2833, 1960, 1734, 1436, 1279, 1242, 1159, 696 cm$^{-1}$; **HRMS** (WATERS): *m/z* calcd for $C_{42}H_{36}FeO_4$ $[M+H]^+$ 661.2041, found 661.2045.



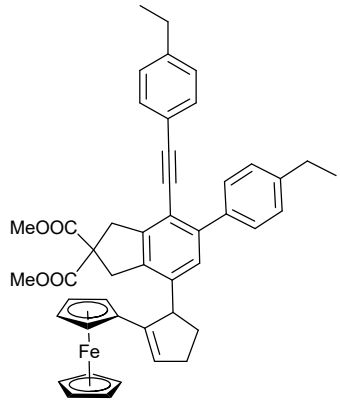

**Diethyl 7-(2- ferroceneyl-2-en-1-yl)-5-phenyl-4-(phenylethynyl)-1H-indene-2, 2(3H)-dicarboxylate (3w)**

White solid; 571 mg (83 % yield); m. p. 138-141 ℃; TLC (petroleum ether/EtOAc = 8:1): $R_f$ = 0.63; **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 7.56 (d, $J$ = 8.0 Hz, 2H), 7.43-7.36 (m, 5H), 7.31-7.30 (m, 3H), 7.03 (s, 1H), 6.05 (s, 1H), 4.45 (s, 1H), 4.33-4.27 (m, 4H), 4.23-4.20 (m, 2H), 4.09-4.07 (m, 7H), 3.90-2.86 (m, 4H), 2.58-2.47 (m, 3H), 1.93-1.89 (m, 1H), 1.37-1.32 (m, 6H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 171.8, 171.7, 143.7, 143.1, 142.2, 142.0, 136.8, 131.4, 127.8, 126.8, 123.7, 115.5, 95.4, 87.5, 69.4, 68.4, 67.8, 66.1, 61.9, 59.9, 41.0, 39.6, 33.7, 31.7, 14.1. **FT-IR** (KBr): $v$ = 3088, 2977, 2933, 2849, 1736, 1492, 1246, 1183, 1067, 762 cm$^{-1}$; **HRMS** (WATERS): *m/z* calcd for $C_{44}H_{40}FeO_4$ $[M+H]^+$ 689.2354, found 689.2349.




**Diisopropyl 7-(2-ferroceneyl-2-en-1-yl)-5-phenyl-4-(phenylethynyl)-1H-indene-2, 2(3H)-dicarboxylate (3x)**

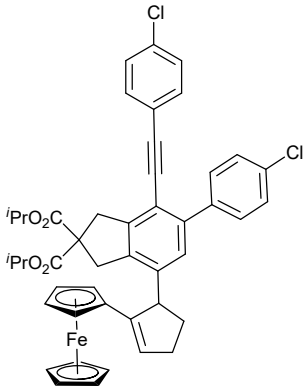
White solid; 587 mg (82 % yield); m. p. 147-151 ℃; TLC (petroleum ether/EtOAc = 8:1): $R_f$ = 0.83; **$^{1}$H NMR** (400 MHz, $CDCl_3$) $\delta$ 7.70 (d, $J$ = 7.2 Hz, 2H), 7.46 (t, $J$ = 7.4 Hz, 2H), 7.40-7.38 (m, 3H), 7.35-7.32 (m, 3H), 7.16 (s, 1H), 5.10-5.04 (m, 2H), 4.13-4.06 (m, 9H), 3.84 (s, 2H), 3.44 (s, 2H), 2.88 (t, $J$ = 7.0 Hz, 3H), 2.73 (t, $J$ = 7.0 Hz, 3H), 2.13-2.06 (m, 2H), 1.28 (d, $J$ = 6.0 Hz, 6H), 1.23 (d, $J$ = 6.0 Hz, 6H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 171.3, 143.9, 142.8, 140.5, 131.4, 128.4, 128.1, 127.3, 123.7, 116.1, 95.7, 87.7, 81.5, 69.2, 68.6, 67.5, 59.3, 41.0, 40.1, 39.6, 36.9, 22.9, 21.6. **FT-IR** (KBr): $v$ = 3083, 3024, 2982, 1724, 1282, 1245, 1106, 814, 696 cm$^{-1}$; **HRMS** (WATERS): *m/z* calcd for $C_{46}H_{44}FeO_4$ $[M+H]^+$ 717.2662, found 717.2667.




**2-ethyl 2-methyl 5-(4-ethylphenyl)-4-((4-ethylphenyl)ethynyl)-7-(2-ferroceneyl-2-en-1-yl)-1H-indene-2, 2(3H)-dicarboxylate (3y)**

White solid; 573 mg (80 % yield); m. p. 90-93 ℃; TLC (petroleum ether/EtOAc = 8:1): $R_f$ = 0.53; **$^{1}$H NMR** (400 MHz, $CDCl_3$) $\delta$ 7.51 (d, $J$ = 8.0 Hz, 2H), 7.31 (d, $J$ = 8.0 Hz, 2H), 7.23 (d, $J$ = 8.0 Hz, 2H), 7.15 (d, $J$ = 8.0 Hz, 2H), 7.02 (s, 1H), 6.04 (s, 1H), 4.44 (s, 1H), 4.22-4.18 (m, 2H), 4.09-4.06 (m, 7H), 3.90-3.88 (m, 2H), 3.86-3.83 (m, 6H), 3.76-3.67 (m, 2H), 2.73-2.63 (m, 4H), 2.58-2.51(m, 2H), 2.47-2.40 (m, 1H), 1.92-1.86 (m, 1H), 1.31-1.23 (m, 6H); **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 172.3, 172.1, 144.5, 143.4, 143.2, 142.9, 142.1, 141.7, 136.4, 131.4, 125.8, 120.9, 115.7, 95.6, 86.9, 69.3, 67.7, 67.5, 66.0, 59.2, 53.1, 41.2, 39.6, 33.7, 31.8, 28.9, 28.6, 15.6, 15.4. **FT-IR** (KBr): $v$ = 3087, 2958, 1737, 1436, 1276,

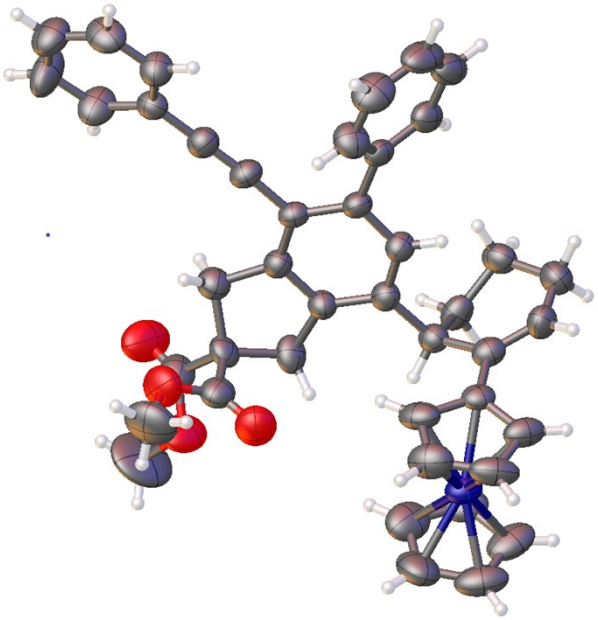
1245, 1198, 1162, 1068, 830 $cm^{-1}$; **HRMS** (WATERS): *m/z* calcd for $C_{46}H_{44}FeO_4$ $[M+H]^+$ 717.2667, found 717.2663.



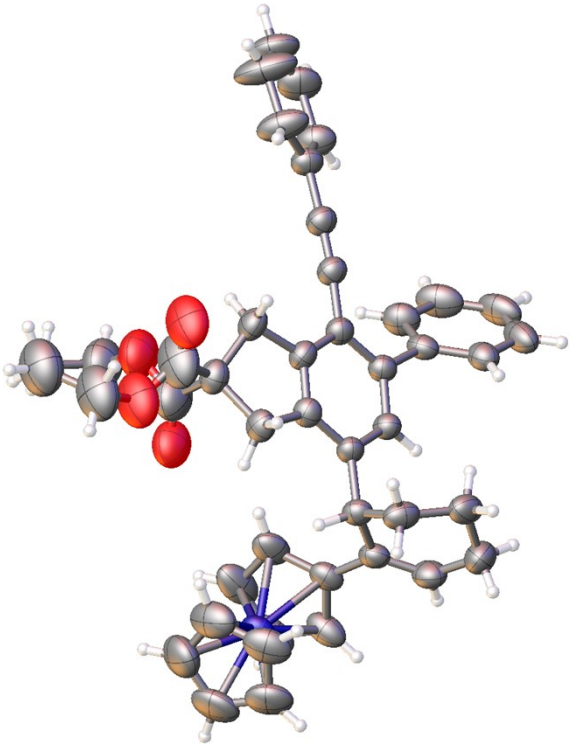

**diisopropyl 5-(4-chlorophenyl)-4-((4-chlorophenyl)ethynyl)-7-(2-ferroceneyl-2-en-1-yl)-1H-indene-2,2(3H)-dicarboxylate (3z)**

White solid; 667 mg (85 % yield); m. p. 100-102 ℃; TLC (petroleum ether/EtOAc = 8:1): $R_f$ = 0.76; **$^1$H NMR** (400 MHz, $CDCl_3$) $\delta$ 7.59 (d, *J* = 8.4 Hz, 2H), 7.40 (d, *J* = 8.4 Hz, 2H), 7.32 (s, 4H), 7.09 (s, 1H), 5.08-5.02 (m, 2H), 4.11-4.08 (m, 7H), 4.01 (s, 2H), 3.80 (s, 2H), 3.42 (s, 2H), 2.87 (t, *J* = 7.2 Hz, 2H), 2.70 (t, *J* = 7.2 Hz, 2H), 2.13-2.05 (m, 2H), 1.45 (s, 2H), 1.26 (d, *J* = 6.4 Hz, 6H), 1.22(d, *J* = 6.4 Hz, 6H) ; **$^{13}$C NMR** (101 MHz, $CDCl_3$) $\delta$ 171.2, 137.3, 136.3, 134.2, 133.6, 133.3, 132.6, 130.7, 128.7, 128.3, 128.0, 115.6, 94.8, 88.2, 81.3, 69.3, 69.1, 68.6, 67.4, 59.3, 39.5, 27.0, 25.3, 22.9, 22.7, 21.7, 20.7, 20.5, 19.5, 18.8, 14.4, 14.2, 11.5. **FT-IR** (KBr): *v* = 3091, 2928, 2848, 1725, 1277, 1250, 1196, 1168, 1100, 885 $cm^{-1}$; **HRMS** (WATERS): *m/z* calcd for $C_{46}H_{42}Cl_2FeO_4$ $[M+H]^+$ 785.1888, found 785.1882.

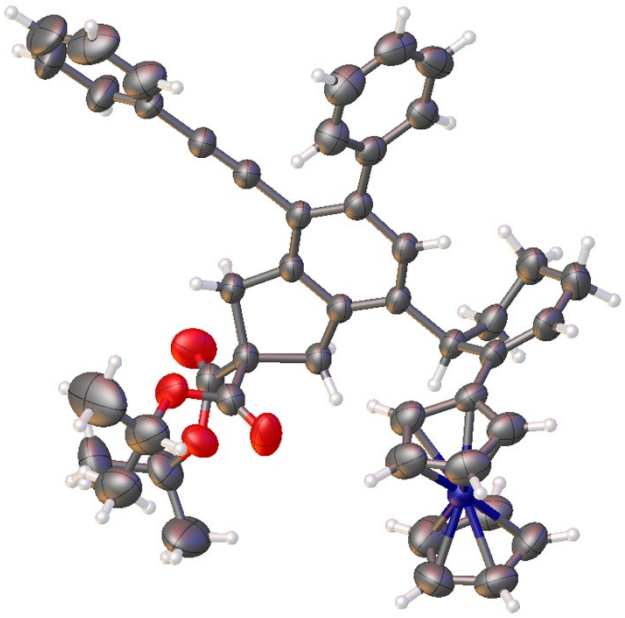
## 4. X-Ray Structure for 3a, 3b, 3c, 3t.



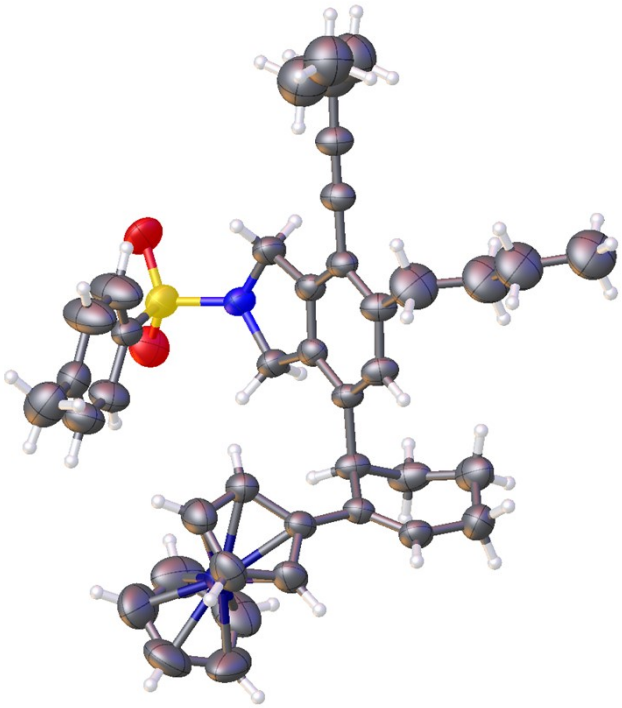
**3a**



**3b**

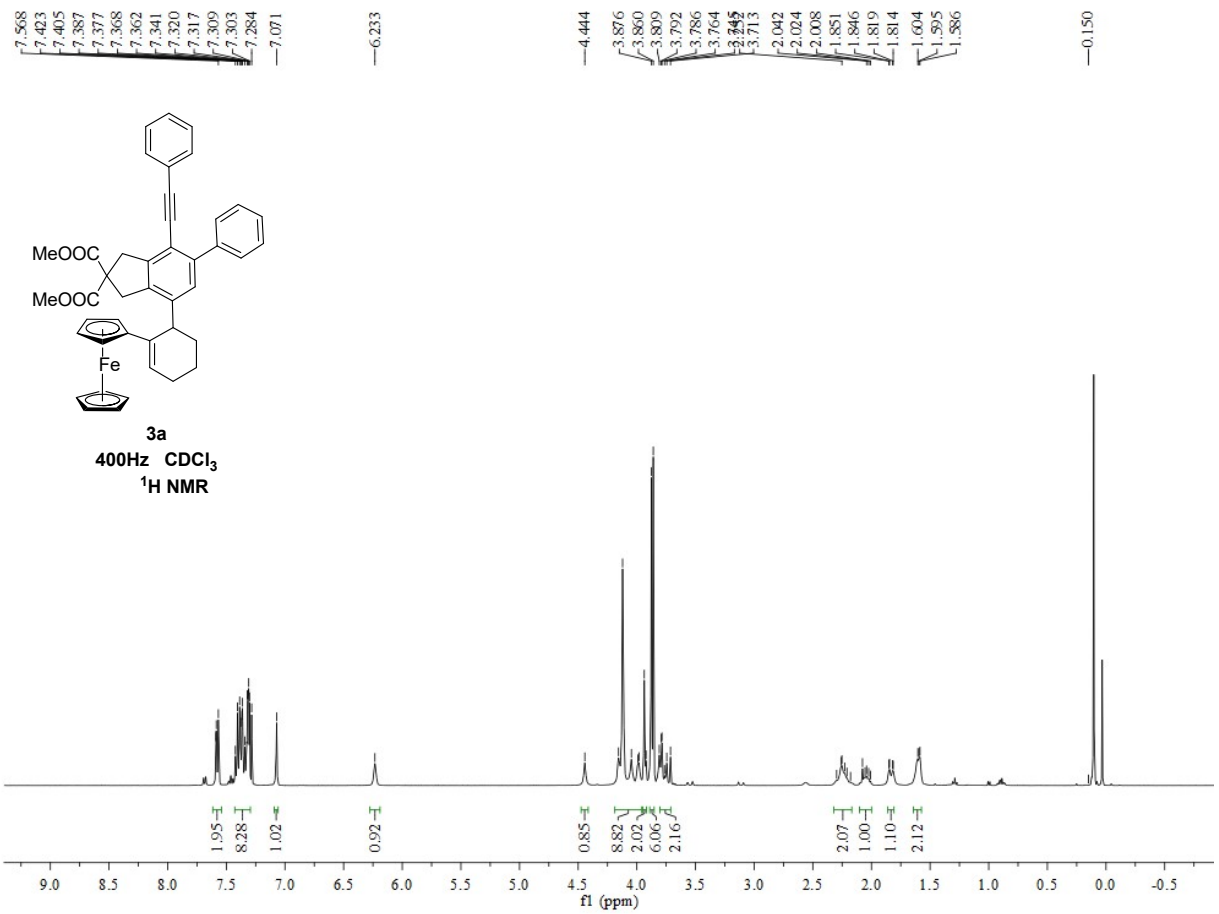


**3c**

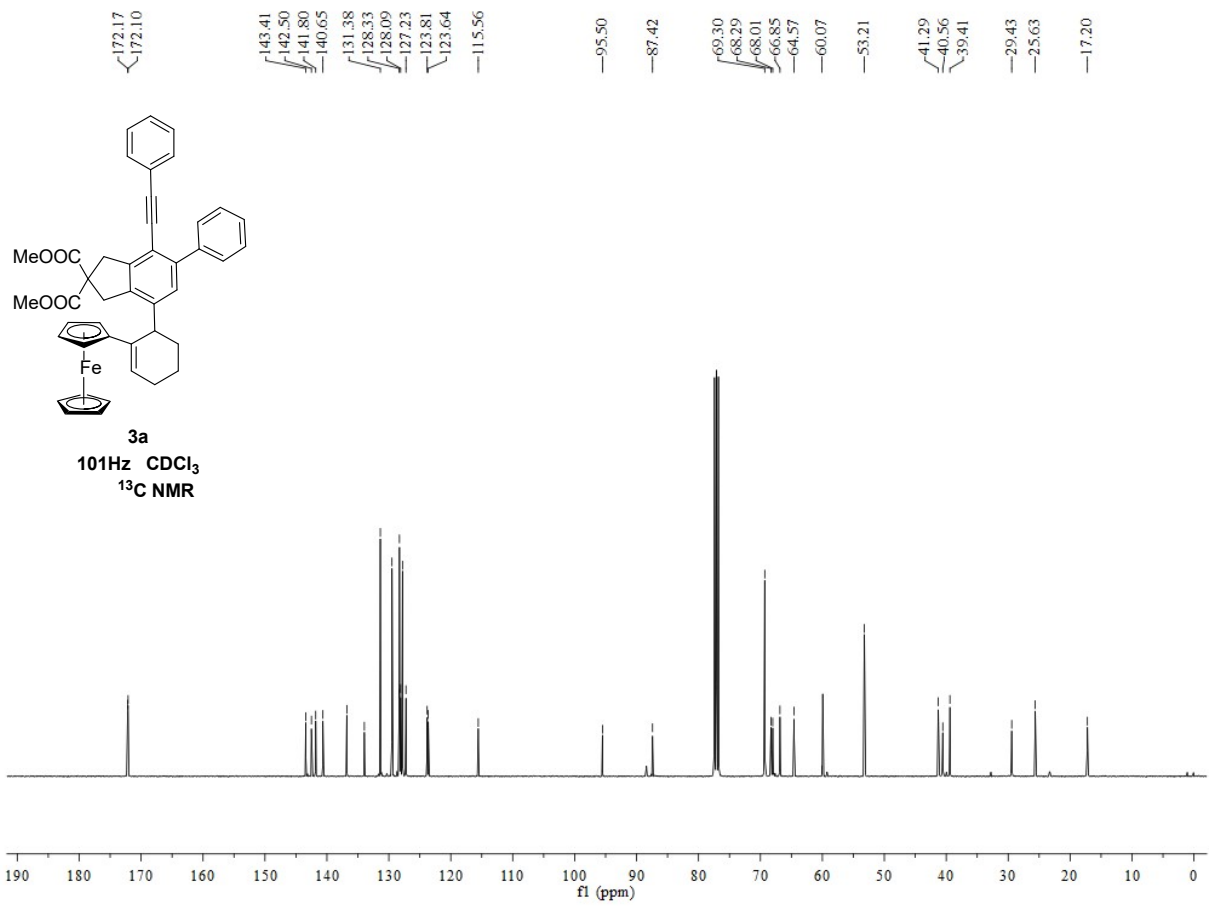


**3t**

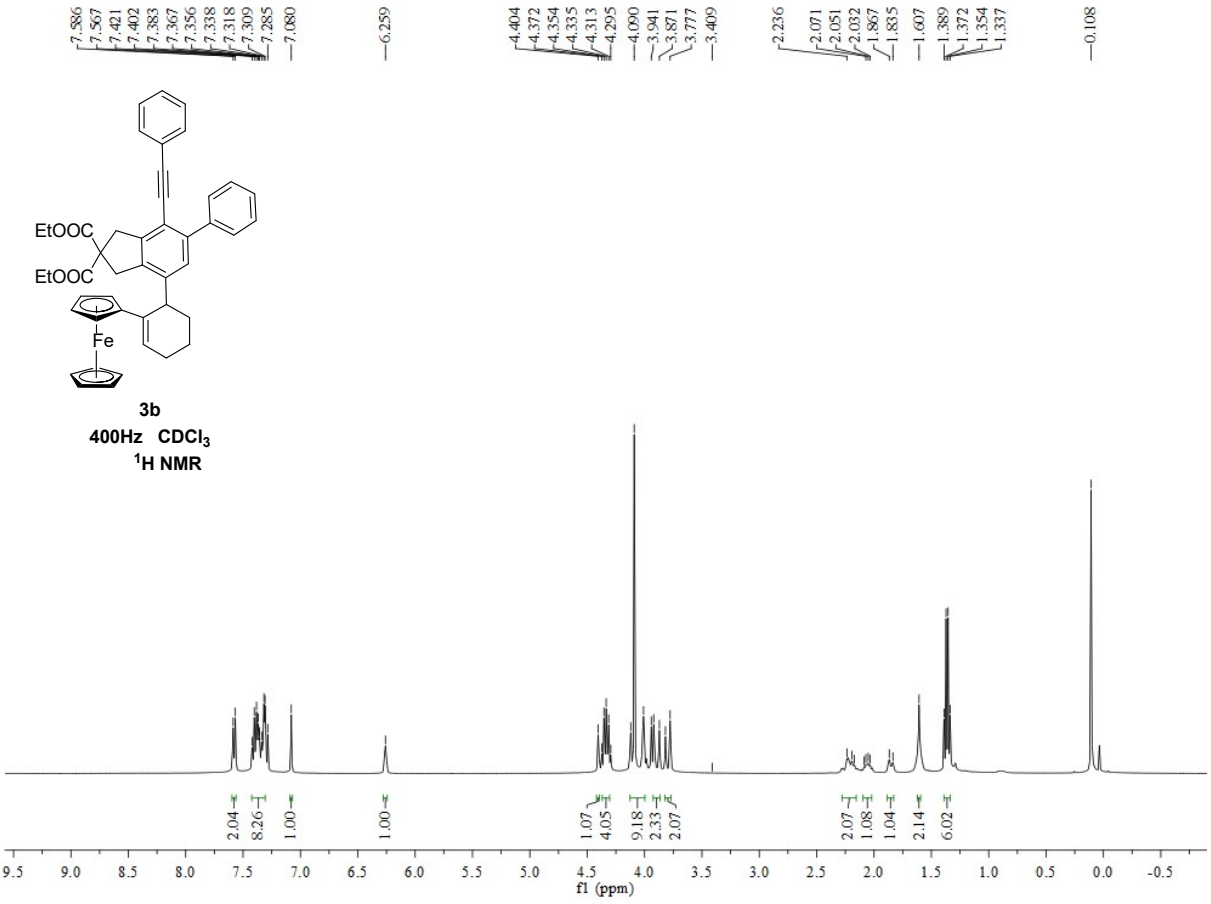
## 5. $^{1}$H NMR & $^{13}$C NMR Spectra for New Compounds



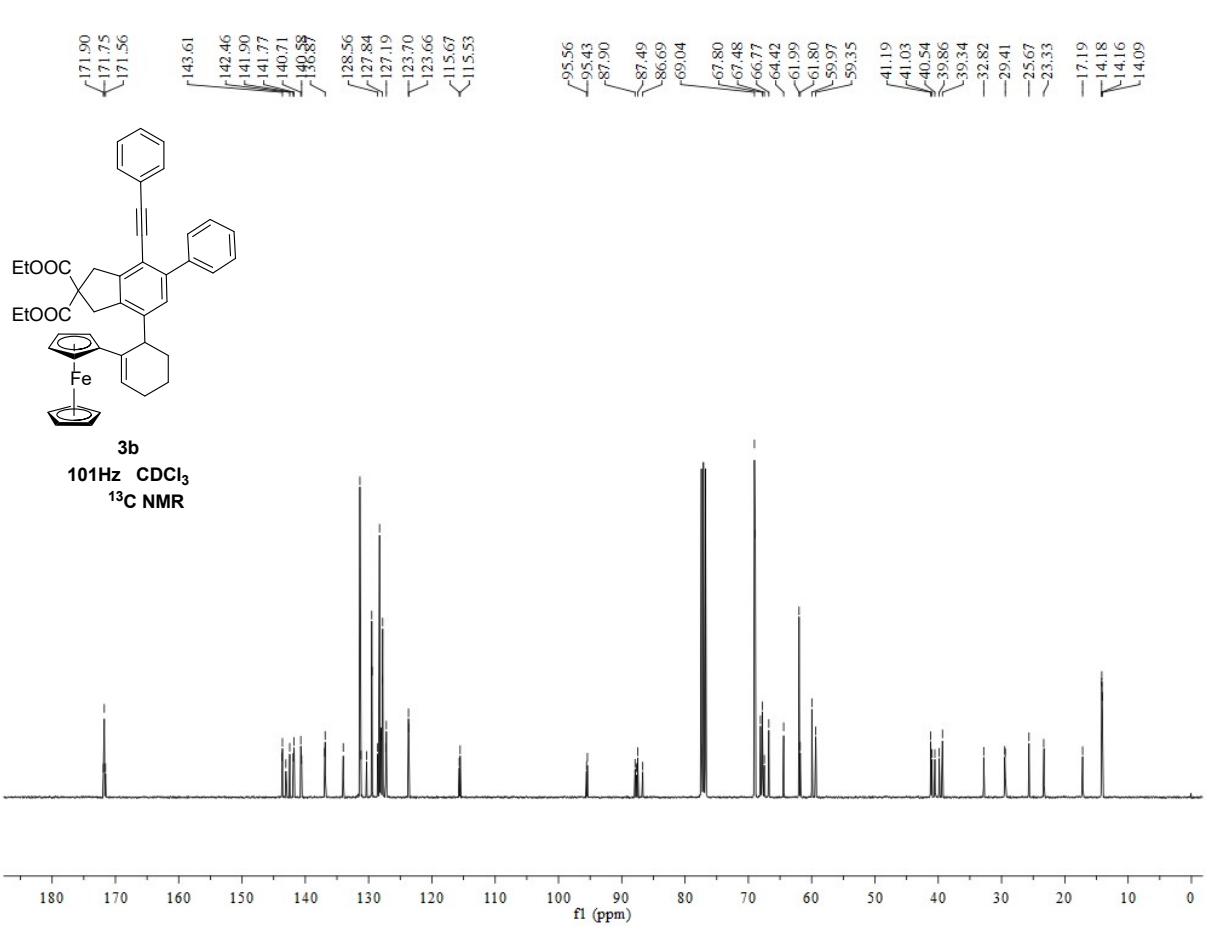

**3a**
**400Hz $CDCl_3$**
**$^1$H NMR**



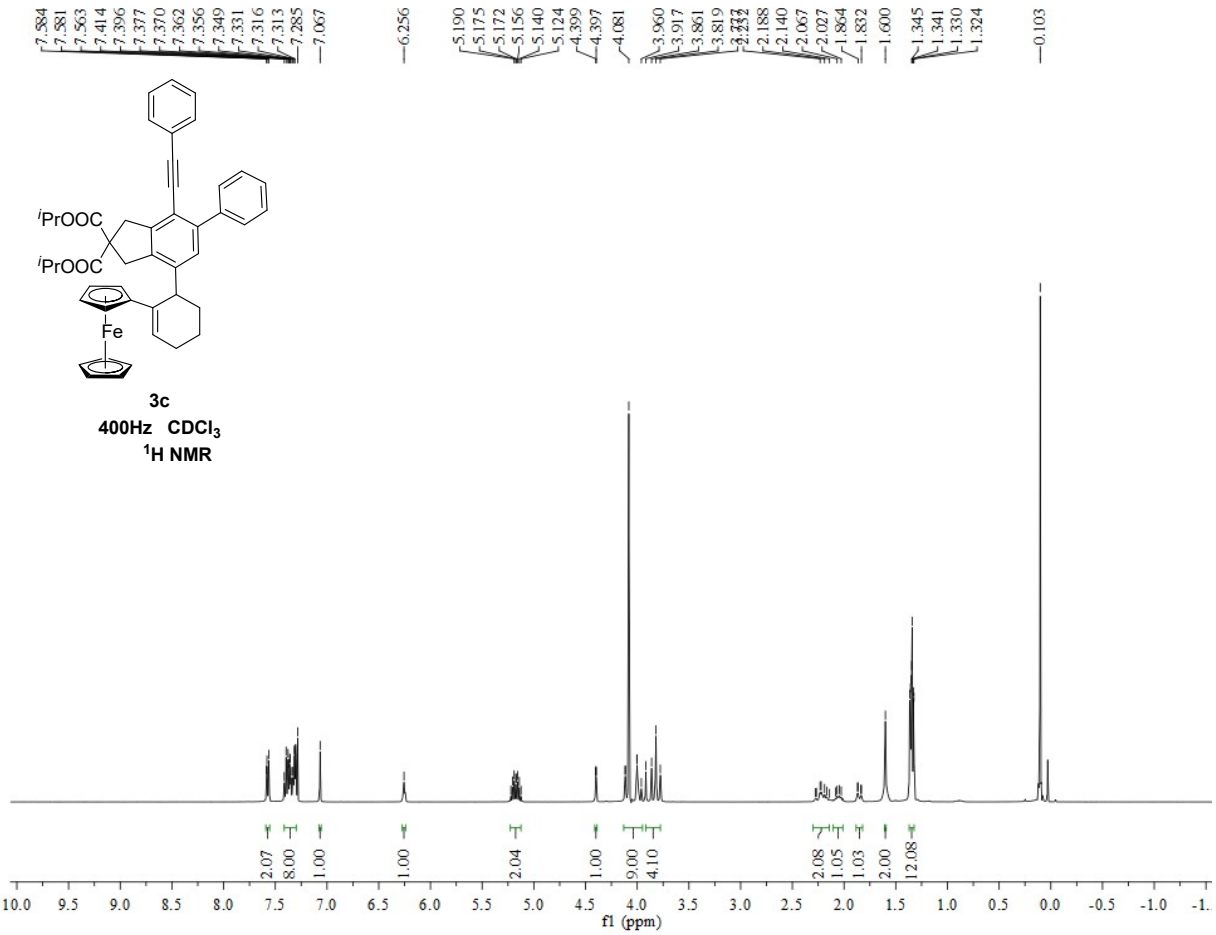

**3a**
**101Hz $CDCl_3$**
**$^{13}$C NMR**



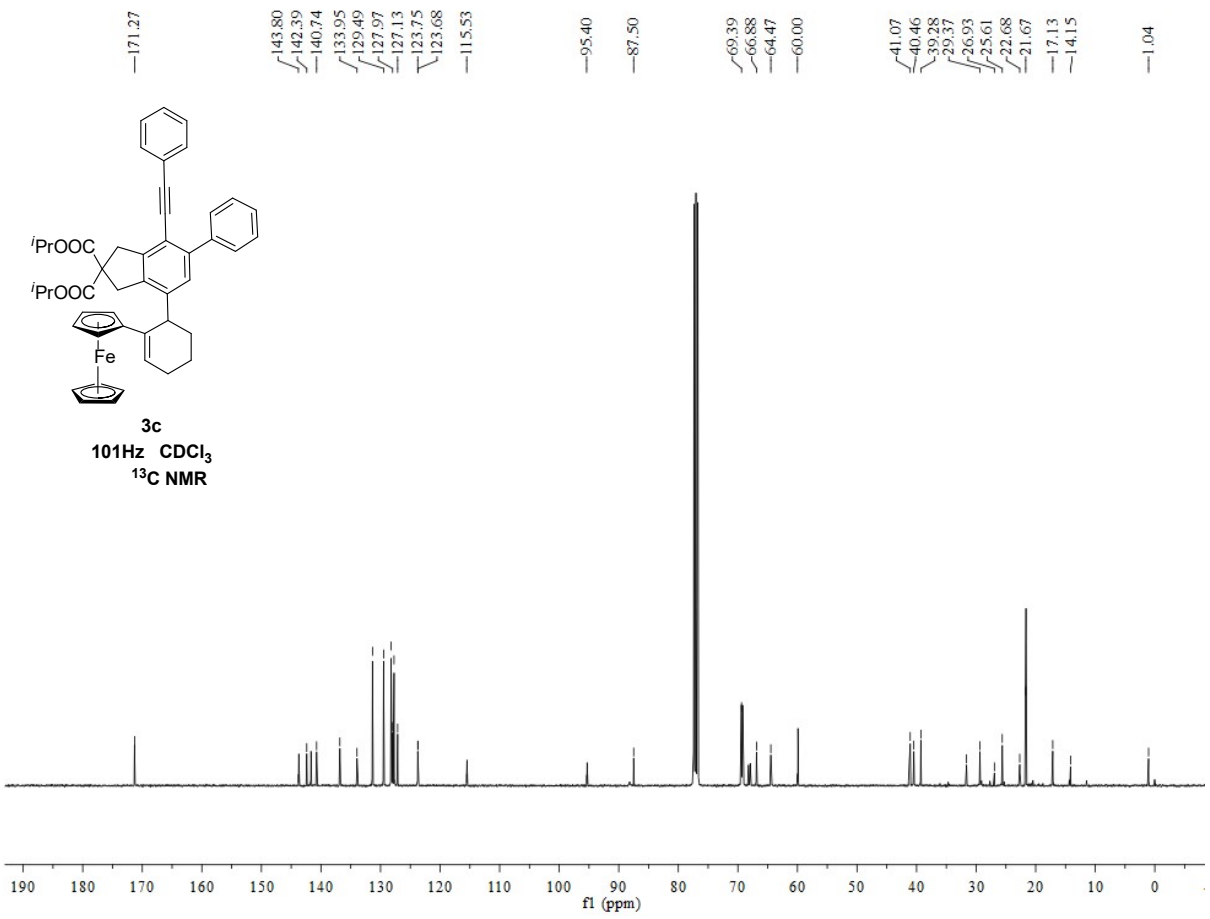

**3b**
**400Hz $CDCl_3$**
**$^1$H NMR**



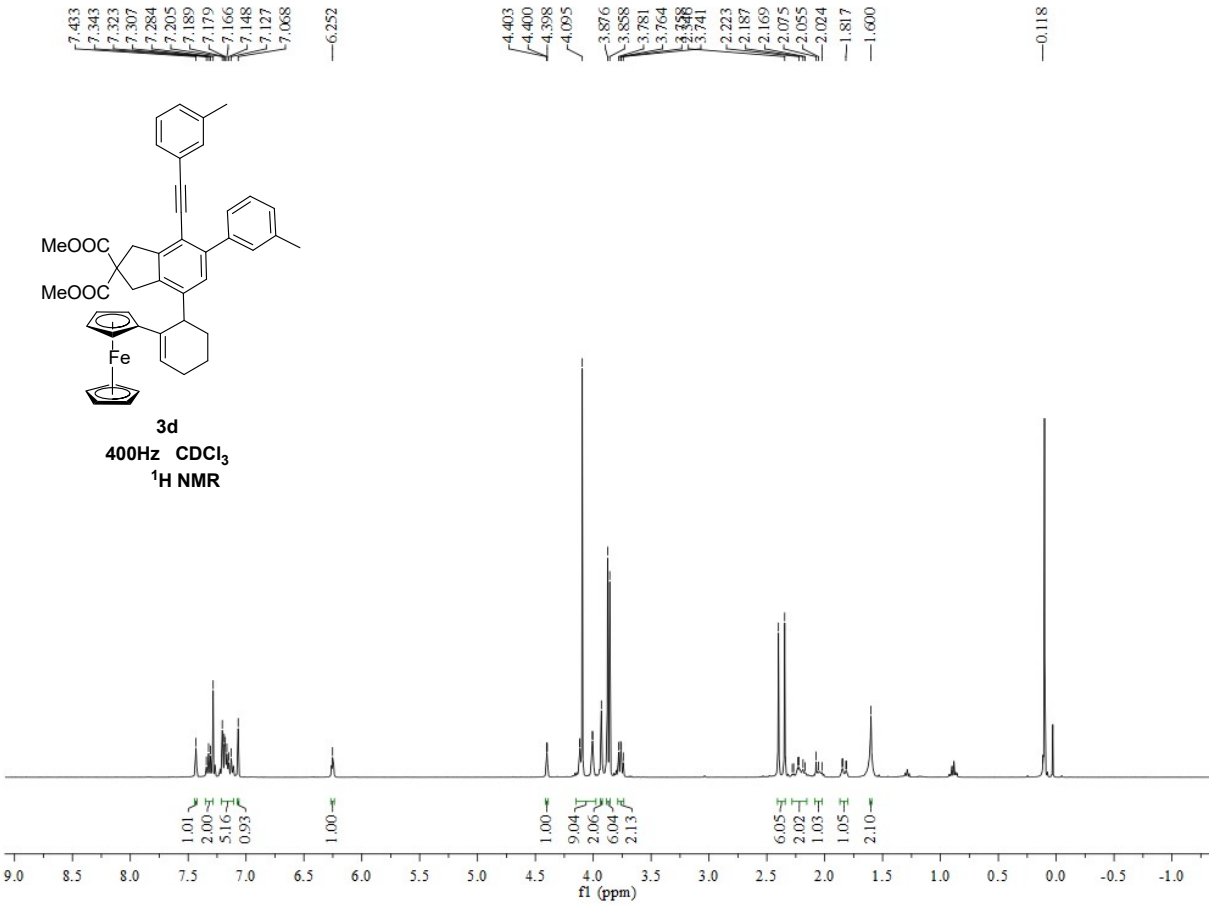

**3b**
**101Hz $CDCl_3$**
**$^{13}$C NMR**



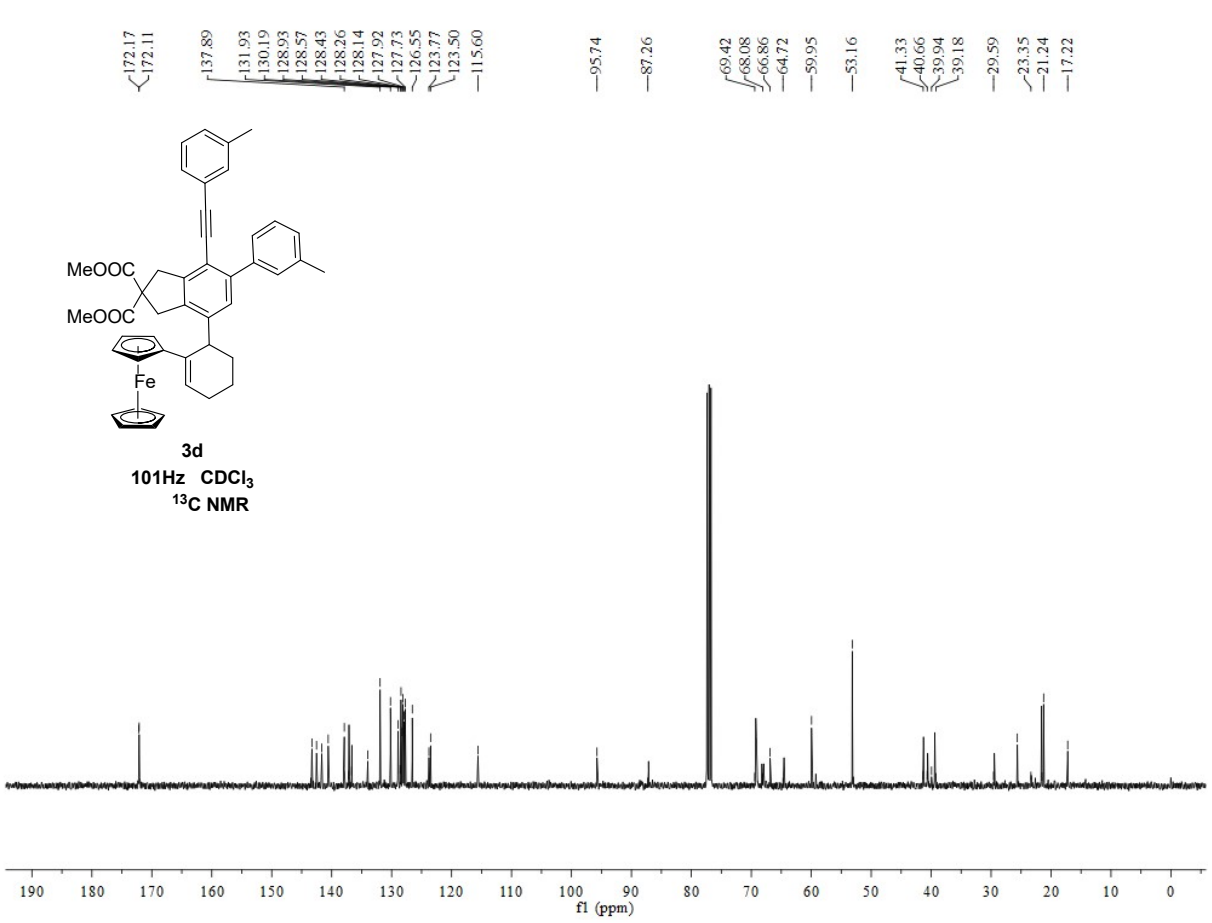

**3c**
**400Hz $CDCl_3$**
**$^1$H NMR**



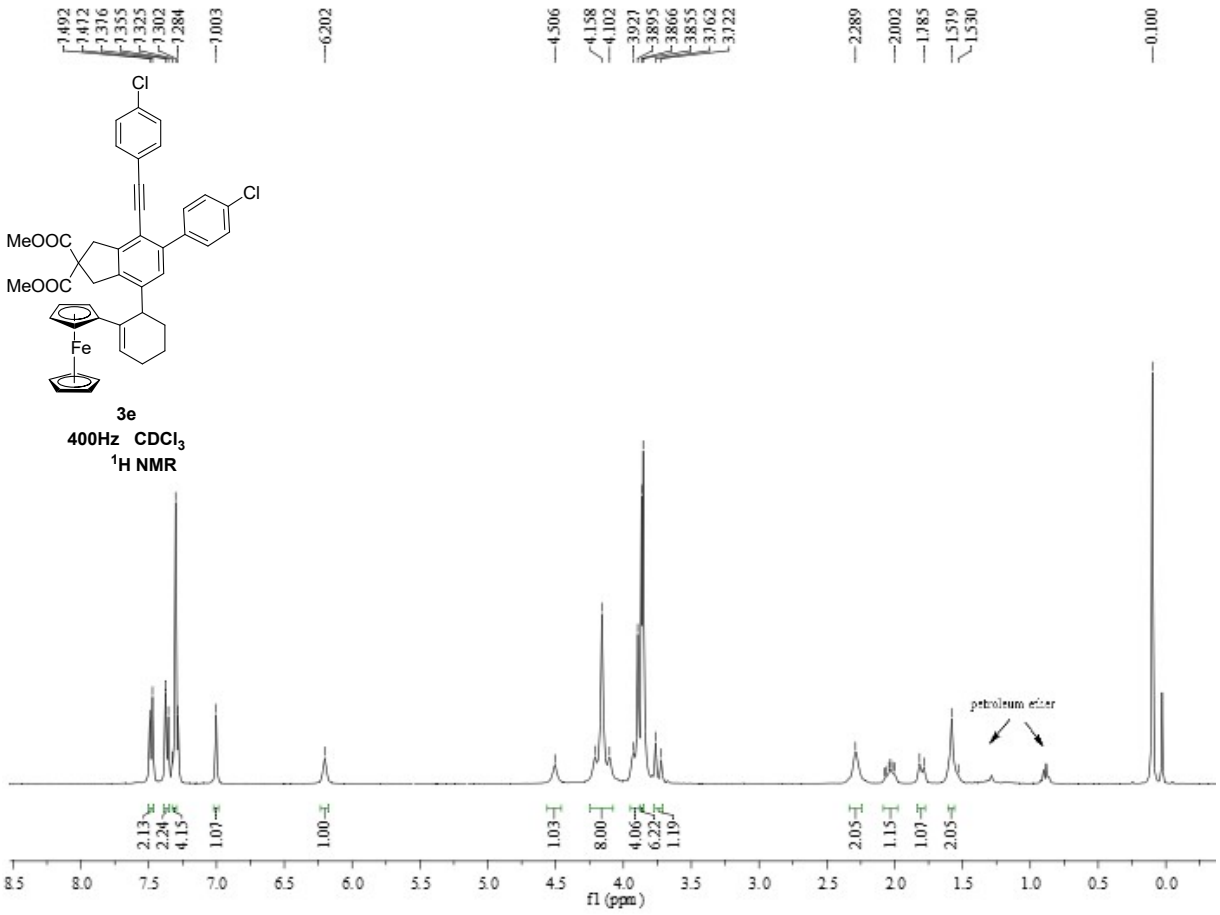

**3c**
**101Hz $CDCl_3$**
**$^{13}$C NMR**




**3d**
**400Hz $CDCl_3$**
**$^{1}H$ NMR**



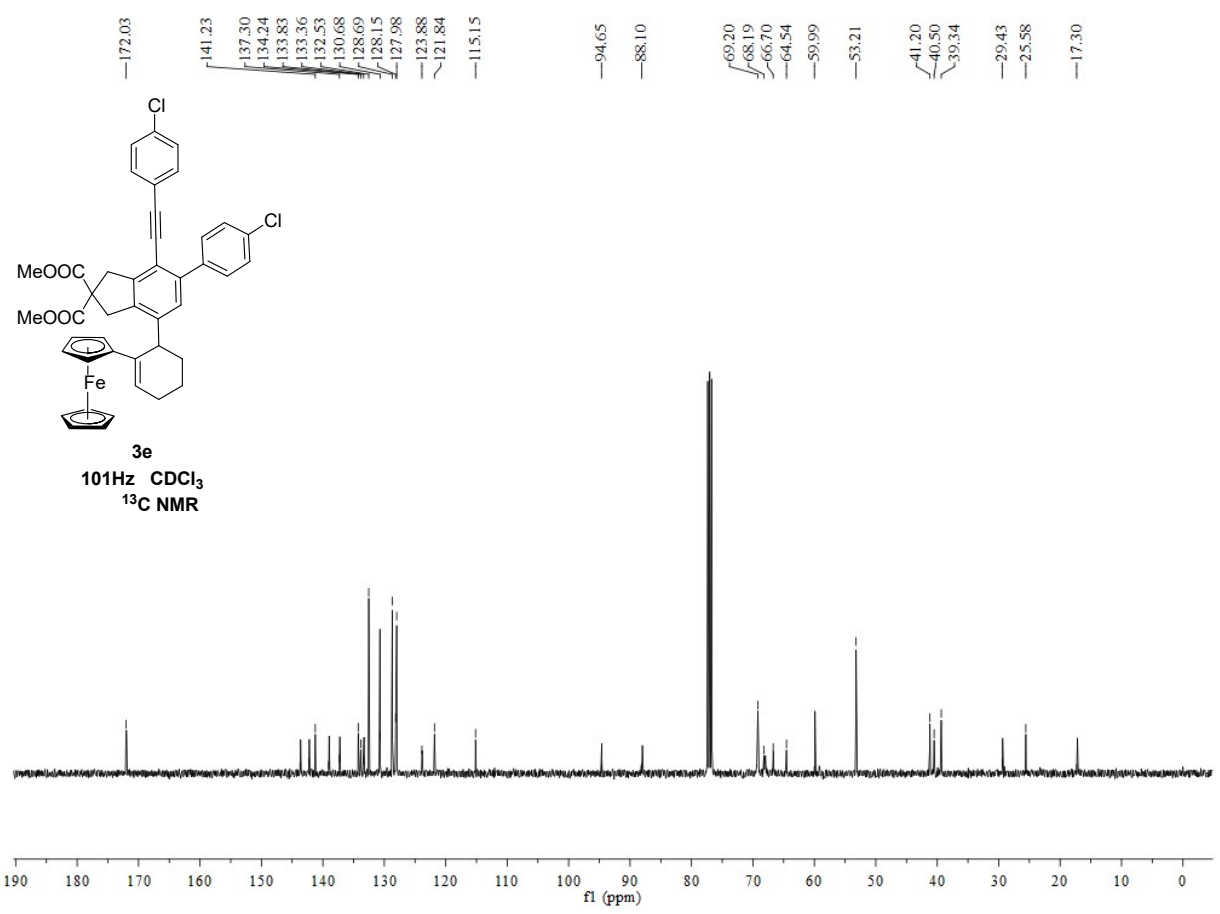

**3d**
**101Hz $CDCl_3$**
**$^{13}C$ NMR**




**3e**

**400Hz $CDCl_3$**

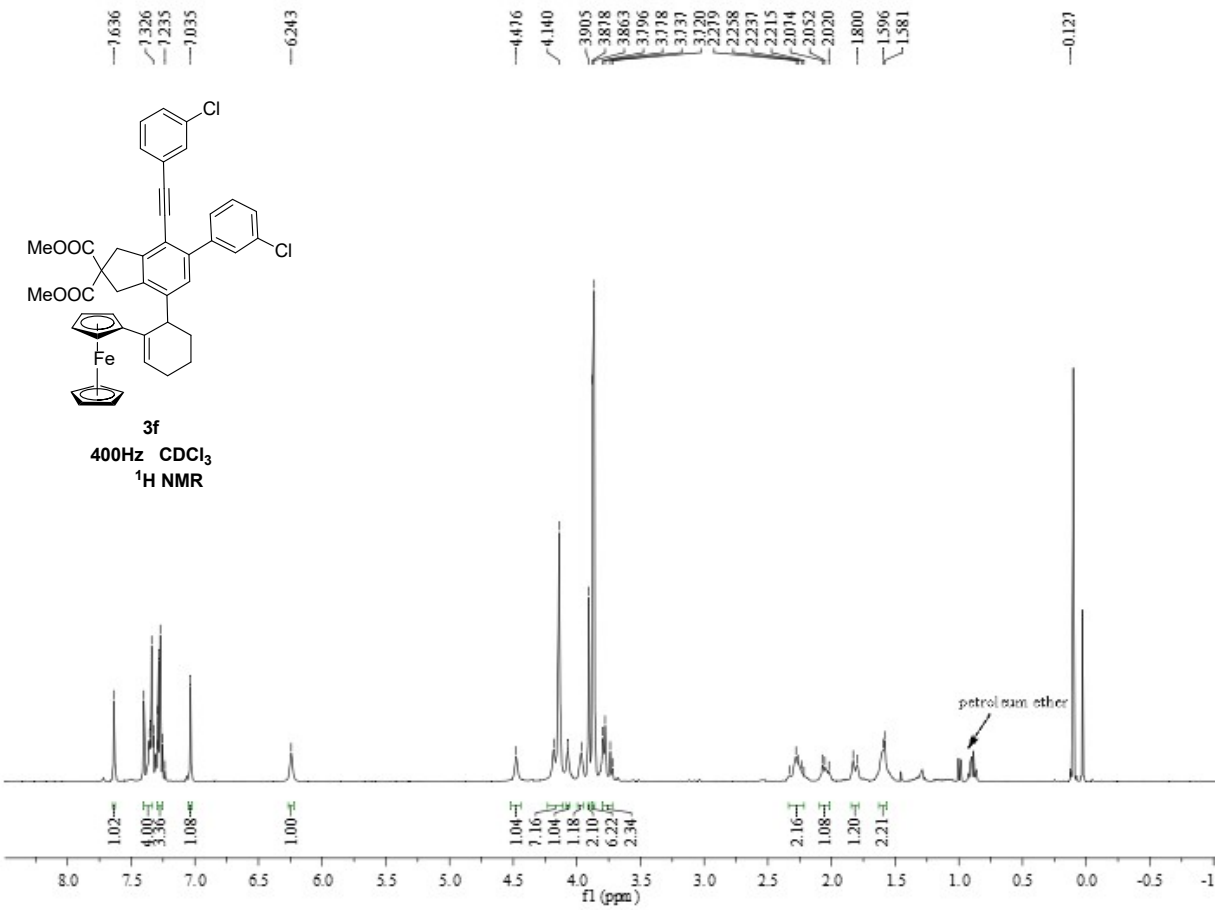
**$^1$H NMR**




**3e**

**101Hz $CDCl_3$**

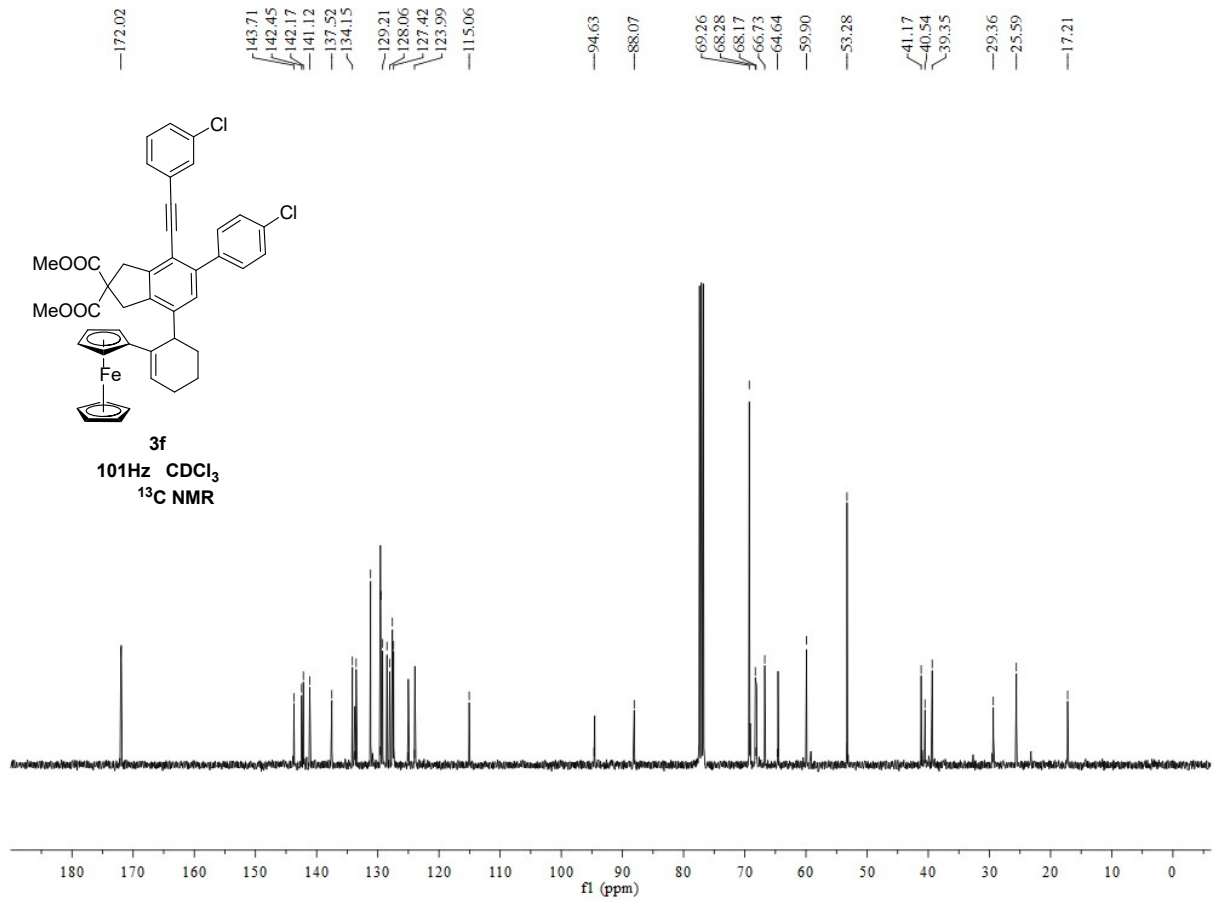
**$^{13}$C NMR**




**3f**

**400Hz $CDCl_3$**

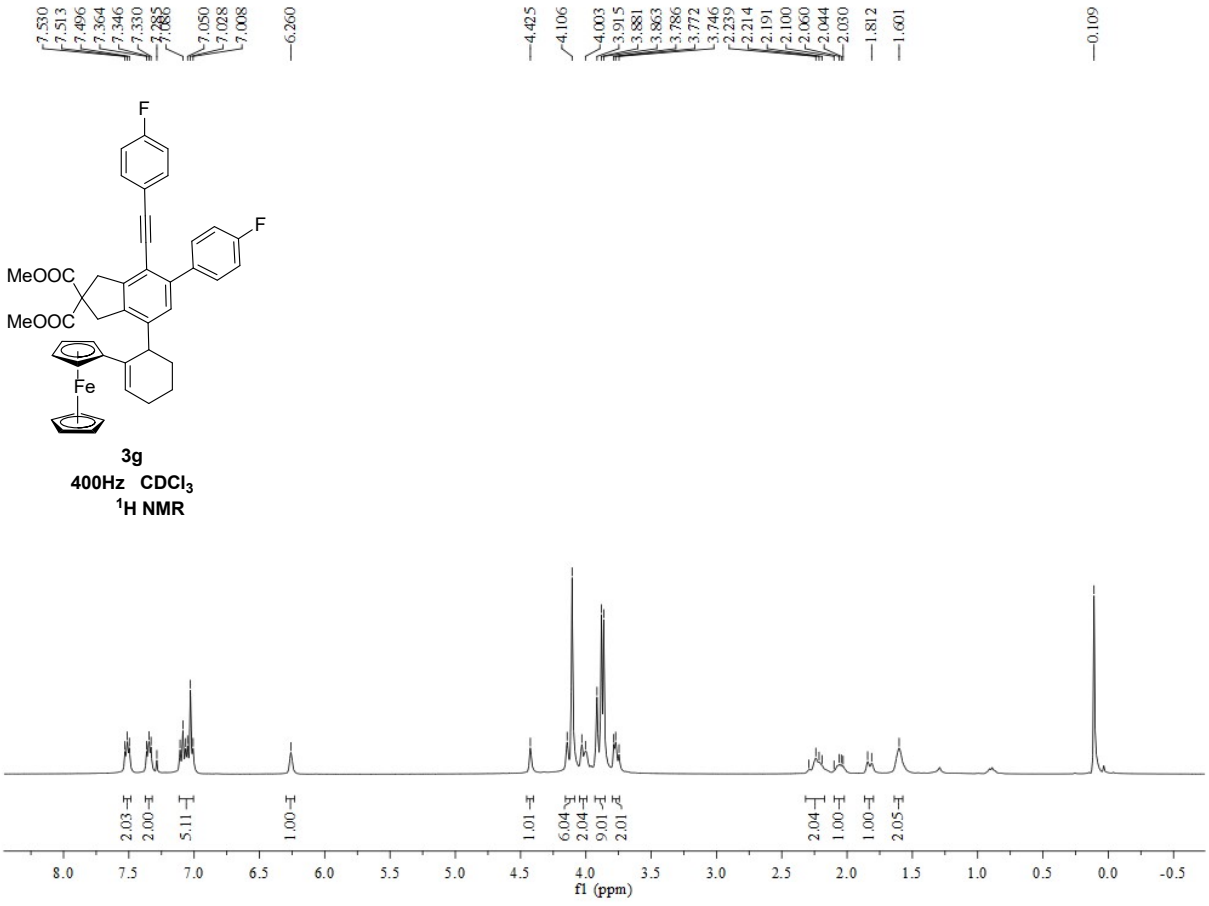
**$^1$H NMR**



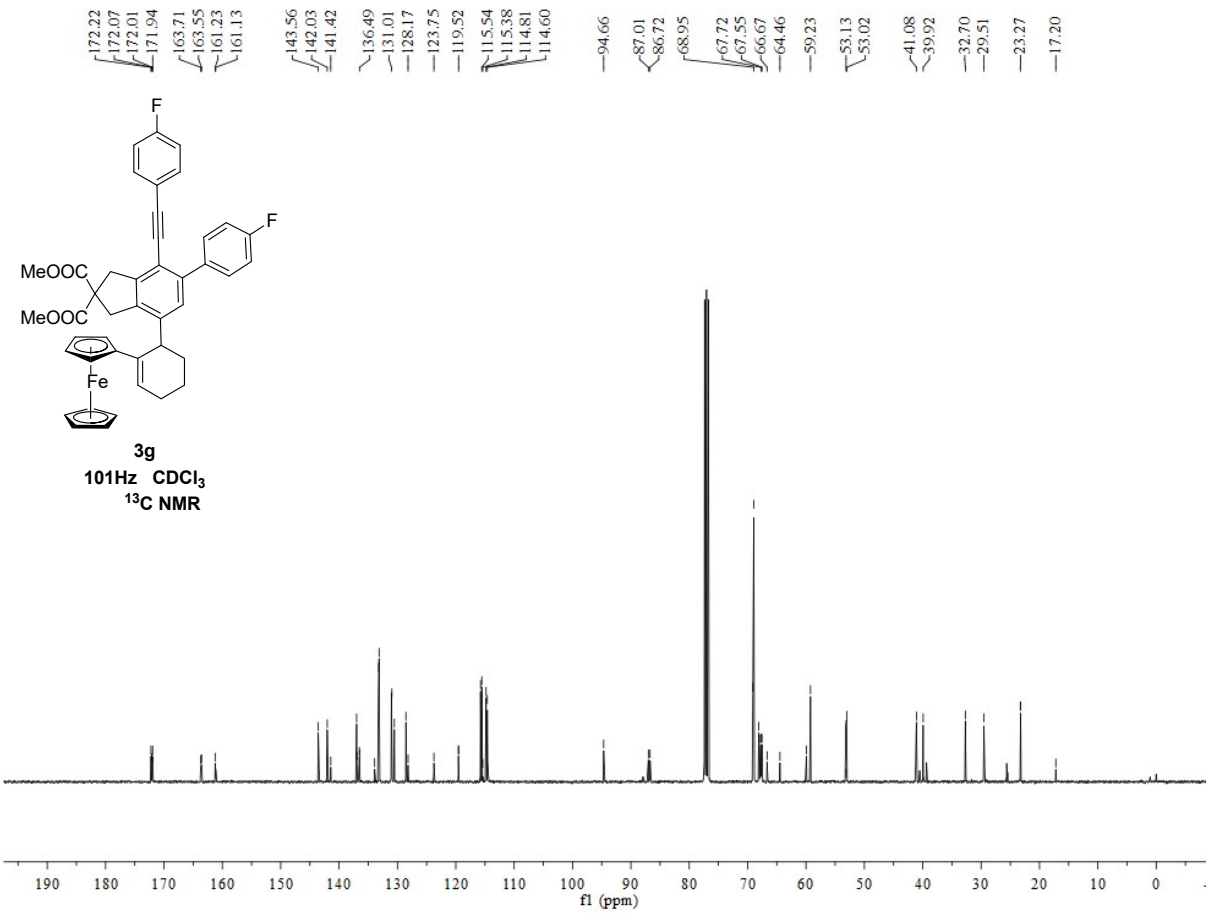

**3f**

**101Hz $CDCl_3$**

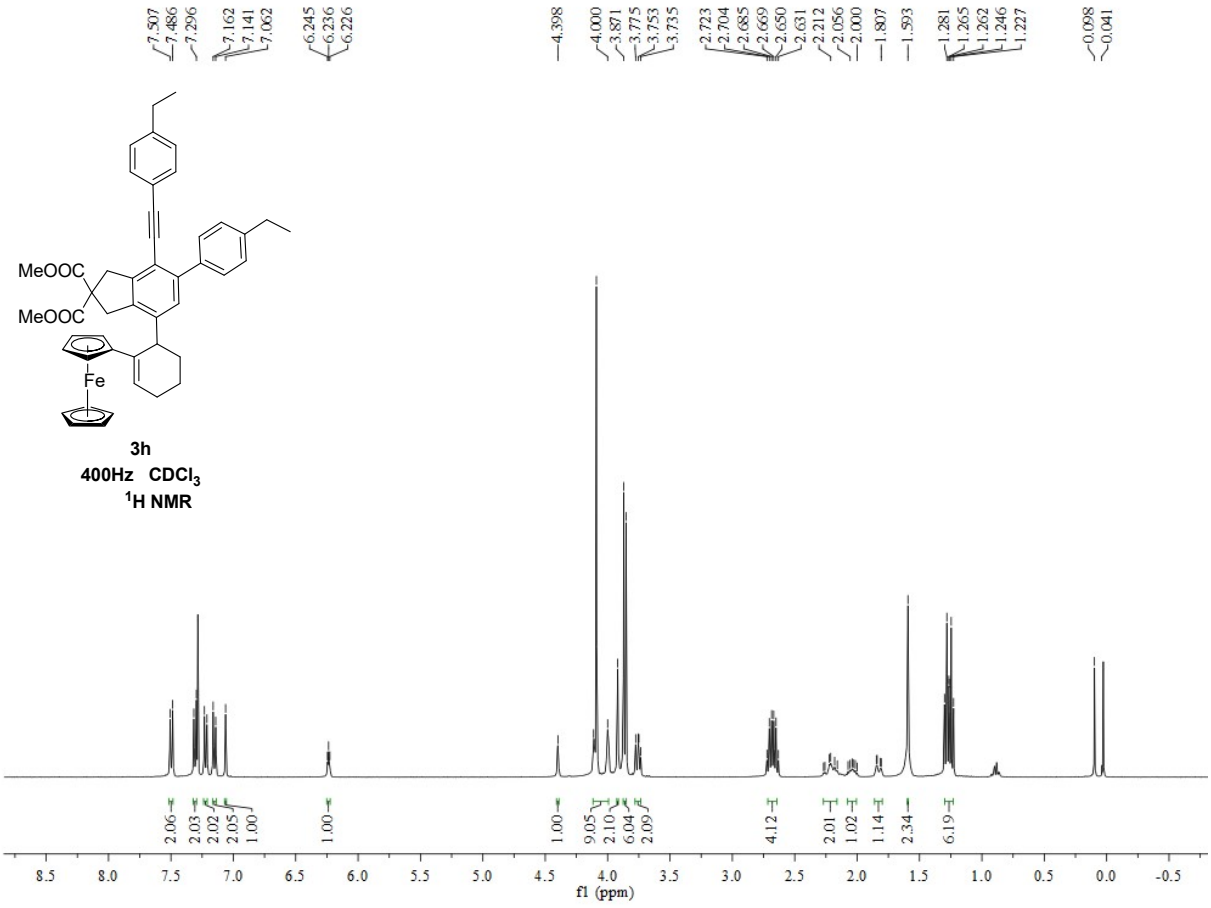
**$^{13}$C NMR**




**3g**
**400Hz $CDCl_3$**
**$^{1}H$ NMR**




**3g**
**101Hz $CDCl_3$**
**$^{13}C$ NMR**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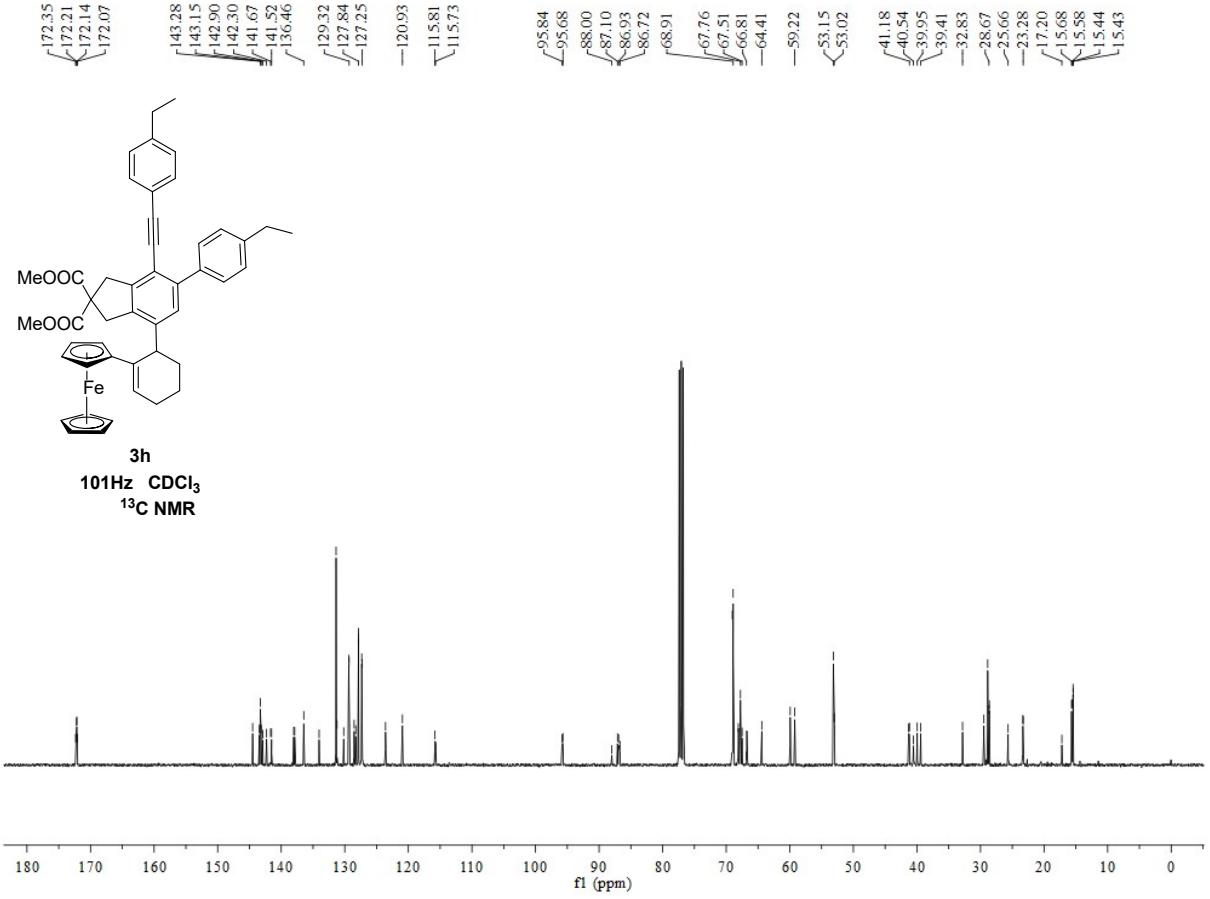
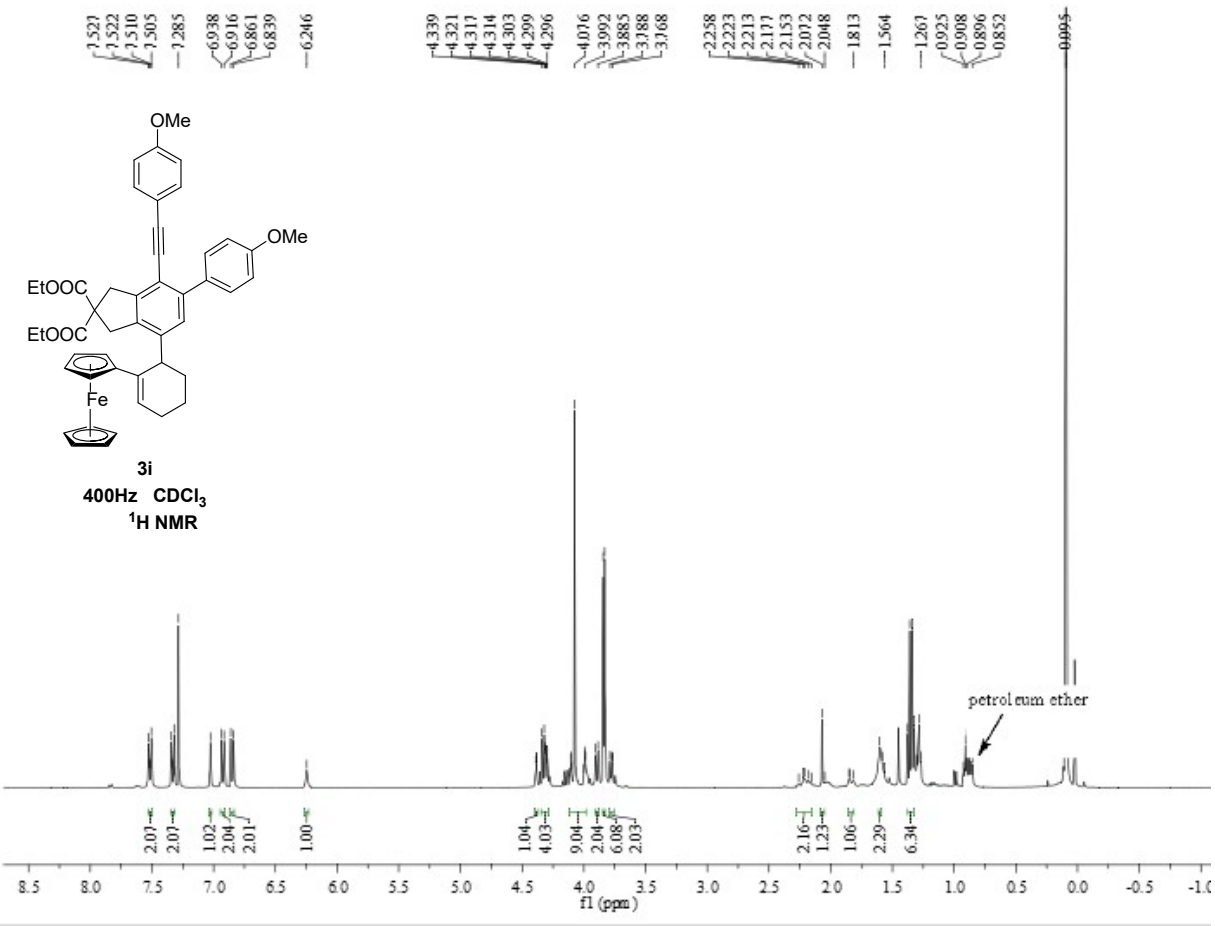
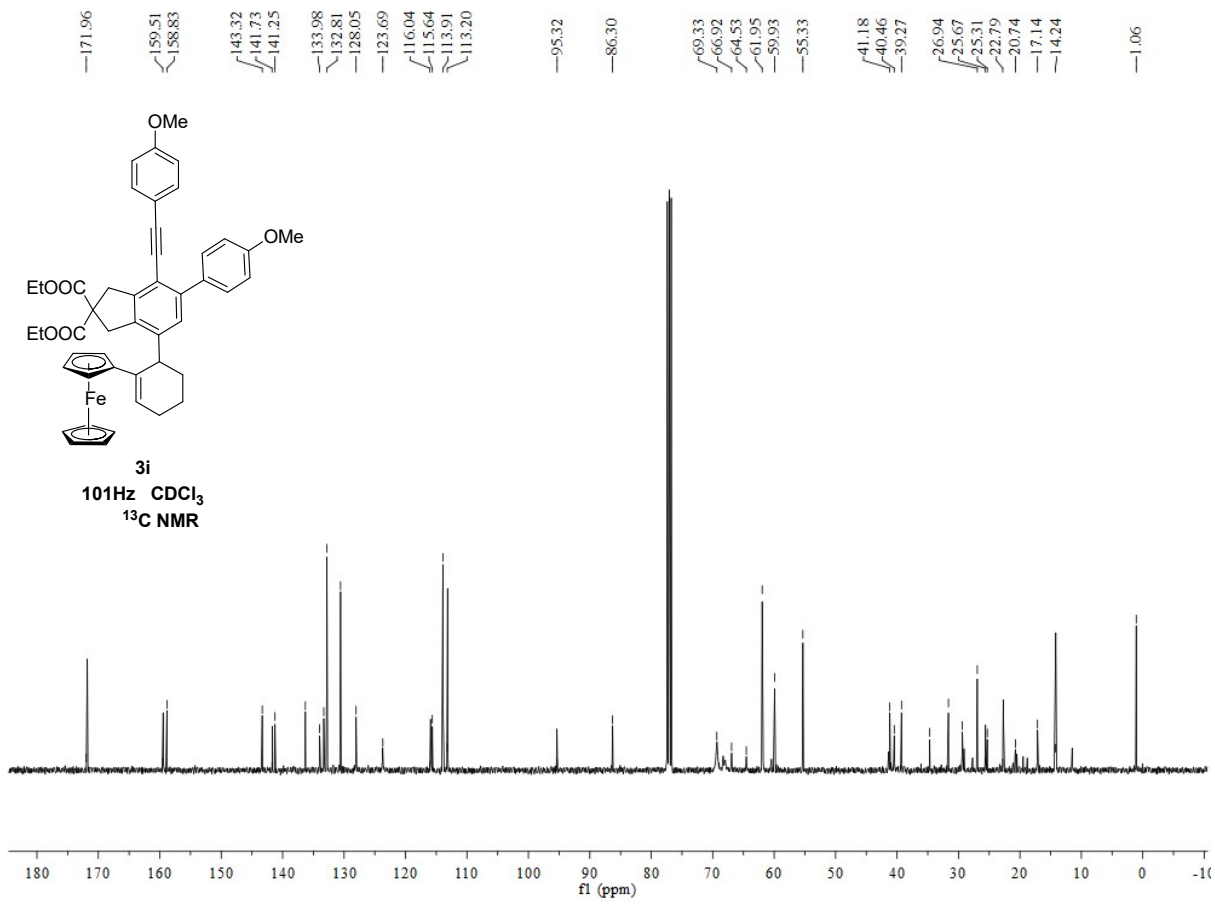
MeOOC
Fe
3h
400Hz CDCl3
1H NMR
f1 (ppm)

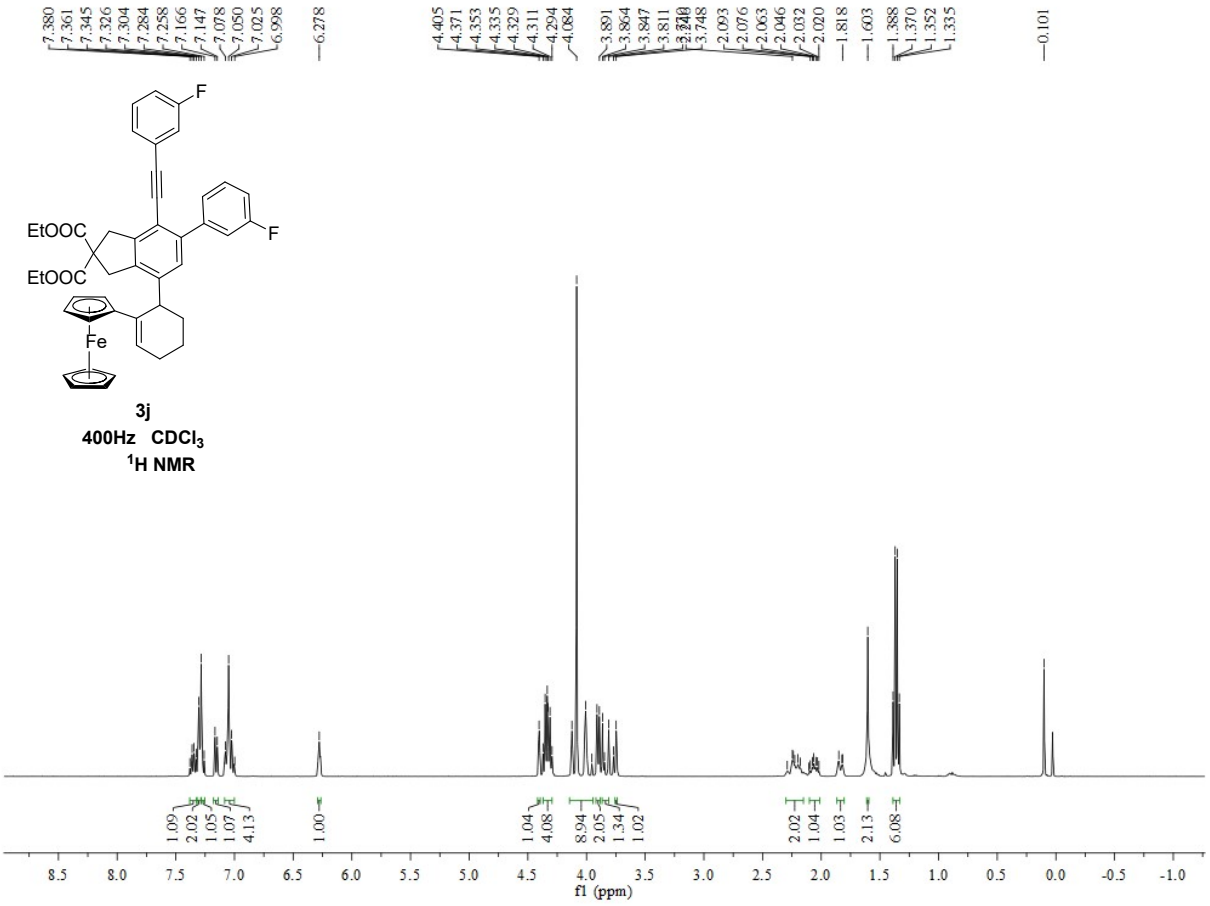

MeOOC
MeOOC
Fe
3h
101Hz CDCl3
13C NMR
f1 (ppm)



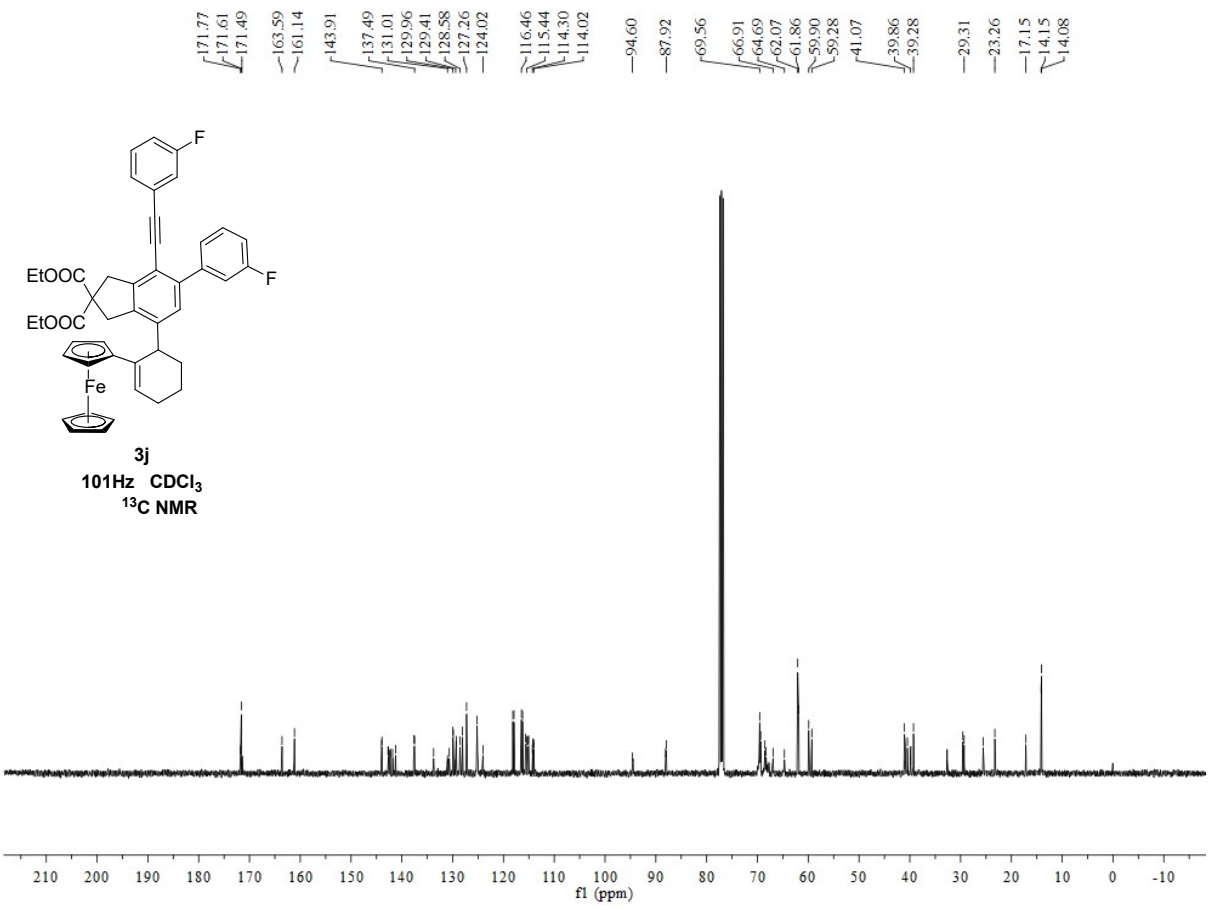

**3i**
**400Hz CDCl$_3$**
**$^1$H NMR**



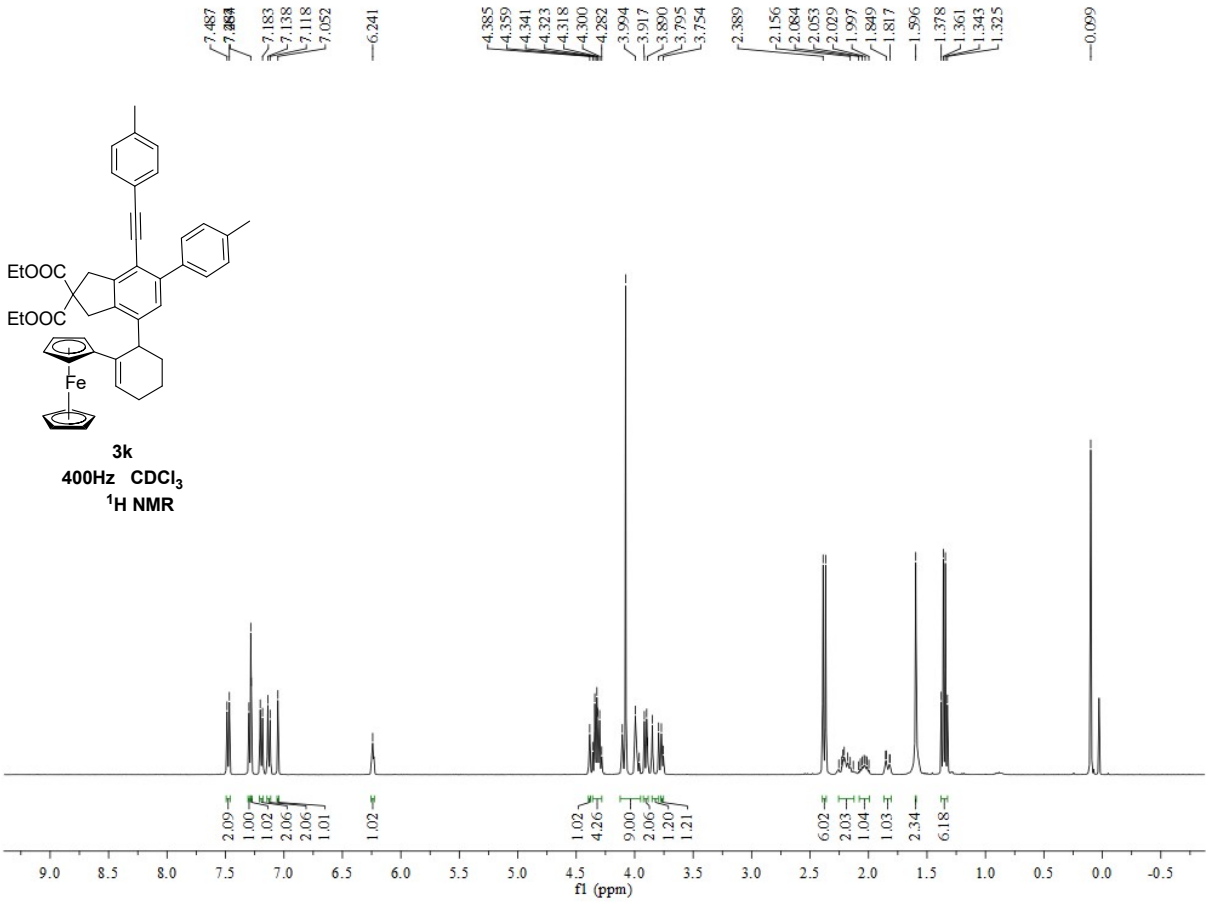

**3i**
**101Hz CDCl$_3$**
**$^{13}$C NMR**

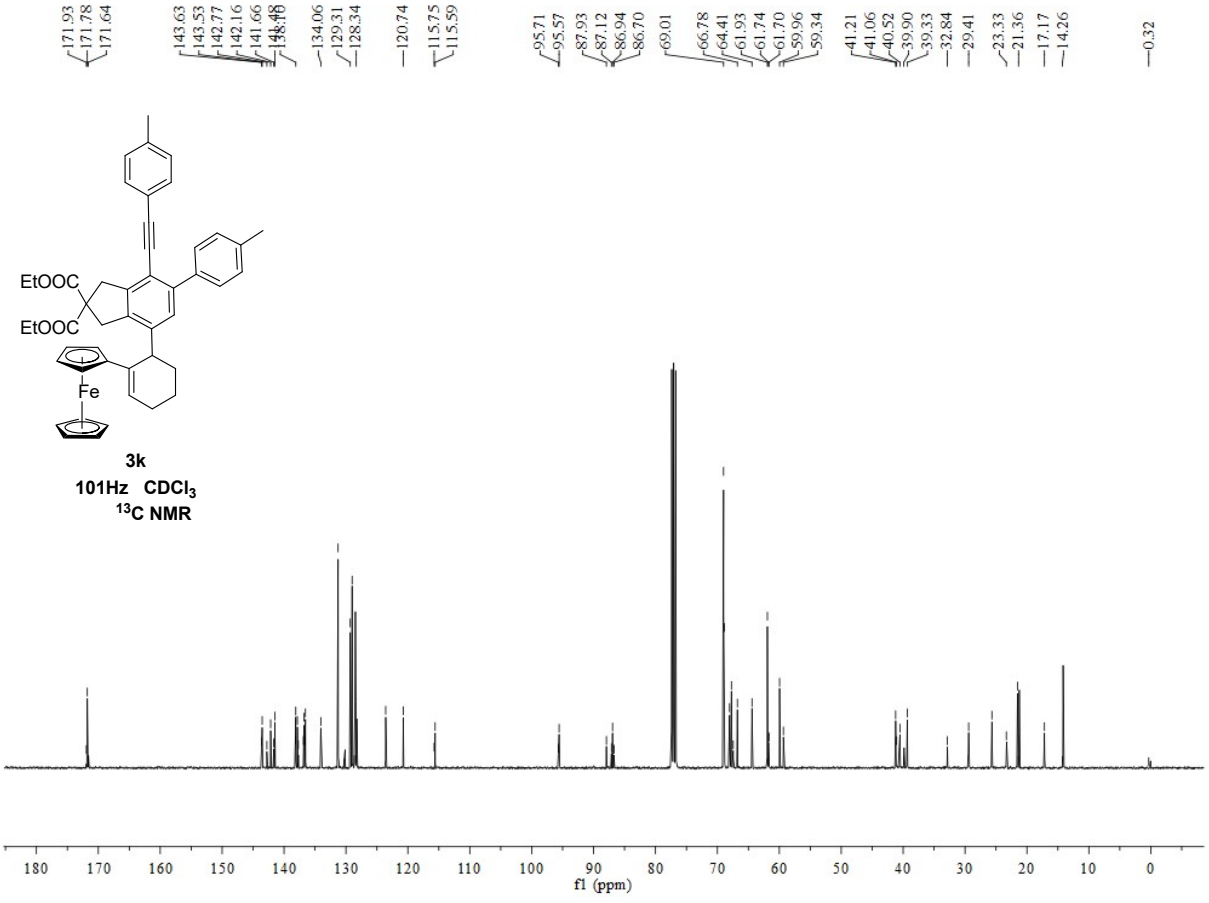


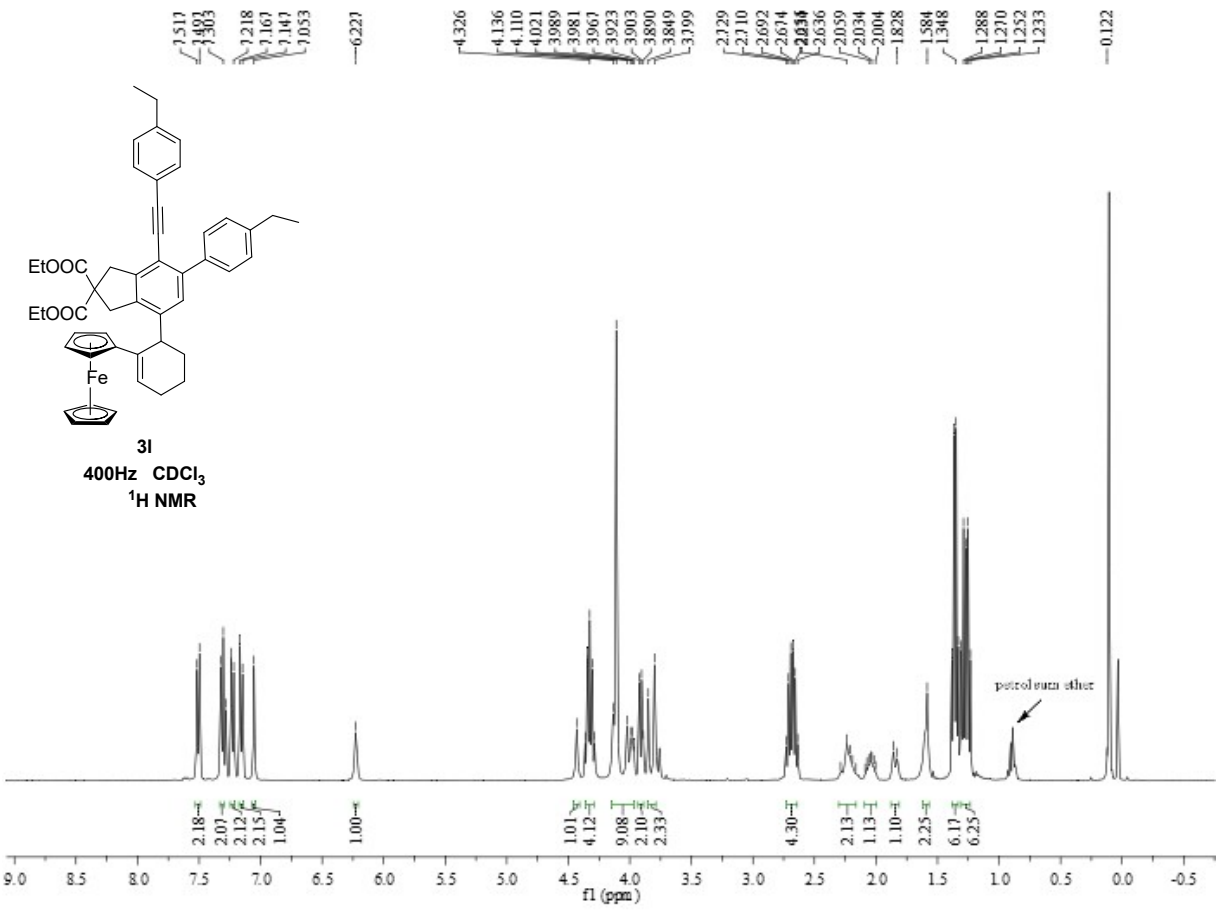

**3j**
**400Hz $CDCl_3$**
**$^1$H NMR**



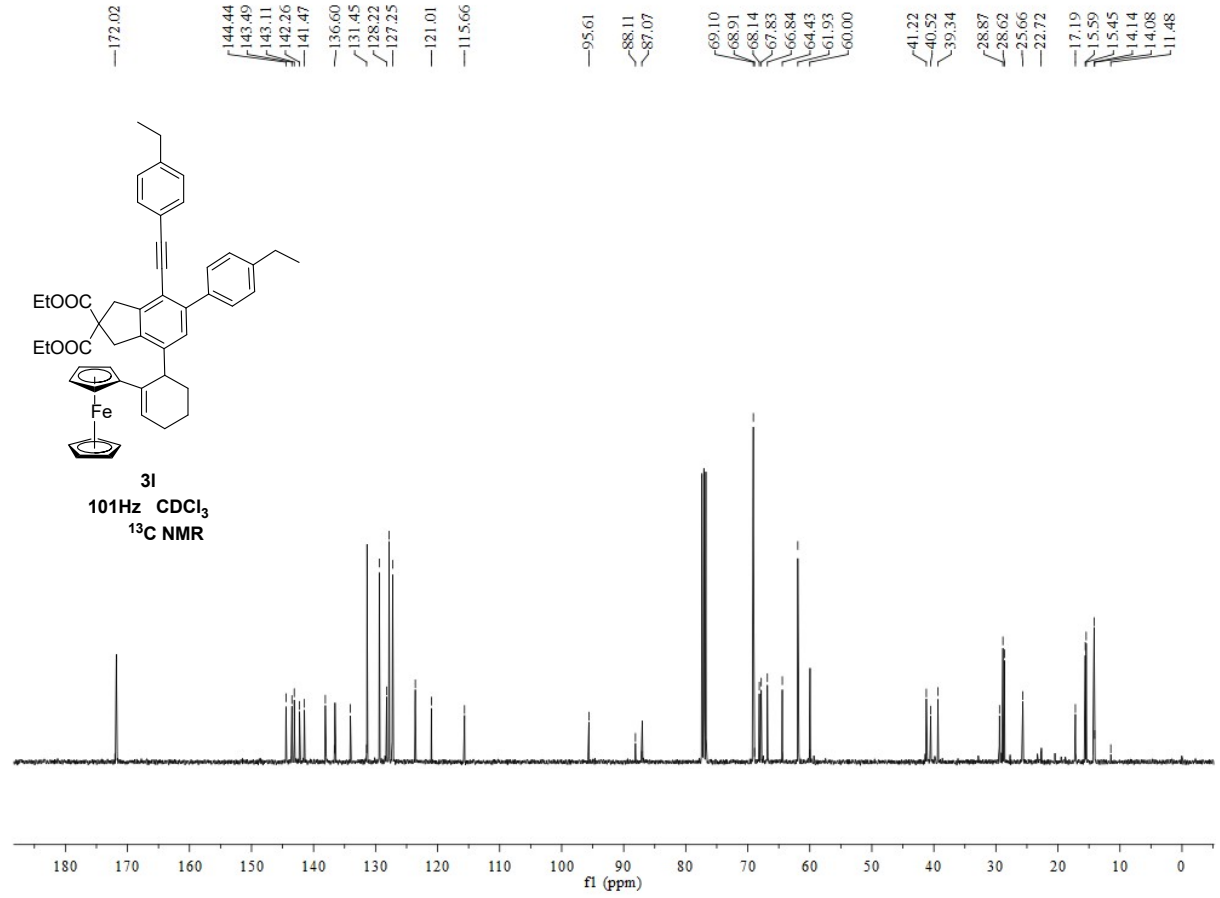

**3j**
**101Hz $CDCl_3$**
**$^{13}$C NMR**


EtOOC
EtOOC
Fe
3k
400Hz CDCl3
1H NMR
f1 (ppm)

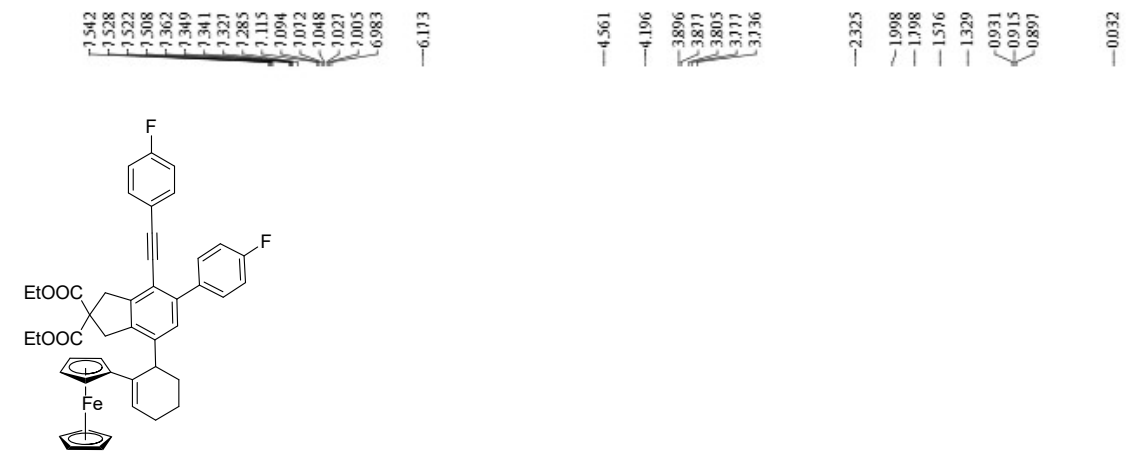

EtOOC
EtOOC
Fe
3k
101Hz CDCl3
13C NMR
f1 (ppm)




**3l**
**400Hz CDCl$_3$**
**$^1$H NMR**



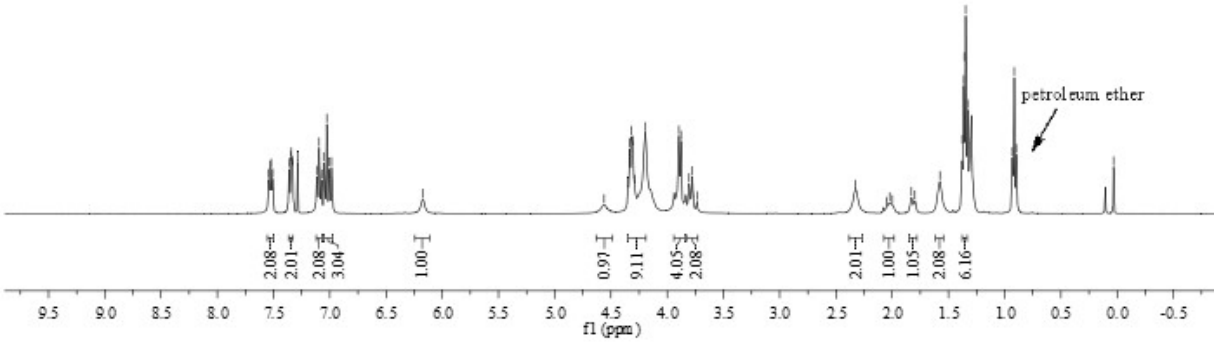

**3l**
**101Hz CDCl$_3$**
**$^{13}$C NMR**

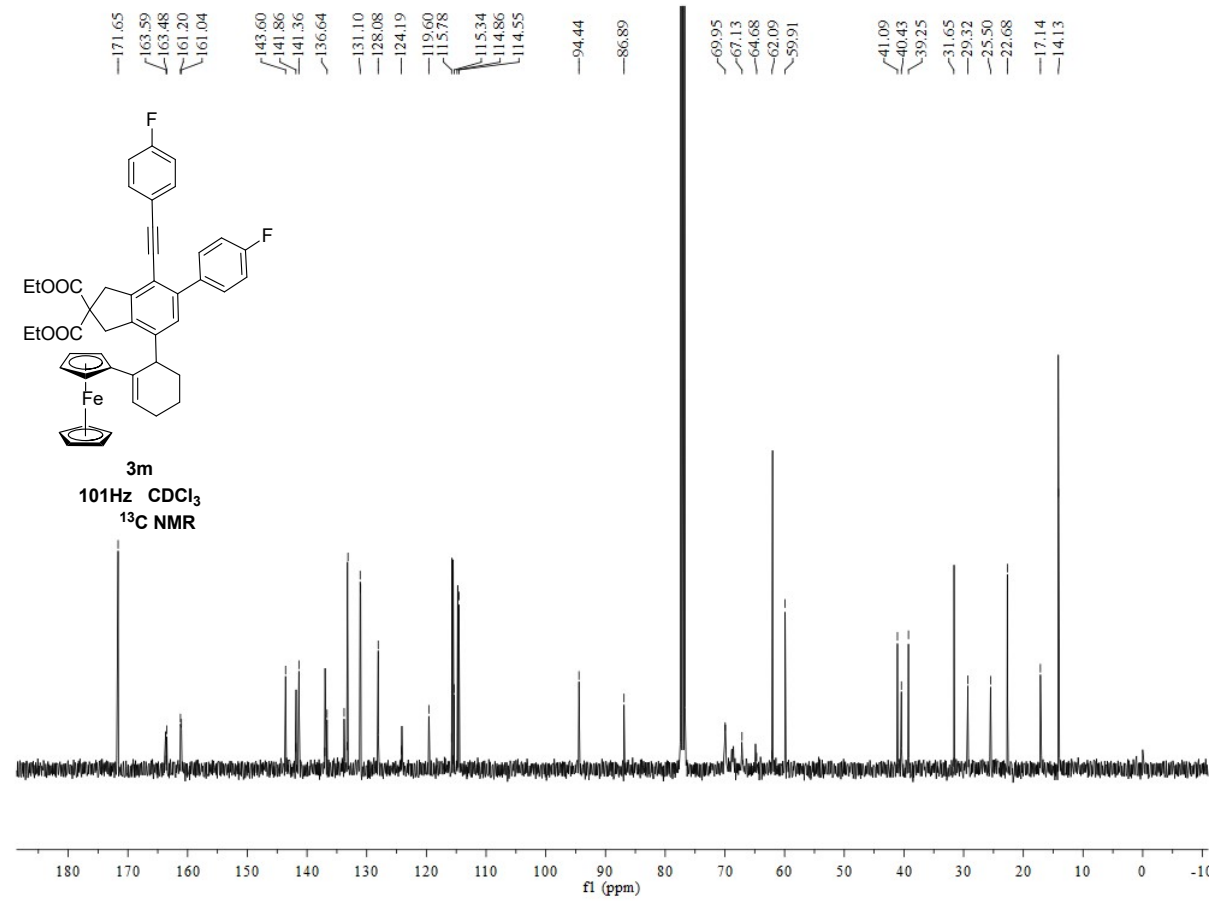






**3m**
**400Hz CDCl$_3$**
**$^1$H NMR**

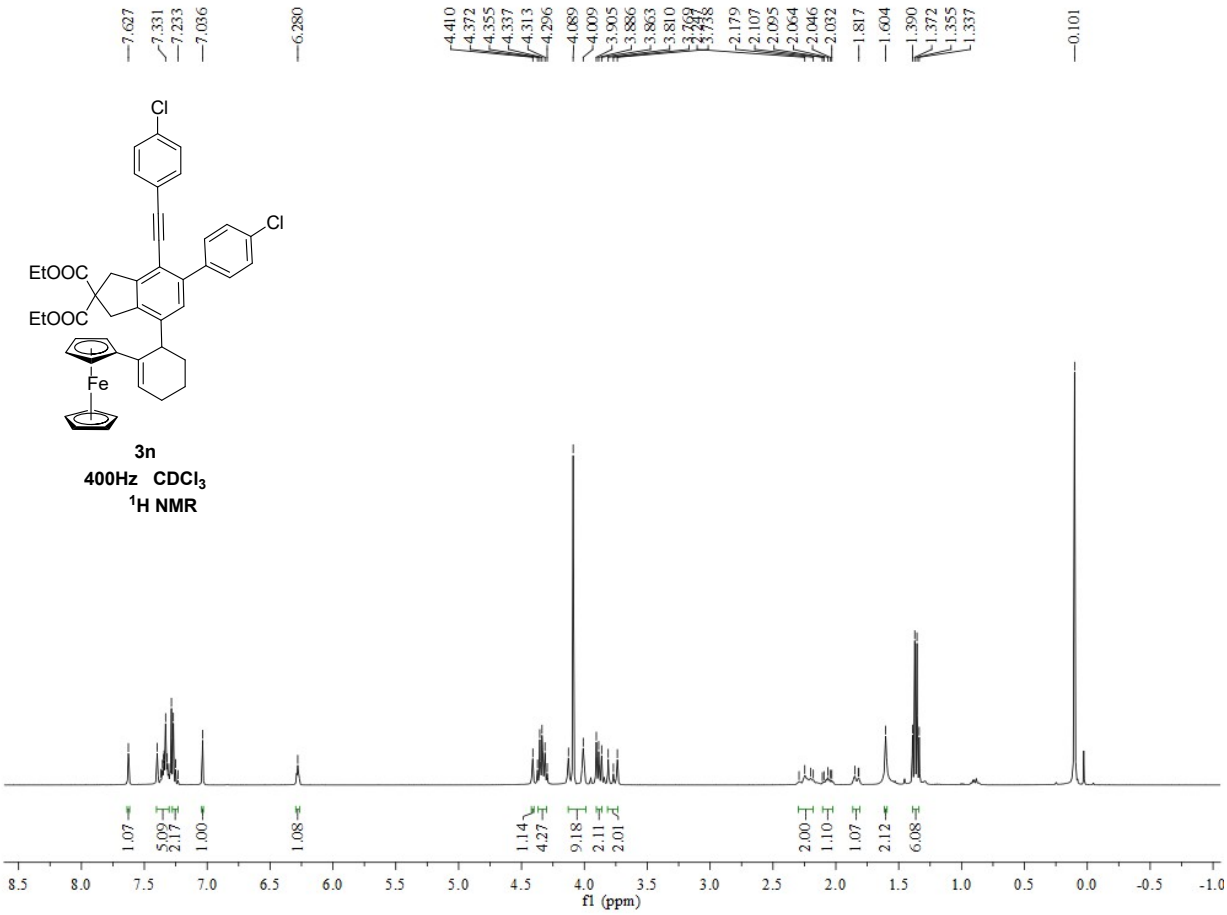






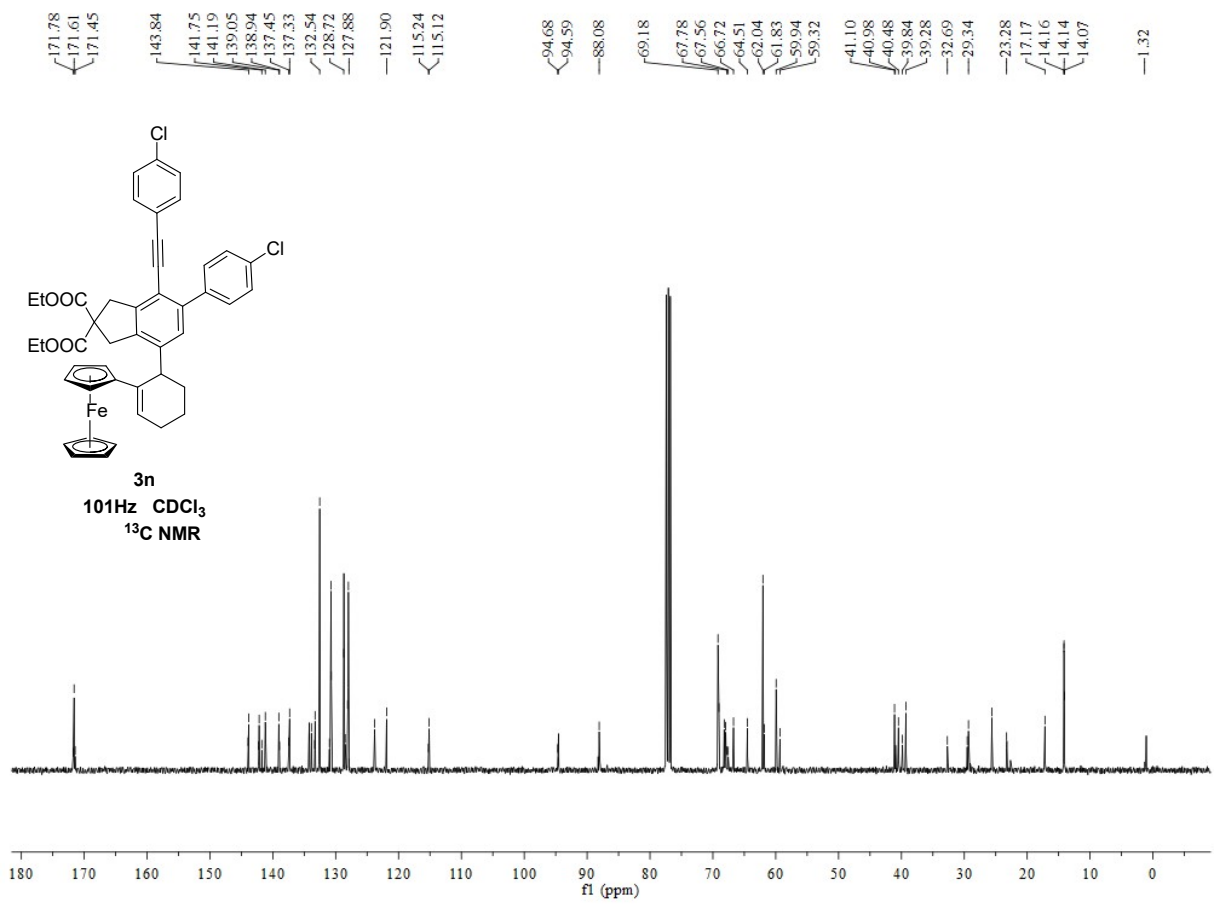
**3m**
**101Hz CDCl$_3$**
**$^{13}$C NMR**




**3n**

**400Hz $CDCl_3$**

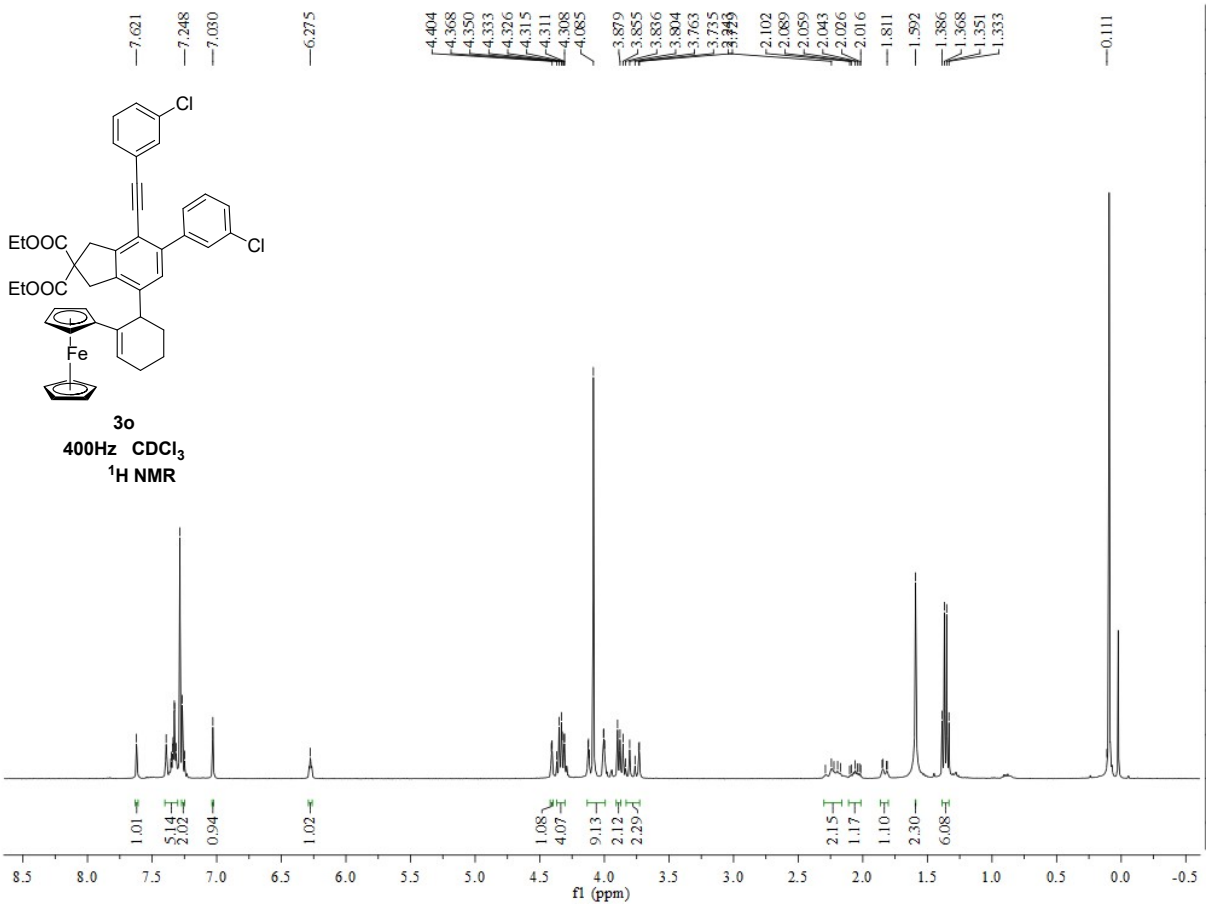
**$^1$H NMR**



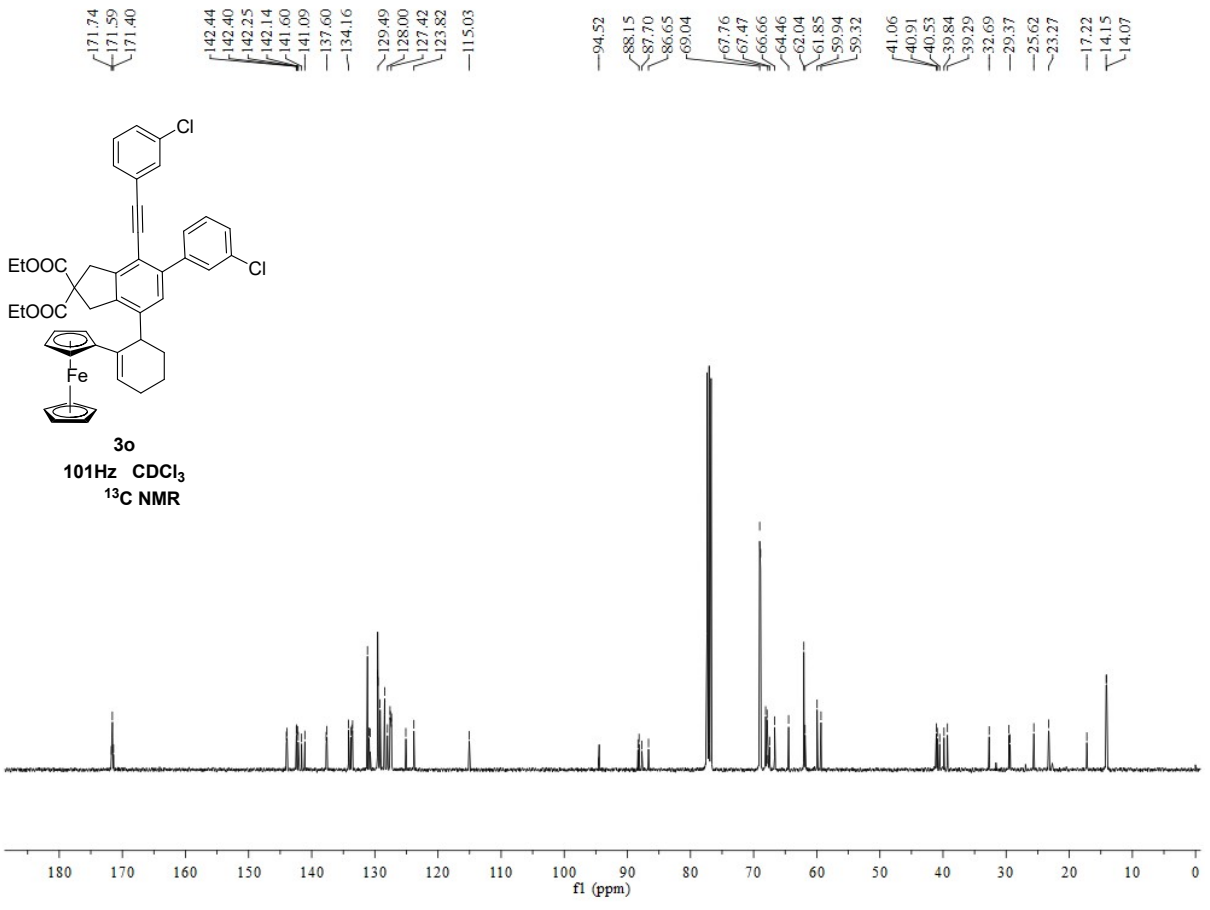

**3n**

**101Hz $CDCl_3$**

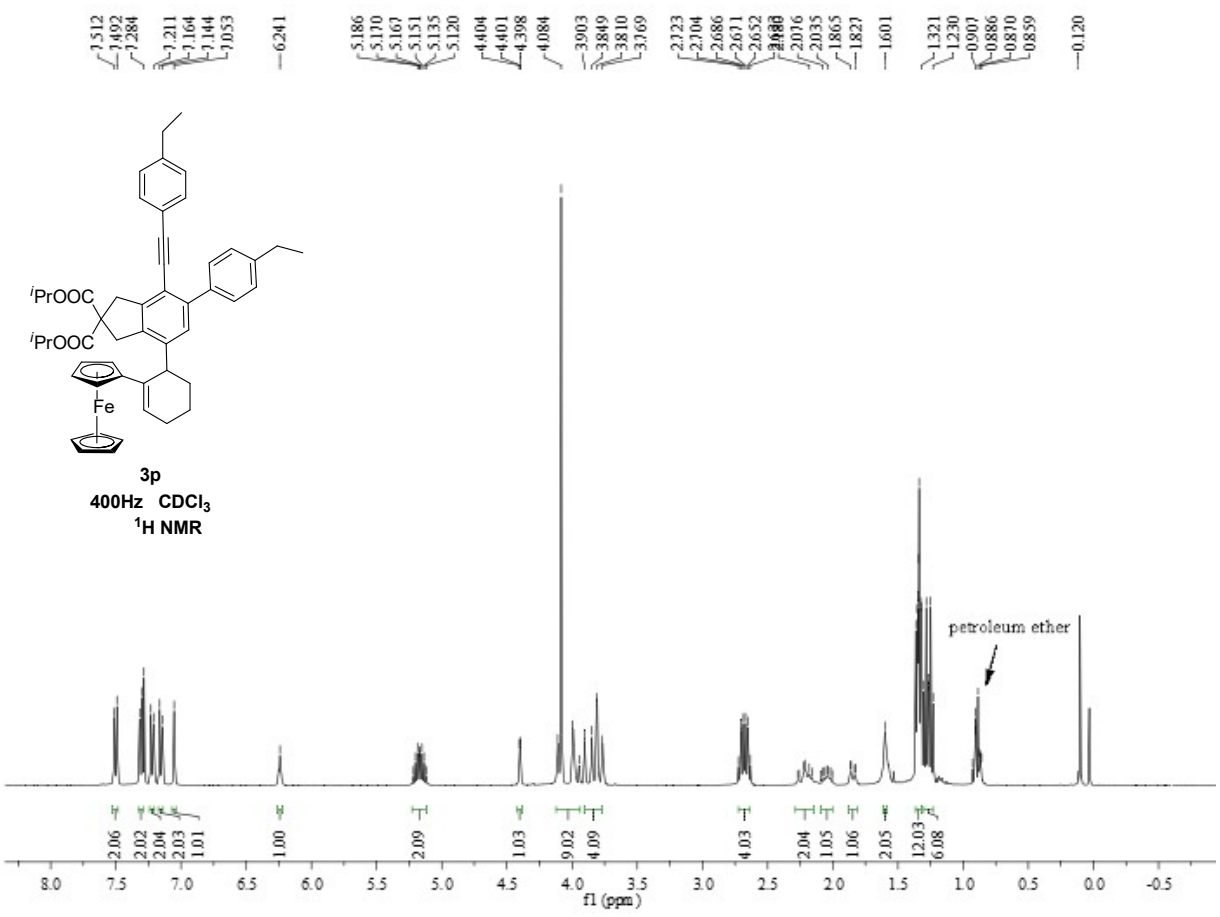
**$^{13}$C NMR**



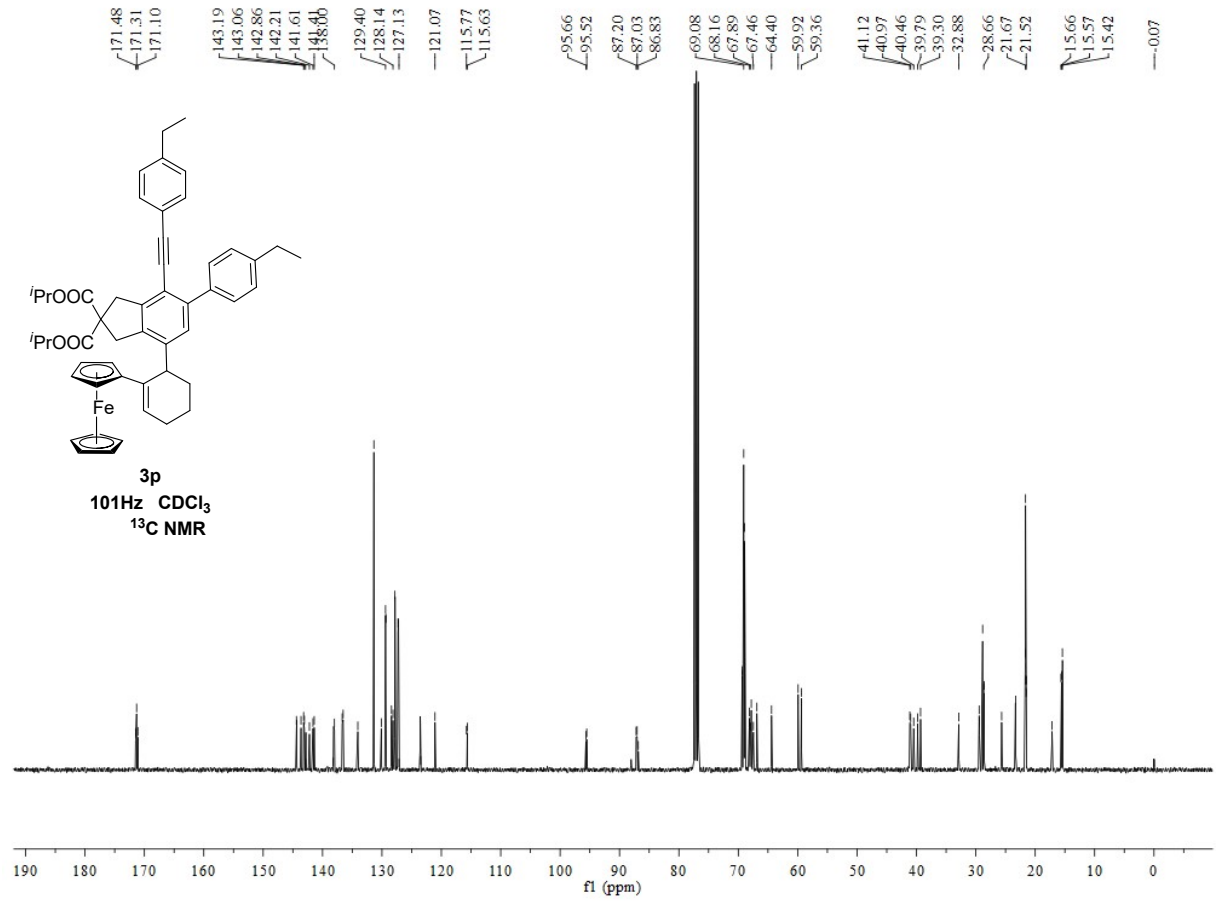

**3o**
**400Hz $CDCl_3$**
**$^{1}H$ NMR**



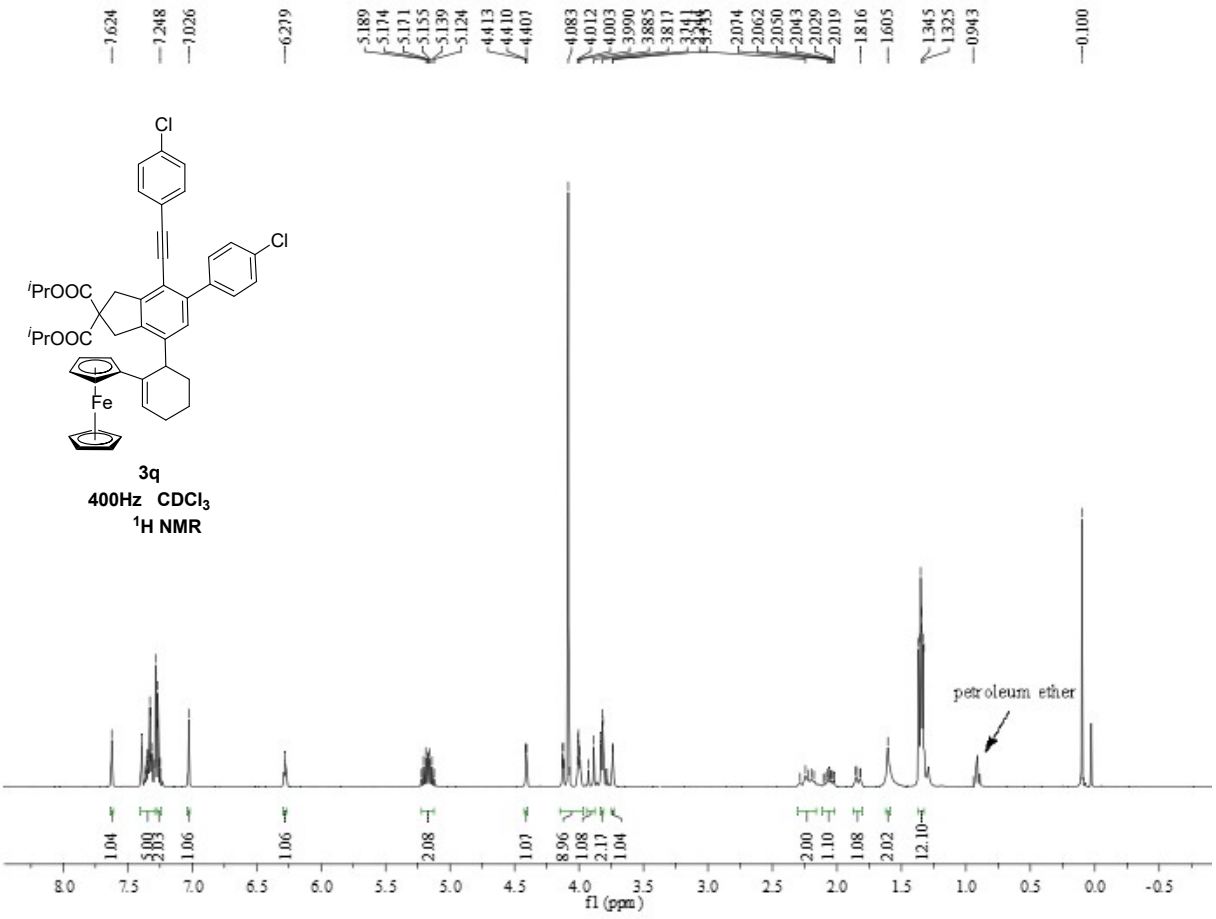

**3o**
**101Hz $CDCl_3$**
**$^{13}C$ NMR**



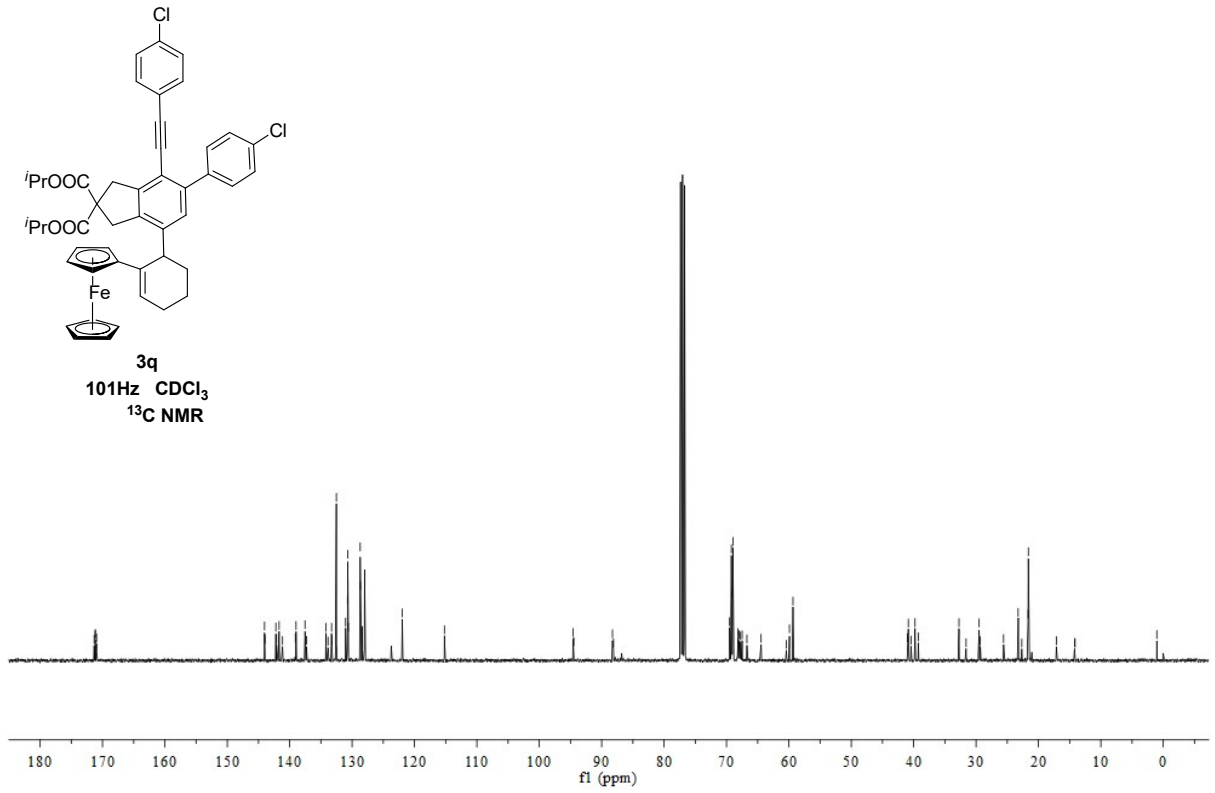

**3p**
**400Hz $CDCl_3$**
**$^1$H NMR**



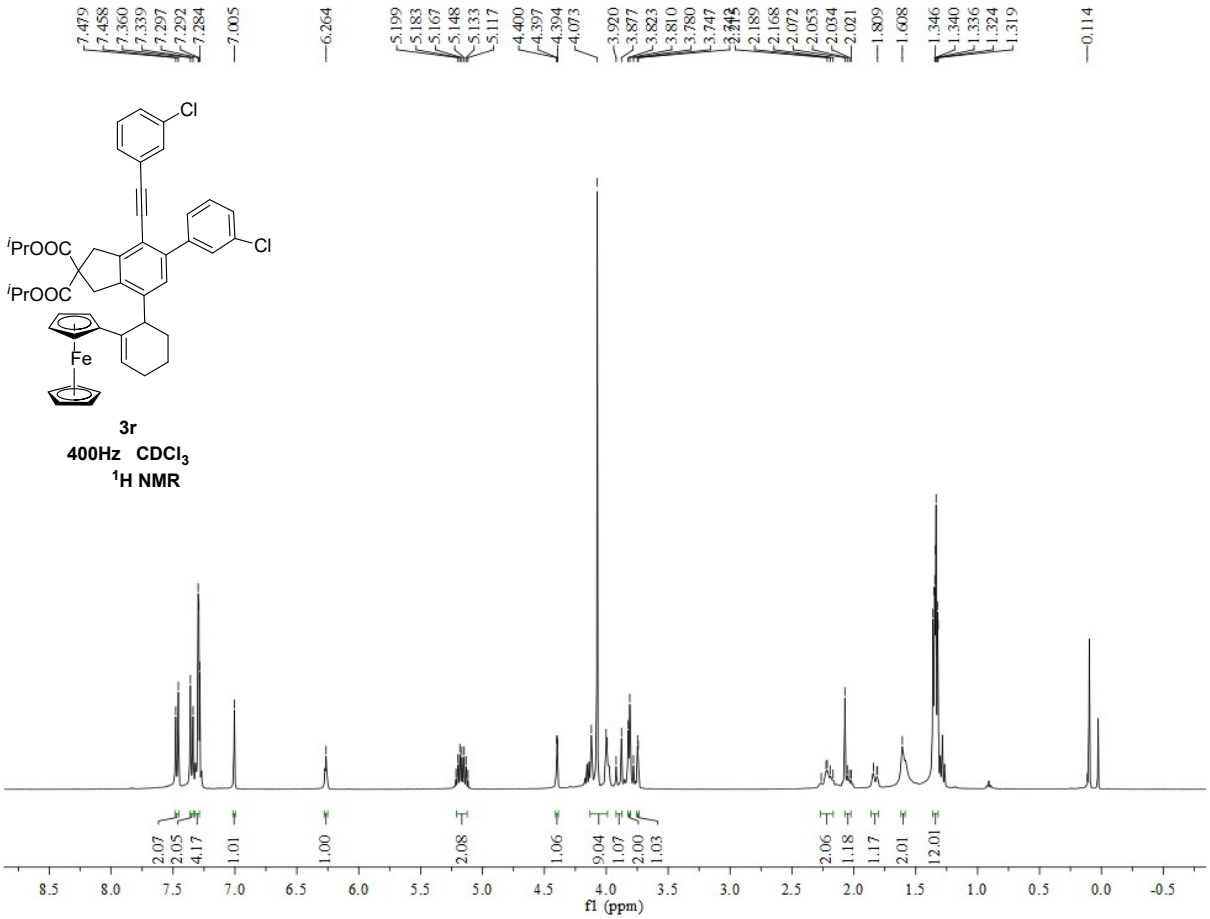

**3p**
**101Hz $CDCl_3$**
**$^{13}$C NMR**



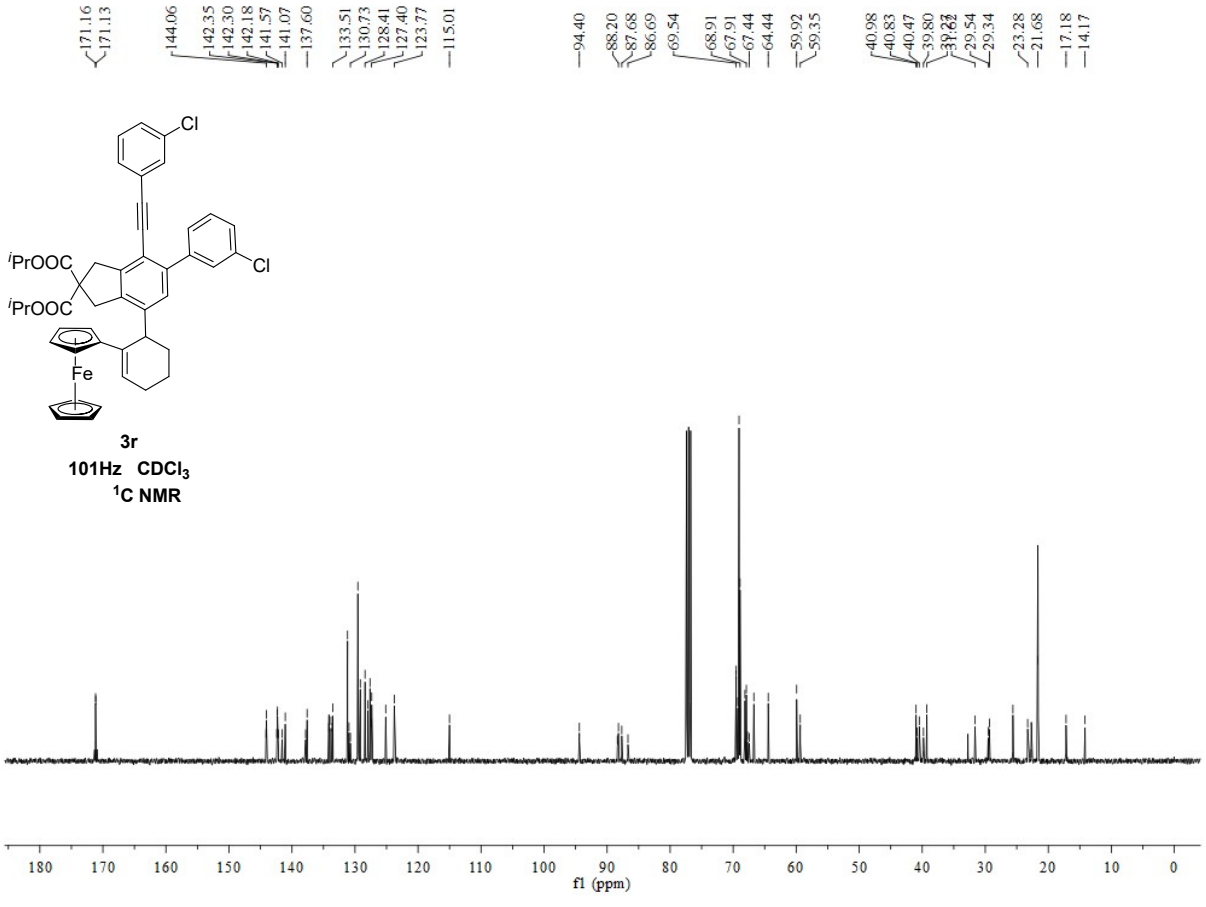

**3q**
**400Hz CDCl$_3$**
**$^1$H NMR**



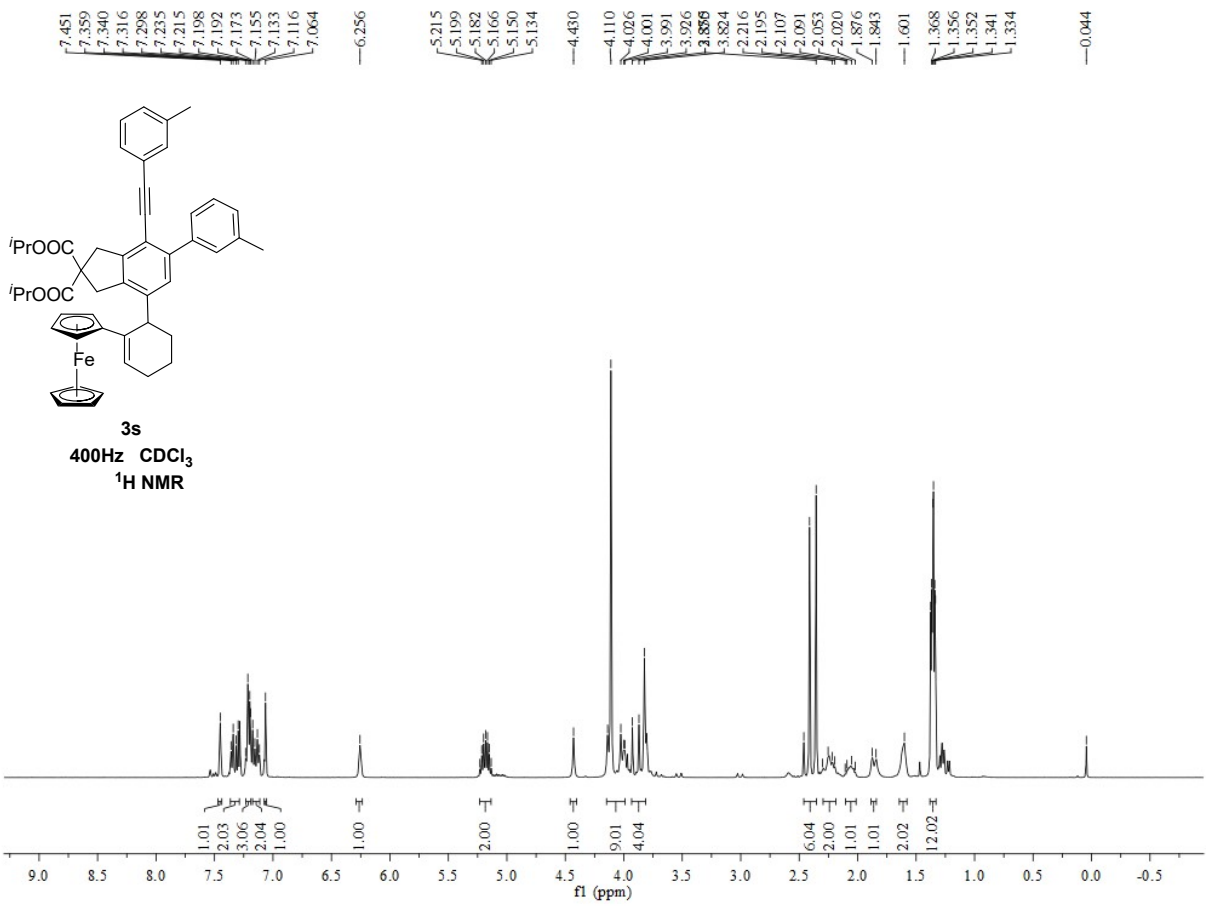

**3q**
**101Hz CDCl$_3$**
**$^{13}$C NMR**



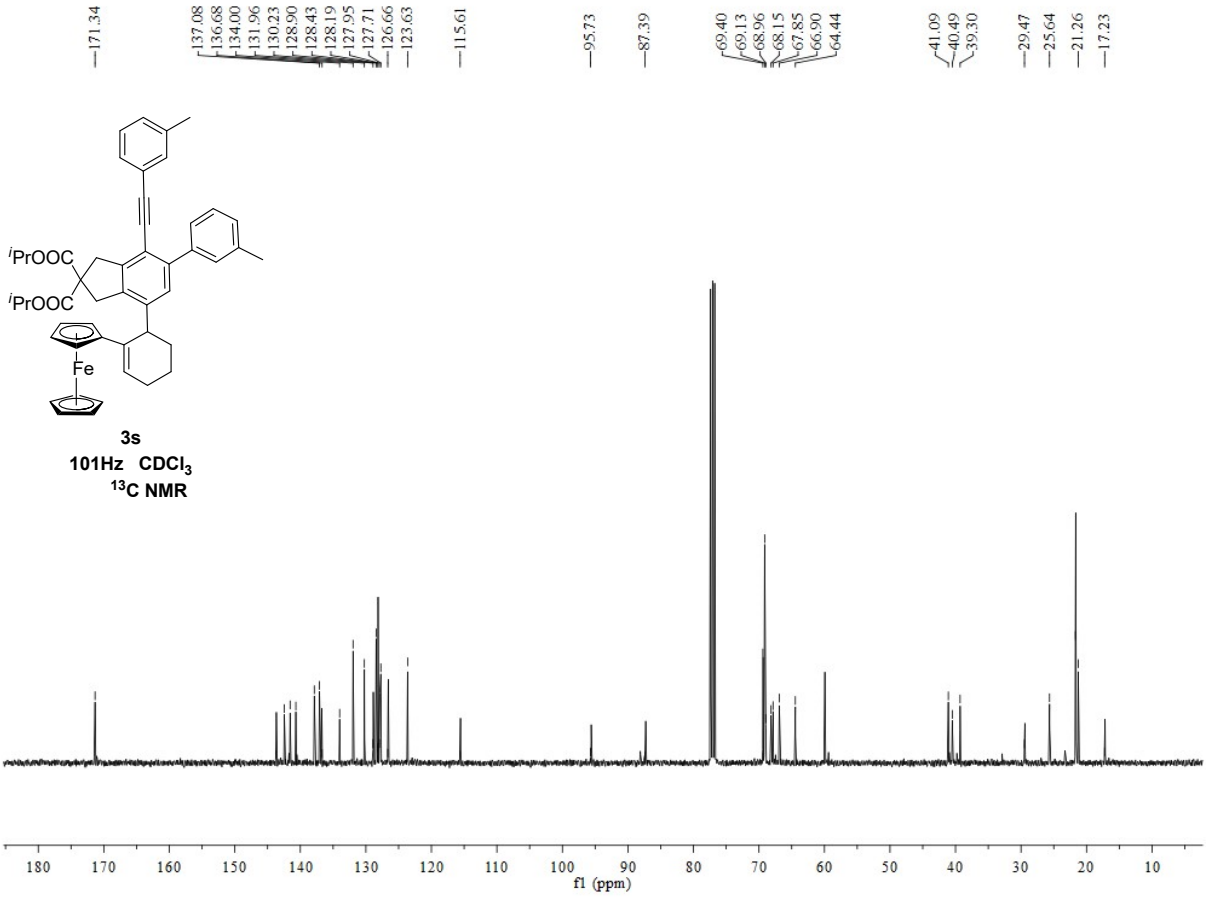

**3r**
**400Hz $CDCl_3$**
**$^1$H NMR**



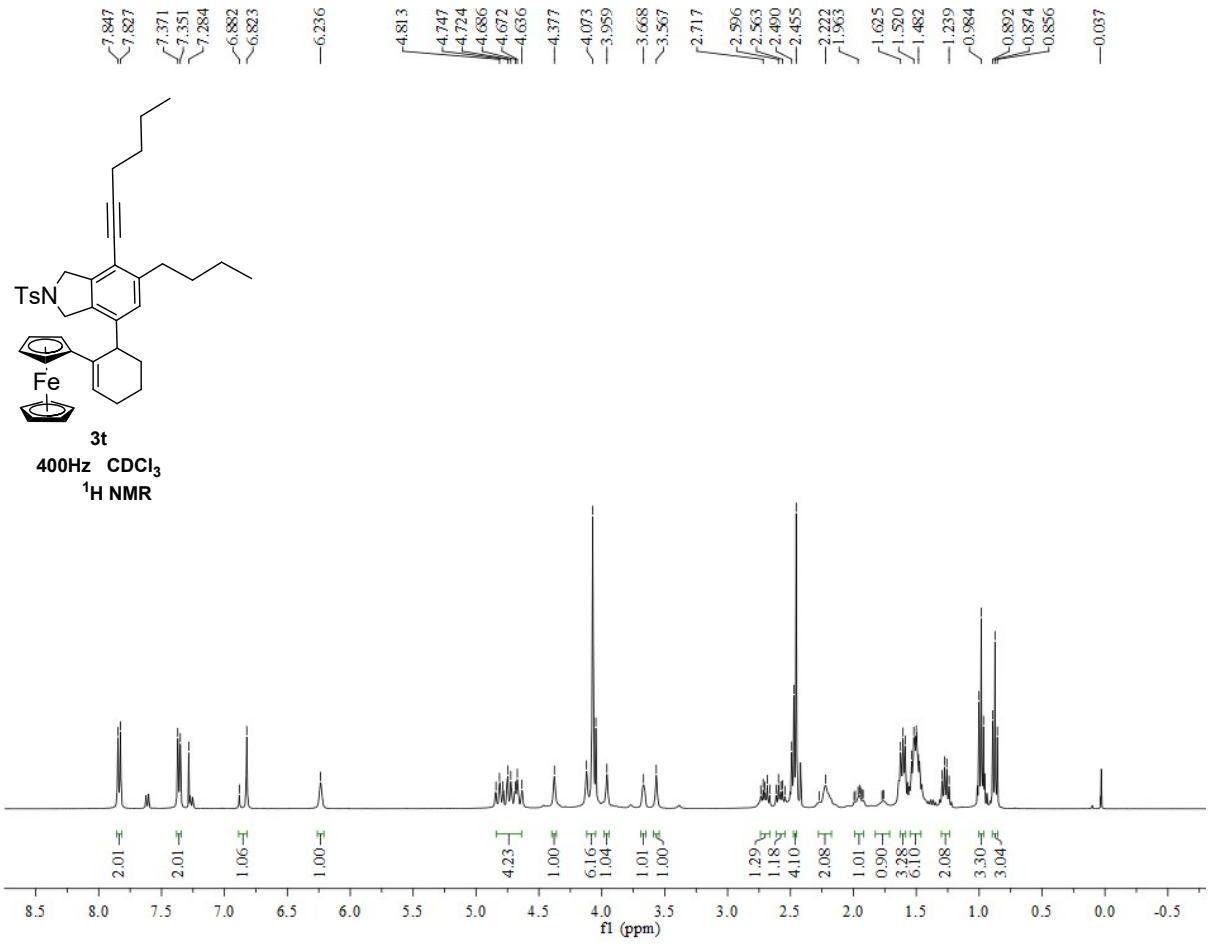

**3r**
**101Hz $CDCl_3$**
**$^1$C NMR**




**3s**
**400Hz $CDCl_3$**
**$^1$H NMR**



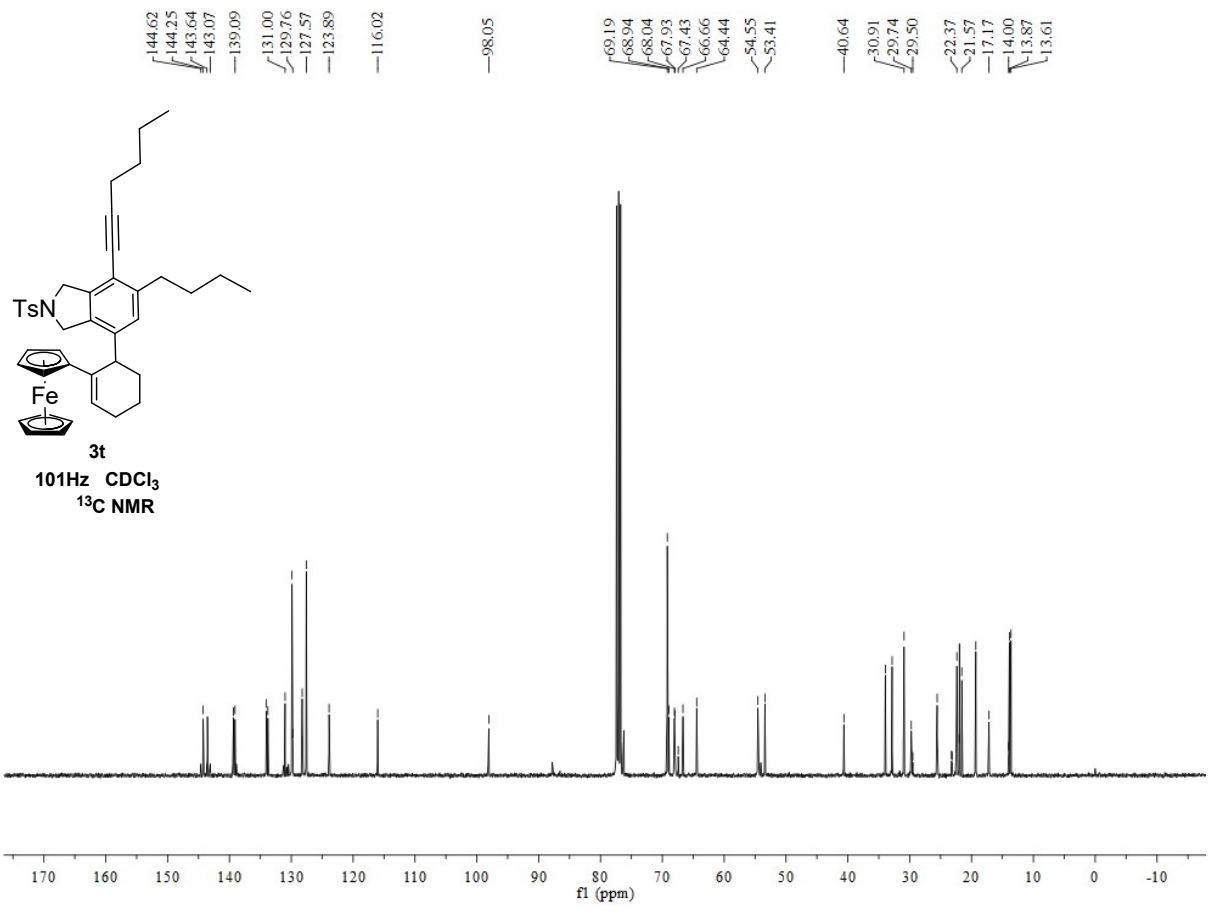

**3s**
**101Hz $CDCl_3$**
**$^{13}$C NMR**




**3t**

**400Hz $CDCl_3$**

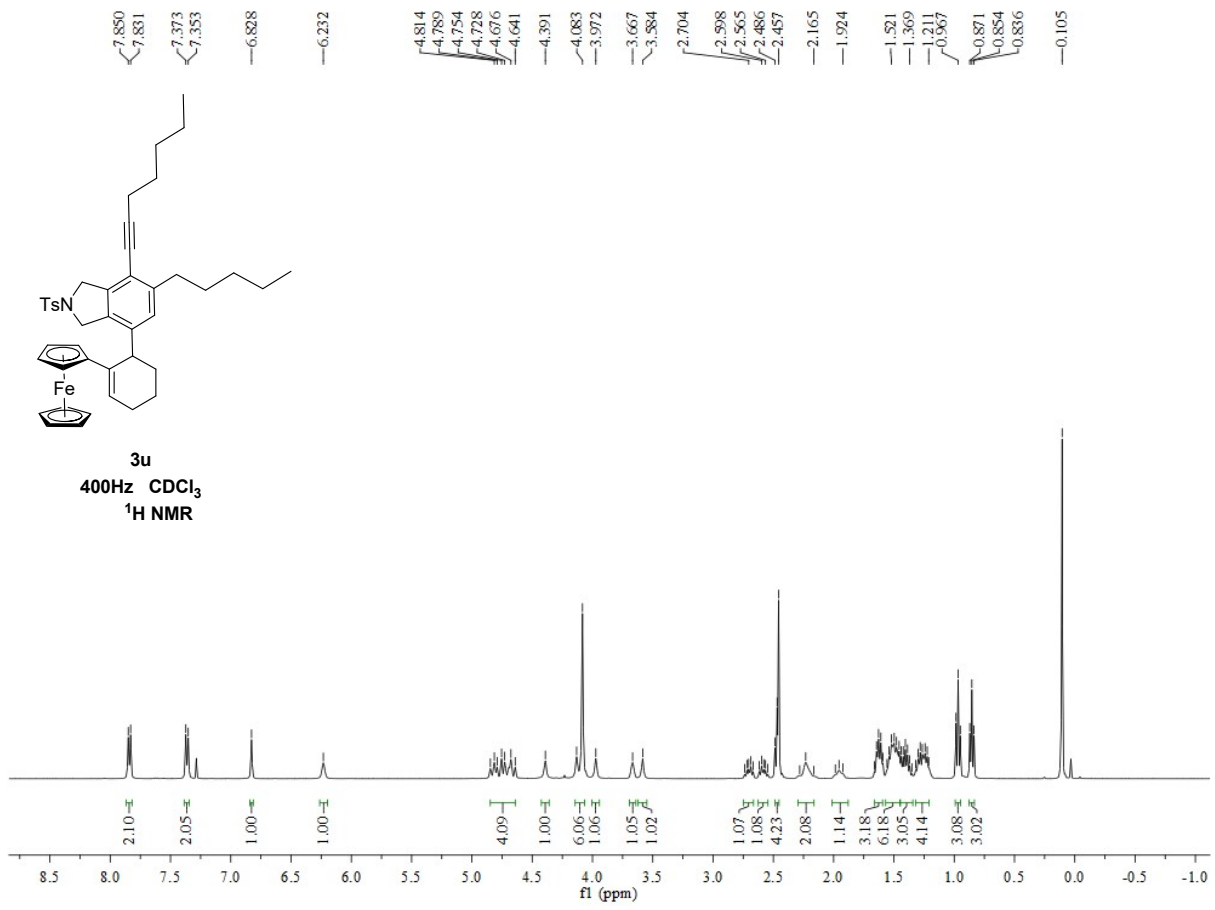
**$^{1}H$ NMR**



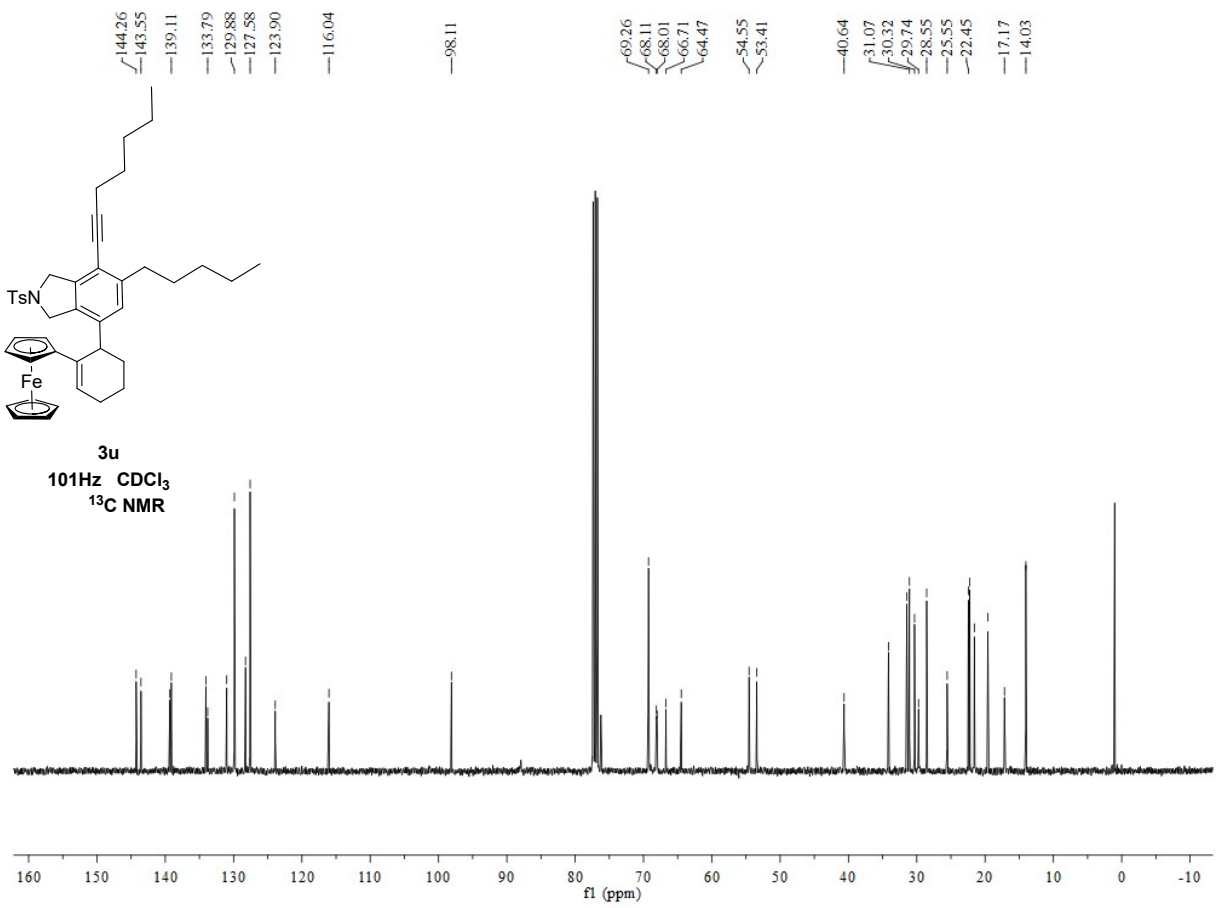

**3t**

**101Hz $CDCl_3$**

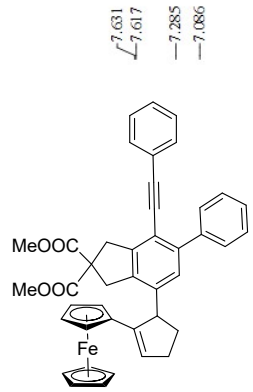
**$^{13}C$ NMR**




**3u**
**400Hz CDCl$_3$**
**$^1$H NMR**

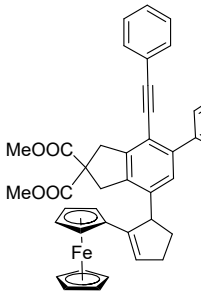



**3u**
**101Hz CDCl$_3$**
**$^{13}$C NMR**

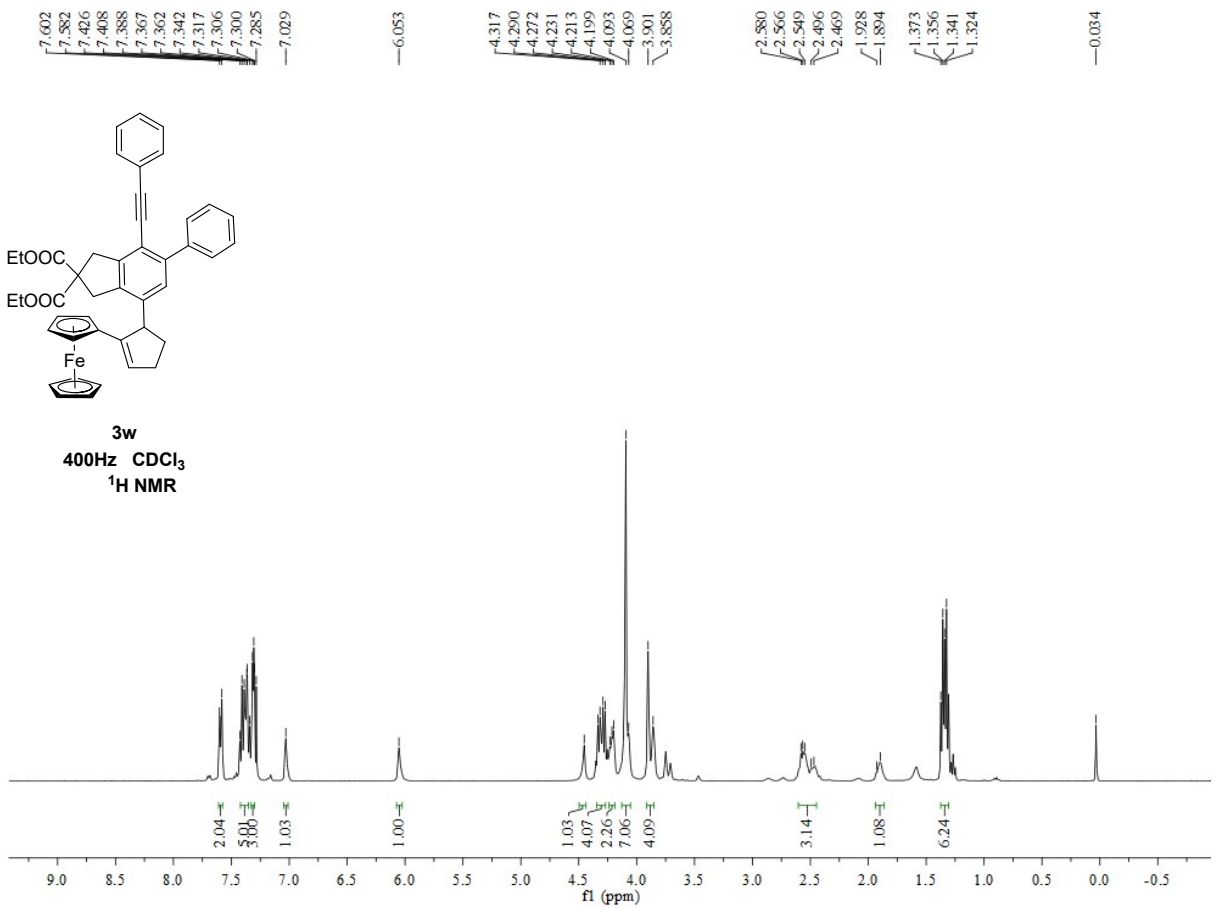



**3v**
**400Hz CDCl$_3$**
**$^1$H NMR**

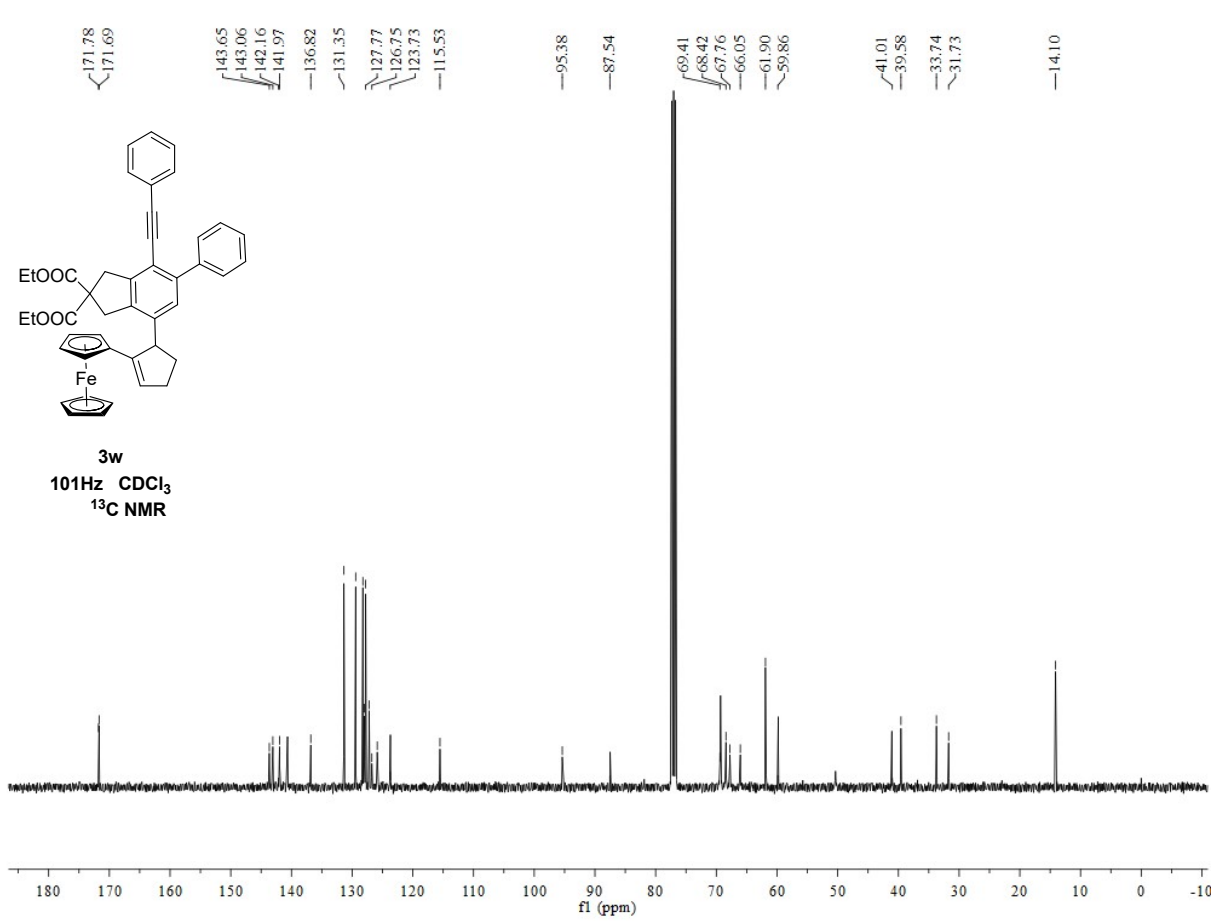


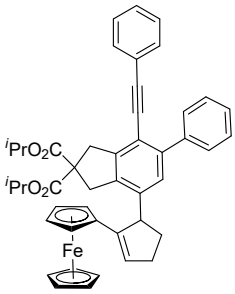

**3v**
**101Hz CDCl$_3$**
**13C NMR**



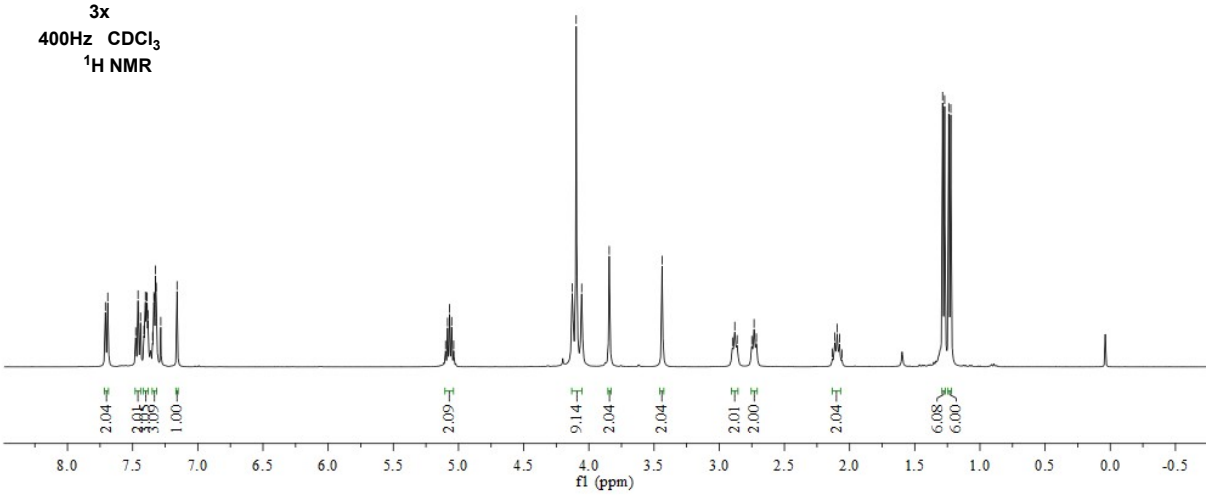

**3w**
**400Hz CDCl$_3$**
**$^1$H NMR**

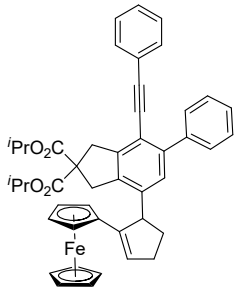



**3w**
**101Hz CDCl$_3$**
**$^{13}$C NMR**

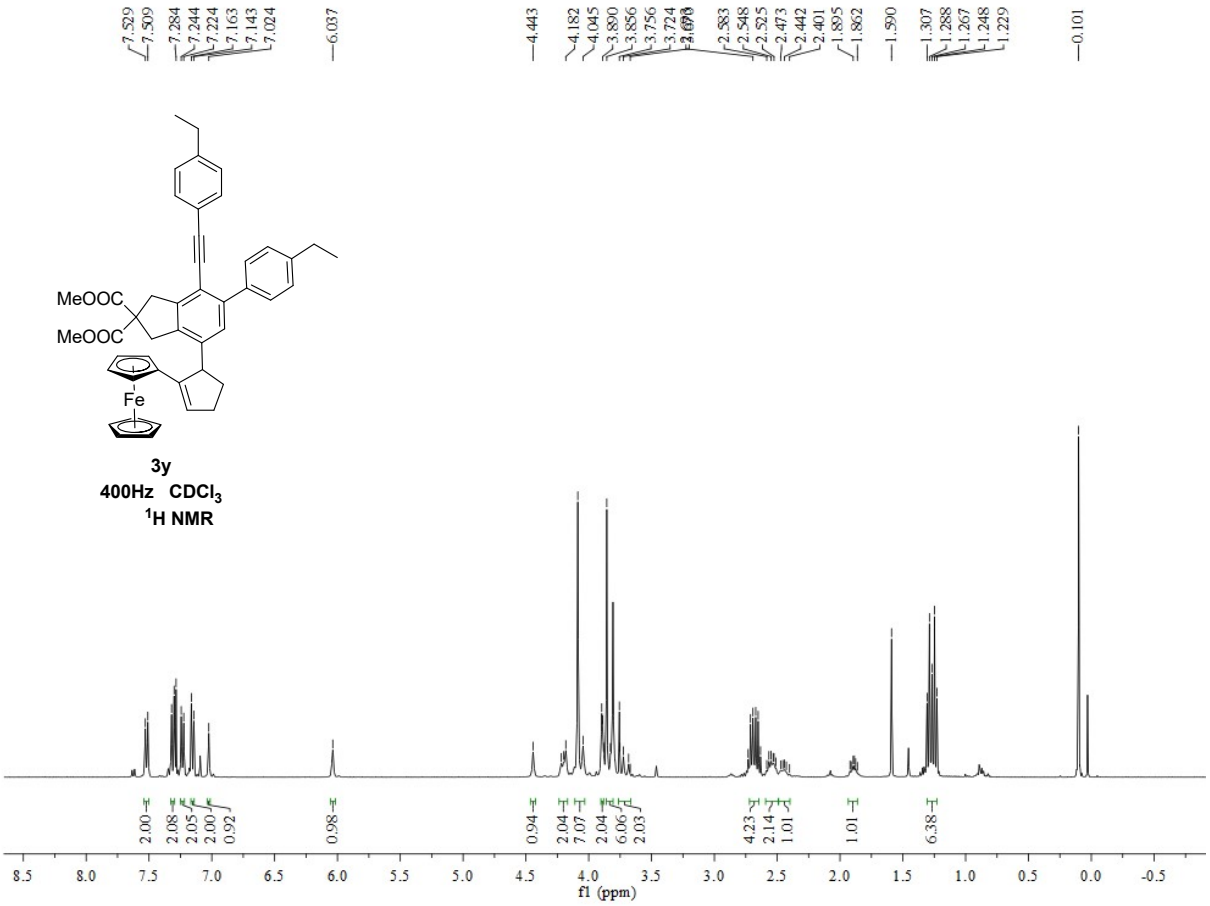


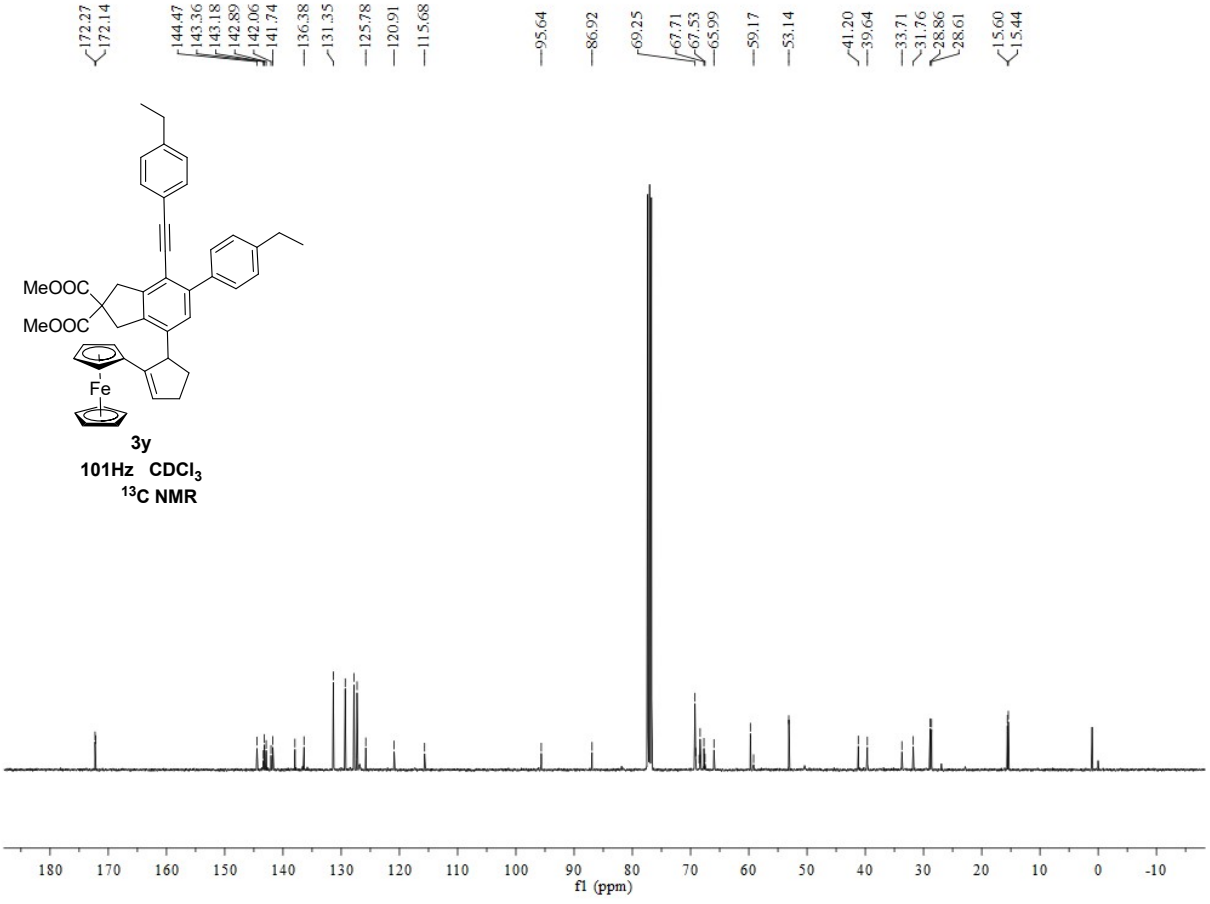

**3x**
**400Hz CDCl$_3$**
**$^1$H NMR**

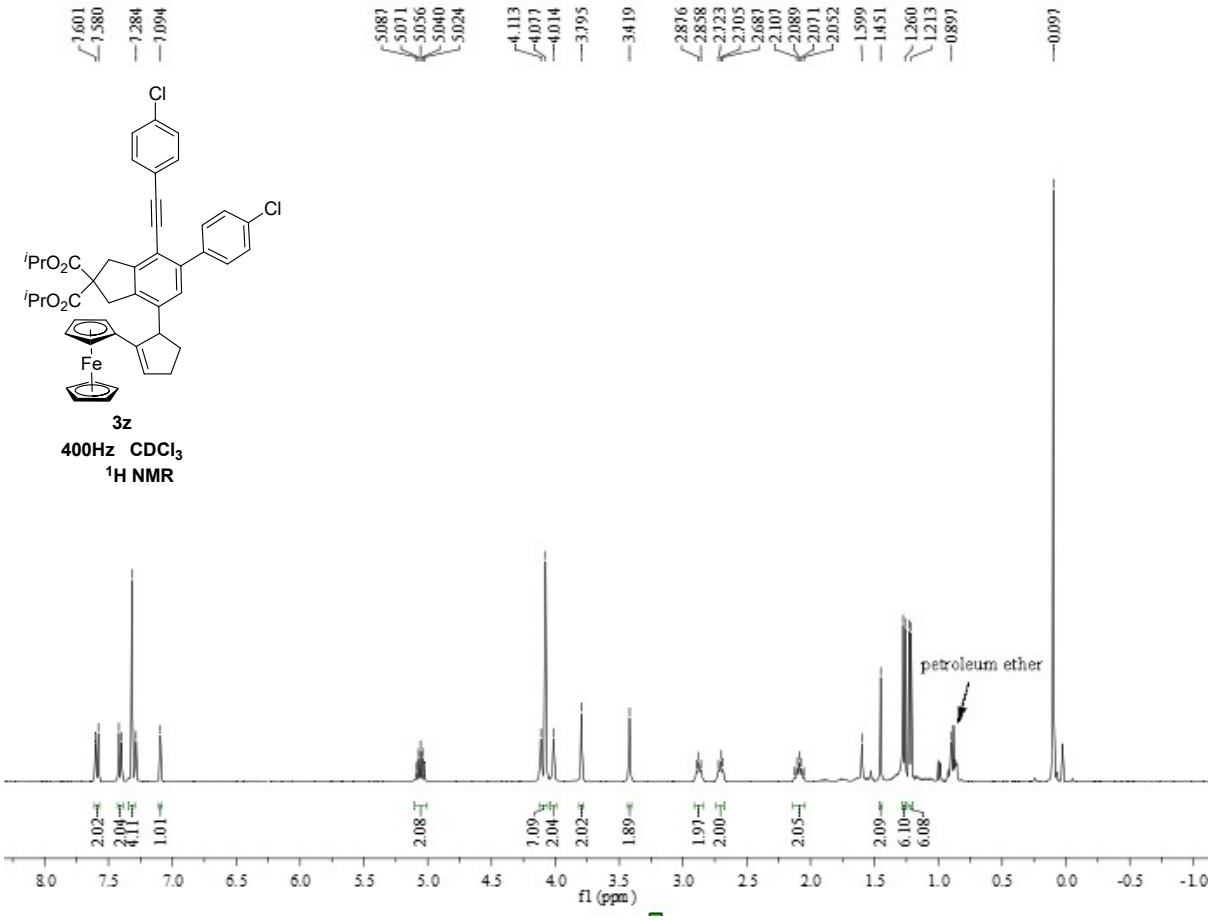



**3x**
**101Hz CDCl$_3$**
**$^{13}$C NMR**


MeOOC
MeOOC
Fe
3y
400Hz CDCl3
1H NMR
f1 (ppm)

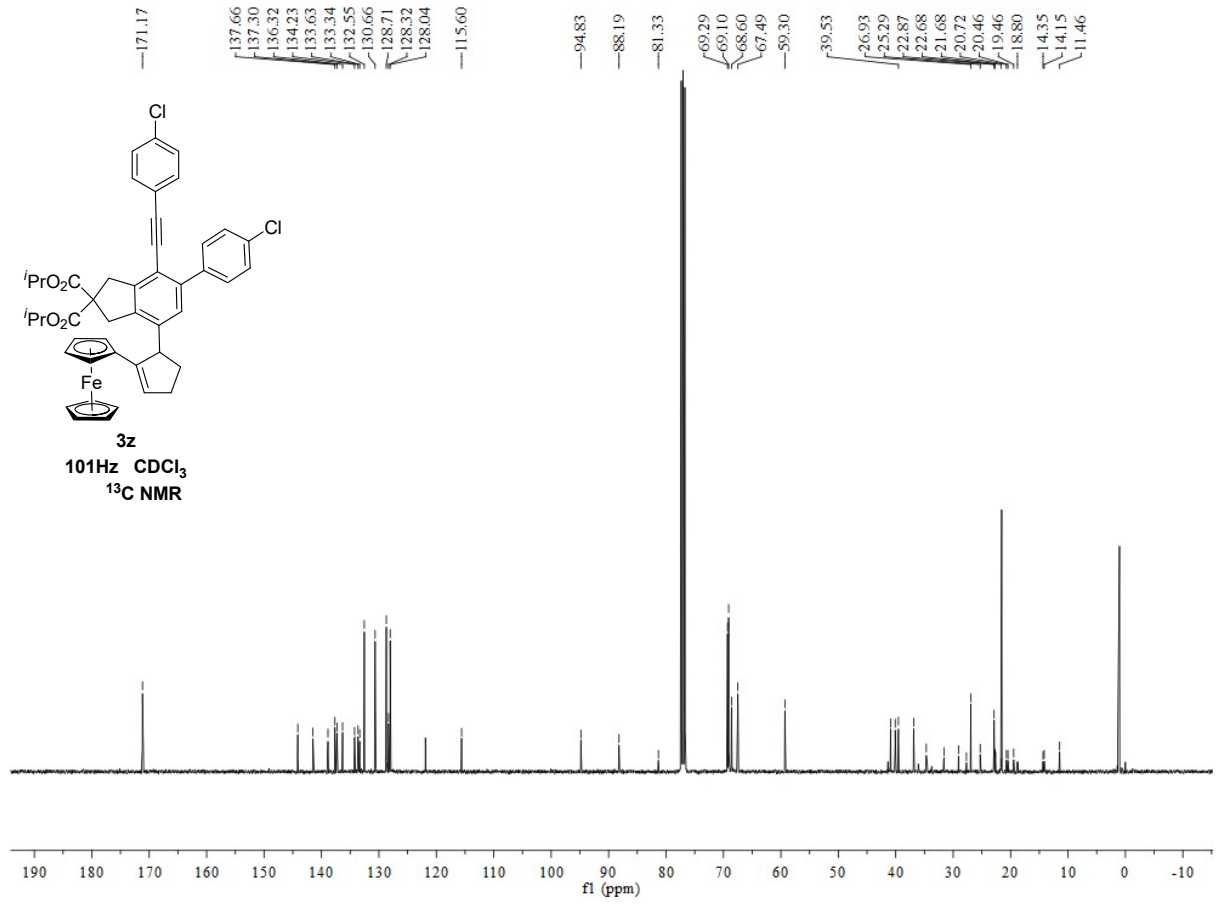

MeOOC
MeOOC
Fe
3y
101Hz CDCl3
13C NMR
f1 (ppm)




**3z**

**400Hz $CDCl_3$**

**$^{1}$H NMR**




**3z**

**101Hz $CDCl_3$**

**$^{13}$C NMR**

## 5. Computational Details

Geometry optimizations, frequency calculations and thermal corrections to the free energy were performed at B3LYP-D3(BJ) method for all of intermediates and transition states, D3 denoting Grimme's dispersion interaction correction, where the def2-SVP basis set was assigned to short-period elements and MDF10 was used for cobalt center.[1-6] All calculations were performed using the Gaussian 16 package.[7]

**References**


[1] A. D. Becke. *J. Chem. Phys.* **1993**, *98*, 5648-5652.

[2] C. Lee, W. Yang, R. G. Parr. *Phys. Rev. B* **1988**, *37*, 785-789.

[3] A. Schäfer, H. Horn, R. Ahlrichs. *J. Chem. Phys*. **1992**, *97*, 2571-2577.

[4] S. Grimme, J. Antony, S. Ehrlich, H. Krieg. *J. Chem. Phys.* **2010**, *132*, 154104.

[5] S. Grimme, S. Ehrlich, L. Goerigk. *J. Comput. Chem*. **2011**, *32*, 1456-1465.

[6] M. Dolg, U. Wedig, H. Stoll, H. Preuss. *J. Chem. Phys*. **1987**, *86*, 866−872.

[7] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A.V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Jr. Montgomery, J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, D. J. Fox. Gaussian 16, *Revision A.01*, *Gaussian, Inc*., Wallingford CT, 2016.

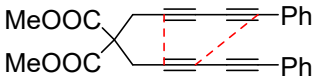

### Calculated Energy Values

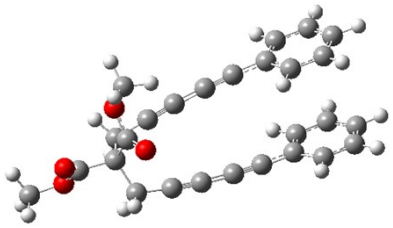
**Table S1**. Energies (in kcal/mol) calculated at B3LYP+D3(BJ)/6-311+G(2d,p)

| Species | $E_{ele}$ / A.U. | $G_{corr}$ / A.U. | *G*/A.U. | D*G*/(kcal/mol) |
|---|---|---|---|---|
| **1a (1v)** | -1340.747916 | 0.327409 | -1340.42 | |
| **2c** | -234.504282 | 0.117076 | -234.387 | |
| **INA** | -1340.810681 | 0.33369 | -1340.48 | -35.4449 |
| **2a** | -744.1037348 | 0.253898 | -743.85 | |
| **3a** | -2085.072543 | 0.615799 | -2084.46 | -116.968 |
| **TSC** | -1575.326153 | 0.472732 | -1574.85 | -28.6829 |
| **TSA** | -2084.930363 | 0.608793 | -2084.32 | -32.1455 |
| **3c** | -1575.469204 | 0.47848 | -1574.99 | -114.842 |

**Cartesian Coordinates for All Species**

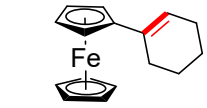
**1a (1v)**

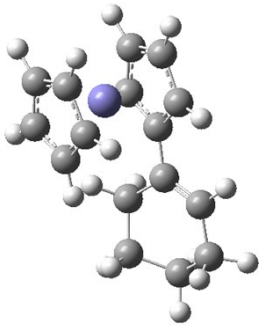




| Atomic Type | Coordinates(Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| C | -3.88156500 | 0.22659800 | 0.06130300 |
| C | -3.45352000 | 1.71145900 | -0.13080700 |
| H | -3.93136700 | 2.07879700 | -1.05345700 |
| H | -3.86669200 | 2.29199900 | 0.71020600 |
| C | -3.25452600 | -0.43441400 | 1.32752900 |
| H | -3.39630800 | 0.25070000 | 2.17839900 |
| H | -3.82708400 | -1.34665800 | 1.55976100 |
| C | -3.55199000 | -0.57295900 | -1.20656400 |
| O | -3.24051300 | -0.08669800 | -2.26113200 |
| O | -3.66763100 | -1.88600300 | -0.98187000 |
| C | -5.40865200 | 0.22194800 | 0.19776200 |
| O | -6.17748400 | -0.13207300 | -0.65889600 |
| O | -5.79038100 | 0.69957000 | 1.39243000 |
| C | -3.39444900 | -2.74151100 | -2.09215500 |
| H | -3.52648300 | -3.76669100 | -1.72686000 |
| H | -4.09079700 | -2.53282200 | -2.91754300 |
| H | -2.36484500 | -2.58978900 | -2.44790100 |
| C | -7.20002500 | 0.77394100 | 1.62337400 |
| H | -7.32169600 | 1.17835400 | 2.63499400 |
| H | -7.67794500 | 1.43322700 | 0.88400900 |
| H | -7.65599600 | -0.22413500 | 1.54923200 |
| C | -2.01728000 | 1.91944300 | -0.21284700 |
| C | -1.84955400 | -0.78937800 | 1.19037600 |
| C | -0.80504100 | 2.04366000 | -0.24427000 |
| C | -0.67588900 | -1.09053700 | 1.05270500 |
| C | 0.56016000 | 2.09245900 | -0.23910800 |
| C | 0.65050600 | -1.35967000 | 0.86219000 |
| C | 1.78279900 | 2.07443500 | -0.20811200 |
| C | 1.84058700 | -1.56489700 | 0.66738500 |
| C | 3.20178000 | 1.98851100 | -0.13470700 |
| C | 3.81760500 | 1.47661700 | 1.02796200 |
| C | 4.01204200 | 2.37590700 | -1.22253300 |
| C | 5.20242000 | 1.35316600 | 1.09403200 |
| H | 3.19037200 | 1.16074000 | 1.86242500 |
| C | 5.39797100 | 2.24955500 | -1.14573400 |
| H | 3.53893600 | 2.76987700 | -2.12381700 |
| C | 5.99675300 | 1.73717300 | 0.00937800 |
| H | 5.66528000 | 0.93766300 | 1.99141700 |
| H | 6.01611900 | 2.55012900 | -1.99512200 |
| H | 7.08260600 | 1.63021600 | 0.06195600 |
| C | 3.22825500 | -1.73824300 | 0.40108300 |
| C | 4.09204700 | -2.28893600 | 1.37017700 |
| C | 3.76500700 | -1.32097000 | -0.83607500 |
| C | 5.45550200 | -2.41206700 | 1.10677100 |
| H | 3.68040600 | -2.61031900 | 2.32863900 |
| C | 5.12761400 | -1.44819700 | -1.08877800 |
| H | 3.10058000 | -0.87929200 | -1.57957400 |
| C | 5.97755000 | -1.99300600 | -0.12064300 |
| H | 6.11633700 | -2.83782100 | 1.86570000 |
| H | 5.53258600 | -1.10687600 | -2.04366700 |
| H | 7.04740800 | -2.08621100 | -0.32122100 |

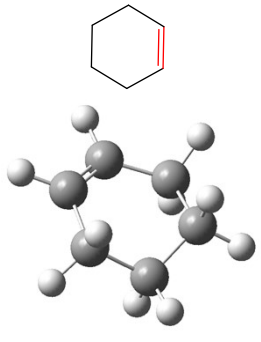
**2a**



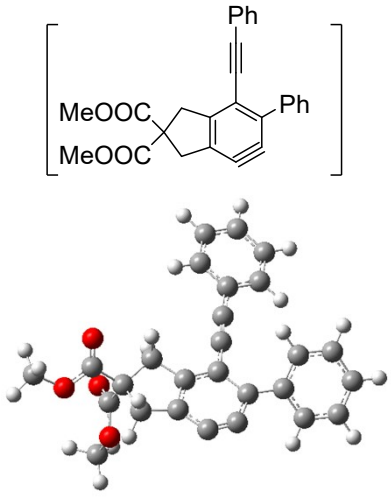
| Atomic Type | Coordinates(Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| C | -1.70322600 | 2.10804500 | 0.28279600 |
| C | -1.68062100 | 1.80304400 | -1.11157500 |
| C | -0.42749400 | 1.18843300 | -1.40614400 |
| C | 0.34342700 | 1.11285400 | -0.19483500 |
| C | -0.46547800 | 1.68100700 | 0.84767800 |
| H | -2.53377500 | 2.55332400 | 0.82751000 |
| H | -2.48682800 | 1.98166400 | -1.82059900 |
| H | -0.11496900 | 0.82461200 | -2.38221200 |
| H | -0.19497700 | 1.74143400 | 1.89944900 |
| Fe | -1.43744500 | 0.07892800 | -0.00118900 |
| C | -0.94011400 | -1.86444800 | 0.47154000 |
| C | -1.67626400 | -1.82756600 | -0.75282300 |
| C | -1.76048000 | -1.30201300 | 1.49630600 |
| H | 0.08163200 | -2.21897200 | 0.59607900 |
| C | -2.95185700 | -1.24267500 | -0.48402300 |
| H | -1.31837500 | -2.16131300 | -1.72529500 |
| C | -3.00386700 | -0.91756700 | 0.90606000 |
| H | -1.47566600 | -1.16290500 | 2.53764300 |
| H | -3.73548800 | -1.05289900 | -1.21534500 |
| H | -3.83428100 | -0.43642200 | 1.41976200 |
| C | 1.68464100 | 0.52010800 | -0.06342000 |
| C | 2.15607400 | -0.36786300 | -1.19766600 |
| C | 2.46631200 | 0.75912700 | 1.00799900 |
| C | 3.35679200 | -1.23526100 | -0.81315900 |
| H | 2.41291000 | 0.26602400 | -2.06716500 |
| H | 1.31978500 | -1.00309900 | -1.53155000 |
| C | 3.84613300 | 0.18992600 | 1.19901800 |
| C | 4.41868700 | -0.40643400 | -0.09019000 |
| H | 3.77757700 | -1.71795900 | -1.70995300 |
| H | 3.01883800 | -2.04926800 | -0.14632300 |
| H | 4.51840700 | 0.97175700 | 1.59382800 |
| H | 3.81259000 | -0.58656300 | 1.98922200 |
| H | 5.31045400 | -1.01456000 | 0.13178200 |
| H | 4.74981600 | 0.41127700 | -0.75498300 |
| H | 2.08994100 | 1.40944000 | 1.80368300 |

**2c**



| Atomic Type | Coordinates(Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| H | -1.88438700 | -0.08934300 | 1.13831000 |
| C | 0.66804400 | 1.30431500 | -0.05608300 |
| C | -0.66692900 | 1.30486400 | 0.05597600 |
| C | 1.49581100 | 0.04569400 | -0.11000400 |
| H | 1.20280400 | 2.25895700 | -0.11212500 |
| C | -1.49570300 | 0.04696400 | 0.11008600 |
| C | 0.69570900 | -1.19046100 | 0.31865700 |
| H | 2.39179700 | 0.16237800 | 0.52460700 |
| H | 1.88458900 | -0.09084900 | -1.13810000 |
| C | -0.69679500 | -1.18984000 | -0.31871000 |
| H | -2.39177600 | 0.16424500 | -0.52427900 |
| H | 1.24438900 | -2.11002800 | 0.05827100 |
| H | 0.58716800 | -1.18817700 | 1.41806700 |
| H | -1.24636100 | -2.10891500 | -0.05844100 |
| H | -0.58826400 | -1.18748100 | -1.41812000 |
| H | -1.20077900 | 2.25999400 | 0.11227800 |

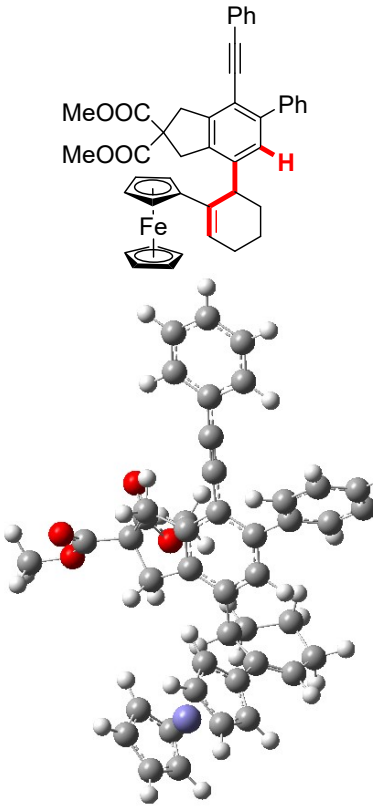
**INA**




| Atomic Type | Coordinates(Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| C | 3.08772900 | -0.00275900 | -0.30320200 |
| C | 3.12230200 | -1.48854500 | -0.77431000 |
| C | 1.68733200 | -1.90566400 | -0.61862500 |
| C | 0.82859700 | -0.78764000 | -0.52702700 |
| C | 1.64347000 | 0.47865300 | -0.60802500 |
| C | 4.13628400 | 0.81826100 | -1.05040700 |
| C | 3.34398800 | 0.16537000 | 1.20160700 |
| O | 3.16940500 | 1.21010500 | 1.77826600 |
| O | 3.92813300 | 1.50858900 | -2.01418900 |
| C | 0.97779400 | -3.09665300 | -0.58160100 |
| C | -0.26529000 | -3.18420100 | -0.44918000 |
| C | -1.23302000 | -2.18885000 | -0.37903600 |
| C | -0.58257000 | -0.89403500 | -0.40423100 |
| C | -2.68223200 | -2.43062200 | -0.25118200 |
| C | -1.32939800 | 0.30684900 | -0.24922800 |
| C | -1.94991400 | 1.34509400 | -0.09711100 |
| C | -2.74706700 | 2.51396800 | 0.07012900 |
| C | -2.18395200 | 3.80265900 | -0.03897600 |
| C | -2.98230500 | 4.93381300 | 0.12034900 |
| C | -4.34858000 | 4.80194100 | 0.38997000 |
| C | -4.91597400 | 3.52800200 | 0.50148000 |
| C | -4.12649300 | 2.39056500 | 0.34500500 |
| C | -3.11813200 | -3.58705300 | 0.42320700 |
| C | -4.47632100 | -3.86735600 | 0.56235300 |
| C | -5.43048500 | -3.00160500 | 0.01865100 |
| C | -5.01104400 | -1.86183700 | -0.67290300 |
| C | -3.65142900 | -1.57662800 | -0.80845400 |

| | | | |
|---|---|---|---|
| O | 3.76906500 | -0.95024100 | 1.80446600 |
| C | 4.02775300 | -0.84605000 | 3.20532600 |
| O | 5.35367900 | 0.62545900 | -0.51761600 |
| C | 6.43649800 | 1.32072000 | -1.13840200 |
| H | 3.83025400 | -2.09278600 | -0.19678700 |
| H | 3.41670100 | -1.53942500 | -1.83753600 |
| H | 1.32191700 | 1.26171200 | 0.09124000 |
| H | 1.60865000 | 0.90819300 | -1.62238400 |
| H | -1.11744200 | 3.90103800 | -0.24961900 |
| H | -2.53554000 | 5.92711000 | 0.03396900 |
| H | -4.97048600 | 5.69145100 | 0.51469200 |
| H | -5.98232100 | 3.42112700 | 0.71444700 |
| H | -4.56137900 | 1.39320300 | 0.43537300 |
| H | -2.37176500 | -4.26169800 | 0.84961800 |
| H | -4.79242000 | -4.76543300 | 1.09842000 |
| H | -6.49571700 | -3.21957900 | 0.12595000 |
| H | -5.74815400 | -1.19077000 | -1.12078400 |
| H | -3.33999500 | -0.69607900 | -1.36793700 |
| H | 4.33349300 | -1.84632500 | 3.53404500 |
| H | 4.82838900 | -0.11584700 | 3.39512300 |
| H | 3.12400500 | -0.52211400 | 3.74185500 |
| H | 7.33601900 | 1.05235600 | -0.57196100 |
| H | 6.53958000 | 1.01705500 | -2.19074200 |
| H | 6.26871800 | 2.40714700 | -1.10145700 |

**3a**

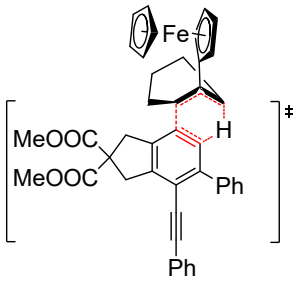


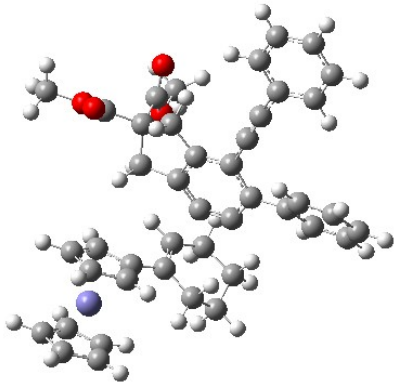

| Atomic Type | Coordinates(Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| C | -0.55266700 | 3.12577500 | 0.12002500 |
| C | 0.67816300 | 2.17752300 | 0.17235100 |
| C | 0.04106900 | 0.81855500 | 0.34618400 |
| C | -1.29704200 | 0.86140300 | -0.05127500 |
| C | -1.67940300 | 2.25133500 | -0.49021800 |
| C | -0.24524200 | 4.35878600 | -0.72271900 |
| C | -1.00925400 | 3.59547900 | 1.50689500 |
| O | -2.00548800 | 4.25197700 | 1.67917100 |
| O | -0.56756200 | 4.52256600 | -1.87088200 |
| C | 0.62427000 | -0.36698600 | 0.80579300 |

| | | | |
|---|---|---|---|
| C | -0.18325700 | -1.51182300 | 0.83797300 |
| C | -1.52737400 | -1.50599700 | 0.43713000 |
| C | -2.10959500 | -0.28604100 | -0.01479400 |
| C | -2.31312900 | -2.76387500 | 0.51526500 |
| C | -3.48143100 | -0.19297100 | -0.38167600 |
| C | -4.65886100 | -0.11745100 | -0.68719900 |
| C | -6.03861500 | -0.12183600 | -1.04202800 |
| C | -6.67871800 | 1.04447500 | -1.51063100 |
| C | -8.02825500 | 1.01458400 | -1.85775600 |
| C | -8.76069800 | -0.17178800 | -1.74475700 |
| C | -8.13481500 | -1.33373500 | -1.28027500 |
| C | -6.78635000 | -1.31453000 | -0.92985500 |
| C | -2.26026700 | -3.55827300 | 1.67391300 |
| C | -2.98563500 | -4.74793400 | 1.76236200 |
| C | -3.77556500 | -5.16946300 | 0.68977600 |
| C | -3.82946300 | -4.39385800 | -0.47253800 |
| C | -3.10685800 | -3.20312400 | -0.55919200 |
| O | -0.21162100 | 3.18918800 | 2.50536300 |
| C | -0.60834400 | 3.57776100 | 3.82131300 |
| O | 0.50137900 | 5.23064300 | -0.02432400 |
| C | 0.88402500 | 6.42689500 | -0.70464100 |
| H | 1.38189300 | 2.46246100 | 0.96113200 |
| H | 1.21822600 | 2.21852600 | -0.79133900 |
| H | -2.67624700 | 2.56923400 | -0.15675400 |
| H | -1.65740900 | 2.34670200 | -1.58834600 |
| H | -6.10365900 | 1.96825400 | -1.59733000 |
| H | -8.51366000 | 1.92427400 | -2.21929700 |
| H | -9.81849100 | -0.19056500 | -2.01748900 |
| H | -8.70393300 | -2.26210900 | -1.18932200 |
| H | -6.29076200 | -2.21637600 | -0.56497400 |
| H | -1.65859200 | -3.22417200 | 2.52214800 |
| H | -2.93830700 | -5.34493800 | 2.67642500 |
| H | -4.34453300 | -6.09983400 | 0.75752400 |
| H | -4.43353600 | -4.72148200 | -1.32235800 |
| H | -3.14672500 | -2.61121300 | -1.47411400 |
| H | 0.12728800 | 3.13585500 | 4.50387400 |
| H | -0.61202100 | 4.67376900 | 3.91455000 |
| H | -1.61771400 | 3.20357200 | 4.04636900 |
| H | 1.47406600 | 7.01038500 | 0.01195000 |
| H | 1.48466000 | 6.19134900 | -1.59580200 |
| H | -0.00518600 | 6.99215700 | -1.02036500 |
| H | 0.25928200 | -2.45563500 | 1.15937500 |
| C | 2.06375800 | -0.36755300 | 1.29336400 |
| C | 2.77382100 | -1.68945800 | 1.06138700 |
| C | 2.14214700 | 0.06434700 | 2.77502800 |
| H | 2.59916000 | 0.38772400 | 0.70019300 |
| C | 3.16572700 | -1.99340400 | -0.32543200 |
| C | 3.03832300 | -2.53286300 | 2.07774100 |
| C | 1.75204300 | -1.08192400 | 3.70492800 |
| H | 1.49450500 | 0.94013800 | 2.93457400 |
| H | 3.17754200 | 0.38001000 | 2.99482800 |
| C | 2.57880000 | -1.43860000 | -1.51551800 |
| C | 4.23570200 | -2.85221200 | -0.74941100 |
| C | 2.69837800 | -2.27183100 | 3.51959200 |
| H | 3.55234500 | -3.47431800 | 1.85945600 |
| H | 1.75708200 | -0.75017400 | 4.75549400 |
| H | 0.71752700 | -1.39041800 | 3.47915200 |
| C | 3.27065600 | -1.96107300 | -2.64733600 |
| H | 1.74657800 | -0.74059400 | -1.54642400 |
| C | 4.29609400 | -2.83400700 | -2.17395500 |
| H | 4.91357500 | -3.39080400 | -0.09081900 |
| H | 2.26721500 | -3.18290000 | 3.97043300 |
| H | 3.63950900 | -2.09414900 | 4.07708200 |
| H | 3.06806600 | -1.71399900 | -3.68772500 |
| Fe | 4.56716500 | -0.93091900 | -1.41494700 |
| H | 5.02153500 | -3.36282900 | -2.78940500 |
| C | 5.31722300 | 0.68463700 | -2.46256000 |

| | | | |
|---|---|---|---|
| C | 4.69316600 | 1.12259200 | -1.25404300 |
| C | 6.37392700 | -0.21094100 | -2.11377800 |
| H | 5.02073400 | 0.96271400 | -3.47231400 |
| C | 5.36519900 | 0.49732100 | -0.15842200 |
| H | 3.83969600 | 1.79463700 | -1.18317900 |
| C | 6.40292700 | -0.32716200 | -0.69004000 |
| H | 7.02409200 | -0.73543300 | -2.81172100 |
| H | 5.11066700 | 0.60036300 | 0.89503700 |
| H | 7.07810300 | -0.95580600 | -0.11232900 |

**TSA**



| Atomic Type | Coordinates(Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
| C | -0.70503200 | 2.96442100 | 0.43917300 |
| C | 0.51152900 | 1.99775200 | 0.53283200 |
| C | -0.15045000 | 0.65025500 | 0.59940000 |
| C | -1.48134500 | 0.71297000 | 0.14065700 |
| C | -1.81918500 | 2.13058900 | -0.25000300 |
| C | -0.33068000 | 4.20901600 | -0.35881600 |
| C | -1.22535700 | 3.42097000 | 1.80794300 |
| O | -2.22456000 | 4.08317200 | 1.93881100 |
| O | -0.60224300 | 4.41481000 | -1.51300000 |
| C | 0.20324700 | -0.63271300 | 0.96088300 |
| C | -0.48472700 | -1.70632200 | 0.89578300 |
| C | -1.80745000 | -1.72647100 | 0.42989900 |
| C | -2.31466100 | -0.43011500 | 0.05342300 |
| C | -2.59518200 | -2.97873500 | 0.35398600 |
| C | -3.65929700 | -0.23965500 | -0.37434500 |
| C | -4.81363000 | -0.05902900 | -0.72277600 |
| C | -6.17200900 | 0.05494400 | -1.13692300 |
| C | -6.69931000 | 1.28287500 | -1.58879300 |
| C | -8.02917500 | 1.36999300 | -1.99683100 |
| C | -8.85437400 | 0.24098600 | -1.96250600 |
| C | -8.34123500 | -0.98127500 | -1.51501900 |
| C | -7.01344500 | -1.07875900 | -1.10372500 |
| C | -2.38642100 | -3.97248200 | 1.32848500 |
| C | -3.09306500 | -5.17389200 | 1.29586000 |
| C | -4.01820700 | -5.41697100 | 0.27564100 |
| C | -4.21897800 | -4.44984900 | -0.71306200 |
| C | -3.51669700 | -3.24351100 | -0.67572800 |
| O | -0.47784800 | 3.00125300 | 2.83746700 |
| C | -0.93511100 | 3.37905100 | 4.13620800 |

| | | | |
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| O | 0.41101400 | 5.04185900 | 0.39288900 |
| C | 0.85040900 | 6.24402500 | -0.23966500 |
| H | 1.15721000 | 2.23044400 | 1.38605800 |
| H | 1.12377500 | 2.06657100 | -0.38220400 |
| H | -2.82184200 | 2.45370900 | 0.06026700 |
| H | -1.75484100 | 2.26995300 | -1.34151500 |
| H | -6.05217200 | 2.16160400 | -1.61447900 |
| H | -8.42618100 | 2.32677700 | -2.34453100 |
| H | -9.89639300 | 0.31388200 | -2.28277000 |
| H | -8.98287700 | -1.86528500 | -1.48466700 |
| H | -6.60697400 | -2.02831800 | -0.74988900 |
| H | -1.66067500 | -3.78039100 | 2.12159200 |
| H | -2.92192600 | -5.92531700 | 2.07084400 |
| H | -4.57253900 | -6.35825400 | 0.24684000 |
| H | -4.92243600 | -4.63769700 | -1.52833300 |
| H | -3.67048800 | -2.50944400 | -1.46544000 |
| H | -0.23152700 | 2.93297000 | 4.84926300 |
| H | -0.94544700 | 4.47439000 | 4.23843100 |
| H | -1.95328400 | 3.00205300 | 4.31193900 |
| H | 1.42491700 | 6.79439100 | 0.51493600 |
| H | 1.48082500 | 6.01585300 | -1.11213800 |
| H | -0.01039700 | 6.84032800 | -0.57649000 |
| H | 1.64564000 | -2.93518800 | 0.23668800 |
| C | 2.36060000 | -0.64688100 | 1.93614100 |
| C | 2.74687300 | -1.21806600 | 0.75652100 |
| C | 2.13190800 | -1.41288200 | 3.21262800 |
| H | 2.40600600 | 0.44098400 | 2.02905400 |
| C | 3.10004100 | -0.39626800 | -0.40133700 |
| C | 2.67324200 | -2.70712600 | 0.59840100 |
| C | 1.95651600 | -2.92055300 | 2.99960200 |
| H | 1.25817600 | -0.99562800 | 3.74012400 |
| H | 2.99894500 | -1.21691600 | 3.87376600 |
| C | 3.63667700 | 0.93759500 | -0.38608400 |
| C | 2.99237700 | -0.79149500 | -1.77971500 |
| C | 2.89912200 | -3.45140800 | 1.91861400 |
| H | 3.37333700 | -3.04661800 | -0.17842000 |
| H | 2.10876000 | -3.45483300 | 3.95099000 |
| H | 0.92024500 | -3.11356900 | 2.68145000 |
| C | 3.84297800 | 1.35515600 | -1.73305400 |
| H | 3.87784600 | 1.51391100 | 0.50420300 |
| C | 3.44210500 | 0.28781800 | -2.59324100 |
| H | 2.62535700 | -1.75092900 | -2.13638300 |
| H | 2.73865100 | -4.53115200 | 1.76981600 |
| H | 3.95054200 | -3.32831900 | 2.23600400 |
| H | 4.26710900 | 2.30612400 | -2.04968300 |
| Fe | 4.94470300 | -0.34574000 | -1.31749600 |
| H | 3.49715900 | 0.28711200 | -3.68011600 |
| C | 6.93840700 | 0.09055900 | -1.63751100 |
| C | 6.72505500 | -0.28300500 | -0.27496000 |
| C | 6.53314600 | -1.00194600 | -2.46346200 |
| H | 7.31691900 | 1.04973800 | -1.98622600 |
| C | 6.18905100 | -1.60659600 | -0.25918200 |
| H | 6.91267000 | 0.34082200 | 0.59709200 |
| C | 6.06902900 | -2.05091700 | -1.61165300 |
| H | 6.54859600 | -1.02147400 | -3.55167400 |
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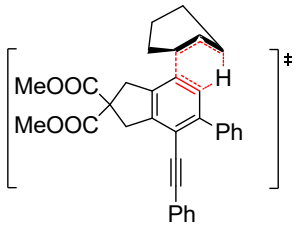
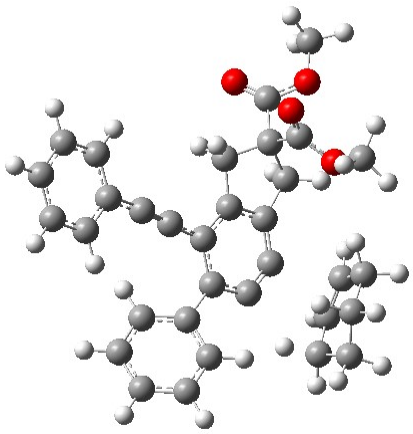
**TSC**





| Atomic Type | Coordinates(Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
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| C | -2.82685600 | -0.74233500 | -1.00798200 |
| C | -1.67168500 | 0.21443500 | -0.89255700 |
| C | -0.45695400 | -0.47453700 | -0.70720000 |
| C | -0.71593100 | -1.96035000 | -0.67174500 |
| C | -2.88553200 | -3.27812800 | -1.00496700 |
| C | -2.43259200 | -2.12672400 | 1.13470700 |
| O | -1.99119300 | -3.03099200 | 1.79817100 |
| O | -2.39461700 | -3.97790000 | -1.85197100 |
| C | -1.50364300 | 1.58442600 | -0.91172600 |
| C | -0.41089900 | 2.23750900 | -0.78308300 |
| C | 0.84255400 | 1.63285200 | -0.63261200 |
| C | 0.78551400 | 0.19311900 | -0.57321800 |
| C | 2.09228700 | 2.41517700 | -0.49474600 |
| C | 1.94444400 | -0.59293400 | -0.31619000 |
| C | 2.92962500 | -1.27048800 | -0.07836700 |
| C | 4.13495200 | -1.98320600 | 0.18448600 |
| C | 4.16339300 | -3.39343300 | 0.20069200 |
| C | 5.35559000 | -4.07002500 | 0.45267700 |
| C | 6.53537400 | -3.35761700 | 0.69211500 |
| C | 6.51731000 | -1.95869600 | 0.67926800 |
| C | 5.33051600 | -1.27261500 | 0.42935000 |
| C | 2.05912100 | 3.63973300 | 0.19775000 |
| C | 3.20986300 | 4.41276000 | 0.34784600 |
| C | 4.42065600 | 3.98411200 | -0.20506200 |
| C | 4.46401600 | 2.78072500 | -0.91464900 |
| C | 3.31341200 | 2.00292400 | -1.05815500 |
| O | -3.11266200 | -1.09434400 | 1.65593000 |
| C | -3.29023600 | -1.11501100 | 3.07364600 |
| O | -4.12359200 | -3.45584300 | -0.51308500 |
| C | -4.85187800 | -4.57618100 | -1.01761700 |
| H | -3.73949700 | -0.41464700 | -0.49838300 |
| H | -3.07405800 | -0.91611200 | -2.07033100 |
| H | -0.12710300 | -2.49913900 | 0.08256200 |
| H | -0.50537100 | -2.43062400 | -1.64622500 |
| H | 3.24076600 | -3.94585900 | 0.01310600 |
| H | 5.36522100 | -5.16258700 | 0.46281100 |
| H | 7.46758200 | -3.89202800 | 0.88972500 |
| H | 7.43634000 | -1.39837500 | 0.86762400 |
| H | 5.30780300 | -0.18106500 | 0.42081500 |
| H | 1.11250700 | 3.97284100 | 0.62834600 |
| H | 3.16263600 | 5.35467600 | 0.90007000 |
| H | 5.32344500 | 4.58894500 | -0.09033200 |
| H | 5.39999400 | 2.44633700 | -1.36937200 |
| H | 3.35887800 | 1.07649200 | -1.62950800 |
| H | -3.82177300 | -0.18998500 | 3.32699400 |
| H | -3.87922000 | -1.99382900 | 3.37453200 |
| H | -2.31686000 | -1.15326000 | 3.58379200 |

| | | | |
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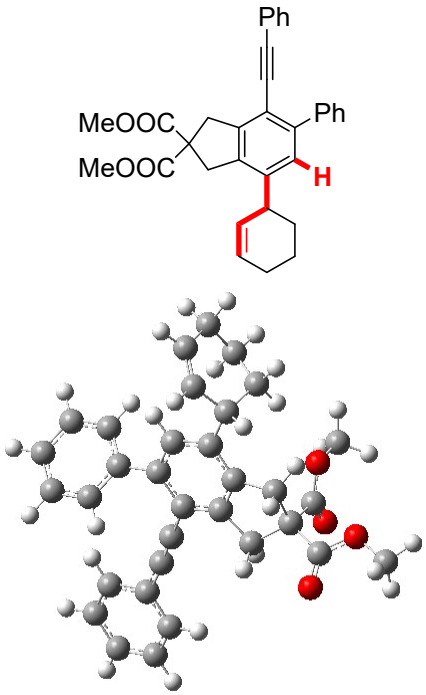
| H | -5.82193200 | -4.56527500 | -0.50666000 |
| H | -4.98926600 | -4.49194500 | -2.10593300 |
| H | -4.31575700 | -5.51244400 | -0.80331400 |
| H | -1.17438200 | 4.15902200 | -0.76304500 |
| C | -3.57568500 | 2.63958700 | -0.46370100 |
| C | -3.13064200 | 3.71428800 | -1.16889300 |
| C | -3.49602200 | 2.55412500 | 1.04247400 |
| H | -4.22461700 | 1.91426100 | -0.96424900 |
| C | -2.18044200 | 4.66569800 | -0.57459400 |
| C | -2.42505400 | 3.47269700 | 1.64787000 |
| H | -3.32396100 | 1.50950000 | 1.34558900 |
| H | -4.49653400 | 2.82091800 | 1.43500900 |
| C | -2.34975900 | 4.83220500 | 0.94155700 |
| H | -2.15036400 | 5.62794200 | -1.10727800 |
| H | -2.61829100 | 3.61167000 | 2.72385000 |
| H | -1.44572500 | 2.97741400 | 1.56559400 |
| H | -1.51250400 | 5.42077200 | 1.35061600 |
| H | -3.26809400 | 5.41230600 | 1.14124000 |
| H | -3.31689300 | 3.75828400 | -2.24645300 |

**3c**




| Atomic Type | Coordinates(Angstroms) | | |
|---|---|---|---|
| | X | Y | Z |
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| C | -1.62161400 | 0.12730200 | -0.76624600 |
| C | -0.38736500 | -0.50830800 | -0.61458700 |
| C | -0.55256700 | -2.00605000 | -0.62240800 |
| C | -2.64521000 | -3.43726000 | -0.97098900 |
| C | -2.24323600 | -2.30226000 | 1.19196000 |
| O | -1.72285700 | -3.17151500 | 1.84525200 |
| O | -2.13240900 | -4.07626600 | -1.85274700 |
| C | -1.72292500 | 1.52411100 | -0.76614300 |
| C | -0.53447700 | 2.25357800 | -0.62265300 |
| C | 0.72256000 | 1.64610300 | -0.48152400 |
| C | 0.80471800 | 0.22426600 | -0.46922600 |
| C | 1.92778400 | 2.49904100 | -0.32003900 |
| C | 2.03541500 | -0.46129900 | -0.26682100 |
| C | 3.09031500 | -1.04394000 | -0.08488600 |
| C | 4.36602100 | -1.64555100 | 0.11597300 |
| C | 4.52059000 | -3.04752000 | 0.13175200 |
| C | 5.77945900 | -3.61397300 | 0.32414100 |

| | | | |
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| C | 6.90142900 | -2.79802800 | 0.50337200 |
| C | 6.75820900 | -1.40630400 | 0.48995500 |
| C | 5.50407200 | -0.82982700 | 0.29923100 |
| C | 1.91546000 | 3.57588700 | 0.58376700 |
| C | 3.03696300 | 4.39196800 | 0.74371200 |
| C | 4.19339900 | 4.14958500 | -0.00199900 |
| C | 4.21618400 | 3.08773700 | -0.91160800 |
| C | 3.09601700 | 2.27034600 | -1.06878500 |
| O | -3.01025400 | -1.33930200 | 1.72387100 |
| C | -3.18250800 | -1.38632400 | 3.14089700 |
| O | -3.85660400 | -3.71074300 | -0.45729500 |
| C | -4.52623300 | -4.85615600 | -0.98576000 |
| H | -3.65993400 | -0.65460000 | -0.42220100 |
| H | -2.93508400 | -1.06411800 | -1.99149200 |
| H | 0.07684400 | -2.53077600 | 0.10861300 |
| H | -0.32528100 | -2.43146900 | -1.61377900 |
| H | 3.64255500 | -3.68074600 | -0.00843100 |
| H | 5.88701400 | -4.70125900 | 0.33483000 |
| H | 7.88627900 | -3.24629300 | 0.65435100 |
| H | 7.63203900 | -0.76553400 | 0.63100300 |
| H | 5.38343100 | 0.25525900 | 0.28933200 |
| H | 1.02064100 | 3.75848100 | 1.18299500 |
| H | 3.00917300 | 5.21701200 | 1.45976100 |
| H | 5.07239600 | 4.78654500 | 0.12274000 |
| H | 5.11117300 | 2.89736900 | -1.50930000 |
| H | 3.12038600 | 1.45143300 | -1.78840400 |
| H | -3.79565700 | -0.51544400 | 3.40171000 |
| H | -3.68822900 | -2.31724800 | 3.43682100 |
| H | -2.20870900 | -1.33941600 | 3.64979100 |
| H | -5.48153200 | -4.92493100 | -0.45201600 |
| H | -4.69683700 | -4.74193800 | -2.06663200 |
| H | -3.92746100 | -5.76379700 | -0.81947900 |
| H | -0.58528700 | 3.34306900 | -0.63820400 |
| C | -3.08623600 | 2.19844900 | -0.83820900 |
| C | -3.02429400 | 3.59992200 | -1.39625400 |
| C | -3.78021000 | 2.18788200 | 0.54702200 |
| H | -3.70416600 | 1.59555000 | -1.52581200 |
| C | -3.22511000 | 4.70233200 | -0.66278400 |
| C | -3.24469800 | 3.30815800 | 1.43915100 |
| H | -3.63868500 | 1.20695100 | 1.02454700 |
| H | -4.86558700 | 2.32553600 | 0.39837700 |
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| H | -2.92108600 | 5.46133500 | 1.32105100 |
| H | -4.57226900 | 4.97126800 | 0.97664600 |
| H | -2.78969000 | 3.69472400 | -2.46158600 |