Supporting Information for

Synthesis of Planar Chiral Ferrocenes via Pd(0)-Catalyzed syn-Carbopalladation/Asymmetric C-H Alkenylation Process

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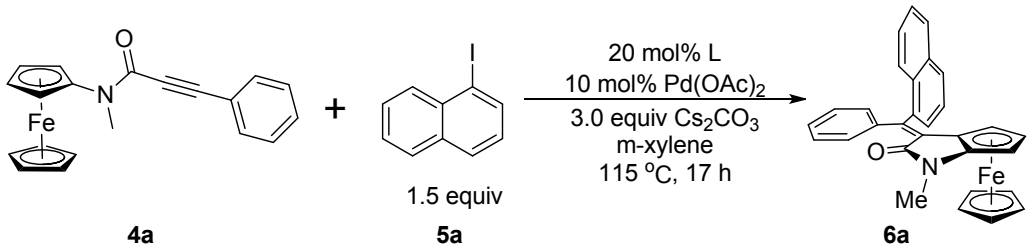
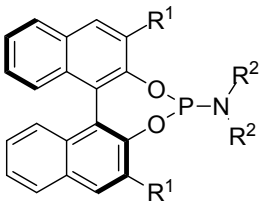
1. General information

Proton nuclear magnetic resonance spectrometers were recorded on Bruker-400 MHz instruments internally referenced to tetramethylsilane (0.0 ppm) or residue of $CDCl_3$ (7.26 ppm) signal. All reactions were performed under an inert atmosphere of dry nitrogen in glassware, unless otherwise stated. Solvents were distilled using standard techniques. Toluene, n-hexane were distilled over sodium under an atmosphere of nitrogen. Dichloromethane were distilled over calcium hydride under an atmosphere of nitrogen. Column chromatography was performed on 200-300 mesh silica gel. Analytical thin-layer chromatography (TLC) was performed on pre-coated, glass-backed silica gel plates.

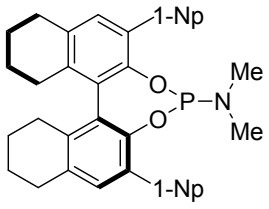
2. Complete optimization data

Table S1. Examination of ligand. [a]

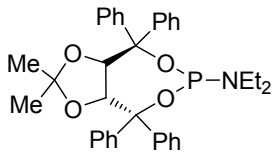




L1: R^1 = 1-Np, R^2 = Me
L2: R^1 = 1-Np, R^2 = Et
L3: R^1 = H, R^2 = Et
L4: R^1 = Ph, R^2 = Me
L5: R^1 = 9-anthracenyl, R^2 = Me



L6



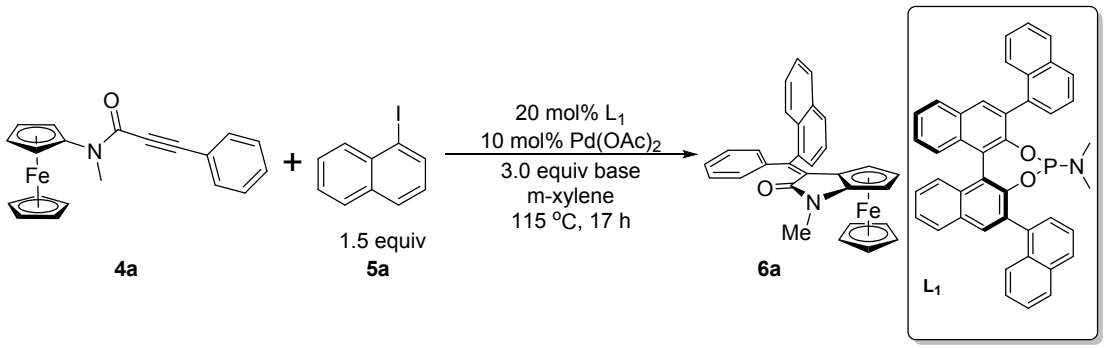
L7

Entry	Ligand	Yeild(%)[b]	Ee(%)[c]
1	$\mathbf{L_1}$	84	82
2	$\mathbf{L_2}$	69	67
3	$\mathbf{L_3}$	60	5
4	$\mathbf{L_4}$	47	42
5	$\mathbf{L_5}$	27	3
6	$\mathbf{L_6}$	42	37
7	$\mathbf{L_7}$	75	35
8	**(S)-BINAP**	15	2

[a] Reaction conditions: amide **4a** (0.10 mmol, 1.0 equiv), **5a** (0.15 mmol, 1.5 equiv), Pd $(OAc)_2$ (10

mol%), L (20 mol%), Cs_2CO_3 (0.30 mmol, 3.0 equiv), m-xylene (1.0 mL), 115 ℃, 17 h. [b] Isolated yield. [c] Determined by chiral HPLC.

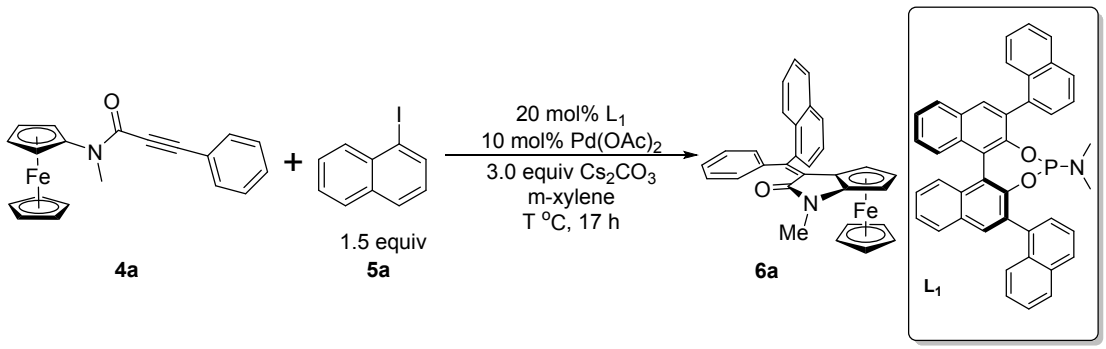
Table S2. Examination of base and additive. [a]



Entry	Base	Yield(%) [b]	Ee(%) [c]
1	Cs_2CO_3	84	82
2	K_3PO_4	21	85
3	Na_2CO_3	5	86
4	$NaHCO_3$	9	89
5[d]	Cs_2CO_3	85	50

[a] Reaction conditions: amide **4a** (0.10 mmol, 1.0 equiv), **5a** (0.15 mmol, 1.5 equiv), Pd $(OAc)_2$ (10 mol%), L_1 (20 mol%), base (0.30 mmol, 3.0 equiv), m-xylene (1.0 mL), 115 ℃, 17 h. [b] Isolated yield. [c] Determined by chiral HPLC. [d] With pivalic acid (30 mol%).

Table S3. Examination of temperature.[a]

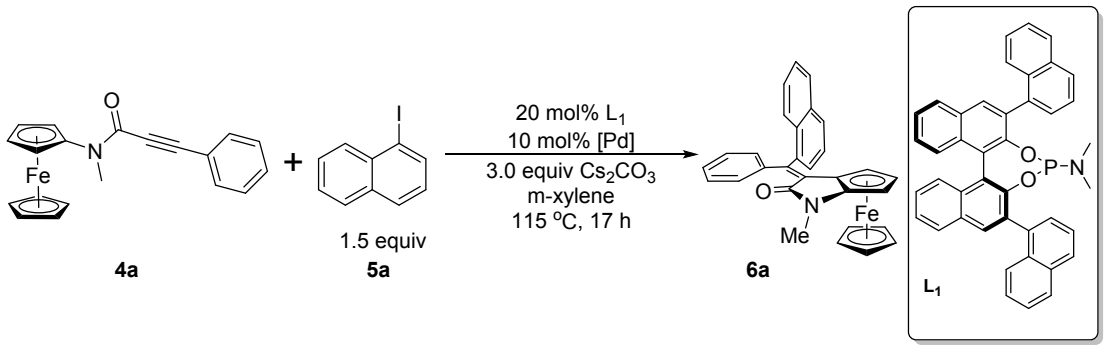


Entry	T(℃)	Yeild(%)[b]	Ee(%)[c]
1	100	58	64
2	115	84	82
3	130	57	32

[a] Reaction conditions: amide **4a** (0.10 mmol, 1.0 equiv), **5a** (0.15 mmol, 1.5 equiv), Pd $(OAc)_2$ (10 mol%), L_1 (20 mol%), Cs_2CO_3 (0.30 mmol, 3.0 equiv), m-xylene (1.0 mL), T ℃, 17 h. [b] Isolated

yield. [c] Determined by chiral HPLC.

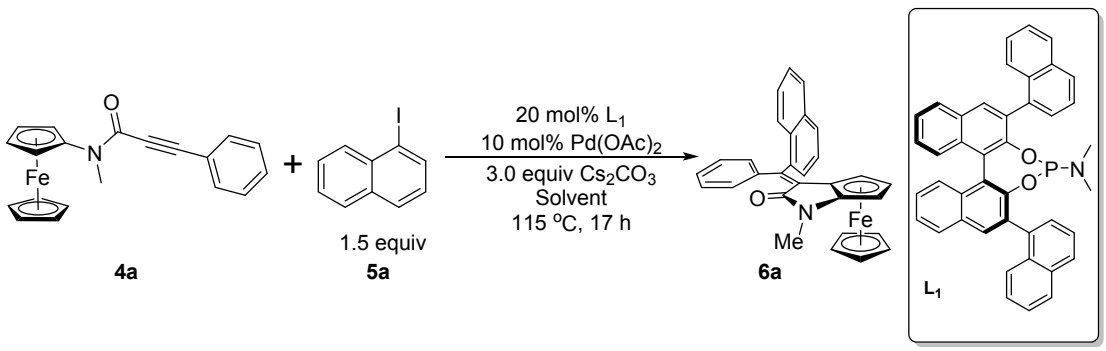
Table S4. Examination of palladium loading. [a]



Entry	[Pd]	Yeild(%)[b]	Ee(%)[c]
1	5% $Pd_2(dba)_3$	82	75
2	10% $Pd(dba)_2$	70	79
3	10% $PdCl_2$	29	76
4	10% $Pd(OAc)_2$	84	82

[a] Reaction conditions: amide **4a** (0.10 mmol, 1.0 equiv), **5a** (0.15 mmol, 1.5 equiv), [Pd] (10 mol%), L_1 (20 mol%), Cs_2CO_3 (0.30 mmol, 3.0 equiv), m-xylene (1.0 mL), 115 ℃, 17 h. [b] Isolated yield. [c] Determined by chiral HPLC.

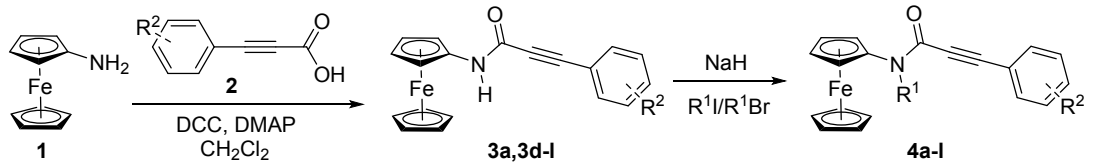
Table S5. Examination of solvent. [a]



Entry	Solvent	Yeild (%)[b]	Ee (%)[c,]
1	DMF	38	-9
2	1,4-Dioxane	59	17
3	Octane	88	91
4	Xylene	84	82

[a] Reaction conditions: amide **4a** (0.10 mmol, 1.0 equiv), **5a** (0.15 mmol, 1.5 equiv), $Pd(OAc)_2$ (10 mol%), L_1 (20 mol%), Cs_2CO_3 (0.30 mmol, 3.0 equiv), m-xylene (1 mL), 115 ℃, 17 h. [b] Isolated yield. [c] Determined by chiral HPLC.

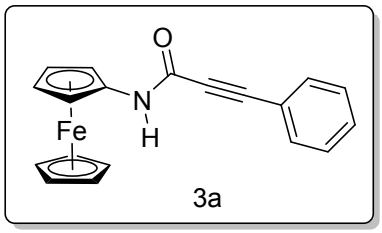
3. General procedure for the synthesis of amide substrates 4a-l. [1-3]



In a flame dried double Schlenk flask, a solution of the corresponding propynoic acid **2** (5.5 mmol, 1.1 equiv) in CH_2Cl_2 (10 mL) was cooled to -20 °C and 4-dimethylaminopyridine (**DMAP**) (0.5 mmol, 0.1 equiv), dicyclohexylcarbodiimide (**DCC**) (5.5 mmol, 1.1 equiv) in CH_2Cl_2 (5 mL) was added dropwise. Then a solution of aminoferrocene **1** (5.0 mmol, 1.0 equiv) in CH_2Cl_2 (5 mL) was added dropwise. The mixture was stirred at room temperature for 12 hours. The crude mixture was filtered and washed with CH_2Cl_2. The filtrate was washed with 0.5 M aqueous HCl, dried over Na_2SO_4, and concentrated. The residue was purified by a silica gel column chromatography (petroleum ether/EtOAc = 4:1) to give **3a, 3d-l** as a yellow / red solid or oil.

Sodium hydride (1.5 equiv) was suspended in dry THF (1.0 M). The reaction mixture was cooled to 0 °C and the amide **3a,3d-l** (1.0 equiv) in solution in dry THF was dropwise added. After 0.5 h, the corresponding alkyl iodide (or Benzyl bromide) was dropwise added and the reaction mixture was stirred overnight at room temperature. The reaction was quenched by slowly pouring in water at 0 °C. The product was extracted with ethyl acetate, washed by brine, dried over $MgSO_4$ and evaporated in vacuo. The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 4/1) to give **4a-l** as a yellow / red solid or oil**.**

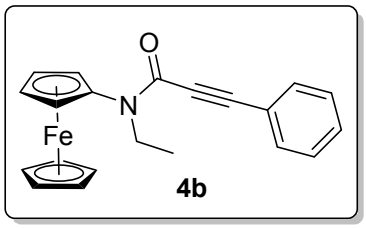
N-ferrocene-3-phenylpropiolamide(3a)



Yellow Solid (80% yield). Analytical data for **3a**: m.p. = 175.1-176.2 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 – 7.28 (m, 6H), 4.68 (s, 1.8H), 4.51 (s, 0.2H), 4.21 (s, 5H), 4.13 (s, 0.2H), 4.04 (s, 1.8H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.06, 132.63, 132.58, 130.43, 130.24, 128.62, 128.56, 120.11, 93.64, 85.38, 83.46, 69.50, 69.44, 65.95, 65.54, 65.02, 61.78. IR (KBr, cm^{-1}): 3227, 3076, 2956, 2918, 2845, 2203, 1623, 1564,

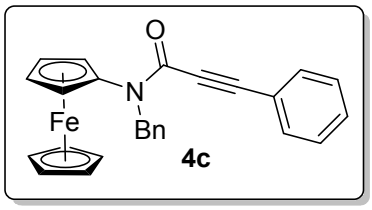
1472, 1388, 1359, 1289, 811, 756, 682. HRMS (ESI): calcd for $C_{19}H_{16}FeNO$ $[M+H]^+$ 330.0576, found 330.0567.

N-ethyl-N-ferrocene-3-phenylpropiolamide(4b)



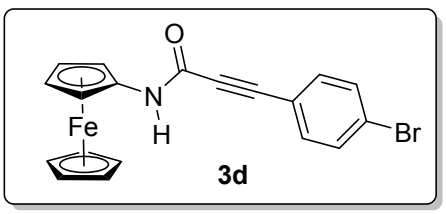
Yellow Solid (64% yield). Analytical data for **4b**: m.p. = 85.0-86.9 ℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 – 7.22 (m, 9.6H), 4.74 (s, 1.8H), 4.48 (s, 2H), 4.26 (s, 5H), 4.19 (s, 6H), 4.13 – 3.97 (m, 6H), 1.47 (t, 2.9H), 1.38 (t, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.27, 153.03, 132.42, 130.07, 129.89, 128.59, 128.38, 120.82, 120.70, 100.92, 98.03, 90.29, 89.67, 83.41, 82.76, 69.30, 65.53, 65.29, 65.07, 62.45, 46.55, 46.38, 15.04, 13.83. HRMS (ESI): calcd for $C_{21}H_{20}FeNO$ $[M+H]^+$ 358.0889, found 358.0891.

N-benzyl-N-ferrocene-3-phenylpropiolamide(4c)



Yellow Solid (47% yield). Analytical data for **4c**: m.p. = 115-117.1 ℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 – 7.15 (m, 10H), 5.27 (d, *J* = 6.2 Hz, 2H), 4.63 (s, 1H), 4.46 (s, 1H), 4.18 (s, 2H), 4.15 (s, 4H), 4.03 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ154.78, 153.97, 137.55, 137.52, 132.51, 132.45, 130.12, 130.09, 128.85, 128.71, 128.49, 128.46, 127.56, 127.16, 126.53, 126.31, 120.70, 120.37, 101.30, 98.85, 91.31, 90.65, 83.22, 82.74, 69.32, 69.25, 65.36, 65.19, 65.04, 63.02, 55.46, 54.25. IR (KBr, cm^{-1}): 3062, 2955, 2924, 2869, 2214, 1634, 1489, 1470, 1376, 1266, 740, 690. HRMS (ESI): calcd for $C_{26}H_{22}FeNO$ $[M+H]^+$ 420.1045, found 420.1041.

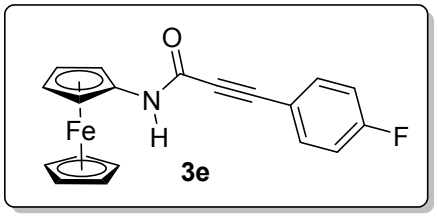
N-ferrocene-3-(4-bromophenyl)propiolamide(3d)



Red Solid (82% yield). Analytical data for **3d**：m.p. = 178.6-181.2 ℃. ^{1}H NMR (400

MHz, $CDCl_3$) δ 7.61 – 7.21 (m, 4H), 7.02 (s, 1H), 4.67 (s, 1.7H), 4.50 (s, 0.3H), 4.23 (s, 5H), 4.14 (s, 0.3H), 4.08 (s, 1.7H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.71, 133.90, 133.87, 132.00, 131.94, 124.92, 119.03, 93.55, 84.33, 84.16, 69.51, 69.47, 66.04, 65.73, 65.09, 61.78. IR (KBr, cm^{-1}): 3223, 2955, 2923, 2853, 2208, 1621, 1596, 1544, 1505, 1474, 1387, 1227, 1155, 833. HRMS (ESI): calcd for $C_{19}H_{15}BrFeNO$ $[M+H]^+$ 407.9681, found 407.9679.

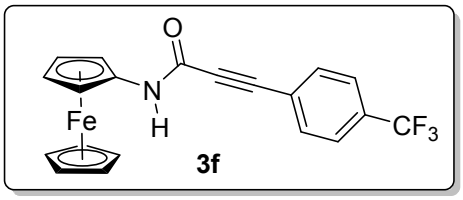
N-ferrocene-3-(4-fluorophenyl)propiolamide(3e)



3e

Red Solid (78% yield). Analytical data for **3e**：m.p. = 170-172.4 ℃. ^1H NMR (400 MHz, $CDCl_3$) δ 7.75 – 6.94 (m, 5H), 4.67 (s, 1.7H), 4.51 (s, 0.3H), 4.22 (s, 5H), 4.14 (s, 0.3H), 4.06 (s, 1.7H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.62 (d, J = 252.9 Hz), 150.86, 134.84 (d, J = 8.8 Hz), 134.74 (d, J = 8.8 Hz), 116.12, 116.11 (d, J = 22.2 Hz), 116.08 (d, J = 22.2 Hz), 93.62, 84.32, 83.26, 69.50, 69.47, 66.01, 65.74, 65.06, 61.76. ^{19}F NMR (376 MHz, $CDCl_3$) δ -106.74, -107.15. IR (KBr, cm^{-1}): 3211, 3076, 2956, 2919, 2870, 2850, 2206, 1730, 1629, 1557, 1504, 1462, 1379, 1230, 846. HRMS (ESI): calcd for $C_{19}H_{15}FFeNO$ $[M+H]^+$ 348.0482, found 348.0477.

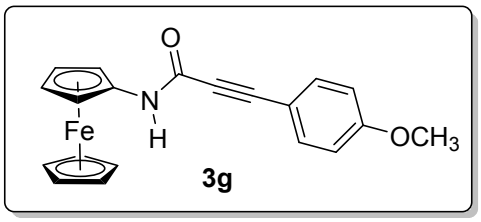
N-ferrocene-3-(4-(trifluoromethyl)phenyl)propiolamide(3f)



3f

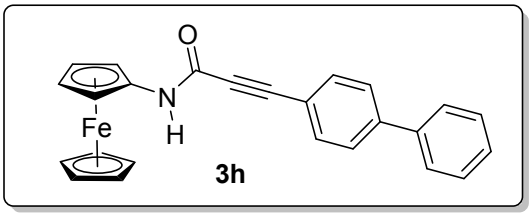
Red Solid (83% yield). Analytical data for **3f**：m.p. = 157.9-160.8 ℃. ^1H NMR (400 MHz, $CDCl_3$) δ 7.75 – 7.45 (m, 4H), 7.31 – 7.15 (s, 1H), 4.67 (s, 1.8H), 4.51 (s, 0.2H), 4.22 (s, 5H), 4.15 (s, 0.2H), 4.07 (s, 1.8H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.40, 132.78, 131.79 (q, J = 33.1 Hz), 125.57 (q, J = 3.7 Hz), 125.53 (q, J = 3.7 Hz), 123.93 (d, J = 1.2 Hz), 123.59 (q, J = 274.0 Hz), 93.30, 85.07, 83.37, 69.54, 69.45, 66.13, 65.85, 65.13, 61.83. ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.05, -63.11. IR (KBr, cm^{-1}): 3233, 3073, 2928, 2851, 2210, 1629, 1555, 1472, 1323, 1129, 1068, 843. HRMS (ESI): calcd for $C_{20}H_{15}F_3FeNO$ $[M+H]^+$ 398.0450, found 398.0445.

N-ferrocene-3-(4-methoxyphenyl)propiolamide(3g)



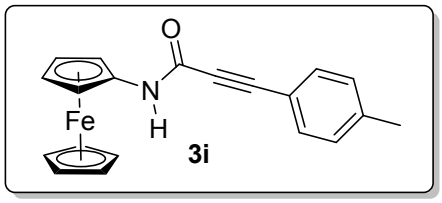
Yellow Solid (84% yield). Analytical data for **3g**: m.p. = 127.2-129.6 ℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 – 6.90 (m, 5H), 4.68 (s, 1.8H), 4.51 (s, 0.2H), 4.21 (s, 5H), 4.13 (s, 0.3H), 4.04 (s, 1.7H), 3.79 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.35, 159.27, 151.06, 129.72, 129.67, 125.04, 121.10, 121.07, 117.26, 117.16, 117.09, 116.95, 93.58, 85.31, 83.23, 69.51, 69.41, 65.93, 65.52, 64.99, 61.80, 55.40. IR (KBr, cm^{-1}): 3236, 3079, 2956, 2922, 2867, 2851, 2209, 1734, 1622, 1555, 1463, 1378, 1228, 734. HRMS (ESI): calcd for $C_{20}H_{18}FeNO_2$ $[M+H]^+$ 360.0681, found 360.0681.

N-ferrocene-3-([1,1'-biphenyl]-4-yl)propiolamide(3h)



Yellow Solid (80% yield). Analytical data for **3h**: m.p. = 173.1-173.9 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 – 7.12 (m, 10H), 4.69 (s, 1.8H), 4.54 (s, 0.2H), 4.22 (s, 5H), 4.15 (s, 0.3H), 4.05 (s, 1.7H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.08, 142.96, 139.86, 133.09, 133.05, 129.00, 128.61, 128.11, 128.03, 127.26, 127.22, 127.12, 127.03, 118.87, 93.62, 85.39, 84.09, 69.51, 69.43, 65.97, 65.57, 65.01, 61.80. HRMS (ESI): calcd for $C_{25}H_{20}FeNO$ $[M+H]^+$ 406.0889, found 406.0875.

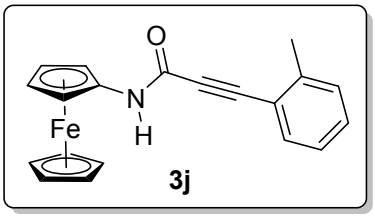
N-ferrocene-3-(p-tolyl)propiolamide(3i)



Yellow Solid (88% yield). Analytical data for **3i**: m.p. = 180.1-180.9 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 – 7.08 (m, 5H), 4.67 (s, 1.8H), 4.51 (s, 0.2H), 4.21 (s, 5H), 4.12 (s, 0.3H), 4.04 (s, 1.7H), 2.38 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.21, 140.75, 132.57, 132.52, 129.38, 129.33, 117.01, 93.68, 85.79, 83.11, 69.47, 69.38, 65.85, 65.40, 64.94, 61.75, 21.71. IR (KBr, cm^{-1}): 3231, 3082, 2955, 2851, 2208, 1625, 1563, 1508, 1475, 1388, 1364, 1295, 1195, 1177, 1105, 815. HRMS (ESI):

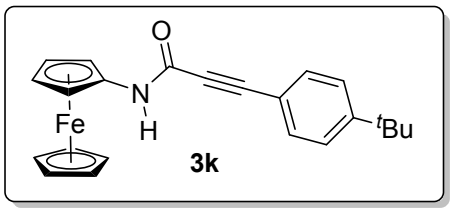
calcd for $C_{20}H_{18}FeNO$ $[M+H]^+$ 344.0732, found 344.0734.

N-ferrocene-3-(o-tolyl)propiolamide (3j)



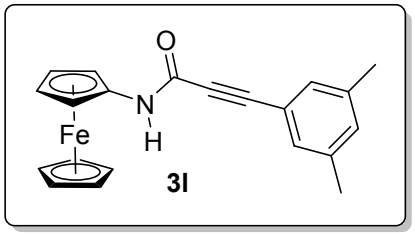
Yellow Solid (76% yield). Analytical data for **3j**: m.p. = 105.8-106.6 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.15 (m, 5H), 4.69 (s, 1.8H), 4.51 (s, 0.2H), 4.21 (s, 5H), 4.13 (s, 0.2H), 4.04 (s, 1.8H), 2.34 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.15, 138.38, 138.34, 133.10, 131.34, 131.14, 129.73, 129.68, 128.49, 128.44, 119.98, 119.92, 93.78, 85.67, 83.21, 69.49, 69.45, 65.90, 65.42, 65.00, 61.77, 21.25. IR (KBr, cm^{-1}):3233, 3082, 2956, 2919, 2870, 2850, 2209, 1738, 1626, 1555, 1462, 1378, 778. HRMS (ESI): calcd for $C_{20}H_{18}FeNO$ $[M+H]^+$ 344.0732, found 344.0732.

N-ferrocene-3-(4-(tert-butyl)phenyl)propiolamide (3k)



Yellow Solid (80% yield). Analytical data for **3k**： m.p. = 177.1-178.8 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 – 7.08 (m, 5H), 4.67 (s, 1.7H), 4.52 (s, 0.3H), 4.21 (s, 5H), 4.12 (s, 0.3H), 4.04 (s, 1.7H), 1.32 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.80, 151.22, 132.46, 132.41, 125.66, 125.61, 117.00, 93.66, 85.77, 83.06, 69.47, 69.39, 65.86, 65.44, 64.94, 61.75, 35.04, 31.10. IR (KBr, cm^{-1}):3227, 3085, 2957, 2924, 2869, 2203, 1630, 1560, 1462, 1356, 742. HRMS (ESI): calcd for $C_{23}H_{24}FeNO$ $[M+H]^+$ 386.1202, found 386.1200.

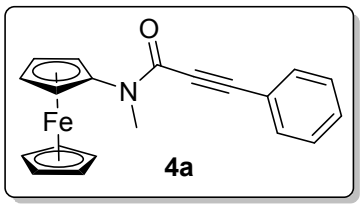
N-ferrocene-3-(3,5-dimethylphenyl)propiolamide(3l)



Yellow Solid (90% yield). Analytical data for **3l**： m.p. = 148.8-149.9 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.00 (m, 4H), 4.68 (s, 1.8H), 4.51 (s, 0.2H), 4.21 (s, 5H),

4.12 (s, 0.2H), 4.03 (s, 1.8H), 2.30 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.20, 138.23, 138.19, 132.38, 132.18, 130.24, 119.71, 93.71, 85.93, 82.92, 69.48, 69.40, 65.86, 65.34, 64.95, 61.75, 21.13. IR (KBr, cm^{-1}): 3229, 3084, 2956, 2923, 2853, 2216, 1627, 1557, 1467, 1387, 1365, 1267, 1105, 852, 687. HRMS (ESI): calcd for $C_{21}H_{20}FeNO$ $[M+H]^+$ 358.0889, found 358.0886.

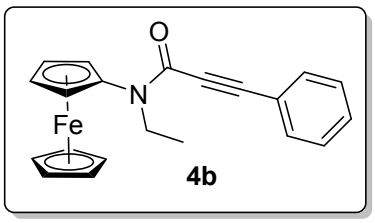
N-ferrocene-N-methyl-3-phenylpropiolamide(4a)



4a

Yellow Solid (98% yield). Analytical data for **4a**: m.p. = 113.8-115 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 – 7.23 (m, 8H), 4.75 (s, 1.2H), 4.54 (s, 2H), 4.27 (s, 5H), 4.21 (s, 3H), 4.18 (s, 2H), 4.10 (s, 1.2H), 3.63 (s, 1.8H), 3.48 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.44, 153.50, 132.43, 132.40, 130.14, 130.00, 128.60, 128.44, 120.72, 120.58, 100.62, 98.58, 91.02, 90.44, 83.13, 82.58, 69.19, 69.06, 65.27, 65.19, 64.60, 62.63, 38.12, 37.37. IR (KBr, cm^{-1}): 3089, 2956, 2924, 2870, 2852, 2209, 1734, 1627, 1555, 1462, 1377,1105, 753, 685, 618. HRMS (ESI): calcd for $C_{20}H_{18}FeNO$ $[M+H]^+$ 344.0732, found 344.0735.

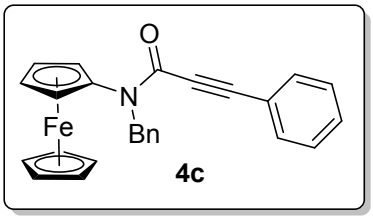
N-ethyl-N-ferrocene-3-phenylpropiolamide(4b)



4b

Yellow Solid (64% yield). Analytical data for **4b**: m.p. = 85.0-86.9 ℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 – 7.22 (m, 9.6H), 4.74 (s, 1.8H), 4.48 (s, 2H), 4.26 (s, 5H), 4.19 (s, 6H), 4.13 – 3.97 (m, 6H), 1.47 (t, 2.9H), 1.38 (t, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.27, 153.03, 132.42, 130.07, 129.89, 128.59, 128.38, 120.82, 120.70, 100.92, 98.03, 90.29, 89.67, 83.41, 82.76, 69.30, 65.53, 65.29, 65.07, 62.45, 46.55, 46.38, 15.04, 13.83. HRMS (ESI): calcd for $C_{21}H_{20}FeNO$ $[M+H]^+$ 358.0889, found 358.0891.

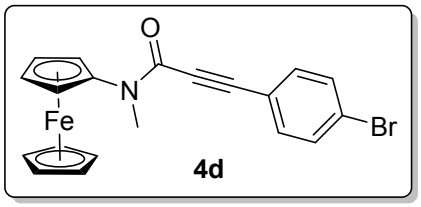
N-benzyl-N-ferrocene-3-phenylpropiolamide(4c)



4c

Red Solid (47% yield). Analytical data for **4c**: m.p. = 115-117.1 ℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 – 7.15 (m, 10H), 5.27 (d, *J* = 6.2 Hz, 2H), 4.63 (s, 1H), 4.46 (s, 1H), 4.18 (s, 2H), 4.15 (s, 4H), 4.03 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ154.78, 153.97, 137.55, 137.52, 132.51, 132.45, 130.12, 130.09, 128.85, 128.71, 128.49, 128.46, 127.56, 127.16, 126.53, 126.31, 120.70, 120.37, 101.30, 98.85, 91.31, 90.65, 83.22, 82.74, 69.32, 69.25, 65.36, 65.19, 65.04, 63.02, 55.46, 54.25. IR (KBr, cm^{-1}): 3062, 2955, 2924, 2869, 2214, 1634, 1489, 1470, 1376, 1266, 740, 690. HRMS (ESI): calcd for $C_{26}H_{22}FeNO$ $[M+H]^+$ 420.1045, found 420.1041.

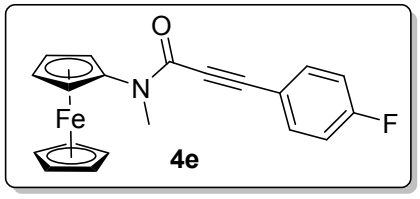
N-ferrocene-3-(4-bromophenyl)-N-methylpropiolamide(4d)



4d

Yellow Solid (94% yield). Analytical data for **4d**： m.p. = 126.2-127.8 ℃.^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 – 7.18 (m, 6.2H), 4.74 (s, 1.2H), 4.52 (s, 2H), 4.28 (s, 5H), 4.21 (s, 3H), 4.18 (s, 2H), 4.11 (s, 1.2H), 3.62 (s, 1.8H), 3.48 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.22, 153.22, 133.74, 133.72, 131.98, 131.82, 124.78, 124.64, 119.62, 119.50, 100.51, 98.44, 89.82, 89.21, 84.02, 83.48, 69.23, 69.08, 65.31, 65.26, 64.63, 62.64, 38.12, 37.46. IR (KBr, cm^{-1}): 2954, 2922, 2850, 2211, 1626, 1581, 1484, 1352, 1335, 1066, 999, 816. HRMS (ESI): calcd for $C_{20}H_{17}BrFeNO$ $[M+H]^+$ 421.9837, found 421.9837.

N-ferrocene-3-(4-fluorophenyl)-N-methylpropiolamide(4e)

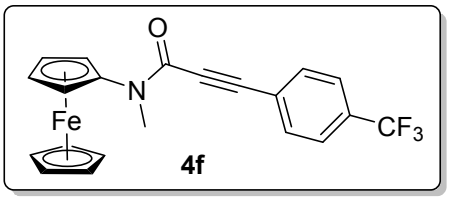


4e

Yellow Solid (95% yield). Analytical data for **4e**： m.p. = 110-113 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (s, 1.1H), 7.39 (s, 2H), 7.09 (s,1.1H), 7.01 (s, 2H), 4.75 (s, 1.1H), 4.53 (s, 2H), 4.28 (s, 5H), 4.21 (s, 2.4H), 4.19 (s, 2H), 4.11 (s, 1.1H), 3.62 (s, 1.7H),

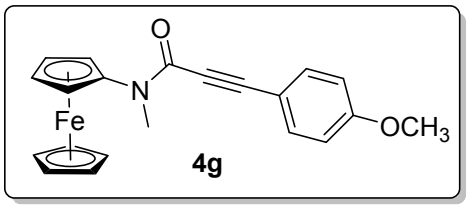
3.48 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.58 (d, *J* = 253.4 Hz), 163.50 (d, *J* = 253.4 Hz), 154.36, 153.37, 134.59 (d, *J* = 8.8 Hz), 134.57 (d, *J* = 8.8 Hz), 116.77 (d, *J* = 11.9 Hz), 116.73 (d, *J* = 11.9 Hz), 116.10 (d, *J* = 22.3 Hz), 115.93 (d, *J* = 22.3 Hz), 100.59, 98.50, 89.99, 89.39, 82.95, 82.42, 69.21, 69.06, 65.27, 65.22, 64.64, 62.63, 38.11, 37.42. ^{19}F NMR (376 MHz, $CDCl_3$) δ -107.39, -107.52. IR (KBr, cm^{-1}): 2955, 2922, 2851, 2215, 1626, 1505, 1464, 1378, 833, 819, 807. HRMS (ESI): calcd for $C_{20}H_{17}FFeNO$ $[M+H]^+$ 362.0638, found 362.0640.

N-ferrocene-N-methyl-3-(4-(trifluoromethyl)phenyl)propiolamide(4f)



Yellow Solid (90% yield). Analytical data for **4f:** m.p. = 137-138.2 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.1 Hz, 2.4H), 7.57 (m, 2H), 7.50 (s, 2H), 4.75 (s, 1.1H), 4.53 (s, 2H), 4.29 (s, 5H), 4.22 (s, 2.6H), 4.19 (s, 2H), 4.13 (s, 1.1H), 3.63 (s, 1.7H), 3.50 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.96, 152.88, 132.57, 131.69 (q, *J* = 33.0 Hz), 131.51 (q, *J* = 32.9 Hz), 125.54 (q, *J* = 3.6 Hz), 125.37 (q, *J* = 3.7 Hz), 124.53 (d, *J* = 1.1 Hz), 124.41 (d, *J* = 1.1 Hz), 123.63 (q, *J* = 273.6 Hz), 100.46, 98.37, 89.01, 88.43, 84.81, 84.25, 69.25, 69.09, 65.37, 65.29, 64.66, 62.65, 38.08, 37.51. ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.03, -63.06. IR (KBr, cm^{-1}): 3095, 2956, 2924, 2848, 2216, 1731, 1555, 1481, 1322, 1128, 839. HRMS (ESI): calcd for $C_{21}H_{17}F_3FeNO$ $[M+H]^+$ 412.0606, found 412.0606.

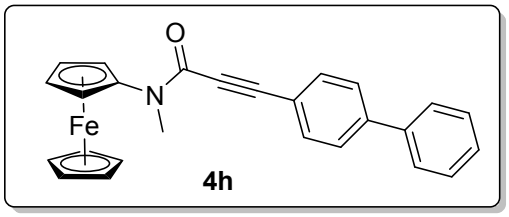
N-ferrocene-3-(4-methoxyphenyl)-N-methylpropiolamide (4g)



Yellow oil (87% yield). Analytical data for **4g:** ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 – 6.82 (m, 6.4H), 4.74 (s, 1.2H), 4.54 (s, 2H), 4.27 (s, 5H), 4.21 (s, 2.8H), 4.18 (s, 2H), 4.10 (s, 1.2H), 3.81 (s, 1.8H), 3.76 (s, 3H), 3.62 (s, 1.8H), 3.47 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.38, 159.22, 154.40, 153.45, 129.72, 129.55, 124.87, 124.84, 121.62, 121.49, 117.10, 117.03, 116.84, 116.70, 100.59, 98.54, 90.95, 90.35, 82.84, 82.28, 69.20, 69.07, 65.28, 65.21, 64.64, 62.65, 55.42, 55.33, 38.16, 37.39. IR (KBr, cm^{-1}): 3091, 2940, 2836, 2211, 1633, 1574, 1482, 1355, 1286, 1223, 1036, 781, 684.

HRMS (ESI): calcd for $C_{21}H_{20}FeNO_2$ $[M+H]^+$ 374.0838, found 374.0835.

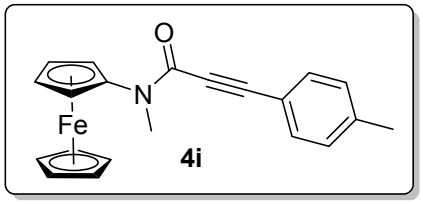
3-([1,1'-biphenyl]-4-yl)-N-ferrocene-N-methylpropiolamide (4h)



4h

Yellow Solid (80% yield). Analytical data for **4h:** m.p. = 168.1-169.3 ℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 – 7.30 (m, 14.4H), 4.76 (s, 1.2H), 4.56 (s, 2H), 4.28 (s, 5H), 4.22 (s, 3H), 4.20 (s, 2H), 4.11 (s, 1.2H), 3.65 (s, 1.8H), 3.49 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.48, 153.55, 142.90, 142.77, 139.96, 139.92, 132.90, 129.00, 128.96, 128.09, 128.02, 127.26, 127.13, 127.10, 119.49, 119.33, 100.65, 98.60, 91.05, 90.46, 83.76, 83.20, 69.21, 69.08, 65.30, 65.22, 64.64, 62.66, 38.17, 37.40. HRMS (ESI): calcd for $C_{26}H_{22}FeNO$ $[M+H]^+$ 420.1045, found 420.1036.

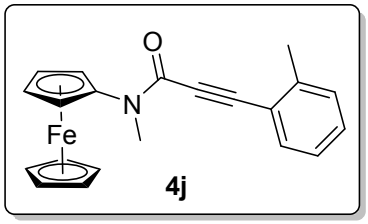
N-ferrocene-N-methyl-3-(p-tolyl)propiolamide(4i)



4i

Yellow Solid (93% yield). Analytical data for **4i**： m.p. = 105.8-117.2℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 – 7.01 (m, 6.6H), 4.75 (s, 1.3H), 4.55 (s, 2H), 4.27 (s, 5H), 4.21 (s, 3H), 4.18 (s, 2H), 4.10 (s, 1.3H), 3.62 (s, 2H), 3.47 (s, 3H), 2.39 (s, 2H), 2.34 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.58, 153.69, 140.68, 140.52, 132.39, 129.38, 129.22, 117.61, 117.46, 100.67, 98.64, 91.47, 90.90, 82.76, 82.21, 69.17, 69.04, 65.22, 65.16, 64.57, 62.63, 38.13, 37.31, 21.73, 21.70. IR (KBr, cm^{-1}): 3092, 2956, 2919, 2848, 2215, 1731, 1634, 1558, 1463, 1378, 1105, 816. HRMS (ESI): calcd for $C_{21}H_{20}FeNO$ $[M+H]^+$ 358.0889, found 358.0891.

N-ferrocene-N-methyl-3-(p-tolyl)propiolamide(4j)

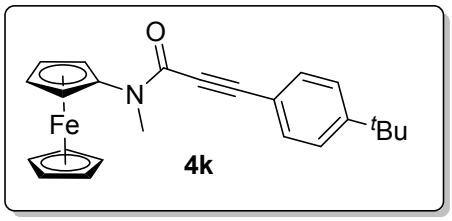


4j

Yellow oil (73% yield). Analytical data for **4j**： ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 –

7.05 (m, 6.5H), 4.74 (s, 1.3H), 4.54 (s, 2H), 4.26 (s, 5H), 4.20 (s, 3H), 4.17 (s, 2H), 4.09 (s, 1.4H), 3.61 (s, 2H), 3.46 (s, 3H), 2.35 (s, 1.9H), 2.29 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.46, 153.57, 138.38, 138.19, 132.90, 131.09, 130.95, 129.55, 129.53, 128.51, 128.35, 120.50, 120.35, 100.62, 98.60, 91.33, 90.76, 82.85, 82.31, 69.19, 69.06, 65.27, 65.19, 64.58, 62.64, 38.14, 37.34, 21.27, 21.24. IR (KBr, cm^{-1}): 2957, 2927, 2847, 2206, 1654, 1630, 1617, 1560, 1483, 1266, 1106, 739, 705, 690. HRMS (ESI): calcd for $C_{21}H_{20}FeNO$ $[M+H]^+$ 358.0889, found 358.0891.

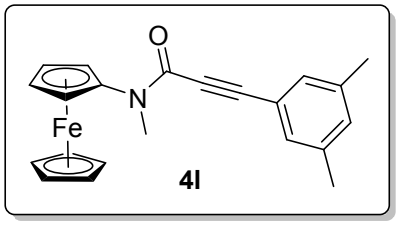
N-ferrocene-3-(4-(tert-butyl)phenyl)-N-methylpropiolamide(4k)



4k

Yellow Solid (80% yield). Analytical data for **4k**: m.p. = 78.2-79.8 ℃, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 – 7.21 (m, 6.4H), 4.75 (s, 1.2H), 4.55 (s, 2H), 4.27 (s, 5H), 4.21 (s, 3H), 4.17 (s, 2H), 4.10 (s, 1.2H), 3.62 (s, 1.8H), 3.48 (s, 3H), 1.33 (s, 5.5H), 1.29 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.62, 153.71, 153.55, 132.28, 132.24, 125.65, 125.49, 117.63, 117.48, 100.68, 98.65, 91.44, 90.87, 82.73, 82.18, 69.17, 69.04, 65.22, 65.16, 64.60, 62.63, 38.14, 37.34, 35.03, 34.98, 31.11, 31.08. IR (KBr, cm^{-1}): 3093, 2962, 2868, 2216, 1633, 1505, 1482, 1428, 1366, 1339, 1097, 836, 726. HRMS (ESI): calcd for $C_{24}H_{26}FeNO$ $[M+H]^+$ 400.1358, found 400.1361.

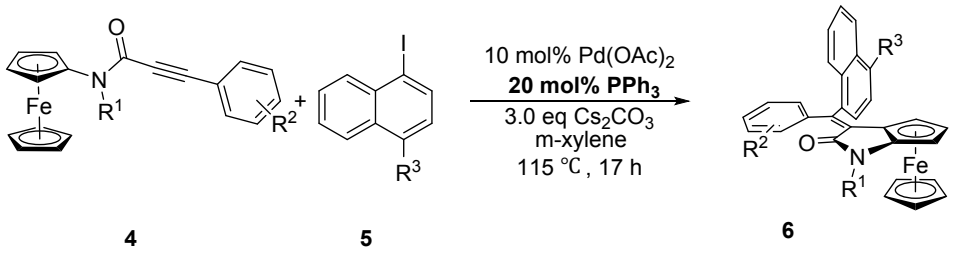
N-ferrocene-3-(3,5-dimethylphenyl)-N-methylpropiolamide(4l)



4l

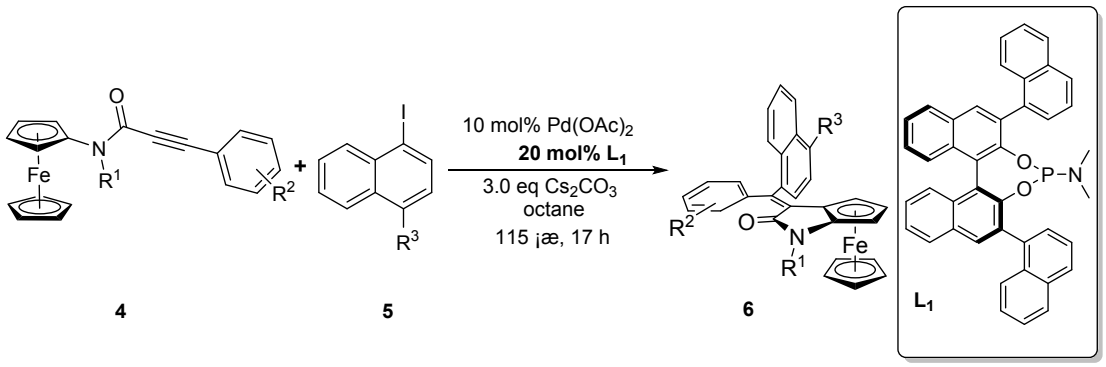
Yellow oil (92% yield). Analytical data for **4l:** ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 – 6.91 (m, 5.2H), 4.73 (s, 1.5H), 4.53 (s, 2H), 4.25 (s, 5H), 4.19 (s, 3.3H), 4.16 (s, 2H), 4.08 (s, 1.5H), 3.59 (s, 2.2H), 3.45 (s, 3H), 2.30 (s, 4.2H), 2.24 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.46, 153.61, 138.24, 138.05, 132.14, 132.00, 130.07, 130.05, 120.30, 120.14, 100.63, 98.64, 91.60, 91.05, 82.60, 82.06, 69.19, 69.06, 65.27, 65.17, 64.55, 62.64, 38.13, 37.28, 21.16, 21.13. IR (KBr, cm^{-1}): 2957, 2927, 2847, 2208, 1654, 1634, 1617, 1560, 1483, 1266, 1106, 739, 687. HRMS (ESI): calcd for $C_{22}H_{22}FeNO$ $[M+H]^+$ 372.1045, found 372.1050.

4. General procedures: preparation of the racemic ferrocene [1,2-d] pyrrolinones derivatives 6.



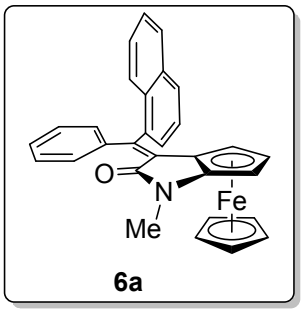
To a 10 mL Schlenk-type sealed tube, substrate **4** (0.1 mmol), Cs_2CO_3 (97.5 mg, 0.30 mmol, 3.0 equiv), Pd $(OAc)_2$ (2.3 mg, 0.01 mmol, 10 mol %), ligand PPh_3 (5.2 mg, 0.02 mmol, 20.0 mol %), Iodonaphthalene **5** (0.15 mmol, 0.15 equiv) were dissolved in m-xylene (1.0 mL) under nitrogen. The reaction mixture was stirred at 115 °C. After the reaction was complete (monitored by TLC), then cooled to the room temperature. The reaction mixture was concentrated under reduced pressure. The residue was purified by silica gel column chromatography (ethyl acetate/petroleum ether = 1/8, v/v) to afford the racemic product **6**.

5. General procedure : enantioselective synthesis of planar chiral ferrocene [1,2-d] pyrrolinones derivatives 6.



To a 10 mL Schlenk-type sealed tube, substrate **4** (0.1 mmol), Cs_2CO_3 (97.5 mg, 0.30 mmol, 3.0 equiv), Pd $(OAc)_2$ (2.3 mg, 0.01 mmol, 10 mol%), ligand L_1 (12.2 mg, 0.02 mmol, 20.0 mol%), Iodonaphthalene **5** (0.15 mmol, 0.15 equiv) were dissolved in n-octane (1.0 mL) under nitrogen. The reaction mixture was stirred at 115 °C. After the reaction was complete (monitored by TLC), then cooled to the room temperature. The reaction mixture was concentrated under reduced pressure. The residue was purified by silica gel column chromatography (ethyl acetate/petroleum ether = 1/8, v/v) to afford desired product **6.**

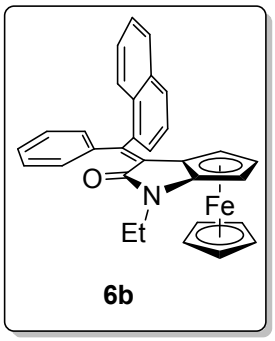
(Z)-1-methyl-3-(naphthalen-1-yl(phenyl)methylene)ferrocene[1,2-d]pyrrol-2(1H)-one(6a)[a]



6a

Purple solid (41.3 mg, 88% yield, 91% ee). Analytical data for **6a**: m.p. = 218.8-220.2 ℃. $[\alpha]_D^{20}$ = -2291 (c = 0.01 $CHCl_3$, 91% ee). ^1H NMR (400 MHz, $CDCl_3$) δ 8.13 – 7.21 (m, 12H), 4.13 (s, 3H), 4.00 (s, 1H), 3.85 (s, 2H), 3.79 (s, 1H), 3.08 (s, 3H), 2.47 (d, *J* = 24.2 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.82, 168.61, 145.33, 144.97, 140.10, 139.77, 138.45, 138.17, 134.10, 133.99, 130.48, 130.46, 130.16, 130.09, 129.29, 129.23, 128.54, 128.51, 128.46, 128.33, 128.23, 127.72, 127.66, 126.59, 126.31, 126.27, 126.18, 126.12, 125.89, 125.84, 125.81, 125.43, 125.27, 106.35, 106.14, 72.78, 72.18, 70.23, 70.08, 64.72, 64.38, 60.69, 60.52, 50.68, 27.89, 27.78. IR (KBr, cm^{-1}): 3055, 2925, 2847, 1695, 1600, 1521, 1505, 1453, 1324, 1228, 1077, 780. HRMS (ESI): calcd for $C_{30}H_{24}FeNO$ $[M+H]^+$ 470.1202, found 470.1184. The enantiomeric excess was determined by Daicel Chiralpak IA-3 (0.46 cm x 25 cm), Hexanes / IPA = 95 / 5, 0.8 mL/min, λ = 250 nm, t (major) = 11.2 min, t (minor) = 16.7 min.

(Z)-1-ethyl-3-(naphthalen-1-yl(phenyl)methylene)ferrocene[1,2-d]pyrrol-2(1H)-one(6b)

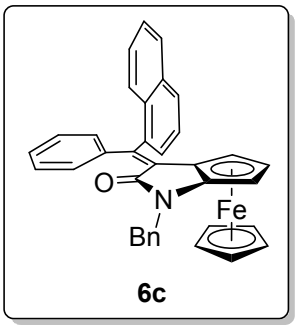


6b

Purple solid (39 mg, 81% yield, 77% ee). Analytical data for **6b**: m.p. = 203.1-204.9℃, $[\alpha]_D^{20}$ = -1395 (c = 0.009 $CHCl_3$, 77% ee). ^1H NMR (400 MHz, $CDCl_3$) δ 8.05 – 7.15 (m, 12H), 4.06 (s, 3H), 3.98 (d, *J* = 6.7 Hz, 1H), 3.79 (s, 2H), 3.76 (s, 1H), 3.63 (s, 1H), 3.50 (s, 1H), 2.39 (s, 3H), 1.39-1.17 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.22, 167.96, 145.35, 144.84, 140.06, 139.90, 138.51, 138.13, 134.15,

133.96, 130.47, 130.45, 130.22, 130.19, 129.28, 129.26, 128.55, 128.51, 128.47, 128.42, 128.34, 128.28, 127.72, 127.67, 126.63, 126.26, 126.23, 126.19, 126.14, 125.88, 125.87, 125.82, 125.45, 125.33, 105.36, 105.15, 72.62, 71.91, 70.56, 70.41, 64.82, 64.48, 60.64, 60.40, 51.22, 51.12, 36.39, 36.23, 13.70. IR (KBr, cm^{-1}): 3054, 2975, 2928, 2853, 1694, 1516, 1454, 1320, 1261, 1089, 795, 695. HRMS (ESI): calcd for $C_{31}H_{26}FeNO$ $[M+H]^+$ 484.1358, found 484.1347. The enantiomeric excess was determined by Daicel Chiralpak IA-3 (0.46 cm x 25 cm), Hexanes / IPA = 95 / 5, 0.8 mL/min, λ = 250 nm, t (major) = 9.0 min, t (minor) = 10.9 min.

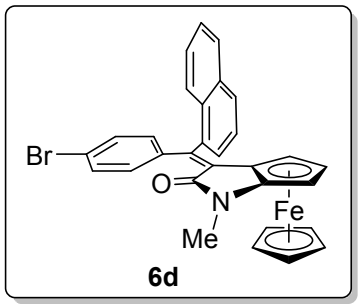
(Z)-1-benzyl-3-(naphthalen-1-yl(phenyl)methylene)ferrocene[1,2-d]pyrrol-2(1H)-one(6c)



6c

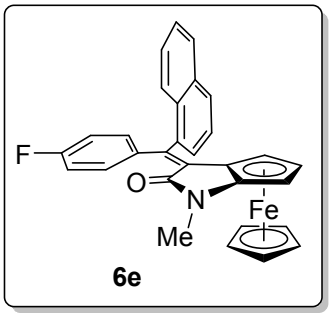
Purple solid (44.8 mg, 82% yield, 74% ee). Analytical data for **6c**: m.p. =235.6-237.2℃. $[\alpha]_D^{20}$ = -1645 (c = 0.008 $CHCl_3$, 74% ee). ^1H NMR (400 MHz, $CDCl_3$) δ 8.20 – 7.10 (m, 17H), 4.70 (dd, *J* = 40.9, 11.8 Hz, 2H), 3.86 (s, 3H), 3.78 (s, 1H), 3.72 (s, 1H), 3.63 (s, 2H), 2.42 (d, *J* = 13.2 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.47, 168.21, 145.62, 145.25, 140.06, 139.77, 138.46, 138.19, 136.68, 136.64, 134.11, 133.97, 130.43, 130.02, 129.99, 129.37, 129.29, 129.06, 128.80, 128.74, 128.72, 128.60, 128.54, 128.33, 128.28, 128.00, 127.91, 127.78, 127.73, 126.62, 126.33, 126.27, 126.19, 126.13, 125.87, 125.85, 125.44, 125.27, 105.05, 104.86, 72.72, 71.99, 70.38, 70.22, 64.91, 64.57, 60.46, 60.12, 51.68, 51.58, 45.88, 45.68. IR (KBr, cm^{-1}): 2923, 2852, 1691, 1630, 1514, 1451, 1384, 1310, 1199, 1104, 695. HRMS (ESI): calcd for $C_{36}H_{28}FeNO$ $[M+H]^+$ 546.1515, found 546.1502. The enantiomeric excess was determined by Daicel Chiralpak IA-3 (0.46 cm x 25 cm), Hexanes / IPA = 95 / 5, 0.8 mL/min, λ = 250 nm, t (major) = 12.4 min, t (minor) = 16.0 min.

(Z)-3-[(4-bromophenyl)(naphthalen-1-yl)methylene]-1-methylferrocene[1,2-d]pyrrol-2(1H)-one(6d)



Purple solid (38.8 mg, 70% yield, 91% ee). Analytical data for **6d**: m.p. = 207.2-208.5℃. $[\alpha]_D^{20}$ = -978 (c = 0.008 $CHCl_3$, 91% ee). ^1H NMR (400 MHz, $CDCl_3$) δ 8.10 – 7.20 (m, 11H), 4.13 (s, 3H), 4.02 (s, 1H), 3.85 (s, 3H), 3.08 (s, 3H), 2.49 (d, *J* = 26.6 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.67, 168.44, 143.56, 143.21, 139.56, 139.23, 137.33, 137.02, 134.13, 134.02, 130.98, 130.92, 130.86, 130.77, 130.69, 130.34, 130.33, 128.77, 128.66, 128.48, 128.43, 126.73, 126.46, 126.42, 126.30, 126.24, 125.95, 125.89, 125.55, 125.26, 125.23, 122.71, 122.69, 106.34, 106.12, 72.50, 71.89, 70.30, 70.16, 64.97, 64.61, 60.85, 60.59, 50.94, 50.90, 27.91, 27.79. IR (KBr, cm^{-1}): 3057, 2923, 2852, 1697, 1520, 1486, 1453,1324, 1073, 1009, 784. HRMS (ESI): calcd for $C_{30}H_{23}BrFeNO$ $[M+H]^+$ 548.0307, found 548.0289. The enantiomeric excess was determined by Daicel Chiralpak IA-3 (0.46 cm x 25 cm), Hexanes / IPA = 95 / 5, 0.8 mL/min, λ = 250 nm, t (major) = 13.1 min, t (minor) = 28.9 min.

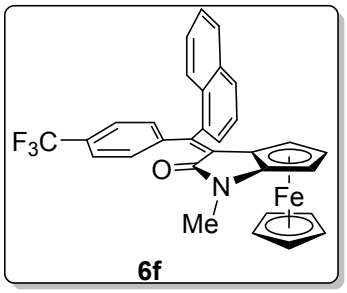
(Z)-3-[(4-fluorophenyl)(naphthalen-1-yl)methylene]-1-methylferrocene[1,2-d] pyrrol-2(1H)-one(6e)



Purple solid (43.5 mg, 89% yield, 93% ee). Analytical data for **6e**: m.p. =210-212℃, $[\alpha]_D^{20}$ = -1785 (c = 0.008 $CHCl_3$, 93% ee). ^1H NMR (400 MHz, $CDCl_3$) δ 8.10 – 7.19 (m, 9H), 6.97 (s, 2H), 4.14 (s, 3H), 4.01 (s, 1H), 3.85 (s, 2H), 3.80 (s, 1H), 3.09 (s, 3H), 2.47 (d, *J* = 24.9 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.81, 168.58, 162.72 (d, *J* = 249.7 Hz), 143.98, 143.64, 139.86, 139.52, 134.35 (d, *J* = 3.4 Hz), 134.14, 134.09 (d, *J* = 3.4 Hz), 134.03, 131.35 (d, *J* = 8.3 Hz), 131.25 (d, *J* = 8.3 Hz), 130.37, 130.20, 130.12, 128.70, 128.63, 128.41, 126.67, 126.42, 126.38, 126.27, 126.20,

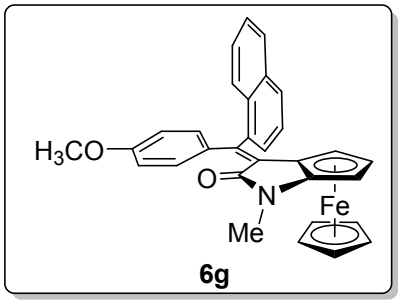
125.90, 125.64, 125.28, 125.27, 114.75 (d, J = 21.6 Hz), 114.69 (d, J = 21.6 Hz), 106.23, 106.02, 72.71, 72.13, 70.25, 70.10, 64.83, 64.46, 60.75, 60.49, 50.80, 50.76, 27.91, 27.79. ^{19}F NMR (376 MHz, $CDCl_3$) δ -112.50, -112.61. IR (KBr, cm^{-1}): 3056, 2925, 1695, 1599,1521, 1505, 1453, 1324,1228, 1077, 782. HRMS (ESI): calcd for $C_{30}H_{23}FFeNO$ $[M+H]^+$ 488.1108, found 488.1094. The enantiomeric excess was determined by Daicel Chiralpak IA-3 (0.46 cm x 25 cm), Hexanes / IPA = 95 / 5, 0.8 mL/min, λ = 250 nm, t (major) = 11.5 min, t (minor) = 21.5 min.

(Z)-1-methyl-3-[naphthalen-1-yl(4-(trifluoromethyl)phenyl)methylene]ferrocene [1,2-d]pyrrol-2(1H)-one(6f)



Purple solid (44.4 mg, 83% yield, 89% ee). Analytical data for **6f**: m.p. = 207.2 - 209.1℃. $[\alpha]_D^{20}$ = -4432 (c = 0.008 $CHCl_3$, 89% ee). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 – 7.11 (m, 11H), 4.07 (s, 3H), 3.97 (s, 1H), 3.80 (s, 3H), 3.01 (s, 3H), 2.47 (d, J = 28.9 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.52, 168.31, 142.78, 142.45, 142.12, 141.78, 139.37, 139.04, 134.14, 134.04, 131.88, 131.80, 130.25, 130.23, 130.05 (d, J = 1.0 Hz), 129.73 (d, J = 1.0 Hz), 129.55, 129.47, 128.91, 128.75, 128.62, 128.52, 126.82, 126.50, 126.41, 126.37, 126.33, 125.94, 125.45, 125.31, 125.13, 124.71 (q, J = 3.8 Hz), 124.67 (q, J = 3.8 Hz), 124.20 (q, J = 273.2 Hz), 106.49, 106.29, 72.07, 71.42, 70.40, 70.25, 65.20, 64.88, 60.98, 60.82, 51.18, 51.17, 27.90, 27.80, 26.94. ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.64, -62.65. IR (KBr, cm^{-1}): 3051, 2923, 2847, 1699, 1520, 1453, 1323, 1123, 1067, 780. HRMS (ESI): calcd for $C_{31}H_{23}F_3FeNO$ $[M+H]^+$ 538.1076, found 538.1072. The enantiomeric excess was determined by Daicel Chiralpak IA-3 (0.46 cm x 25 cm), Hexanes / IPA = 95 / 5, 0.8 mL/min, λ = 250 nm, t (major) = 9.6 min, t (minor) = 20.1 min.

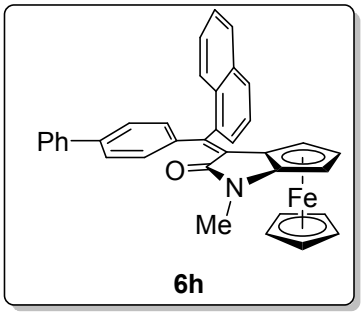
(Z)-3-((4-methoxyphenyl)(naphthalen-1-yl)methylene)-1-methylferrocene[1,2-d] pyrrol-2(1H)-one(6g)



6g

Purple solid (34.6 mg, 69% yield, 88% ee). Analytical data for **6g**: m.p. = 161-162.6 ℃. $[\alpha]_D^{20}$ = -2329 (c = 0.009 $CHCl_3$, 88% ee). ^1H NMR (400 MHz, $CDCl_3$) δ 8.07-7.06 (m, 10H), 6.84 (s, 1H), 4.12 (s, 3H), 3.98 (s, 1H), 3.84 (s, 2H), 3.77 (s, 1H), 3.73 (s, 3H), 3.07 (s, 3H), 2.45 (d, *J* = 24.5 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ168.68, 168.47, 158.95, 158.90, 144.92, 144.57, 139.99, 139.78, 139.64, 139.51, 134.09, 133.98, 130.47, 130.37, 128.63, 128.56, 128.53, 128.51, 128.32, 128.22, 126.58, 126.26, 126.22, 126.18, 126.12, 125.89, 125.80, 125.72, 125.39, 125.27, 122.06, 122.00, 115.36, 115.28, 113.46, 113.36, 106.40, 106.17, 72.72, 72.11, 70.22, 70.08, 64.74, 64.39, 60.74, 60.53, 55.23, 50.67, 27.94, 27.81. IR (KBr, cm^{-1}): 3055, 2956, 2930, 2828, 1697, 1595, 1576, 1520, 1457, 1324, 1282, 1076, 783. HRMS (ESI): calcd for $C_{31}H_{26}FeNO_2$ $[M+H]^+$ 500.1307, found 500.1298. The enantiomeric excess was determined by Daicel Chiralpak IA-3 (0.46 cm x 25 cm), Hexanes / IPA = 95 / 5, 0.8 mL/min, λ = 250 nm, t (major) = 14.4 min, t (minor) = 18.5 min.

(Z)-3-([1,1'-biphenyl]-4-yl(naphthalen-1-yl)methylene)-1-methylferrocene[1,2-d]pyrrol-2(1H)-one(6h)

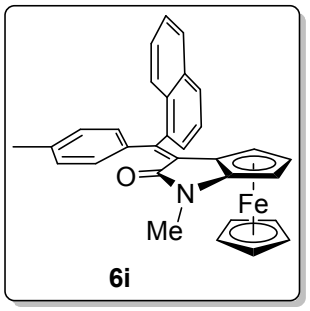


6h

Purple solid (38.3 mg, 70% yield, 91% ee). Analytical data for **6h**: m.p. = 234.6-236.1 ℃. $[\alpha]_D^{20}$ = -1186 (c = 0.010 $CHCl_3$, 91% ee). ^1H NMR (400 MHz, $CDCl_3$) δ 8.08 – 6.96 (m, 16H), 4.07 (s, 3H), 3.94 (s, 1H), 3.78 (s, 2H), 3.73 (s, 1H), 3.03 (s, 3H), 2.39 (d, *J* = 22.7 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.89, 168.68, 144.86, 144.50, 141.15, 141.11, 140.85, 140.08, 139.73, 137.34, 137.10, 134.13, 134.02, 130.55, 130.53, 130.24, 130.16, 129.90, 129.85, 128.74, 128.58, 128.36, 128.30, 127.33, 127.07, 127.05, 126.66, 126.41, 126.37, 126.34, 126.24, 126.18, 125.95,

125.91, 125.87, 125.44, 125.32, 106.29, 106.08, 72.93, 72.32, 70.27, 70.11, 64.81, 64.47, 60.75, 60.56, 50.75, 27.94, 27.83. HRMS (ESI): calcd for $C_{36}H_{28}FeNO$ $[M+H]^+$ 546.1515, found 546.1504. The enantiomeric excess was determined by Daicel Chiralpak IA-3 (0.46 cm x 25 cm), Hexanes / IPA = 95 / 5, 0.8 mL/min, λ = 250 nm, t (major) = 23.5 min, t (minor) = 49.0 min.

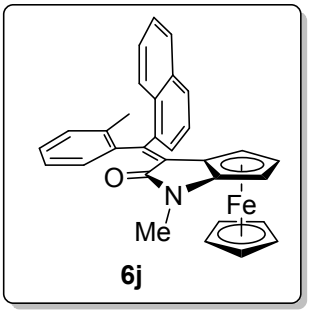
(Z)-1-methyl-3-(naphthalen-1-yl(p-tolyl)methylene)ferrocene[1,2-d]pyrrol-2(1H)-one(6i)



6i

Purple solid (43 mg, 89% yield, 87% ee). Analytical data for **6i**: m.p. =235.8-237.8 ℃. $[\alpha]_D^{20}$ = -1770 (c = 0.008 $CHCl_3$, 87% ee). ^1H NMR (400 MHz, $CDCl_3$) δ 8.16 – 7.20 (m, 9H), 7.10 (s, 2H), 4.12 (s, 2H), 3.98 (s, 1H), 3.83 (s, 2H), 3.76 (s, 1H), 3.08 (s, 3H), 2.44 (d, *J* = 22.9 Hz, 1H), 2.29 (s, 3H). NMR (101 MHz, $CDCl_3$) δ 168.92, 168.70, 145.62, 145.25, 140.22, 139.87, 138.62, 138.56, 135.56, 135.31, 134.10, 133.99, 130.55, 130.54, 129.59, 129.51, 129.31, 129.26, 128.53, 128.49, 128.44, 128.32, 128.17, 126.58, 126.32, 126.26, 126.17, 126.11, 125.90, 125.89, 125.80, 125.48, 125.29, 106.24, 106.04, 73.04, 72.46, 70.20, 70.05, 64.62, 64.28, 60.62, 60.41, 50.58, 50.57, 27.90, 27.78, 21.53, 21.52. IR (KBr, cm^{-1}): 2955, 2923, 2952, 1698, 1521, 1455, 1324, 1289, 1076, 781. HRMS (ESI): calcd for $C_{31}H_{26}FeNO$ $[M+H]^+$ 484.1358, found 484.1343. The enantiomeric excess was determined by Daicel Chiralpak IA-3 (0.46 cm x 25 cm), Hexanes / IPA = 95 / 5, 0.8 mL/min, λ = 250 nm, t (major) = 12.1 min, t (minor) = 20.7 min.

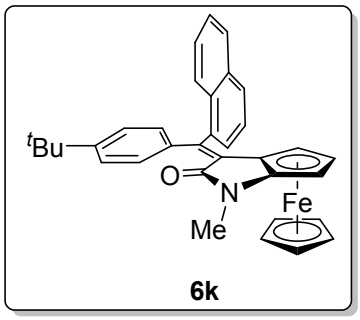
(Z)-1-methyl-3-(naphthalen-1-yl(o-tolyl)methylene)ferrocene[1,2-d]pyrrol-2(1H)-one(6j)



6j

Purple solid (32.2 mg, 67% yield, 89% ee). Analytical data for **6j**: m.p. =198.6-199.9℃. $[\alpha]_D^{20}$ = -1713 (c = 0.008 $CHCl_3$, 89% ee). ^1H NMR (400 MHz, $CDCl_3$) δ 8.15 – 6.98 (m, 11H), 4.12 (s, 3H), 3.98 (s, 1H), 3.85 (s, 2H), 3.77 (s, 1H), 3.08 (s, 3H), 2.44 (d, *J* = 23.3 Hz, 1H), 2.28 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.81, 168.61, 145.61, 145.23, 140.19, 139.86, 138.41, 138.14, 137.24, 137.20, 134.09, 133.97, 130.50, 130.48, 130.07, 130.00, 129.48, 129.44, 129.38, 129.32, 128.54, 128.43, 128.32, 128.15, 127.53, 127.48, 126.67, 126.59, 126.25, 126.22, 126.17, 126.11, 125.92, 125.89, 125.72, 125.47, 125.32, 106.34, 106.15, 72.81, 72.23, 70.21, 70.06, 64.65, 64.32, 60.63, 60.51, 50.62, 27.93, 27.81, 26.95, 21.55. IR (KBr, cm^{-1}): 3045, 2923, 2854, 1697,1521, 1452, 1384, 1324, 1289, 1076, 783. HRMS (ESI): calcd for $C_{31}H_{26}FeNO$ $[M+H]^+$ 484.1358, found 484.1347. The enantiomeric excess was determined by Daicel Chiralpak IA-3 (0.46 cm x 25 cm), Hexanes / IPA = 95 / 5, 0.8 mL/min, λ = 250 nm, t (major) = 9.7 min, t (minor) = 12.8 min.

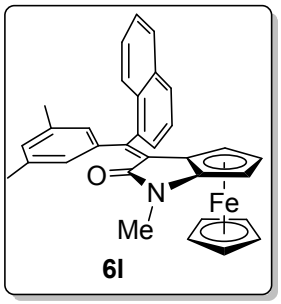
(Z)-3-((4-(tert-butyl)phenyl)(naphthalen-1-yl)methylene)-1-methylferrocene [1,2-d]pyrrol-2(1H)-one(6k)



6k

Purple solid (21.9 mg, 41% yield, 89% ee). Analytical data for **6k**: m.p. =124-126℃. $[\alpha]_D^{20}$ = -1395 (c = 0.01 $CHCl_3$, 89% ee). ^1H NMR (400 MHz, $CDCl_3$) δ 8.15 – 7.20 (m, 11H), 4.12 (s, 3H), 3.99 (s, 1H), 3.83 (s, 2H), 3.77 (s, 1H), 3.09 (s, 3H), 2.41 (d, *J* = 26.0 Hz, 1H), 1.28 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.94, 168.74, 151.56, 151.53, 145.61, 145.31, 140.31, 139.88, 135.20, 135.06, 134.06, 133.97, 130.56, 130.53, 129.54, 129.47, 129.10, 129.07, 128.49, 128.38, 128.28, 128.08, 126.54, 126.20, 126.18, 126.16, 126.09, 126.05, 125.95, 125.70, 125.50, 125.28, 124.65, 124.60, 106.14, 105.96, 73.09, 72.48, 70.19, 69.99, 64.61, 64.29, 60.55, 60.43, 50.56, 50.52, 34.73, 31.22, 27.91, 27.81. IR (KBr, cm^{-1}): 3055, 2960, 2866, 1698, 1521, 1453, 1324, 1290, 1076, 777. HRMS (ESI): calcd for $C_{34}H_{32}FeNO$ $[M+H]^+$ 526.1828, found 526.1818. The enantiomeric excess was determined by Daicel Chiralpak IA-3 (0.46 cm x 25 cm), Hexanes / IPA = 95 / 5, 0.8 mL/min, λ = 250 nm, t (major) = 8.6 min, t (minor) = 13.6 min.

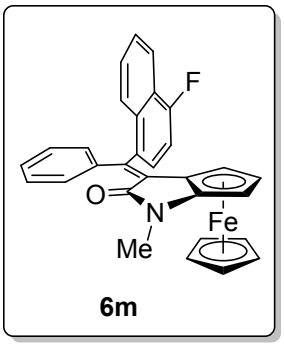
(Z)-3-((3,5-dimethylphenyl)(naphthalen-1-yl)methylene)-1-methylferrocene[1,2-d] pyrrol-2(1H)-one(6l)



6l

Purple solid (40.8 mg, 82% yield, 82% ee). Analytical data for **6l**: m.p. = 208.9-210.5℃. $[\alpha]_D^{20}$ = -2292 (c = 0.008 $CHCl_3$, 82% ee) .^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 – 7.10 (m, 9H), 6.93 (s, 1H), 4.11 (s, 3H), 3.97 (s, 1H), 3.85 (s, 2H), 3.74 (s, 1H), 3.07 (s, 3H), 2.39 (d, *J* = 20.8 Hz, 1H), 2.27 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.76, 168.58, 145.87, 145.47, 140.33, 140.02, 138.36, 138.10, 136.99, 136.94, 134.07, 133.94, 130.51, 130.48, 130.39, 130.31, 129.94, 129.87, 128.51, 128.31, 128.30, 128.04, 126.87, 126.82, 126.57, 126.23, 126.14, 126.10, 126.09, 125.94, 125.60, 125.51, 125.36, 106.36, 106.20, 72.83, 72.31, 70.19, 70.01, 64.55, 64.24, 60.53, 60.52, 50.53, 50.50, 27.97, 27.85, 21.46. IR (KBr, cm^{-1}): 2956, 2917, 1698, 1567, 1518, 1450, 1384, 1324, 1127, 876, 781, 618. HRMS (ESI): calcd for $C_{32}H_{28}FeNO$ $[M+H]^+$ 498.1515, found 498.1502. The enantiomeric excess was determined by Daicel Chiralpak IA-3 (0.46 cm x 25 cm), Hexanes / IPA = 95 / 5, 0.8 mL/min, λ = 250 nm, t (major) = 7.8 min, t (minor) = 9.8 min.

(Z)-3-((4-fluoronaphthalen-1-yl)(phenyl)methylene)-1-methylferrocene[1,2-d] pyrrol-2(1H)-one(6m)

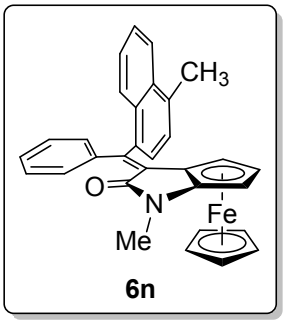


6m

Purple solid (40 mg, 82% yield, 89% ee). Analytical data for **6m**: m.p. = 222-224 ℃. $[\alpha]_D^{20}$ = -1306 (c = 0.012 $CHCl_3$, 89% ee). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 – 7.07 (m, 11H), 4.13 (s, 3H), 4.02 (s, 1H), 3.86 (s, 2H), 3.83 (s, 1H), 3.08 (s, 3H), 2.57 (d, *J* = 19.8 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.62, 168.51, 158.7 (d, *J* = 254.4 Hz), 158.5 (d, *J* = 254.0 Hz), 144.38, 144.03, 138.46, 138.15, 136.10 (d, *J* = 4.6 Hz),

135.81 (d, *J* = 4.6 Hz), 131.95, 131.90, 130.70, 130.56, 129.30, 129.23, 128.62, 128.57, 127.78, 127.72, 127.60, 127.26, 126.54 (d, *J* = 1.8 Hz), 126.51 (d, *J* = 1.8 Hz), 126.26 (d, *J* = 8.3 Hz), 125.84 (d, *J* = 8.3 Hz), 125.79 (d, *J* = 2.6 Hz), 125.50 (d, *J* = 2.6 Hz), 124.29 (d, *J* = 16.4 Hz), 124.19 (d, *J* = 16.3 Hz), 121.16 (d, *J* = 5.5 Hz), 120.88 (d, *J* = 5.5 Hz), 109.58 (d, *J* = 20.1 Hz), 109.00 (d, *J* = 20.2 Hz), 106.41, 106.20, 72.62, 72.02, 70.26, 70.14, 64.86, 64.52, 60.73, 60.46, 50.88, 50.83, 27.93, 27.80. ^{19}F NMR (376 MHz, $CDCl_3$) δ -121.86, -122.31. IR (KBr, cm^{-1}): 3063, 2929, 1599, 1520, 1455, 1391, 1324, 1289, 1078, 763, 734, 695. HRMS (ESI): calcd for $C_{30}H_{23}FFeNO$ $[M+H]^+$ 488.1108, found 488.1103. The enantiomeric excess was determined by Daicel Chiralpak AD-H (0.46 cm x 25 cm), Hexanes / IPA = 95 / 5, 0.8 mL/min, λ = 250 nm, t (major) = 10.3 min, t (minor) = 16.7 min.

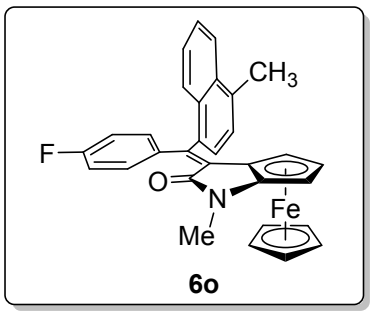
(Z)-1-methyl-3-((4-methylnaphthalen-1-yl)(phenyl)methylene)ferrocene[1,2-d] pyrrol-2(1H)-one(6n)



6n

Purple solid (36.1 mg, 75% yield, 95% ee). Analytical data for **6n**: m.p. = 230-232.1 ℃. $[\alpha]_D^{20}$ = -1690 (c = 0.01 $CHCl_3$, 95% ee). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 – 7.15 (m, 11H), 4.14 (s, 3H), 4.00 (s, 1H), 3.86 (s, 2H), 3.79 (s, 1H), 3.08 (s, 3H), 2.78 (s, 3H), 2.54 (d, *J* = 33.8 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.91, 168.70, 145.78, 145.43, 138.70, 138.47, 138.42, 138.10, 134.96, 134.65, 133.18, 133.09, 130.49, 130.06, 129.95, 129.31, 129.23, 128.45, 128.40, 127.68, 127.63, 126.63, 126.44, 126.19, 126.11, 126.07, 126.03, 125.99, 125.93, 125.89, 125.51, 124.71, 124.47, 106.30, 106.08, 72.96, 72.40, 70.23, 70.09, 64.67, 64.32, 60.81, 60.55, 50.65, 50.63, 27.91, 27.79, 19.84, 19.72. IR (KBr, cm^{-1}): 3055, 2956, 2926, 2847, 1698, 1633, 1520, 1454, 1384, 1324, 1289, 1077, 755. HRMS (ESI): calcd for $C_{31}H_{26}FeNO$ $[M+H]^+$ 484.1358, found 484.1348. The enantiomeric excess was determined by Daicel Chiralpak IA-3 (0.46 cm x 25 cm), Hexanes / IPA = 95 / 5, 0.8 mL/min, λ = 250 nm, t (major) = 10.6 min, t (minor) = 13.7 min.

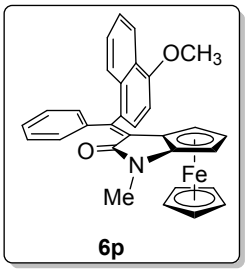
(Z)-3-((4-fluorophenyl)(4-methylnaphthalen-1-yl)methylene)-1-methylferrocene [1,2-d]pyrrol-2(1H)-one(6o)



6o

Purple solid (37.1 mg, 75% yield, 91% ee). Analytical data for **6o**: m.p. = 211.7-213.5 ℃. $[\alpha]_D^{20}$ = -2469 (c = 0.008 $CHCl_3$, 92% ee). ^1H NMR (400 MHz, $CDCl_3$) δ 8.19 – 7.15 (m, 8H), 6.96 (s, 2H), 4.14 (s, 3H), 4.01 (s, 1H), 3.85 (s, 2H), 3.81 (s, 1H), 3.09 (s, 3H), 2.79 (s, 3H), 2.54 (d, *J* = 33.5 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.90, 168.68, 162.69 (d, *J* = 248.6 Hz), 144.43, 144.08, 138.22, 137.85, 135.19, 134.86, 134.62, 134.59, 134.37, 134.33, 133.23, 133.15, 131.39, 131.31, 131.24, 130.40, 130.10, 129.98, 126.62, 126.25, 126.20, 126.06, 126.00, 125.97, 125.92, 125.60, 124.78, 124.53, 114.68 (d, *J* = 21.7 Hz), 114.63 (d, *J* = 21.7 Hz), 106.19, 105.98, 72.90, 72.34, 70.24, 70.10, 64.76, 64.38, 60.86, 60.52, 50.75, 50.69, 27.91, 27.78, 19.81, 19.69. ^{19}F NMR (376 MHz, $CDCl_3$) δ -112.67, -112.79. IR (KBr, cm-1): 2955, 2922, 1694, 1586, 1520, 1461, 1324, 1238, 1079, 765, 695. HRMS (ESI): calcd for $C_{31}H_{26}FeNO_2$ [M+H]+ 502.1264, found 502.1247. The enantiomeric excess was determined by Daicel Chiralpak AZ-H (0.46 cm x 25 cm), Hexanes / IPA = 97 / 3, 0.8 mL/min, λ = 250 nm, t (major) = 30.6 min, t (minor) = 39.7 min.

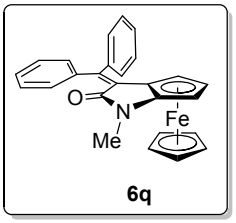
(Z)-3-((4-methoxynaphthalen-1-yl)(phenyl)methylene)-1-methylferrocene[1,2-d] pyrrol-2(1H)-one(6p)



6p

Purple solid (36 mg, 72% yield, 89% ee). Analytical data for **6p**: m.p. =176.1-178.3℃. $[\alpha]_D^{20}$ = -2191 (c = 0.012 $CHCl_3$, 89% ee). ^1H NMR (400 MHz, $CDCl_3$) δ 8.44 – 6.77 (m, 11H), 4.20 – 3.95 (m, 7H), 3.85 (s, 2H), 3.81 (s, 1H), 3.08 (s, 3H), 2.66 (d, *J* = 37.7 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.97, 168.80, 155.67, 155.41, 145.76, 145.46, 139.02, 138.66, 132.49, 132.08, 131.51, 130.23, 129.94, 129.39, 129.29, 128.45, 128.38, 127.67, 127.62, 127.04, 126.80, 126.78, 126.14, 126.03, 125.94, 125.59, 125.51, 125.41, 125.34, 122.45, 122.24, 106.32, 106.07, 103.62, 103.02,

73.18, 72.63, 70.18, 70.13, 64.65, 64.25, 60.89, 60.58, 55.70, 55.63, 50.65, 50.59, 27.92, 27.78. IR (KBr, cm^{-1}): 2955, 2922, 1694, 1586, 1520, 1461, 1324, 1238, 1079, 765, 695. HRMS (ESI): calcd for $C_{31}H_{26}FeNO_2$ $[M+H]^+$ 500.1307, found 500.1295. The enantiomeric excess was determined by Daicel Chiralpak IA-3 (0.46 cm x 25 cm), Hexanes / IPA = 95 / 5, 0.8 mL/min, λ = 250 nm, t (major) = 12.7 min, t (minor) = 16.0 min.

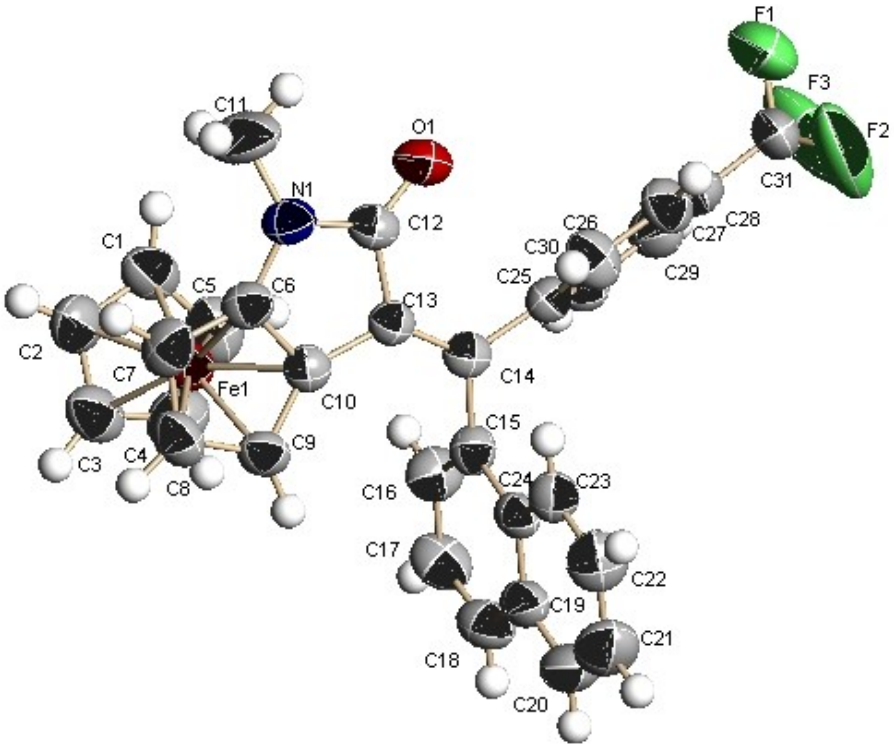


6q

Purple solid (40% yield, 86% ee); Analytical data for 6q: $[\alpha]_D^{20}$ = -1669 (c = 0.012 $CHCl_3$, 86% ee). Mp: 235.8-237.8 ℃. ^1H NMR (400 MHz, $CDCl_3$) δ 7.53 – 7.48 (m, 2H), 7.45 – 7.38 (m, 2H), 7.36 – 7.33 (m, 3H), 7.32 – 7.28 (m, 2H), 4.23 (s, 5H), 4.11 (dd, *J* = 2.4, 0.8 Hz, 1H), 4.06 (t, *J* = 2.4 Hz, 1H), 3.66 (dd, *J* = 2.4, 0.8 Hz, 1H), 3.05 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.12, 146.54, 142.17, 140.02, 129.63, 129.40, 128.37, 128.22, 128.14, 127.79, 107.18, 71.68, 70.19, 64.76, 60.07, 50.70, 27.88. IR (KBr, cm^{-1}): 3045, 2920, 2850, 1700, 1598, 1523, 1445, 1288, 1078, 750, 679. HRMS (ESI): calcd for $C_{26}H_{22}FeNO$ $[M+H]^+$ 420.1045, found 420.1044.

[a] The number of carbons is more than those of molecular formula, and there are two N-Me carbons in **6a-q**. The NMR spectra seems to indicate the existence of the diastereomers of planar and axial chirality. The variable-temperature H-NMR of **6a** were carried out in CD_2Cl_2 to investigate the stability of the axial chirality. There is obvious change on the spectrums of ^{1}HNMR from 183K to 308K. The result indicates that the axial chirality in our products is not stable.

6. X-ray crystal structure of enantiopure 6d



The crystal of enantiopure **6f** was obtained through slow evaporation from its solution in diethyl ether and *n*-hexane. The structure and absolute configuration of **6f**were then determined by X-ray crystallography.

Table 1. Crystal data and structure refinement for 1.

Identification code	1
Empirical formula	C31 H22 F3 Fe N O
Formula weight	537.35
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 10.501(2) A alpha = 90 deg.
	b = 12.436(3) A beta = 90 deg.

	c = 19.235(4) A gamma = 90 deg.
Volume	2511.9(9) A^3
Z, Calculated density	4, 1.421 Mg/m^3
Absorption coefficient	0.648 mm^-1
F(000)	1104
Crystal size	? x ? x ? mm
Theta range for data collection	1.95 to 28.33 deg.
Limiting indices	-13<=h<=13, -16<=k<=16, -25<=l<=25
Reflections collected / unique	22786 / 6212 [R(int) = 0.0454]
Completeness to theta = 28.33	99.7 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6212 / 0 / 334
Goodness-of-fit on F^2	1.023
Final R indices [I>2sigma(I)]	R1 = 0.0478, wR2 = 0.1157
R indices (all data)	R1 = 0.0931, wR2 = 0.1346
Absolute structure parameter	0.00(2)
Largest diff. peak and hole	0.338 and -0.224 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 1. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Fe(1)	3908(1)	2976(1)	7717(1)	61(1)
C(24)	7838(3)	1994(3)	6000(2)	54(1)
C(13)	6774(3)	3601(2)	7340(2)	50(1)
C(10)	5846(3)	2825(2)	7603(2)	53(1)
C(23)	8960(4)	1779(3)	6376(2)	62(1)
O(1)	7540(3)	5227(2)	7937(1)	73(1)
N(1)	6198(3)	4047(2)	8480(1)	63(1)
C(15)	7016(3)	2859(3)	6163(2)	56(1)
C(14)	7354(3)	3647(3)	6726(2)	52(1)
C(6)	5537(3)	3112(3)	8293(2)	60(1)
C(25)	8305(3)	4486(3)	6538(2)	58(1)
C(31)	10932(5)	6975(4)	6047(2)	88(1)
C(29)	8906(5)	6005(3)	5842(2)	75(1)
C(1)	2885(4)	4369(3)	7758(3)	84(1)
C(12)	6924(3)	4395(3)	7931(2)	57(1)
C(16)	5904(4)	2988(3)	5799(2)	71(1)
C(30)	8061(4)	5193(3)	6000(2)	64(1)

C(27)	10298(4)	5403(3)	6732(2)	76(1)
C(17)	5582(4)	2294(3)	5255(2)	78(1)
C(3)	2050(4)	2753(4)	7462(3)	88(1)
C(26)	9447(3)	4599(3)	6898(2)	75(1)
C(9)	5211(3)	1830(3)	7458(2)	61(1)
C(19)	7520(4)	1299(3)	5442(2)	65(1)
C(8)	4531(4)	1551(3)	8073(2)	73(1)
C(21)	9441(5)	276(4)	5636(3)	96(2)
C(7)	4730(4)	2340(3)	8588(2)	75(1)
C(22)	9749(4)	943(4)	6200(2)	84(1)
C(5)	3264(4)	4152(4)	7075(3)	88(1)
C(20)	8336(5)	450(4)	5273(2)	87(1)
C(28)	10036(4)	6103(3)	6205(2)	68(1)
C(2)	2141(4)	3516(4)	8001(3)	86(1)
C(4)	2705(4)	3146(4)	6892(2)	87(1)
C(18)	6365(4)	1490(3)	5067(2)	73(1)
F(1)	11022(4)	7721(3)	6496(2)	170(2)
C(11)	5931(6)	4712(4)	9078(2)	111(2)
F(2)	12092(4)	6660(3)	5979(4)	229(3)
F(3)	10740(6)	7478(4)	5485(2)	227(3)

Table 3. Bond lengths [A] and angles [deg] for 1.

Fe(1)-C(8)	2.010(4)
Fe(1)-C(5)	2.030(4)
Fe(1)-C(3)	2.031(4)
Fe(1)-C(9)	2.038(3)
Fe(1)-C(4)	2.038(4)
Fe(1)-C(1)	2.040(4)
Fe(1)-C(6)	2.045(4)
Fe(1)-C(7)	2.045(4)
Fe(1)-C(2)	2.048(4)
Fe(1)-C(10)	2.055(3)
C(24)-C(23)	1.408(5)
C(24)-C(15)	1.415(5)
C(24)-C(19)	1.416(5)
C(13)-C(14)	1.330(4)
C(13)-C(10)	1.462(4)
C(13)-C(12)	1.514(4)
C(10)-C(6)	1.412(4)

C(10)-C(9)	1.433(4)
C(23)-C(22)	1.371(5)
C(23)-H(23A)	0.9300
O(1)-C(12)	1.221(4)
N(1)-C(12)	1.371(4)
N(1)-C(6)	1.402(5)
N(1)-C(11)	1.444(5)
C(15)-C(16)	1.370(5)
C(15)-C(14)	1.504(4)
C(14)-C(25)	1.490(5)
C(6)-C(7)	1.401(5)
C(25)-C(30)	1.382(5)
C(25)-C(26)	1.392(5)
C(31)-F(3)	1.265(6)
C(31)-F(1)	1.272(5)
C(31)-F(2)	1.287(6)
C(31)-C(28)	1.467(5)
C(29)-C(30)	1.379(5)
C(29)-C(28)	1.382(6)
C(29)-H(29A)	0.9300
C(1)-C(5)	1.400(6)
C(1)-C(2)	1.398(6)
C(1)-H(1A)	0.9800
C(16)-C(17)	1.399(5)
C(16)-H(16A)	0.9300
C(30)-H(30A)	0.9300
C(27)-C(28)	1.364(5)
C(27)-C(26)	1.379(6)
C(27)-H(27A)	0.9300
C(17)-C(18)	1.344(6)
C(17)-H(17A)	0.9300
C(3)-C(4)	1.383(6)
C(3)-C(2)	1.408(6)
C(3)-H(3A)	0.9800
C(26)-H(26A)	0.9300
C(9)-C(8)	1.425(5)
C(9)-H(9A)	0.9800
C(19)-C(20)	1.398(6)
C(19)-C(18)	1.432(5)
C(8)-C(7)	1.409(6)
C(8)-H(8A)	0.9800
C(21)-C(20)	1.372(6)
C(21)-C(22)	1.404(6)
C(21)-H(21A)	0.9300

C(7)-H(7A)	0.9800
C(22)-H(22A)	0.9300
C(5)-C(4)	1.427(7)
C(5)-H(5A)	0.9800
C(20)-H(20A)	0.9300
C(2)-H(2A)	0.9800
C(4)-H(4A)	0.9800
C(18)-H(18A)	0.9300
C(11)-H(11A)	0.9600
C(11)-H(11B)	0.9600
C(11)-H(11C)	0.9600

C(8)-Fe(1)-C(5)	162.06(19)
C(8)-Fe(1)-C(3)	105.93(17)
C(5)-Fe(1)-C(3)	68.40(19)
C(8)-Fe(1)-C(9)	41.22(15)
C(5)-Fe(1)-C(9)	125.39(18)
C(3)-Fe(1)-C(9)	119.37(16)
C(8)-Fe(1)-C(4)	123.95(18)
C(5)-Fe(1)-C(4)	41.06(18)
C(3)-Fe(1)-C(4)	39.73(18)
C(9)-Fe(1)-C(4)	107.37(16)
C(8)-Fe(1)-C(1)	155.09(19)
C(5)-Fe(1)-C(1)	40.22(18)
C(3)-Fe(1)-C(1)	67.65(17)
C(9)-Fe(1)-C(1)	163.19(17)
C(4)-Fe(1)-C(1)	67.42(19)
C(8)-Fe(1)-C(6)	67.39(15)
C(5)-Fe(1)-C(6)	123.27(18)
C(3)-Fe(1)-C(6)	161.01(18)
C(9)-Fe(1)-C(6)	68.20(14)
C(4)-Fe(1)-C(6)	158.66(18)
C(1)-Fe(1)-C(6)	110.43(17)
C(8)-Fe(1)-C(7)	40.67(16)
C(5)-Fe(1)-C(7)	156.6(2)
C(3)-Fe(1)-C(7)	123.39(19)
C(9)-Fe(1)-C(7)	69.27(15)
C(4)-Fe(1)-C(7)	159.95(18)
C(1)-Fe(1)-C(7)	121.26(19)
C(6)-Fe(1)-C(7)	40.06(15)
C(8)-Fe(1)-C(2)	119.54(18)
C(5)-Fe(1)-C(2)	67.93(19)
C(3)-Fe(1)-C(2)	40.40(17)
C(9)-Fe(1)-C(2)	154.55(17)

C(4)-Fe(1)-C(2)	67.16(19)
C(1)-Fe(1)-C(2)	40.00(17)
C(6)-Fe(1)-C(2)	125.90(16)
C(7)-Fe(1)-C(2)	106.90(18)
C(8)-Fe(1)-C(10)	68.46(14)
C(5)-Fe(1)-C(10)	109.35(16)
C(3)-Fe(1)-C(10)	155.94(16)
C(9)-Fe(1)-C(10)	40.99(13)
C(4)-Fe(1)-C(10)	122.73(16)
C(1)-Fe(1)-C(10)	127.12(15)
C(6)-Fe(1)-C(10)	40.27(13)
C(7)-Fe(1)-C(10)	68.50(14)
C(2)-Fe(1)-C(10)	162.89(16)
C(23)-C(24)-C(15)	122.8(3)
C(23)-C(24)-C(19)	118.0(3)
C(15)-C(24)-C(19)	119.2(3)
C(14)-C(13)-C(10)	129.9(3)
C(14)-C(13)-C(12)	126.2(3)
C(10)-C(13)-C(12)	103.9(3)
C(6)-C(10)-C(9)	107.1(3)
C(6)-C(10)-C(13)	108.1(3)
C(9)-C(10)-C(13)	144.4(3)
C(6)-C(10)-Fe(1)	69.47(19)
C(9)-C(10)-Fe(1)	68.84(19)
C(13)-C(10)-Fe(1)	129.5(2)
C(22)-C(23)-C(24)	121.6(4)
C(22)-C(23)-H(23A)	119.2
C(24)-C(23)-H(23A)	119.2
C(12)-N(1)-C(6)	109.9(3)
C(12)-N(1)-C(11)	122.7(3)
C(6)-N(1)-C(11)	125.7(3)
C(16)-C(15)-C(24)	119.7(3)
C(16)-C(15)-C(14)	119.5(3)
C(24)-C(15)-C(14)	120.8(3)
C(13)-C(14)-C(25)	123.6(3)
C(13)-C(14)-C(15)	120.3(3)
C(25)-C(14)-C(15)	116.1(3)
N(1)-C(6)-C(7)	139.9(3)
N(1)-C(6)-C(10)	109.7(3)
C(7)-C(6)-C(10)	110.3(3)
N(1)-C(6)-Fe(1)	128.4(2)
C(7)-C(6)-Fe(1)	70.0(2)
C(10)-C(6)-Fe(1)	70.26(19)
C(30)-C(25)-C(26)	118.0(4)

C(30)-C(25)-C(14)	120.2(3)
C(26)-C(25)-C(14)	121.8(3)
F(3)-C(31)-F(1)	103.4(5)
F(3)-C(31)-F(2)	102.4(5)
F(1)-C(31)-F(2)	102.7(5)
F(3)-C(31)-C(28)	116.2(5)
F(1)-C(31)-C(28)	116.5(4)
F(2)-C(31)-C(28)	113.8(4)
C(30)-C(29)-C(28)	120.4(4)
C(30)-C(29)-H(29A)	119.8
C(28)-C(29)-H(29A)	119.8
C(5)-C(1)-C(2)	109.0(4)
C(5)-C(1)-Fe(1)	69.5(2)
C(2)-C(1)-Fe(1)	70.3(2)
C(5)-C(1)-H(1A)	125.5
C(2)-C(1)-H(1A)	125.5
Fe(1)-C(1)-H(1A)	125.5
O(1)-C(12)-N(1)	123.7(3)
O(1)-C(12)-C(13)	127.9(3)
N(1)-C(12)-C(13)	108.3(3)
C(15)-C(16)-C(17)	121.0(4)
C(15)-C(16)-H(16A)	119.5
C(17)-C(16)-H(16A)	119.5
C(29)-C(30)-C(25)	120.7(4)
C(29)-C(30)-H(30A)	119.6
C(25)-C(30)-H(30A)	119.6
C(28)-C(27)-C(26)	120.3(4)
C(28)-C(27)-H(27A)	119.8
C(26)-C(27)-H(27A)	119.8
C(18)-C(17)-C(16)	120.8(4)
C(18)-C(17)-H(17A)	119.6
C(16)-C(17)-H(17A)	119.6
C(4)-C(3)-C(2)	108.1(4)
C(4)-C(3)-Fe(1)	70.4(2)
C(2)-C(3)-Fe(1)	70.4(2)
C(4)-C(3)-H(3A)	125.9
C(2)-C(3)-H(3A)	125.9
Fe(1)-C(3)-H(3A)	125.9
C(27)-C(26)-C(25)	121.1(4)
C(27)-C(26)-H(26A)	119.5
C(25)-C(26)-H(26A)	119.5
C(8)-C(9)-C(10)	106.3(3)
C(8)-C(9)-Fe(1)	68.4(2)
C(10)-C(9)-Fe(1)	70.18(18)

C(8)-C(9)-H(9A)	126.8
C(10)-C(9)-H(9A)	126.8
Fe(1)-C(9)-H(9A)	126.8
C(20)-C(19)-C(24)	119.5(4)
C(20)-C(19)-C(18)	121.8(4)
C(24)-C(19)-C(18)	118.7(4)
C(7)-C(8)-C(9)	109.9(3)
C(7)-C(8)-Fe(1)	71.0(2)
C(9)-C(8)-Fe(1)	70.4(2)
C(7)-C(8)-H(8A)	125.1
C(9)-C(8)-H(8A)	125.1
Fe(1)-C(8)-H(8A)	125.1
C(20)-C(21)-C(22)	119.7(4)
C(20)-C(21)-H(21A)	120.2
C(22)-C(21)-H(21A)	120.2
C(6)-C(7)-C(8)	106.4(3)
C(6)-C(7)-Fe(1)	70.0(2)
C(8)-C(7)-Fe(1)	68.3(2)
C(6)-C(7)-H(7A)	126.8
C(8)-C(7)-H(7A)	126.8
Fe(1)-C(7)-H(7A)	126.8
C(23)-C(22)-C(21)	119.9(4)
C(23)-C(22)-H(22A)	120.1
C(21)-C(22)-H(22A)	120.1
C(1)-C(5)-C(4)	106.4(4)
C(1)-C(5)-Fe(1)	70.3(2)
C(4)-C(5)-Fe(1)	69.8(3)
C(1)-C(5)-H(5A)	126.8
C(4)-C(5)-H(5A)	126.8
Fe(1)-C(5)-H(5A)	126.8
C(21)-C(20)-C(19)	121.2(4)
C(21)-C(20)-H(20A)	119.4
C(19)-C(20)-H(20A)	119.4
C(27)-C(28)-C(29)	119.5(4)
C(27)-C(28)-C(31)	119.8(4)
C(29)-C(28)-C(31)	120.7(4)
C(1)-C(2)-C(3)	107.7(4)
C(1)-C(2)-Fe(1)	69.7(2)
C(3)-C(2)-Fe(1)	69.2(2)
C(1)-C(2)-H(2A)	126.2
C(3)-C(2)-H(2A)	126.2
Fe(1)-C(2)-H(2A)	126.2
C(3)-C(4)-C(5)	108.7(4)
C(3)-C(4)-Fe(1)	69.9(3)

C(5)-C(4)-Fe(1)	69.2(3)
C(3)-C(4)-H(4A)	125.7
C(5)-C(4)-H(4A)	125.7
Fe(1)-C(4)-H(4A)	125.7
C(17)-C(18)-C(19)	120.4(4)
C(17)-C(18)-H(18A)	119.8
C(19)-C(18)-H(18A)	119.8
N(1)-C(11)-H(11A)	109.5
N(1)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
N(1)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 1. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Fe(1)	58(1)	51(1)	75(1)	1(1)	5(1)	1(1)
C(24)	61(2)	48(2)	52(2)	6(2)	3(1)	-9(2)
C(13)	49(2)	47(2)	55(2)	-1(2)	-3(2)	3(1)
C(10)	53(2)	49(2)	57(2)	3(2)	0(1)	4(2)
C(23)	63(2)	54(2)	68(2)	6(2)	3(2)	4(2)
O(1)	82(2)	56(1)	83(2)	-9(1)	-4(1)	-4(1)
N(1)	75(2)	62(2)	53(2)	-7(1)	-2(2)	-1(2)
C(15)	54(2)	63(2)	50(2)	4(2)	0(1)	-1(2)
C(14)	50(2)	51(2)	57(2)	0(2)	-5(2)	5(2)
C(6)	70(2)	54(2)	56(2)	-1(2)	-1(2)	3(2)
C(25)	56(2)	56(2)	61(2)	-7(2)	6(2)	2(2)
C(31)	91(3)	72(3)	100(3)	-15(3)	33(3)	-28(3)
C(29)	102(3)	60(2)	64(2)	4(2)	14(2)	-10(3)
C(1)	61(2)	56(2)	134(4)	-8(3)	1(3)	10(2)
C(12)	59(2)	52(2)	59(2)	-3(2)	-9(2)	-1(2)
C(16)	66(2)	75(2)	72(2)	-2(2)	-12(2)	8(2)

C(30)	69(2)	67(2)	57(2)	-4(2)	-6(2)	-4(2)
C(27)	50(2)	76(3)	101(3)	-8(2)	-2(2)	-5(2)
C(17)	78(3)	85(3)	71(2)	5(2)	-26(2)	-13(2)
C(3)	59(2)	73(3)	133(4)	-8(3)	-4(2)	0(2)
C(26)	53(2)	74(3)	97(3)	11(2)	-12(2)	1(2)
C(9)	65(2)	46(2)	72(2)	-3(2)	-1(2)	1(2)
C(19)	81(2)	56(2)	59(2)	-1(2)	11(2)	-13(2)
C(8)	70(2)	58(2)	89(3)	13(2)	3(2)	-8(2)
C(21)	113(4)	61(3)	116(4)	-4(3)	16(3)	12(3)
C(7)	92(3)	70(3)	63(2)	17(2)	13(2)	6(2)
C(22)	82(3)	74(3)	96(3)	12(2)	-4(2)	17(2)
C(5)	68(3)	83(3)	114(4)	22(3)	-2(3)	12(2)
C(20)	109(3)	67(3)	85(3)	-16(2)	13(3)	-13(3)
C(28)	72(2)	55(2)	76(2)	-12(2)	17(2)	2(2)
C(2)	62(2)	82(3)	114(3)	-11(3)	13(2)	7(2)
C(4)	80(3)	94(3)	87(3)	-6(3)	-7(2)	20(3)
C(18)	88(3)	67(2)	64(2)	-2(2)	-11(2)	-15(2)
F(1)	190(3)	127(3)	193(3)	-61(3)	65(3)	-86(3)
C(11)	173(5)	96(3)	63(2)	-22(2)	11(3)	-12(4)
F(2)	117(3)	106(3)	463(9)	10(4)	130(4)	-22(2)
F(3)	291(7)	231(5)	158(3)	77(3)	-44(4)	-186(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 1.

	x	y	z	U(eq)
H(23A)	9171	2214	6751	74
H(29A)	8715	6491	5490	90
H(1A)	3116	5010	8026	101
H(16A)	5354	3546	5917	85
H(30A)	7318	5119	5741	77
H(27A)	11053	5469	6981	91
H(17A)	4816	2389	5020	93
H(3A)	1585	2070	7483	106
H(26A)	9640	4124	7256	90
H(9A)	5246	1418	7024	73
H(8A)	4004	907	8130	87
H(21A)	9983	-282	5509	116

H(7A)	4379	2344	9060	89
H(22A)	10487	818	6455	101
H(5A)	3780	4616	6774	106
H(20A)	8125	-5	4907	105
H(2A)	1757	3456	8464	103
H(4A)	2790	2784	6442	104
H(18A)	6155	1056	4691	88
H(11A)	6512	5308	9087	166
H(11B)	6031	4295	9494	166
H(11C)	5074	4976	9050	166

Table 6. Torsion angles [deg] for 1.

C(14)-C(13)-C(10)-C(6)	178.7(3)
C(12)-C(13)-C(10)-C(6)	-2.6(3)
C(14)-C(13)-C(10)-C(9)	7.0(7)
C(12)-C(13)-C(10)-C(9)	-174.3(4)
C(14)-C(13)-C(10)-Fe(1)	-103.3(4)
C(12)-C(13)-C(10)-Fe(1)	75.4(3)
C(8)-Fe(1)-C(10)-C(6)	-80.0(2)
C(5)-Fe(1)-C(10)-C(6)	119.0(2)
C(3)-Fe(1)-C(10)-C(6)	-160.8(4)
C(9)-Fe(1)-C(10)-C(6)	-118.9(3)
C(4)-Fe(1)-C(10)-C(6)	162.6(2)
C(1)-Fe(1)-C(10)-C(6)	77.5(3)
C(7)-Fe(1)-C(10)-C(6)	-36.1(2)
C(2)-Fe(1)-C(10)-C(6)	41.3(6)
C(8)-Fe(1)-C(10)-C(9)	38.9(2)
C(5)-Fe(1)-C(10)-C(9)	-122.1(2)
C(3)-Fe(1)-C(10)-C(9)	-41.9(5)
C(4)-Fe(1)-C(10)-C(9)	-78.5(3)
C(1)-Fe(1)-C(10)-C(9)	-163.6(2)
C(6)-Fe(1)-C(10)-C(9)	118.9(3)
C(7)-Fe(1)-C(10)-C(9)	82.7(2)
C(2)-Fe(1)-C(10)-C(9)	160.2(5)
C(8)-Fe(1)-C(10)-C(13)	-177.0(3)
C(5)-Fe(1)-C(10)-C(13)	22.0(4)
C(3)-Fe(1)-C(10)-C(13)	102.2(5)
C(9)-Fe(1)-C(10)-C(13)	144.1(4)
C(4)-Fe(1)-C(10)-C(13)	65.6(4)
C(1)-Fe(1)-C(10)-C(13)	-19.5(4)

C(6)-Fe(1)-C(10)-C(13)	-97.0(4)
C(7)-Fe(1)-C(10)-C(13)	-133.2(3)
C(2)-Fe(1)-C(10)-C(13)	-55.7(7)
C(15)-C(24)-C(23)-C(22)	-179.1(3)
C(19)-C(24)-C(23)-C(22)	1.8(5)
C(23)-C(24)-C(15)-C(16)	-176.5(3)
C(19)-C(24)-C(15)-C(16)	2.6(5)
C(23)-C(24)-C(15)-C(14)	4.1(5)
C(19)-C(24)-C(15)-C(14)	-176.8(3)
C(10)-C(13)-C(14)-C(25)	-178.8(3)
C(12)-C(13)-C(14)-C(25)	2.8(5)
C(10)-C(13)-C(14)-C(15)	4.3(5)
C(12)-C(13)-C(14)-C(15)	-174.1(3)
C(16)-C(15)-C(14)-C(13)	76.1(4)
C(24)-C(15)-C(14)-C(13)	-104.5(4)
C(16)-C(15)-C(14)-C(25)	-101.0(4)
C(24)-C(15)-C(14)-C(25)	78.4(4)
C(12)-N(1)-C(6)-C(7)	175.5(5)
C(11)-N(1)-C(6)-C(7)	-19.4(7)
C(12)-N(1)-C(6)-C(10)	0.7(4)
C(11)-N(1)-C(6)-C(10)	165.9(4)
C(12)-N(1)-C(6)-Fe(1)	-79.3(4)
C(11)-N(1)-C(6)-Fe(1)	85.9(5)
C(9)-C(10)-C(6)-N(1)	176.3(3)
C(13)-C(10)-C(6)-N(1)	1.3(4)
Fe(1)-C(10)-C(6)-N(1)	-125.0(3)
C(9)-C(10)-C(6)-C(7)	-0.1(4)
C(13)-C(10)-C(6)-C(7)	-175.1(3)
Fe(1)-C(10)-C(6)-C(7)	58.6(3)
C(9)-C(10)-C(6)-Fe(1)	-58.7(2)
C(13)-C(10)-C(6)-Fe(1)	126.3(2)
C(8)-Fe(1)-C(6)-N(1)	-177.2(4)
C(5)-Fe(1)-C(6)-N(1)	19.2(4)
C(3)-Fe(1)-C(6)-N(1)	-104.4(5)
C(9)-Fe(1)-C(6)-N(1)	138.2(3)
C(4)-Fe(1)-C(6)-N(1)	56.2(6)
C(1)-Fe(1)-C(6)-N(1)	-23.9(4)
C(7)-Fe(1)-C(6)-N(1)	-138.6(4)
C(2)-Fe(1)-C(6)-N(1)	-66.2(4)
C(10)-Fe(1)-C(6)-N(1)	99.9(4)
C(8)-Fe(1)-C(6)-C(7)	-38.6(2)
C(5)-Fe(1)-C(6)-C(7)	157.8(3)
C(3)-Fe(1)-C(6)-C(7)	34.2(6)
C(9)-Fe(1)-C(6)-C(7)	-83.3(2)

C(4)-Fe(1)-C(6)-C(7)	-165.2(4)
C(1)-Fe(1)-C(6)-C(7)	114.7(3)
C(2)-Fe(1)-C(6)-C(7)	72.4(3)
C(10)-Fe(1)-C(6)-C(7)	-121.5(3)
C(8)-Fe(1)-C(6)-C(10)	82.9(2)
C(5)-Fe(1)-C(6)-C(10)	-80.7(3)
C(3)-Fe(1)-C(6)-C(10)	155.7(4)
C(9)-Fe(1)-C(6)-C(10)	38.22(19)
C(4)-Fe(1)-C(6)-C(10)	-43.7(6)
C(1)-Fe(1)-C(6)-C(10)	-123.8(2)
C(7)-Fe(1)-C(6)-C(10)	121.5(3)
C(2)-Fe(1)-C(6)-C(10)	-166.1(2)
C(13)-C(14)-C(25)-C(30)	-117.2(4)
C(15)-C(14)-C(25)-C(30)	59.7(4)
C(13)-C(14)-C(25)-C(26)	61.8(5)
C(15)-C(14)-C(25)-C(26)	-121.2(4)
C(8)-Fe(1)-C(1)-C(5)	-162.1(4)
C(3)-Fe(1)-C(1)-C(5)	-82.5(3)
C(9)-Fe(1)-C(1)-C(5)	35.7(7)
C(4)-Fe(1)-C(1)-C(5)	-39.4(3)
C(6)-Fe(1)-C(1)-C(5)	117.8(3)
C(7)-Fe(1)-C(1)-C(5)	161.0(3)
C(2)-Fe(1)-C(1)-C(5)	-120.3(4)
C(10)-Fe(1)-C(1)-C(5)	75.4(3)
C(8)-Fe(1)-C(1)-C(2)	-41.9(5)
C(5)-Fe(1)-C(1)-C(2)	120.3(4)
C(3)-Fe(1)-C(1)-C(2)	37.7(3)
C(9)-Fe(1)-C(1)-C(2)	155.9(5)
C(4)-Fe(1)-C(1)-C(2)	80.9(3)
C(6)-Fe(1)-C(1)-C(2)	-122.0(3)
C(7)-Fe(1)-C(1)-C(2)	-78.8(3)
C(10)-Fe(1)-C(1)-C(2)	-164.3(2)
C(6)-N(1)-C(12)-O(1)	175.6(3)
C(11)-N(1)-C(12)-O(1)	9.9(6)
C(6)-N(1)-C(12)-C(13)	-2.4(4)
C(11)-N(1)-C(12)-C(13)	-168.1(4)
C(14)-C(13)-C(12)-O(1)	4.0(6)
C(10)-C(13)-C(12)-O(1)	-174.8(3)
C(14)-C(13)-C(12)-N(1)	-178.2(3)
C(10)-C(13)-C(12)-N(1)	3.0(4)
C(24)-C(15)-C(16)-C(17)	-1.8(5)
C(14)-C(15)-C(16)-C(17)	177.6(3)
C(28)-C(29)-C(30)-C(25)	2.4(6)
C(26)-C(25)-C(30)-C(29)	-2.2(5)

C(14)-C(25)-C(30)-C(29)	176.9(3)
C(15)-C(16)-C(17)-C(18)	-1.0(6)
C(8)-Fe(1)-C(3)-C(4)	-124.4(3)
C(5)-Fe(1)-C(3)-C(4)	37.6(3)
C(9)-Fe(1)-C(3)-C(4)	-81.9(3)
C(1)-Fe(1)-C(3)-C(4)	81.1(3)
C(6)-Fe(1)-C(3)-C(4)	169.1(4)
C(7)-Fe(1)-C(3)-C(4)	-165.3(3)
C(2)-Fe(1)-C(3)-C(4)	118.5(4)
C(10)-Fe(1)-C(3)-C(4)	-51.7(5)
C(8)-Fe(1)-C(3)-C(2)	117.1(3)
C(5)-Fe(1)-C(3)-C(2)	-80.9(3)
C(9)-Fe(1)-C(3)-C(2)	159.6(3)
C(4)-Fe(1)-C(3)-C(2)	-118.5(4)
C(1)-Fe(1)-C(3)-C(2)	-37.4(3)
C(6)-Fe(1)-C(3)-C(2)	50.6(6)
C(7)-Fe(1)-C(3)-C(2)	76.3(3)
C(10)-Fe(1)-C(3)-C(2)	-170.2(3)
C(28)-C(27)-C(26)-C(25)	-0.5(6)
C(30)-C(25)-C(26)-C(27)	1.3(6)
C(14)-C(25)-C(26)-C(27)	-177.8(4)
C(6)-C(10)-C(9)-C(8)	0.1(4)
C(13)-C(10)-C(9)-C(8)	171.8(4)
Fe(1)-C(10)-C(9)-C(8)	-59.1(2)
C(6)-C(10)-C(9)-Fe(1)	59.1(2)
C(13)-C(10)-C(9)-Fe(1)	-129.1(5)
C(5)-Fe(1)-C(9)-C(8)	-163.7(3)
C(3)-Fe(1)-C(9)-C(8)	-80.5(3)
C(4)-Fe(1)-C(9)-C(8)	-122.1(3)
C(1)-Fe(1)-C(9)-C(8)	168.8(6)
C(6)-Fe(1)-C(9)-C(8)	80.1(2)
C(7)-Fe(1)-C(9)-C(8)	37.0(2)
C(2)-Fe(1)-C(9)-C(8)	-48.9(5)
C(10)-Fe(1)-C(9)-C(8)	117.7(3)
C(8)-Fe(1)-C(9)-C(10)	-117.7(3)
C(5)-Fe(1)-C(9)-C(10)	78.6(3)
C(3)-Fe(1)-C(9)-C(10)	161.8(2)
C(4)-Fe(1)-C(9)-C(10)	120.2(2)
C(1)-Fe(1)-C(9)-C(10)	51.1(6)
C(6)-Fe(1)-C(9)-C(10)	-37.57(18)
C(7)-Fe(1)-C(9)-C(10)	-80.7(2)
C(2)-Fe(1)-C(9)-C(10)	-166.6(4)
C(23)-C(24)-C(19)-C(20)	-1.7(5)
C(15)-C(24)-C(19)-C(20)	179.2(3)

C(23)-C(24)-C(19)-C(18)	178.4(3)
C(15)-C(24)-C(19)-C(18)	-0.7(5)
C(10)-C(9)-C(8)-C(7)	0.0(4)
Fe(1)-C(9)-C(8)-C(7)	-60.2(3)
C(10)-C(9)-C(8)-Fe(1)	60.2(2)
C(5)-Fe(1)-C(8)-C(7)	168.1(5)
C(3)-Fe(1)-C(8)-C(7)	-123.1(3)
C(9)-Fe(1)-C(8)-C(7)	120.3(3)
C(4)-Fe(1)-C(8)-C(7)	-162.6(3)
C(1)-Fe(1)-C(8)-C(7)	-52.0(5)
C(6)-Fe(1)-C(8)-C(7)	38.0(2)
C(2)-Fe(1)-C(8)-C(7)	-81.6(3)
C(10)-Fe(1)-C(8)-C(7)	81.6(2)
C(5)-Fe(1)-C(8)-C(9)	47.8(6)
C(3)-Fe(1)-C(8)-C(9)	116.6(2)
C(4)-Fe(1)-C(8)-C(9)	77.1(3)
C(1)-Fe(1)-C(8)-C(9)	-172.3(4)
C(6)-Fe(1)-C(8)-C(9)	-82.2(2)
C(7)-Fe(1)-C(8)-C(9)	-120.3(3)
C(2)-Fe(1)-C(8)-C(9)	158.2(2)
C(10)-Fe(1)-C(8)-C(9)	-38.64(19)
N(1)-C(6)-C(7)-C(8)	-174.6(4)
C(10)-C(6)-C(7)-C(8)	0.1(4)
Fe(1)-C(6)-C(7)-C(8)	58.9(3)
N(1)-C(6)-C(7)-Fe(1)	126.4(5)
C(10)-C(6)-C(7)-Fe(1)	-58.8(2)
C(9)-C(8)-C(7)-C(6)	-0.1(4)
Fe(1)-C(8)-C(7)-C(6)	-60.0(3)
C(9)-C(8)-C(7)-Fe(1)	59.9(3)
C(8)-Fe(1)-C(7)-C(6)	117.9(3)
C(5)-Fe(1)-C(7)-C(6)	-52.9(5)
C(3)-Fe(1)-C(7)-C(6)	-167.4(2)
C(9)-Fe(1)-C(7)-C(6)	80.4(2)
C(4)-Fe(1)-C(7)-C(6)	164.3(5)
C(1)-Fe(1)-C(7)-C(6)	-85.0(3)
C(2)-Fe(1)-C(7)-C(6)	-126.2(2)
C(10)-Fe(1)-C(7)-C(6)	36.3(2)
C(5)-Fe(1)-C(7)-C(8)	-170.7(4)
C(3)-Fe(1)-C(7)-C(8)	74.8(3)
C(9)-Fe(1)-C(7)-C(8)	-37.5(2)
C(4)-Fe(1)-C(7)-C(8)	46.4(6)
C(1)-Fe(1)-C(7)-C(8)	157.1(2)
C(6)-Fe(1)-C(7)-C(8)	-117.9(3)
C(2)-Fe(1)-C(7)-C(8)	115.9(3)

C(10)-Fe(1)-C(7)-C(8)	-81.5(2)
C(24)-C(23)-C(22)-C(21)	-0.3(6)
C(20)-C(21)-C(22)-C(23)	-1.5(7)
C(2)-C(1)-C(5)-C(4)	1.4(5)
Fe(1)-C(1)-C(5)-C(4)	60.8(3)
C(2)-C(1)-C(5)-Fe(1)	-59.3(3)
C(8)-Fe(1)-C(5)-C(1)	155.2(5)
C(3)-Fe(1)-C(5)-C(1)	80.5(3)
C(9)-Fe(1)-C(5)-C(1)	-168.1(2)
C(4)-Fe(1)-C(5)-C(1)	116.9(4)
C(6)-Fe(1)-C(5)-C(1)	-82.6(3)
C(7)-Fe(1)-C(5)-C(1)	-44.7(6)
C(2)-Fe(1)-C(5)-C(1)	36.8(3)
C(10)-Fe(1)-C(5)-C(1)	-125.1(3)
C(8)-Fe(1)-C(5)-C(4)	38.3(7)
C(3)-Fe(1)-C(5)-C(4)	-36.4(3)
C(9)-Fe(1)-C(5)-C(4)	75.0(3)
C(1)-Fe(1)-C(5)-C(4)	-116.9(4)
C(6)-Fe(1)-C(5)-C(4)	160.5(3)
C(7)-Fe(1)-C(5)-C(4)	-161.6(4)
C(2)-Fe(1)-C(5)-C(4)	-80.1(3)
C(10)-Fe(1)-C(5)-C(4)	118.0(3)
C(22)-C(21)-C(20)-C(19)	1.6(7)
C(24)-C(19)-C(20)-C(21)	0.0(6)
C(18)-C(19)-C(20)-C(21)	179.9(4)
C(26)-C(27)-C(28)-C(29)	0.6(6)
C(26)-C(27)-C(28)-C(31)	178.2(4)
C(30)-C(29)-C(28)-C(27)	-1.5(6)
C(30)-C(29)-C(28)-C(31)	-179.1(4)
F(3)-C(31)-C(28)-C(27)	168.7(5)
F(1)-C(31)-C(28)-C(27)	-69.1(6)
F(2)-C(31)-C(28)-C(27)	50.1(6)
F(3)-C(31)-C(28)-C(29)	-13.8(7)
F(1)-C(31)-C(28)-C(29)	108.4(6)
F(2)-C(31)-C(28)-C(29)	-132.4(6)
C(5)-C(1)-C(2)-C(3)	-0.1(5)
Fe(1)-C(1)-C(2)-C(3)	-58.9(3)
C(5)-C(1)-C(2)-Fe(1)	58.8(3)
C(4)-C(3)-C(2)-C(1)	-1.3(5)
Fe(1)-C(3)-C(2)-C(1)	59.3(3)
C(4)-C(3)-C(2)-Fe(1)	-60.6(3)
C(8)-Fe(1)-C(2)-C(1)	161.2(3)
C(5)-Fe(1)-C(2)-C(1)	-37.0(3)
C(3)-Fe(1)-C(2)-C(1)	-119.2(4)

C(9)-Fe(1)-C(2)-C(1)	-164.1(4)
C(4)-Fe(1)-C(2)-C(1)	-81.6(3)
C(6)-Fe(1)-C(2)-C(1)	78.9(3)
C(7)-Fe(1)-C(2)-C(1)	118.8(3)
C(10)-Fe(1)-C(2)-C(1)	47.1(7)
C(8)-Fe(1)-C(2)-C(3)	-79.7(3)
C(5)-Fe(1)-C(2)-C(3)	82.2(3)
C(9)-Fe(1)-C(2)-C(3)	-44.9(5)
C(4)-Fe(1)-C(2)-C(3)	37.6(3)
C(1)-Fe(1)-C(2)-C(3)	119.2(4)
C(6)-Fe(1)-C(2)-C(3)	-161.9(3)
C(7)-Fe(1)-C(2)-C(3)	-122.0(3)
C(10)-Fe(1)-C(2)-C(3)	166.3(5)
C(2)-C(3)-C(4)-C(5)	2.2(5)
Fe(1)-C(3)-C(4)-C(5)	-58.4(3)
C(2)-C(3)-C(4)-Fe(1)	60.6(3)
C(1)-C(5)-C(4)-C(3)	-2.3(5)
Fe(1)-C(5)-C(4)-C(3)	58.8(3)
C(1)-C(5)-C(4)-Fe(1)	-61.1(3)
C(8)-Fe(1)-C(4)-C(3)	73.0(3)
C(5)-Fe(1)-C(4)-C(3)	-120.3(4)
C(9)-Fe(1)-C(4)-C(3)	115.3(3)
C(1)-Fe(1)-C(4)-C(3)	-81.7(3)
C(6)-Fe(1)-C(4)-C(3)	-170.3(4)
C(7)-Fe(1)-C(4)-C(3)	38.3(6)
C(2)-Fe(1)-C(4)-C(3)	-38.2(3)
C(10)-Fe(1)-C(4)-C(3)	157.6(2)
C(8)-Fe(1)-C(4)-C(5)	-166.7(3)
C(3)-Fe(1)-C(4)-C(5)	120.3(4)
C(9)-Fe(1)-C(4)-C(5)	-124.4(3)
C(1)-Fe(1)-C(4)-C(5)	38.6(3)
C(6)-Fe(1)-C(4)-C(5)	-50.0(6)
C(7)-Fe(1)-C(4)-C(5)	158.6(5)
C(2)-Fe(1)-C(4)-C(5)	82.1(3)
C(10)-Fe(1)-C(4)-C(5)	-82.1(3)
C(16)-C(17)-C(18)-C(19)	2.9(6)
C(20)-C(19)-C(18)-C(17)	178.1(4)
C(24)-C(19)-C(18)-C(17)	-2.0(5)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for 1 [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)

7. Reference ：

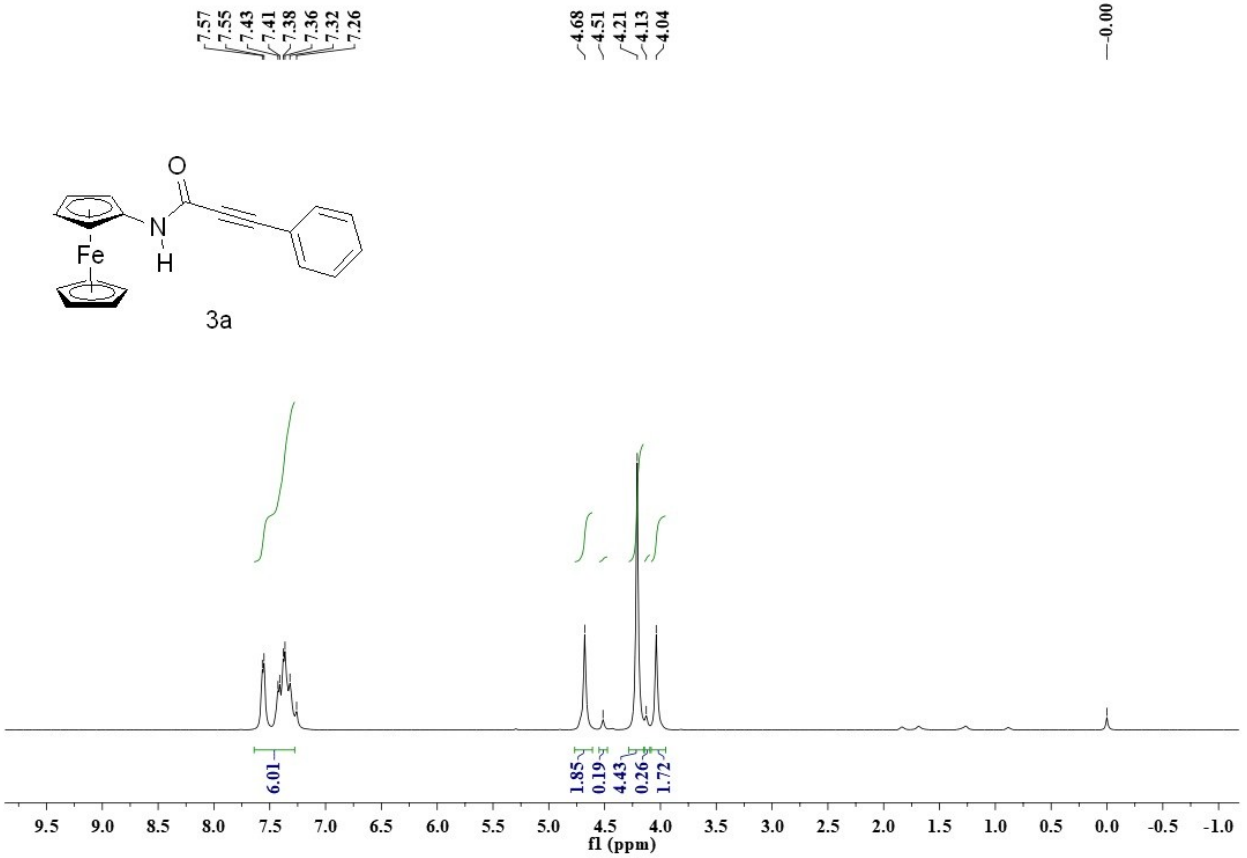
[1] Qian, D.; Zhang, J. Chem. Common. 2012, 48, 7082-7084.

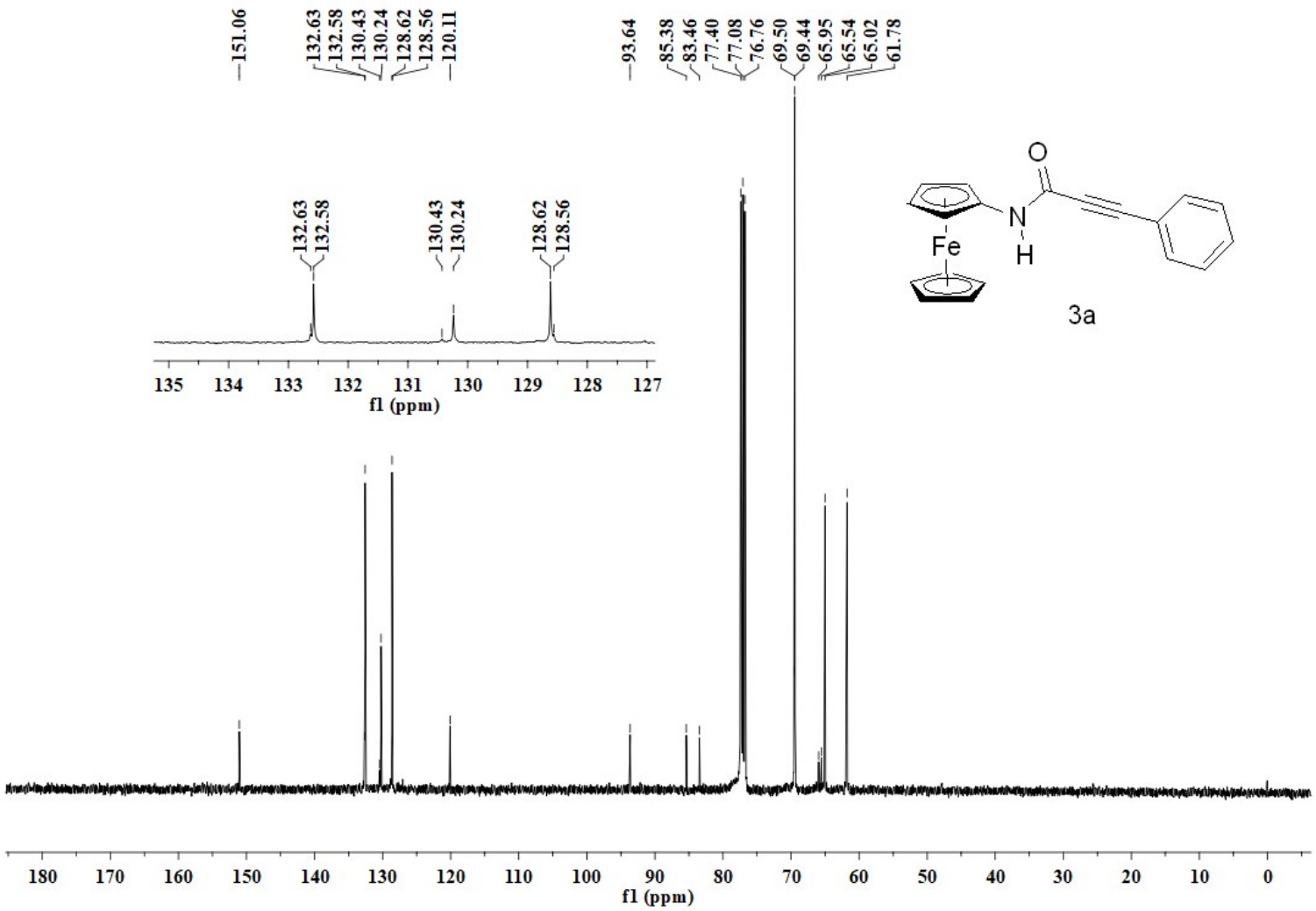
[2] Pinto, A.; Neuville, L.; Retailleau, P.; Zhu, J. Org. Lett. 2006, 8, 4927-4930.

[3] Tang, S.; Peng, P.; Zhong, P.; Li J.-H. J. Org. Chem. 2008, 73, 5476–5480.

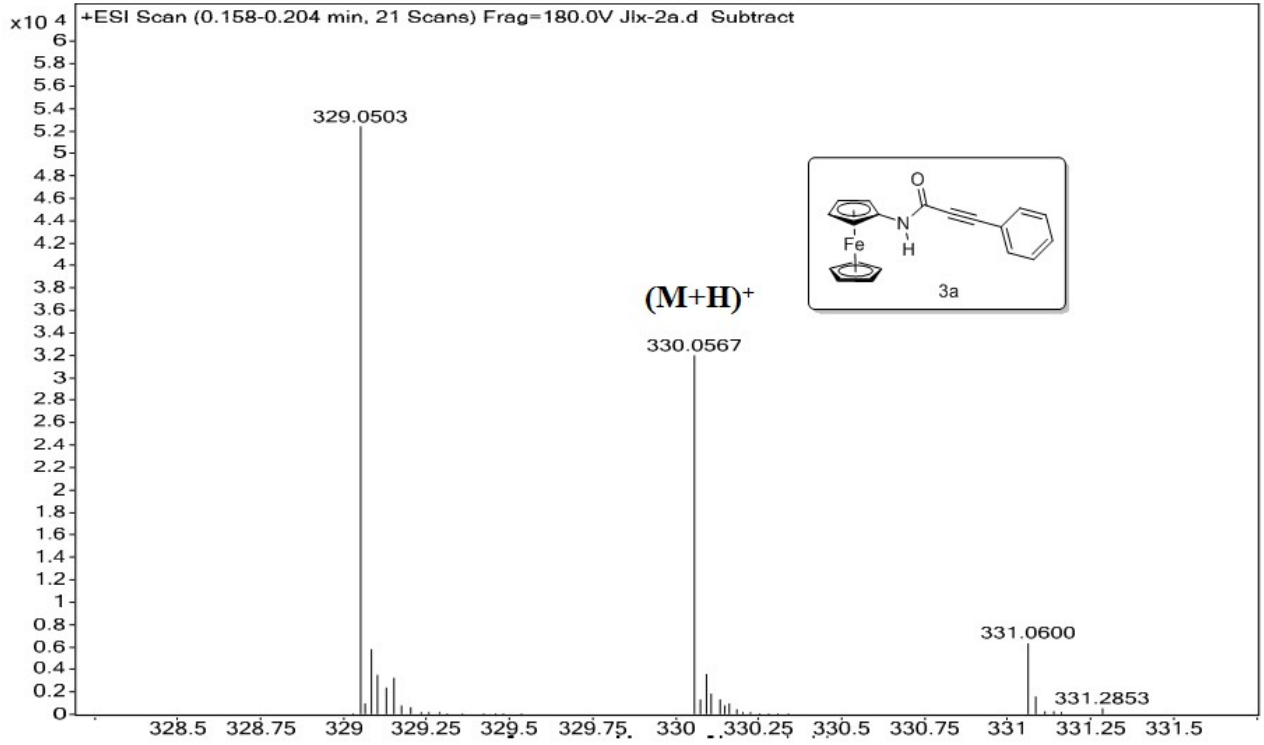
8. NMR 、HMRS Spectra and HPLC Chromatographs

NMR and HMRS Spectra of **3a**

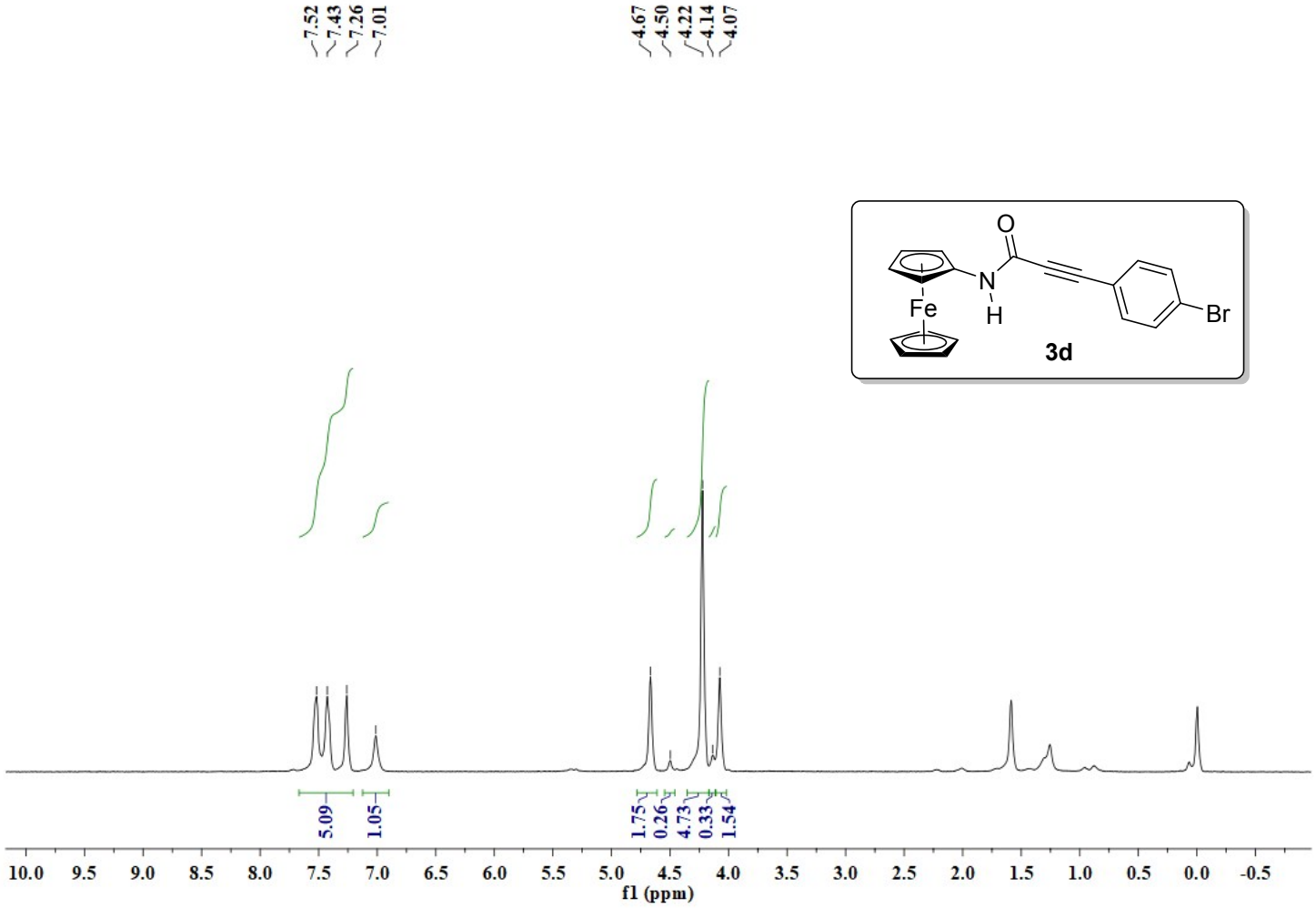


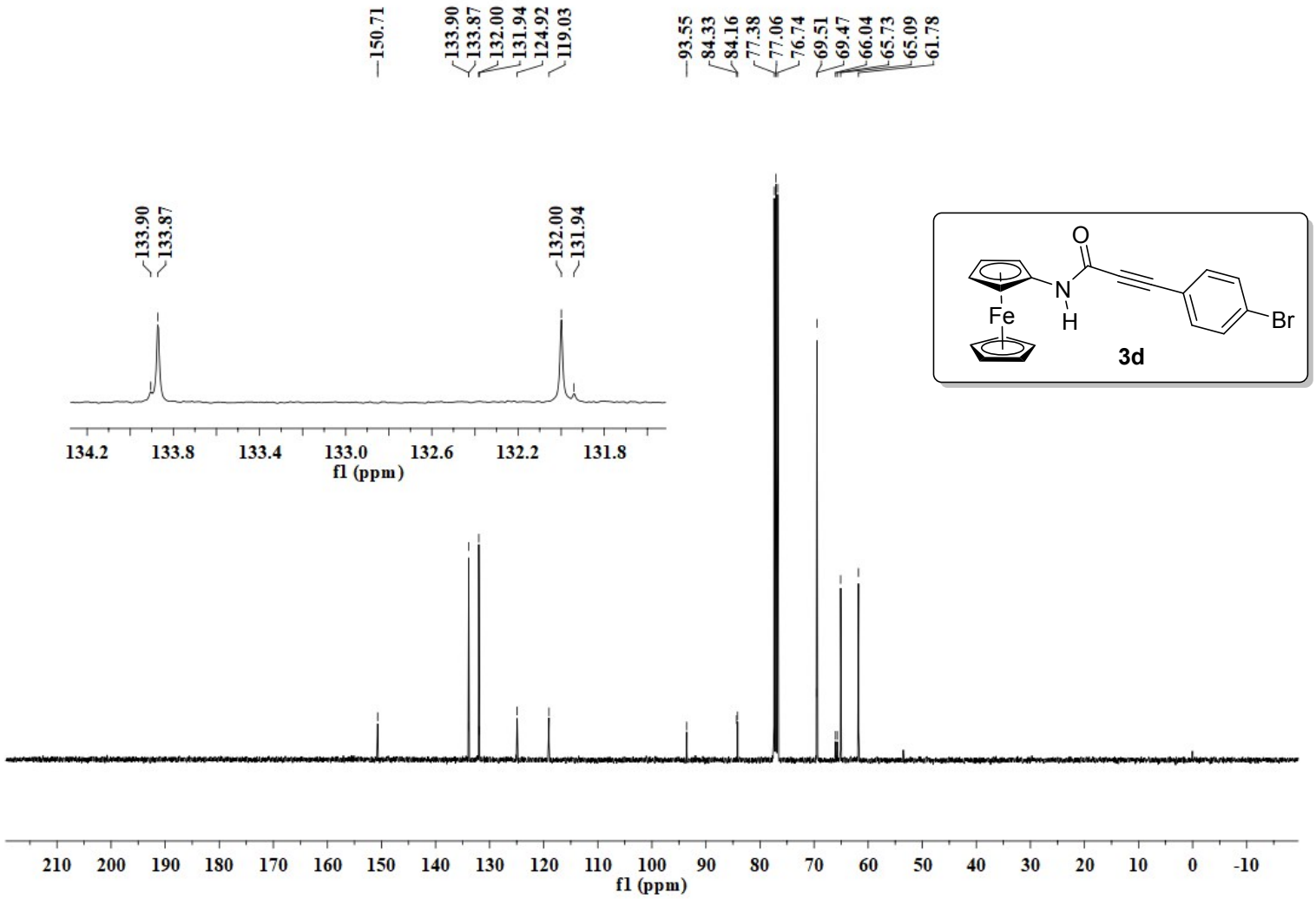

151.06
132.63
132.58
130.43
130.24
128.62
128.56
120.11
93.64
85.38
83.46
77.40
77.08
76.76
69.50
69.44
65.95
65.54
65.02
61.78
O
N
H
Fe
3a
f1 (ppm)
f1 (ppm)

Sample Name	Jlx-2a	**Position**	P1-A1	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	Jlx-2a.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	3/20/18 Tue 16:22:57

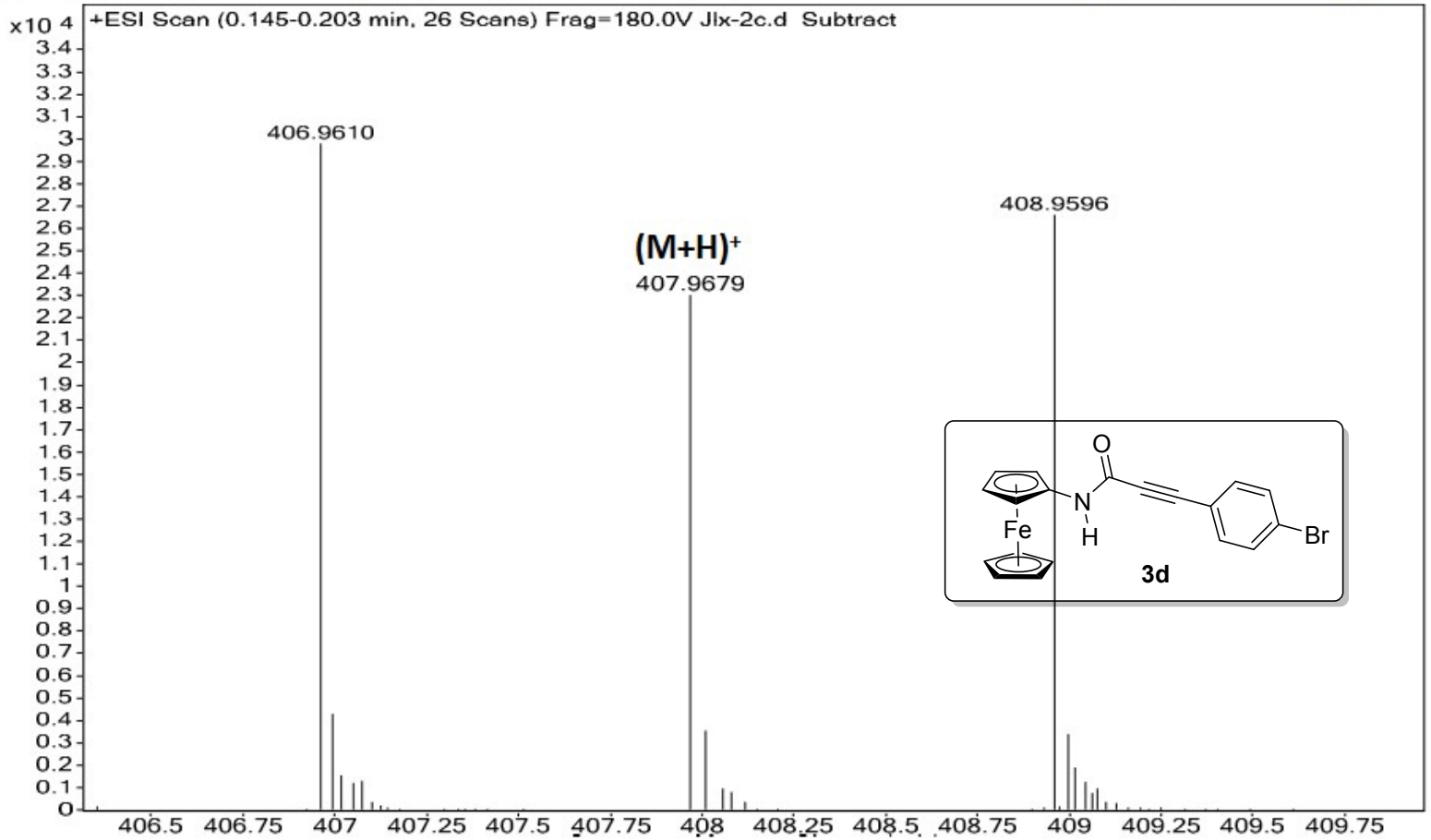


NMR and HMRS Spectra of **3d**

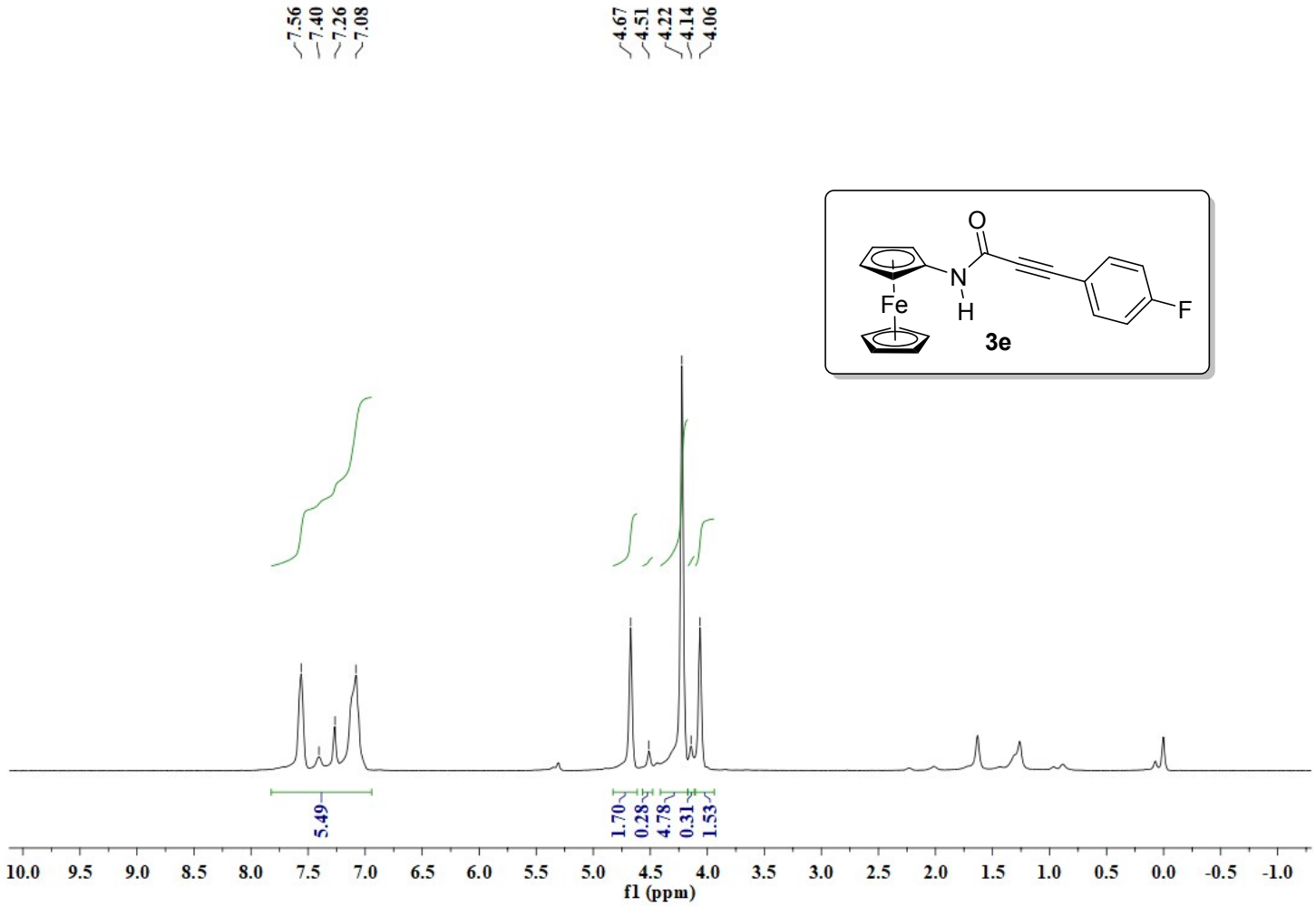


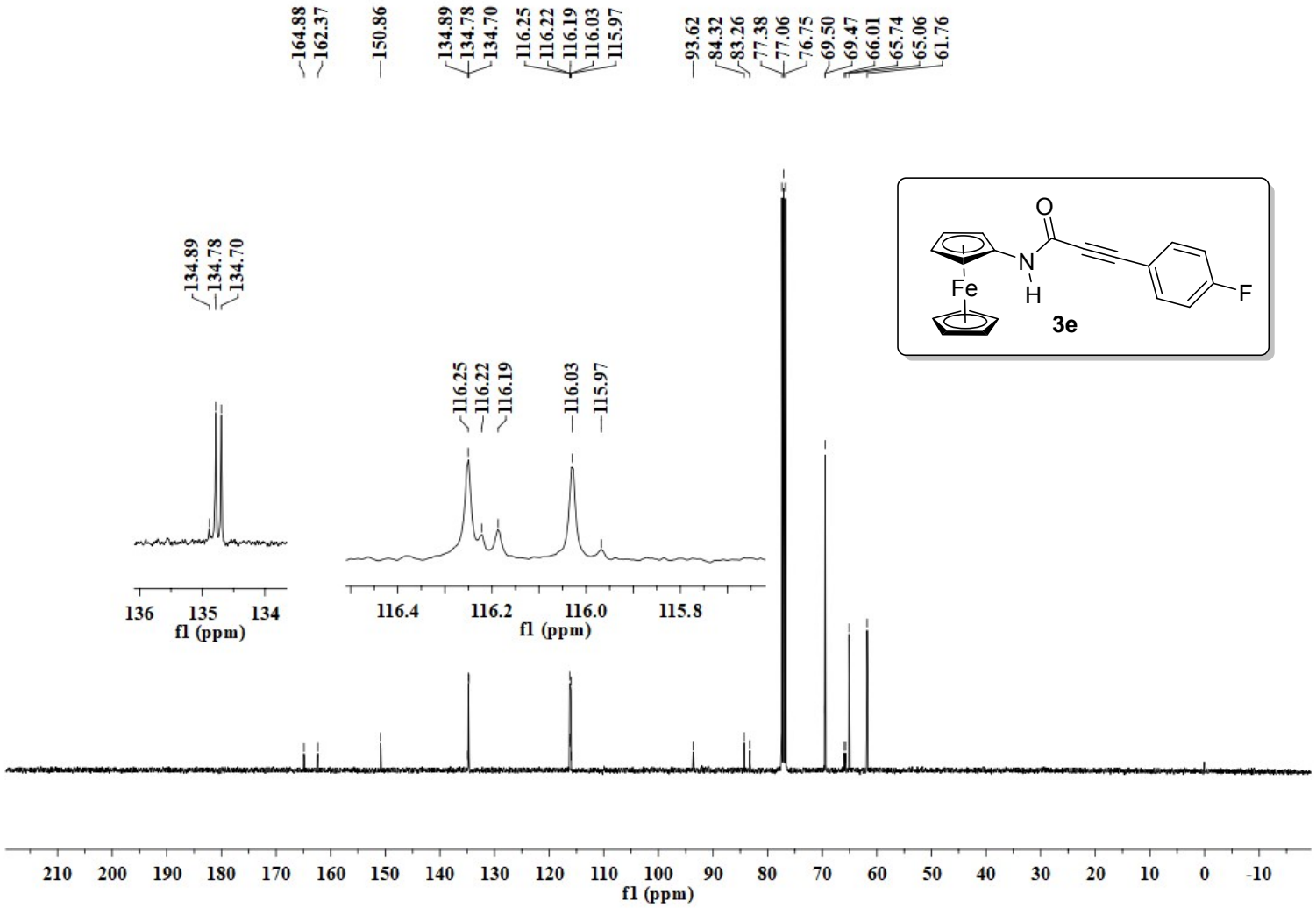

150.71
133.90
133.87
132.00
131.94
124.92
119.03
93.55
84.33
84.16
77.38
77.06
76.74
69.51
69.47
66.04
65.73
65.09
61.78
133.90
133.87
132.00
131.94
134.2
133.8
133.4
133.0
132.6
132.2
131.8
f1 (ppm)
O
N
H
Fe
Br
3d
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

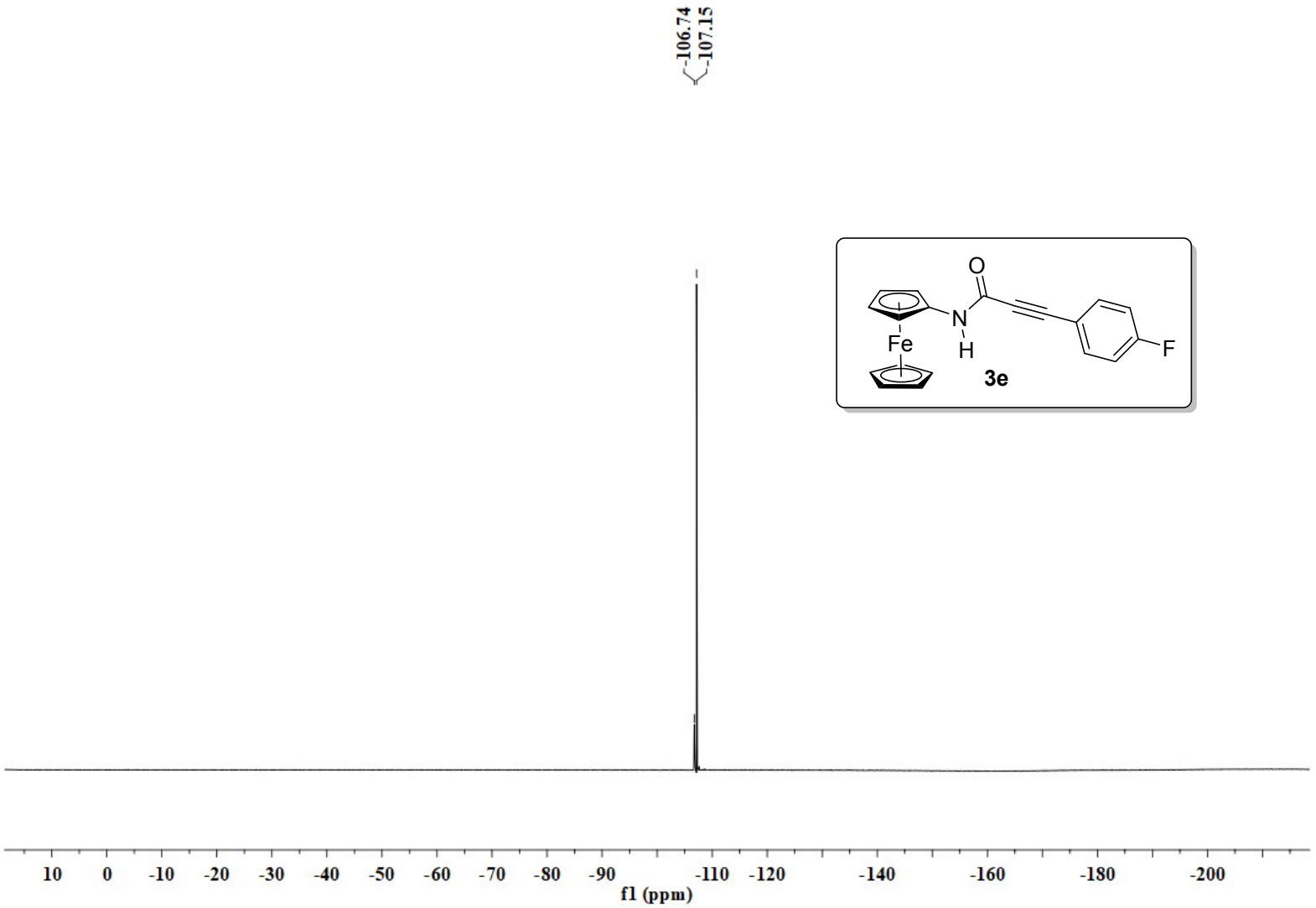
Sample Name	Jlx-2c	**Position**	P1-A3	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	Jlx-2c.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	3/20/18 Tue 16:25:29



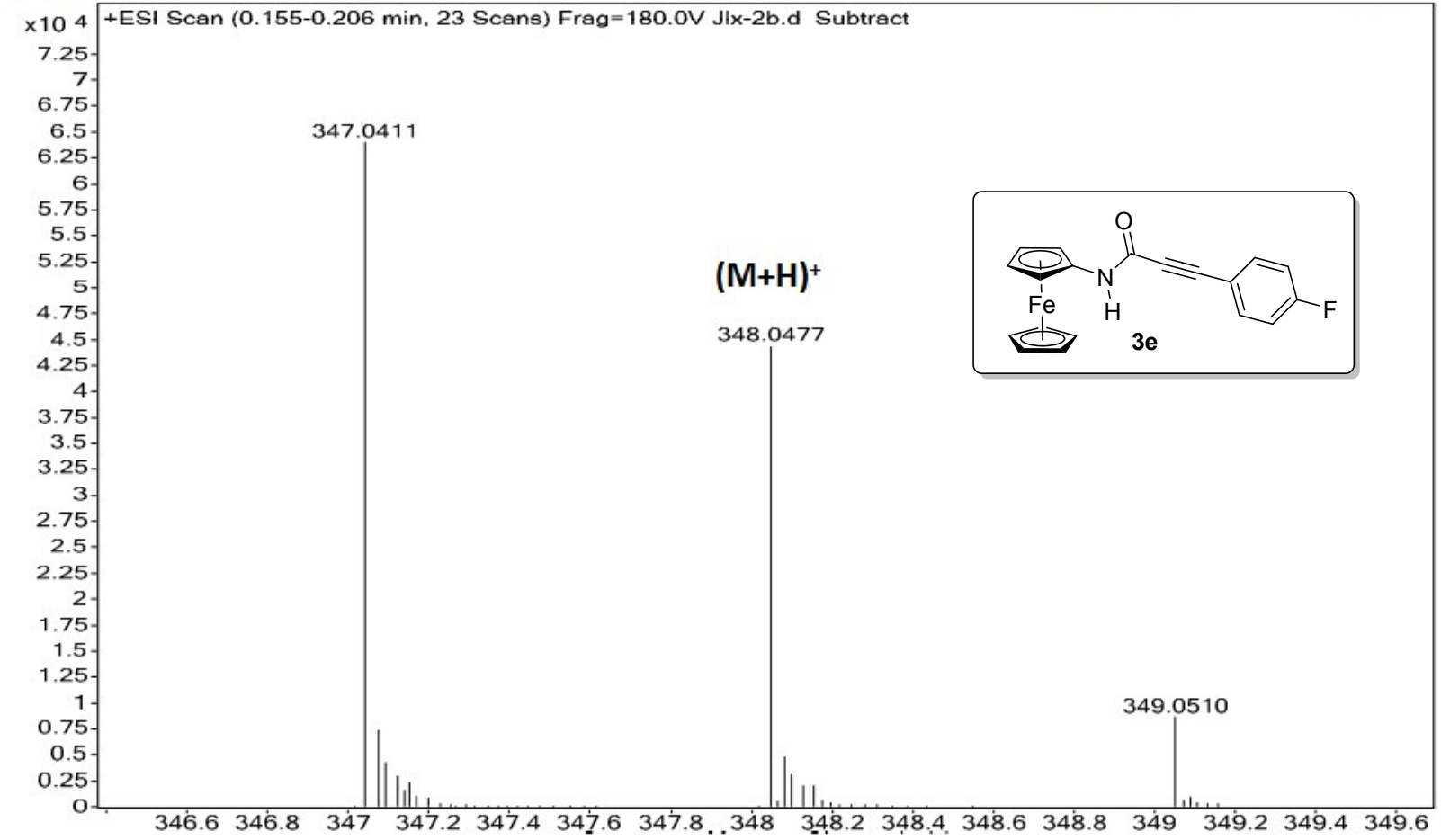
NMR and HMRS Spectra of **3e**



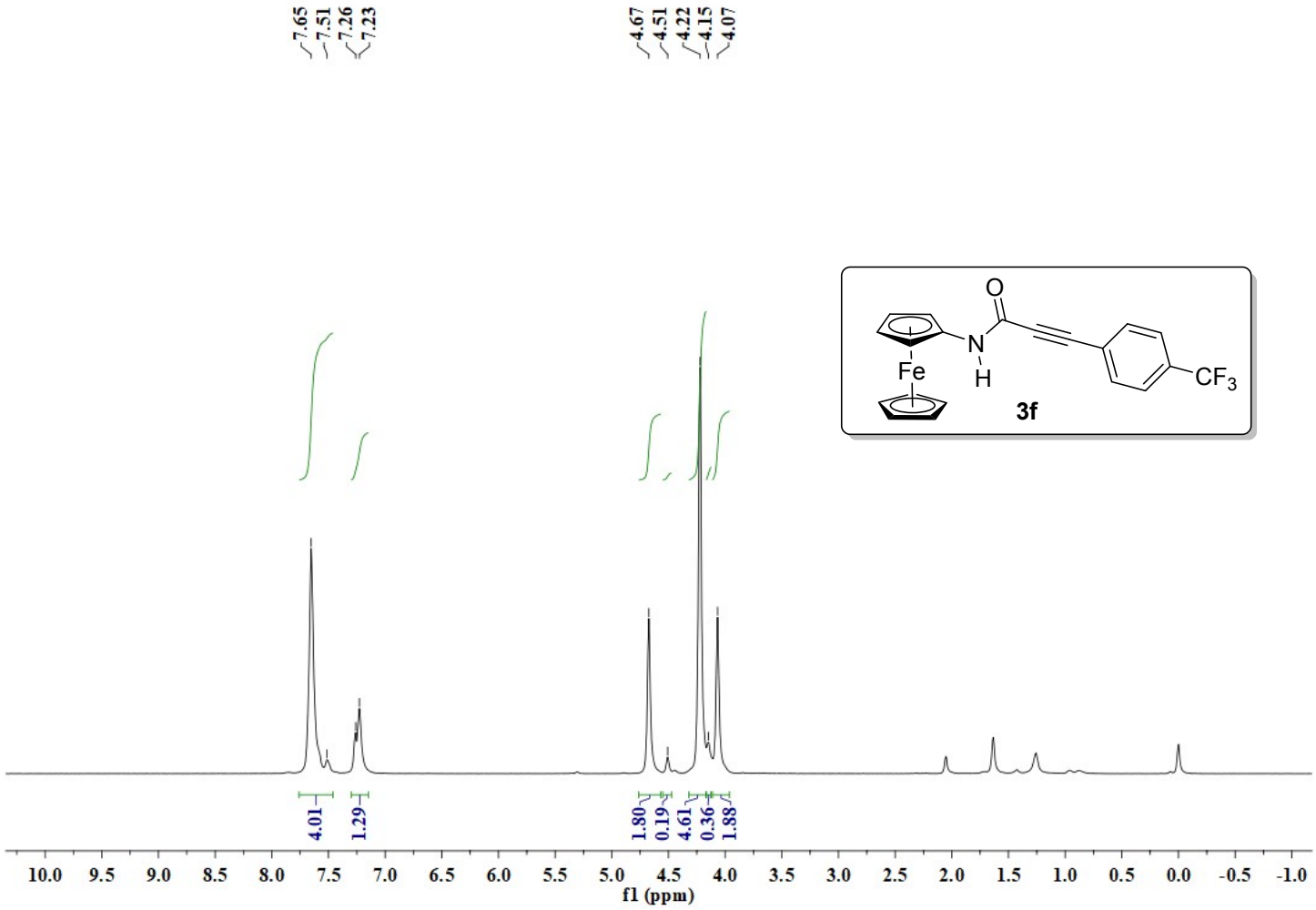

164.88
162.37
150.86
134.89
134.78
134.70
116.25
116.22
116.19
116.03
115.97
93.62
84.32
83.26
77.38
77.06
76.75
69.50
69.47
66.01
65.74
65.06
61.76
O
N
H
Fe
F
3e
fl (ppm)
fl (ppm)
fl (ppm)

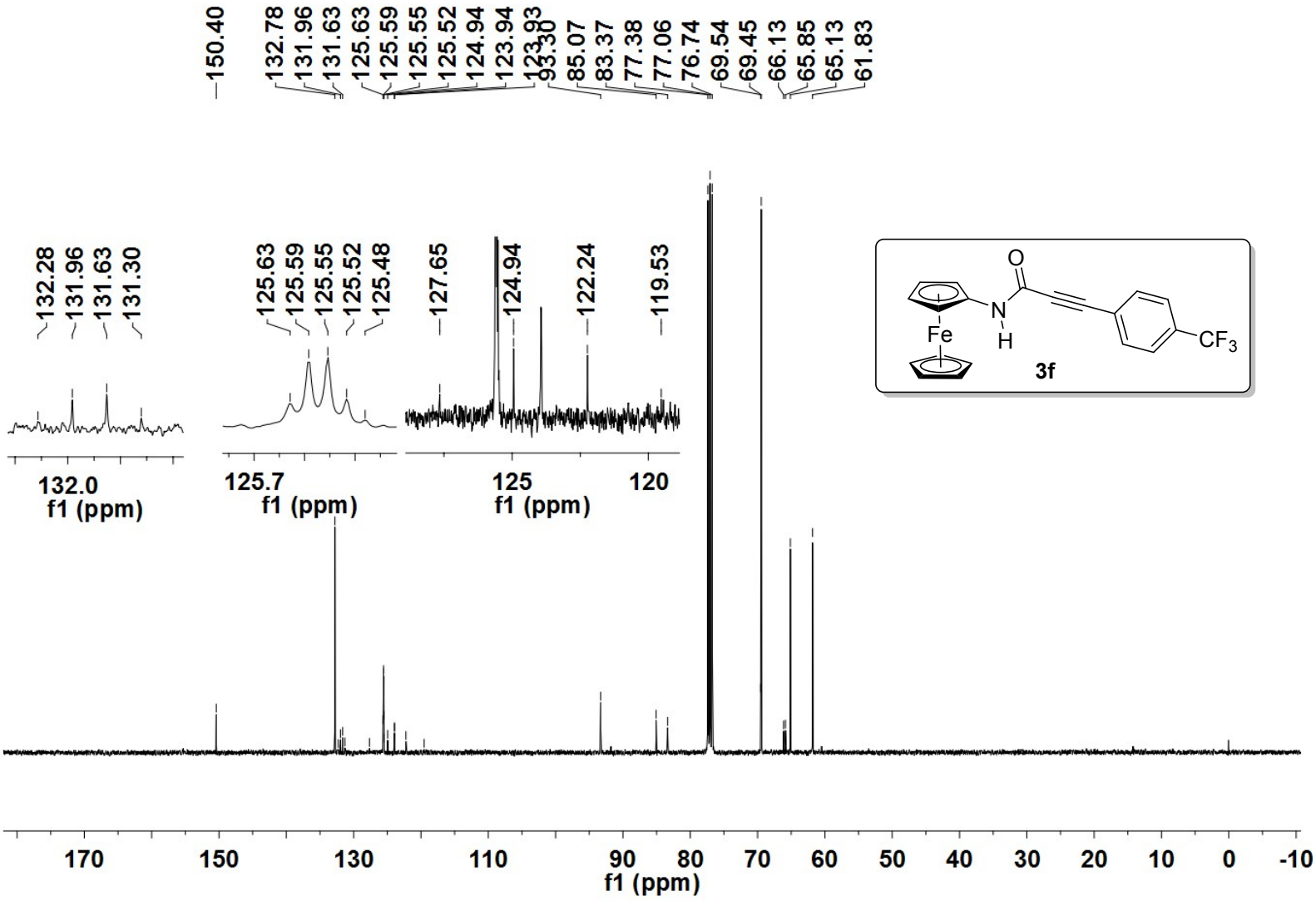

-106.74
-107.15
O
N
H
Fe
F
3e
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-110
-120
-140
-160
-180
-200
f1 (ppm)

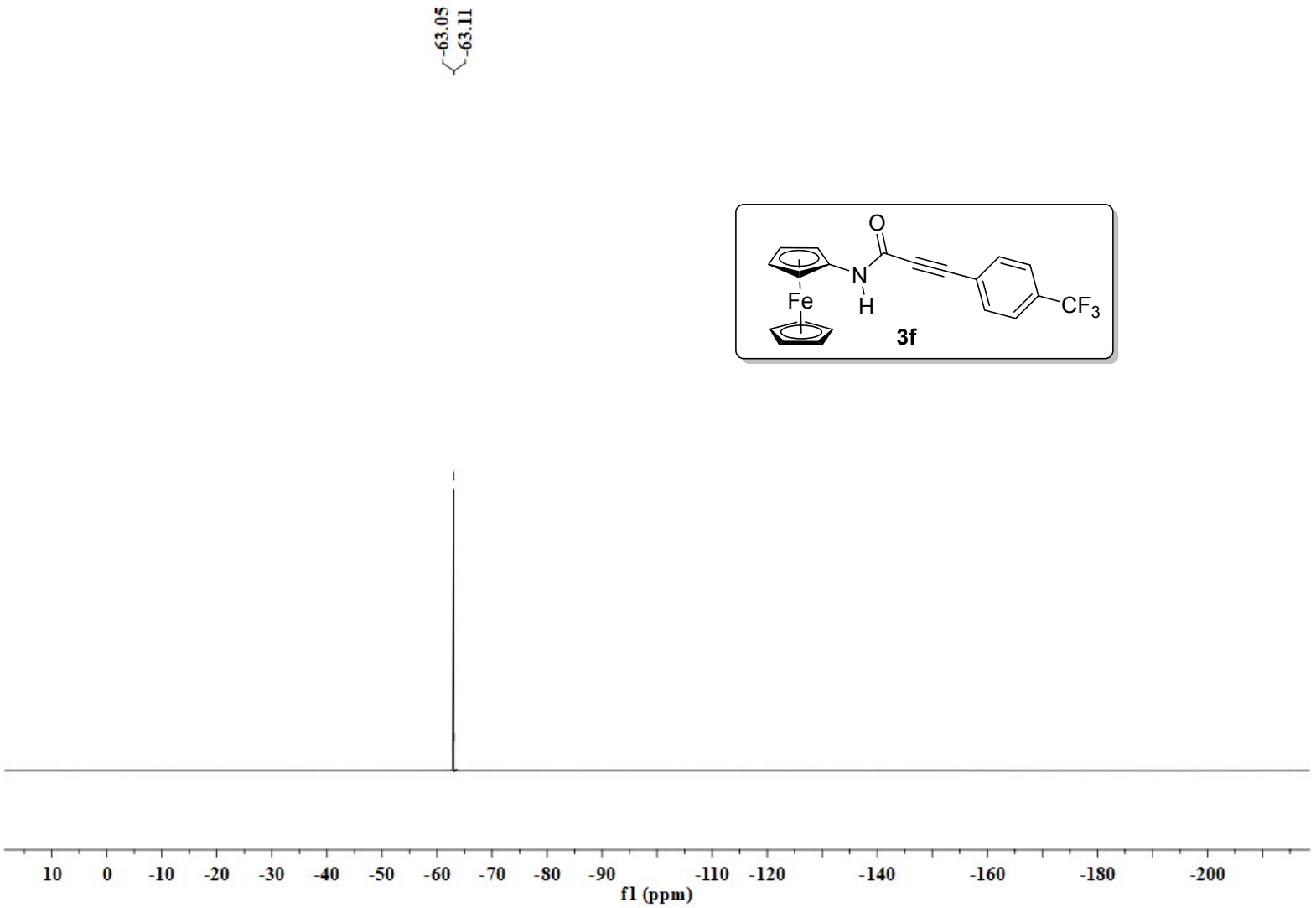
Sample Name	Jlx-2b	**Position**	P1-A2	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	Jlx-2b.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	3/20/18 Tue 16:24:12



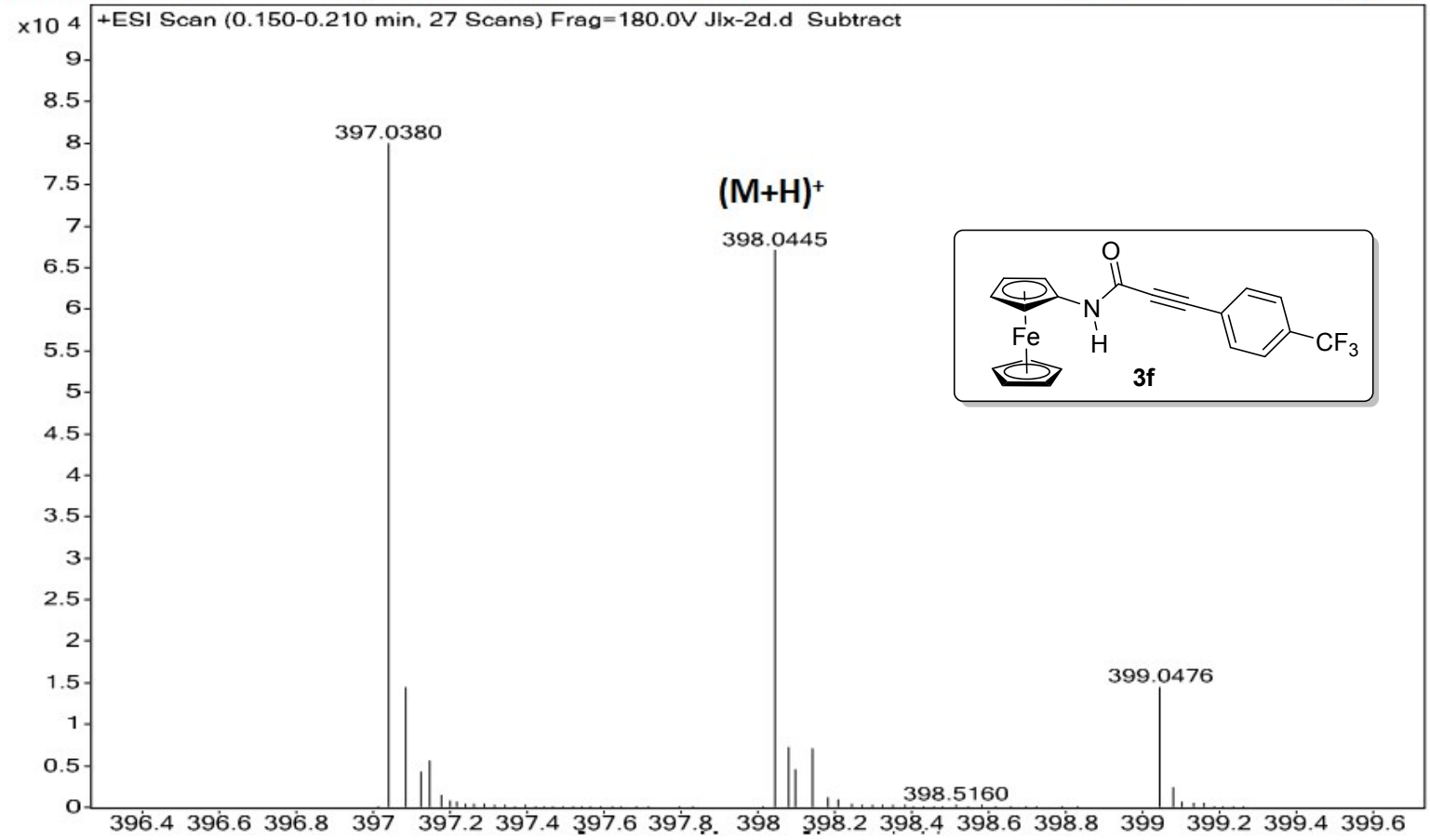
NMR and HMRS Spectra of **3f**



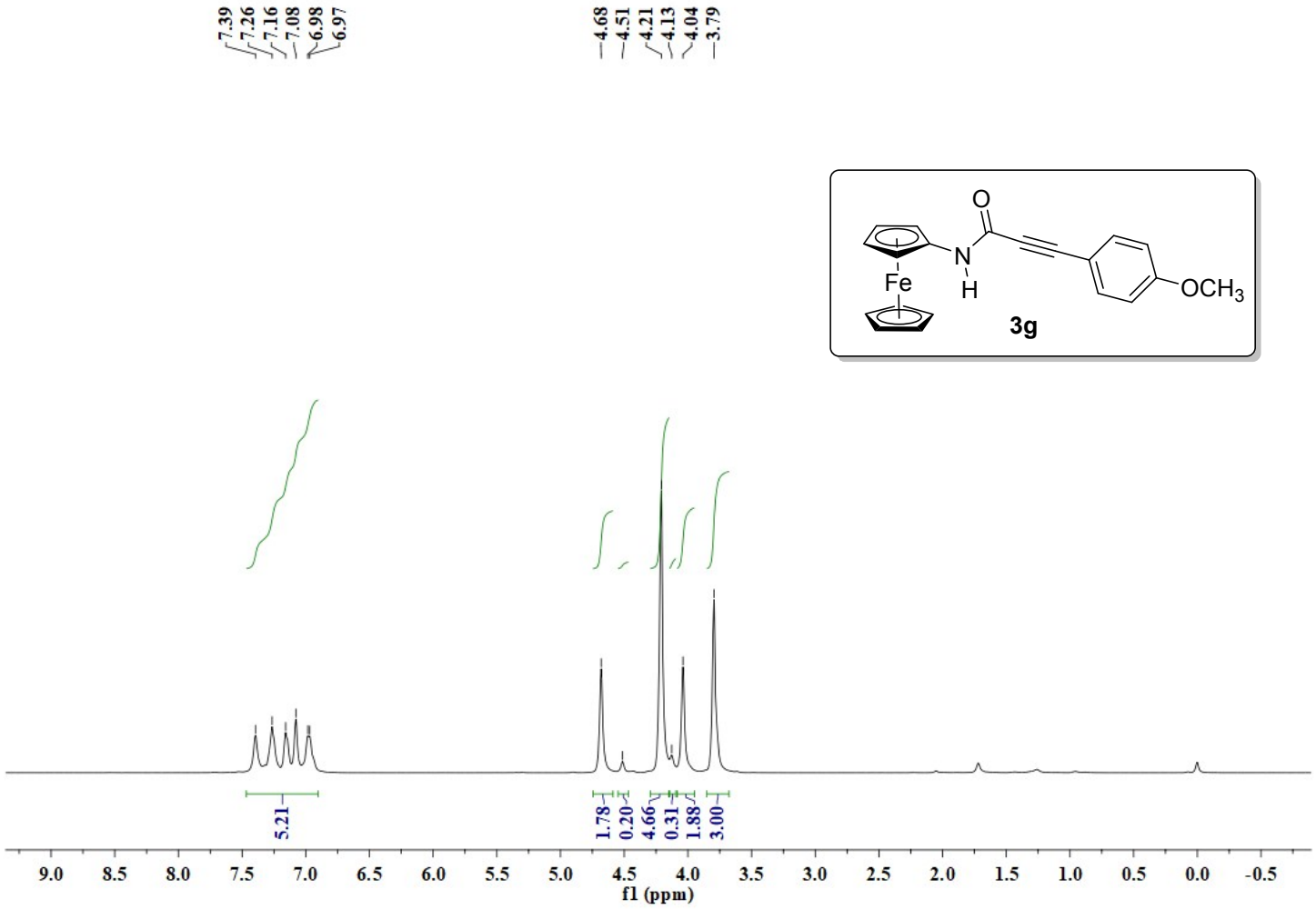

150.40
132.78
131.96
131.63
125.63
125.59
125.55
125.52
124.94
123.94
123.93
93.30
85.07
83.37
77.38
77.06
76.74
69.54
69.45
66.13
65.85
65.13
61.83
132.28
131.96
131.63
131.30
125.63
125.59
125.55
125.52
125.48
127.65
124.94
122.24
119.53
132.0
f1 (ppm)
125.7
f1 (ppm)
125
120
f1 (ppm)
O
N
H
Fe
CF3
3f
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

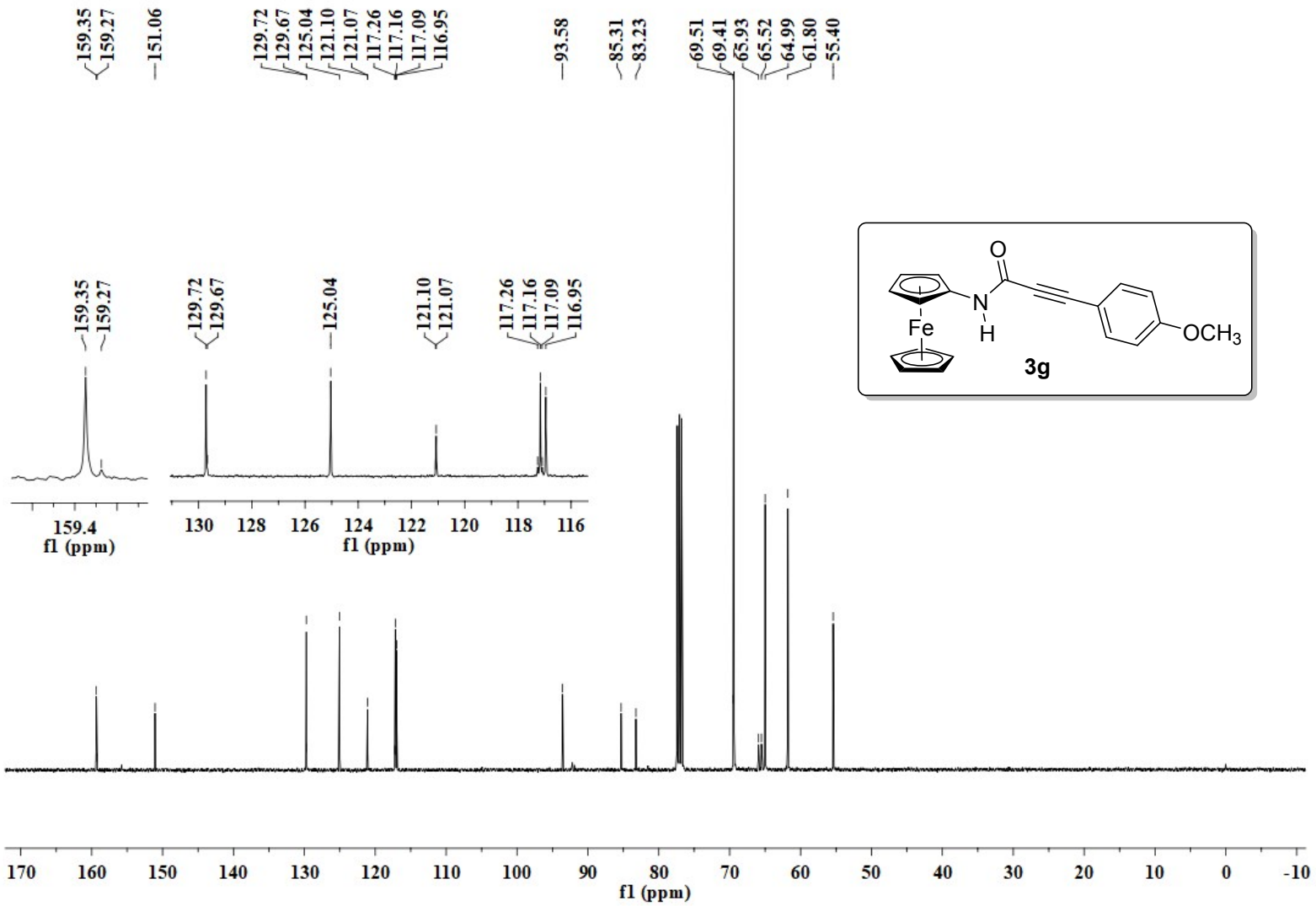

-63.05
-63.11
O
N
H
Fe
CF3
3f
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-110
-120
-140
-160
-180
-200
f1 (ppm)

Sample Name	Jlx-2d	**Position**	P1-A4	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	Jlx-2d.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	3/20/18 Tue 16:26:45

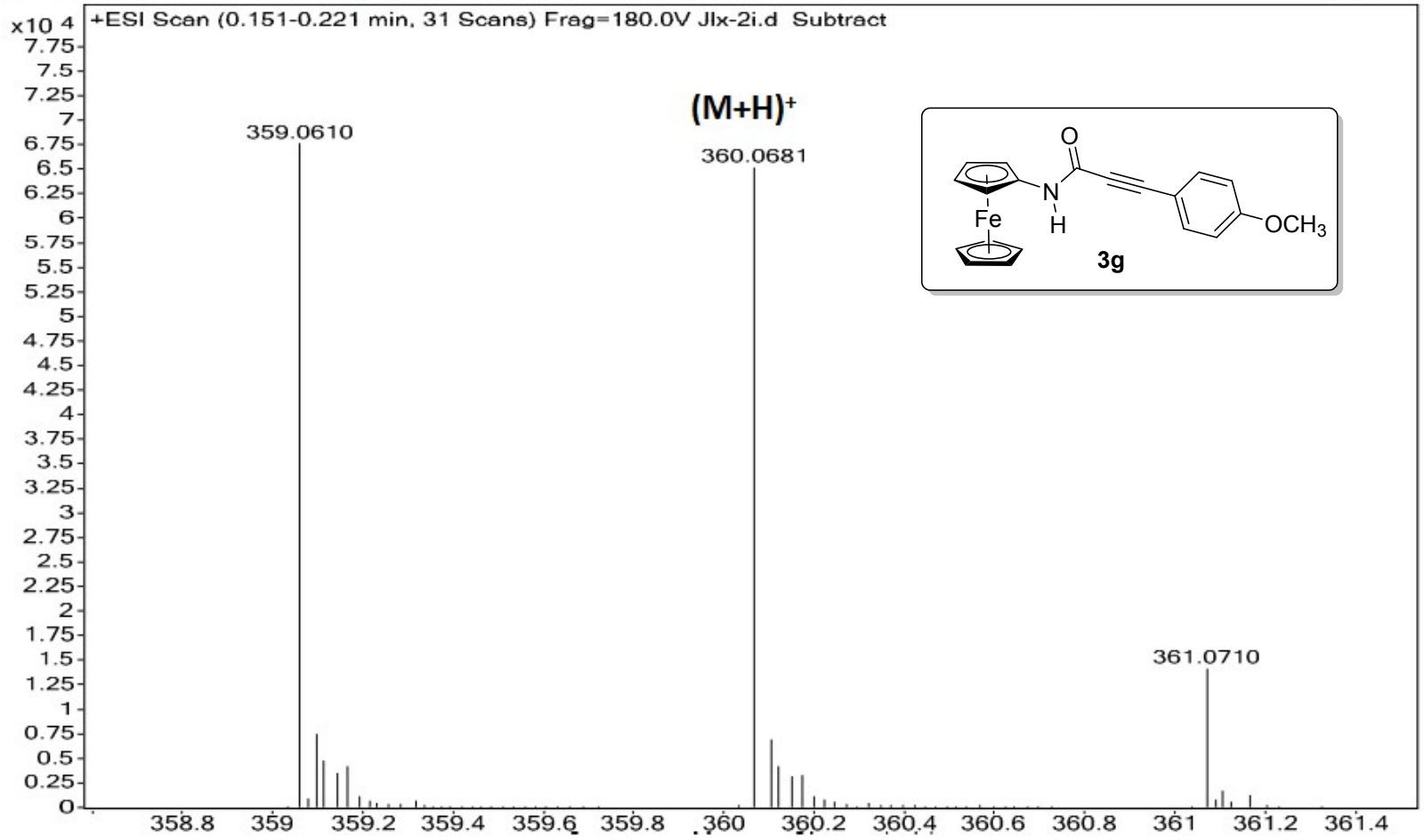


NMR and HMRS Spectra of **3g**

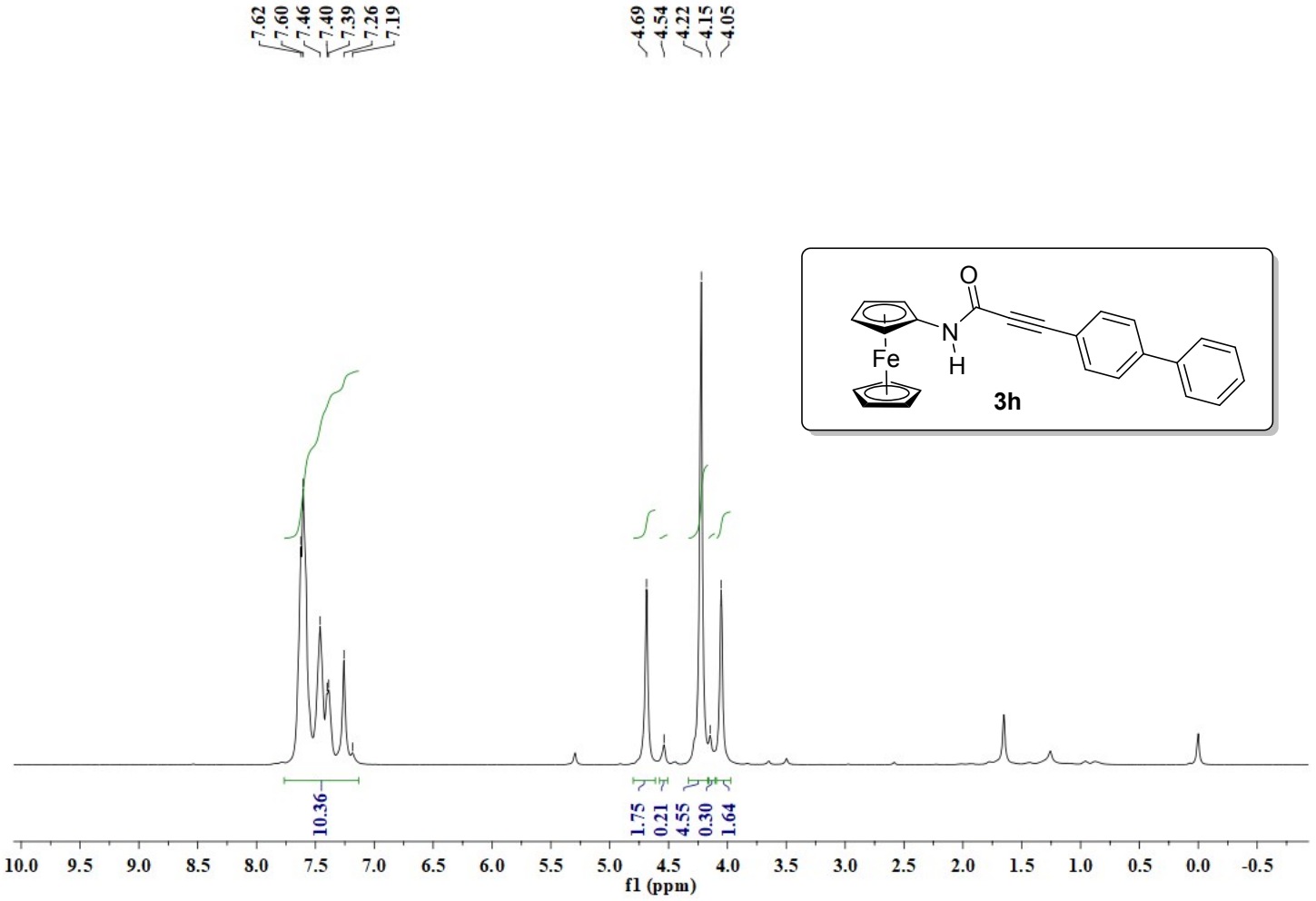


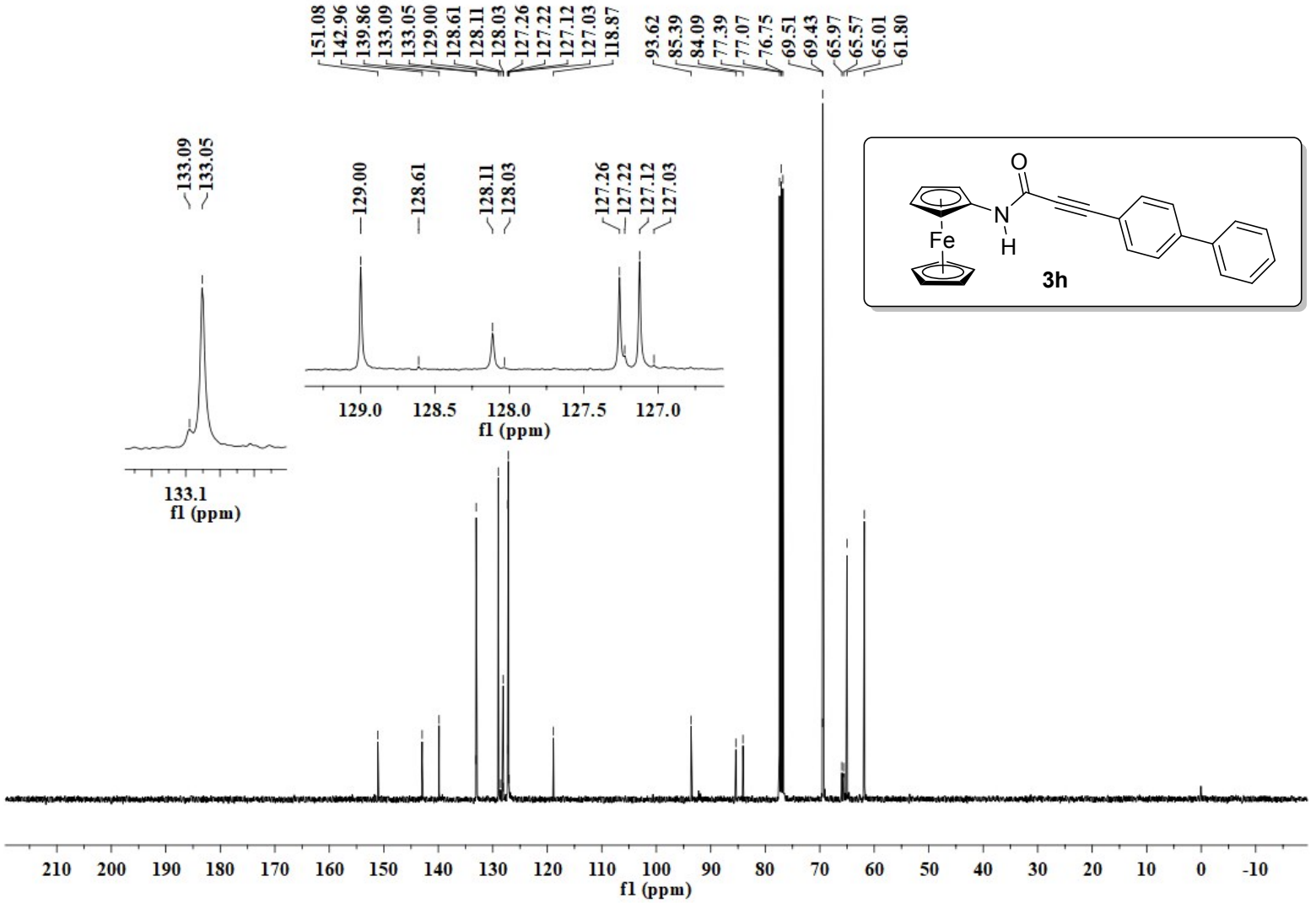

159.35
159.27
151.06
129.72
129.67
125.04
121.10
121.07
117.26
117.16
117.09
116.95
93.58
85.31
83.23
69.51
69.41
65.93
65.52
64.99
61.80
55.40
O
N
H
Fe
OCH3
3g
159.4
f1 (ppm)
130
128
126
124
122
120
118
116
f1 (ppm)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

Sample Name	Jlx-2i	**Position**	P1-A9	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	Jlx-2i.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	3/20/18 Tue 16:33:06

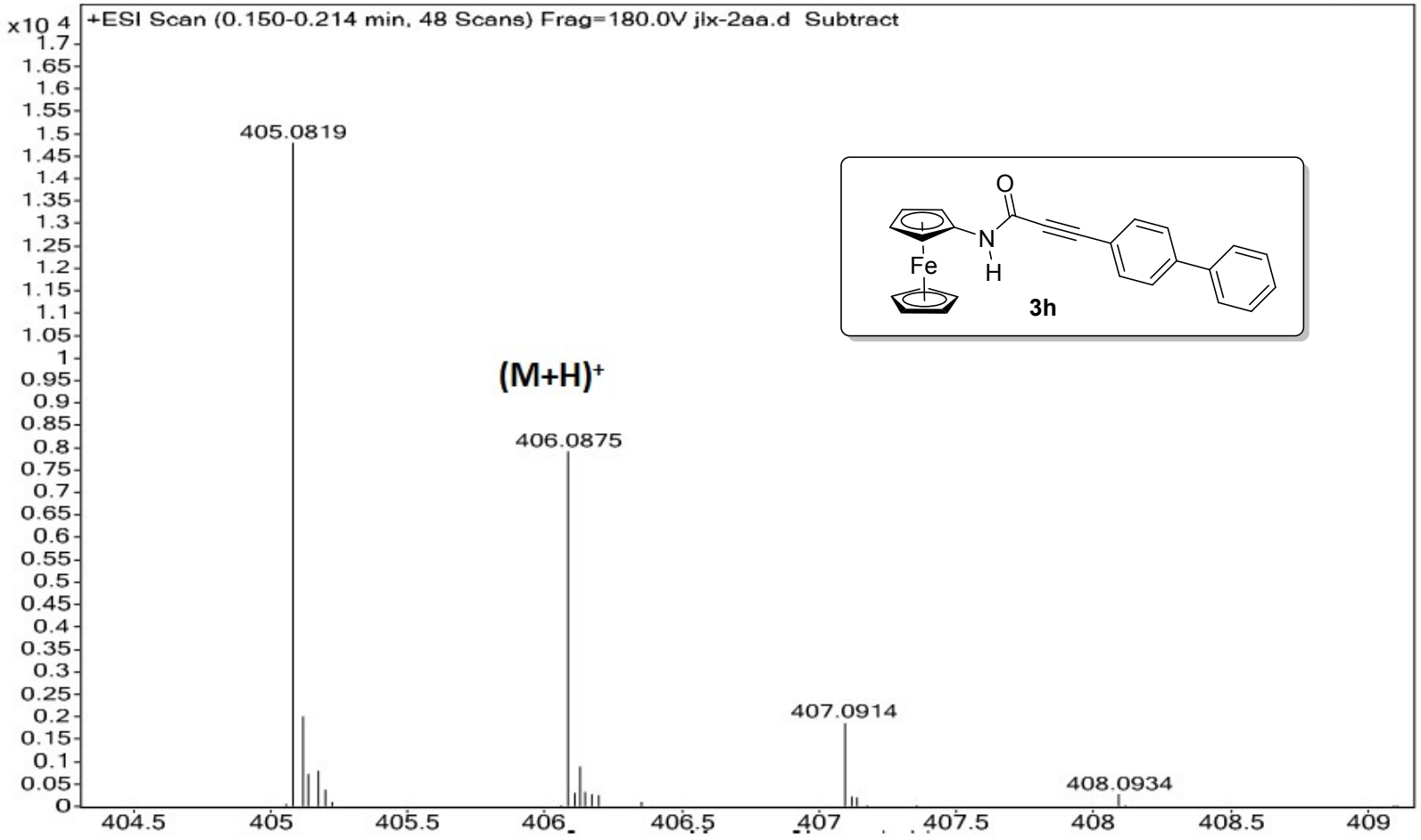


NMR and HMRS Spectra of **3h**

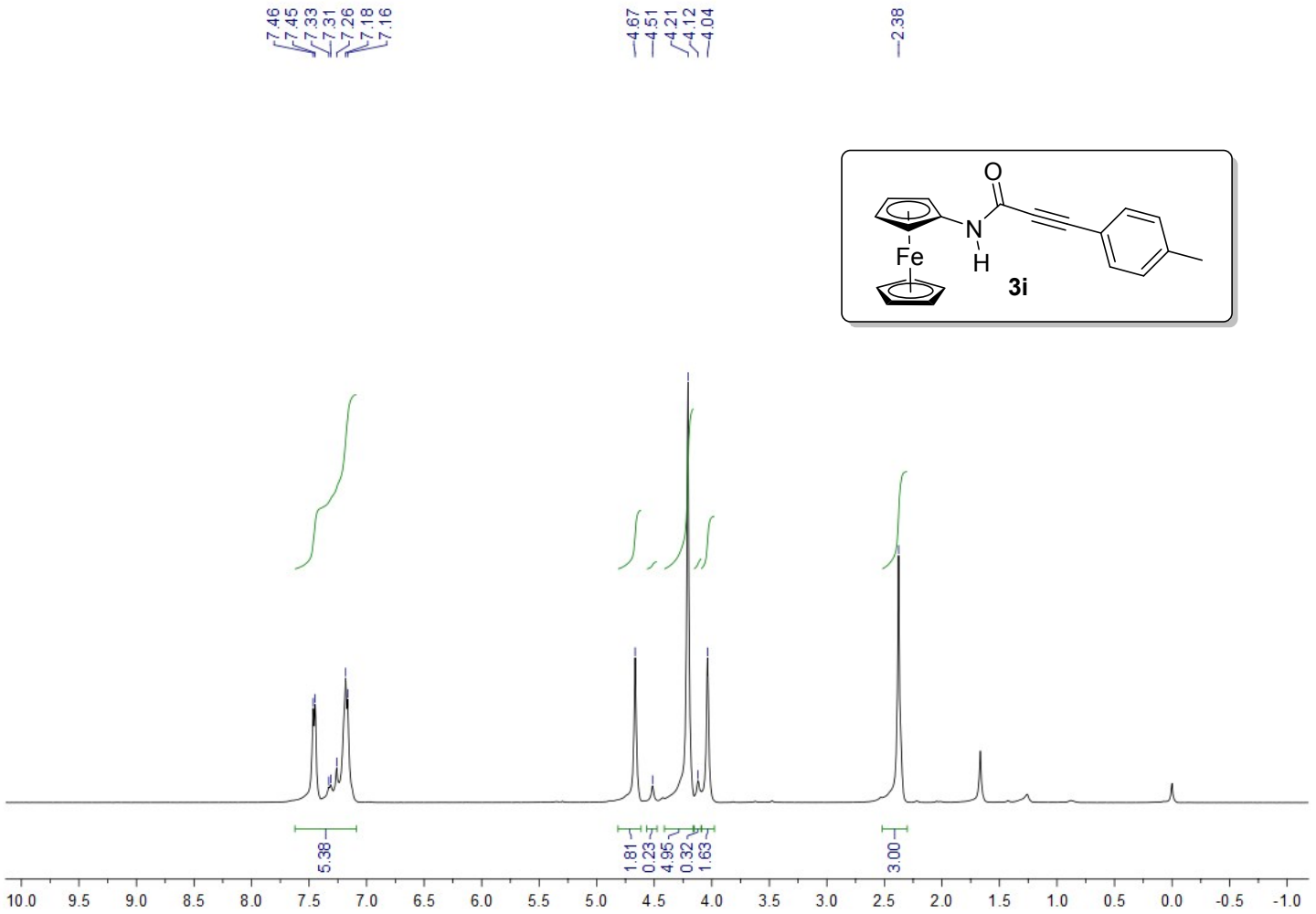


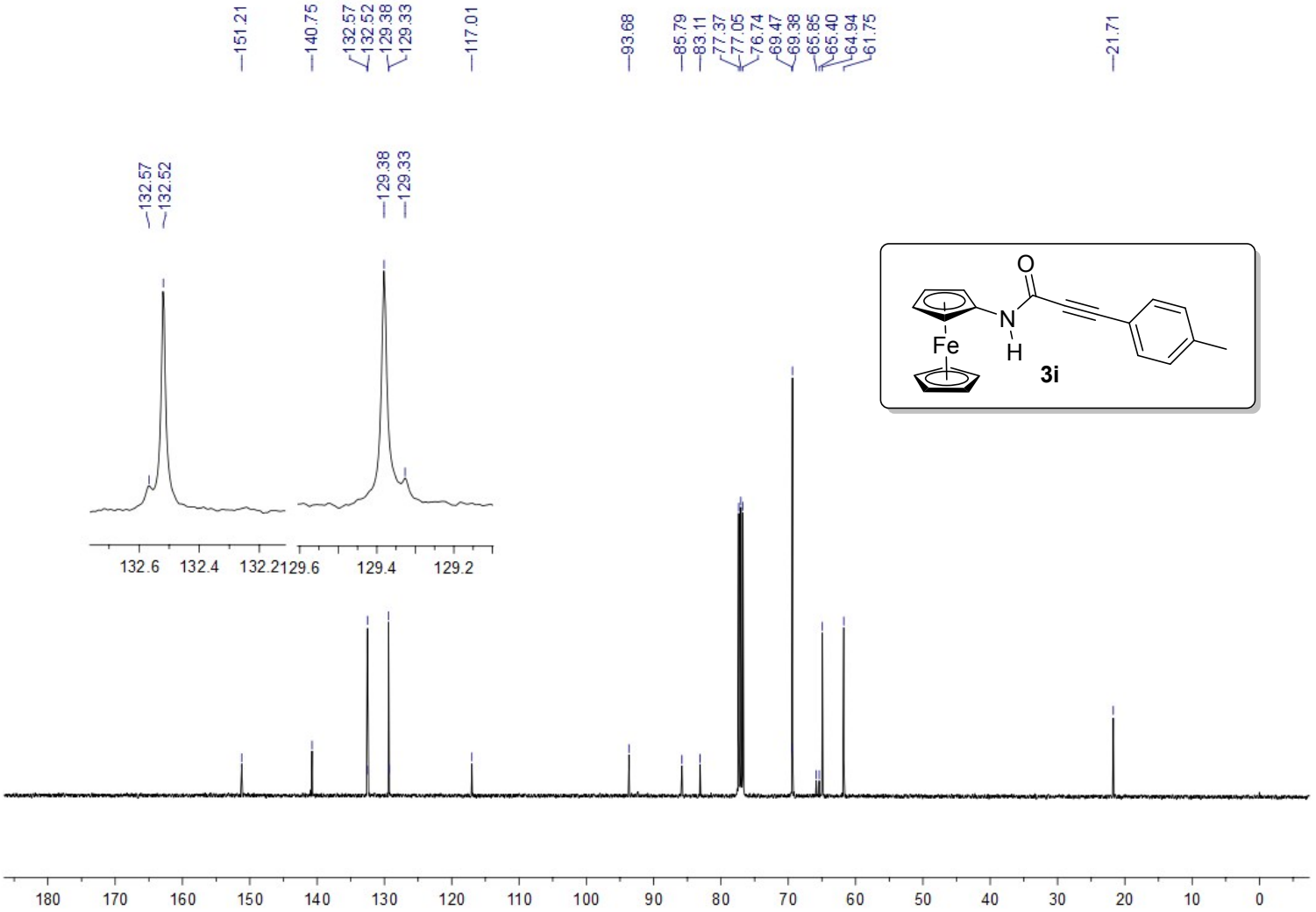

151.08
142.96
139.86
133.09
133.05
129.00
128.61
128.11
128.03
127.26
127.22
127.12
127.03
118.87
93.62
85.39
84.09
77.39
77.07
76.75
69.51
69.43
65.97
65.57
65.01
61.80
133.09
133.05
129.00
128.61
128.11
128.03
127.26
127.22
127.12
127.03
129.0
128.5
128.0
127.5
127.0
f1 (ppm)
133.1
f1 (ppm)
O
N
H
Fe
3h
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

Sample Name	jlx-2aa	**Position**	P1-A1	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
Data Filename	jlx-2aa.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	5/24/18 Thu 10:32:31

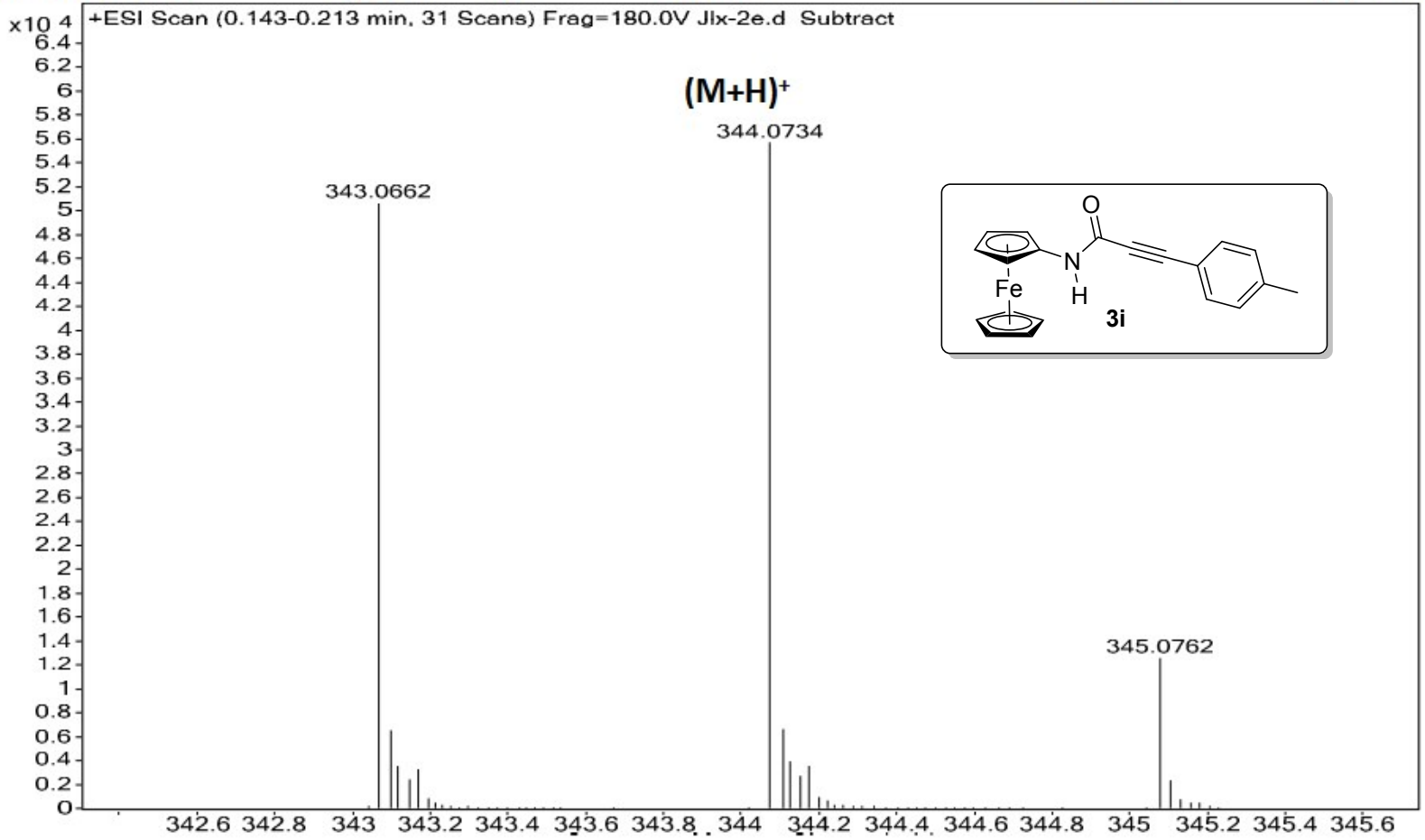


NMR and HMRS Spectra of **3i**

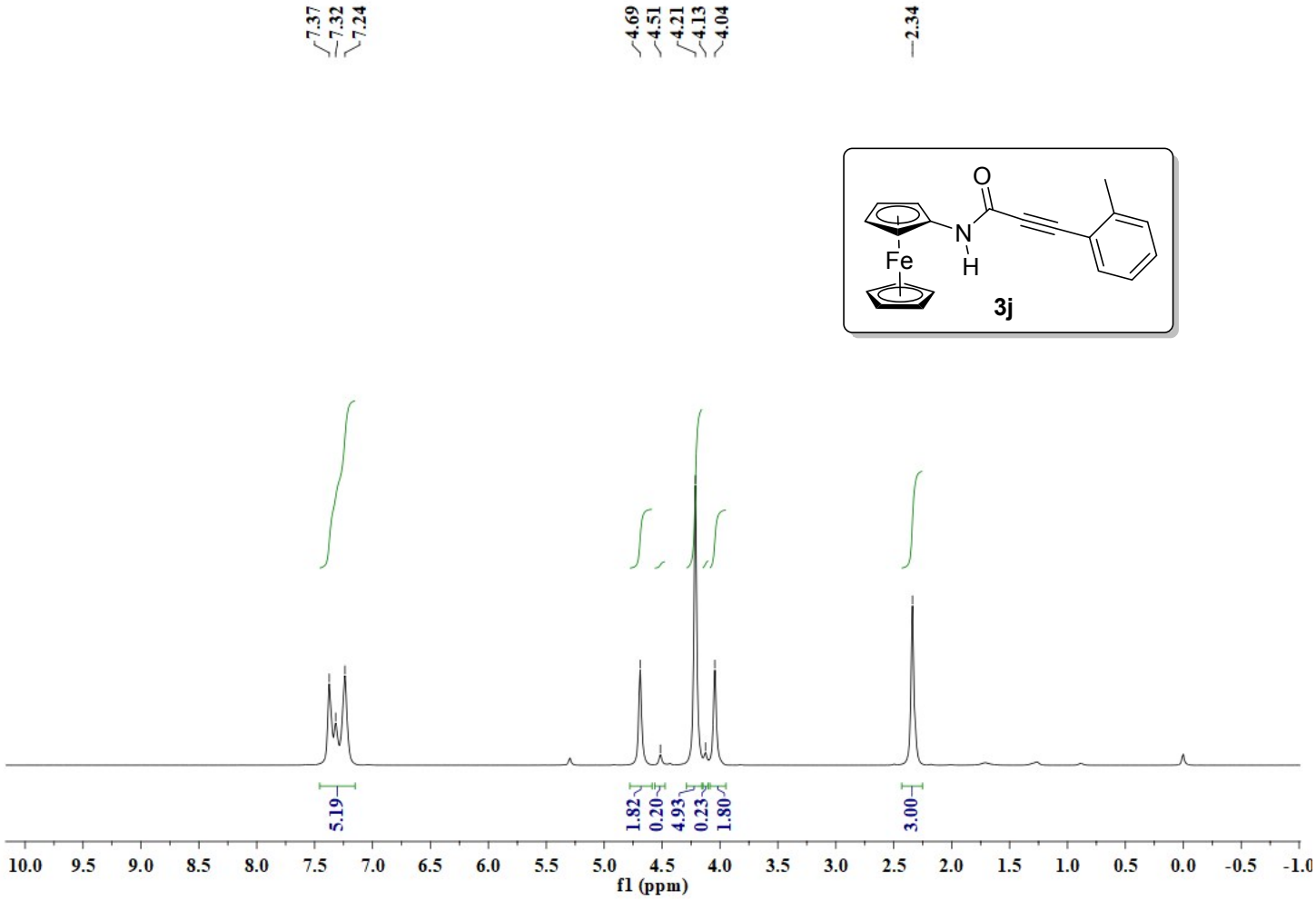


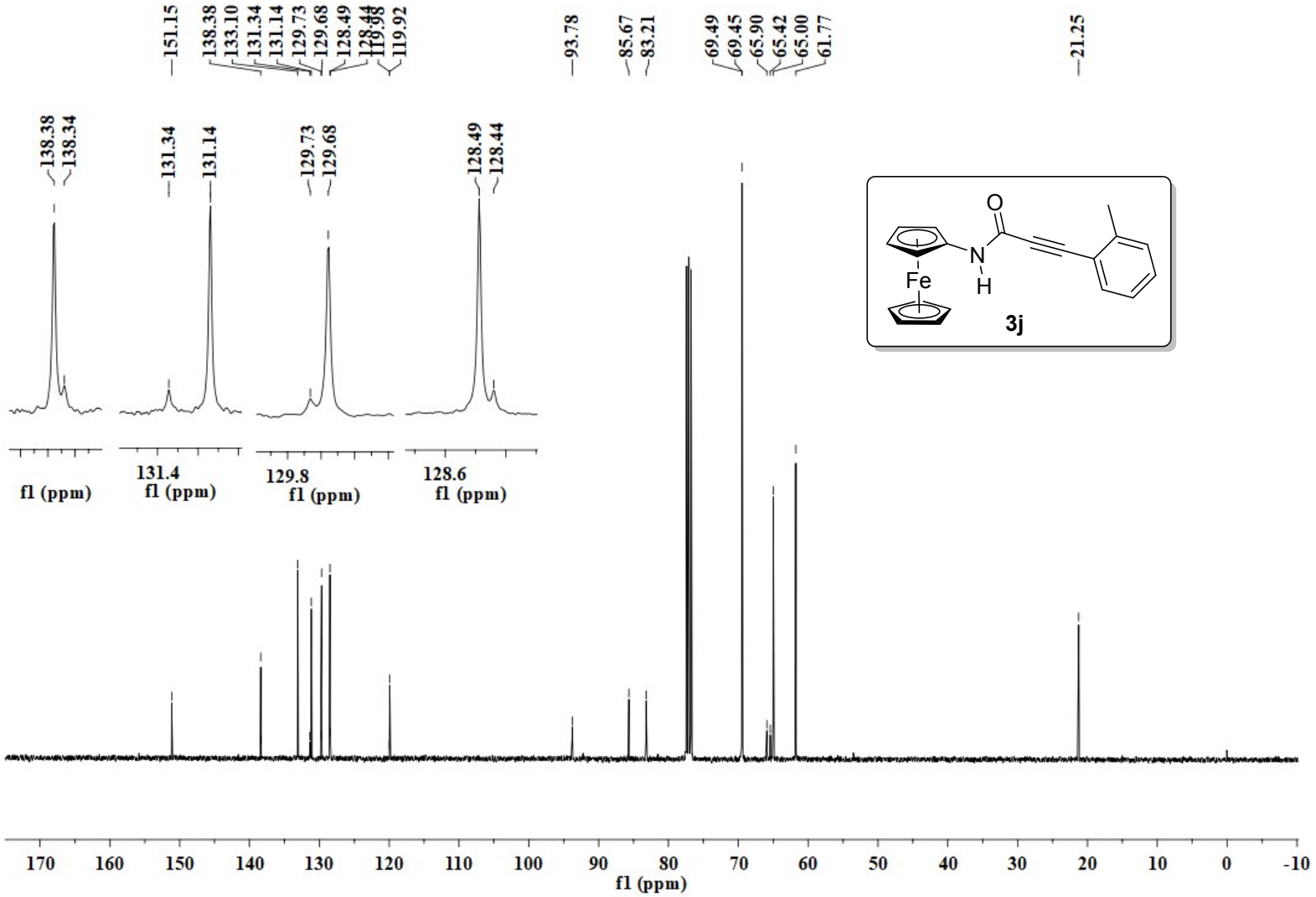

151.21
140.75
132.57
132.52
129.38
129.33
117.01
93.68
85.79
83.11
77.37
77.05
76.74
69.47
69.38
65.85
65.40
64.94
61.75
21.71
132.57
132.52
129.38
129.33
132.6
132.4
132.2
129.6
129.4
129.2
O
N
H
Fe
3i
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

Sample Name	Jlx-2e	**Position**	P1-A5	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.05	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	Jlx-2e.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	3/20/18 Tue 16:45:35

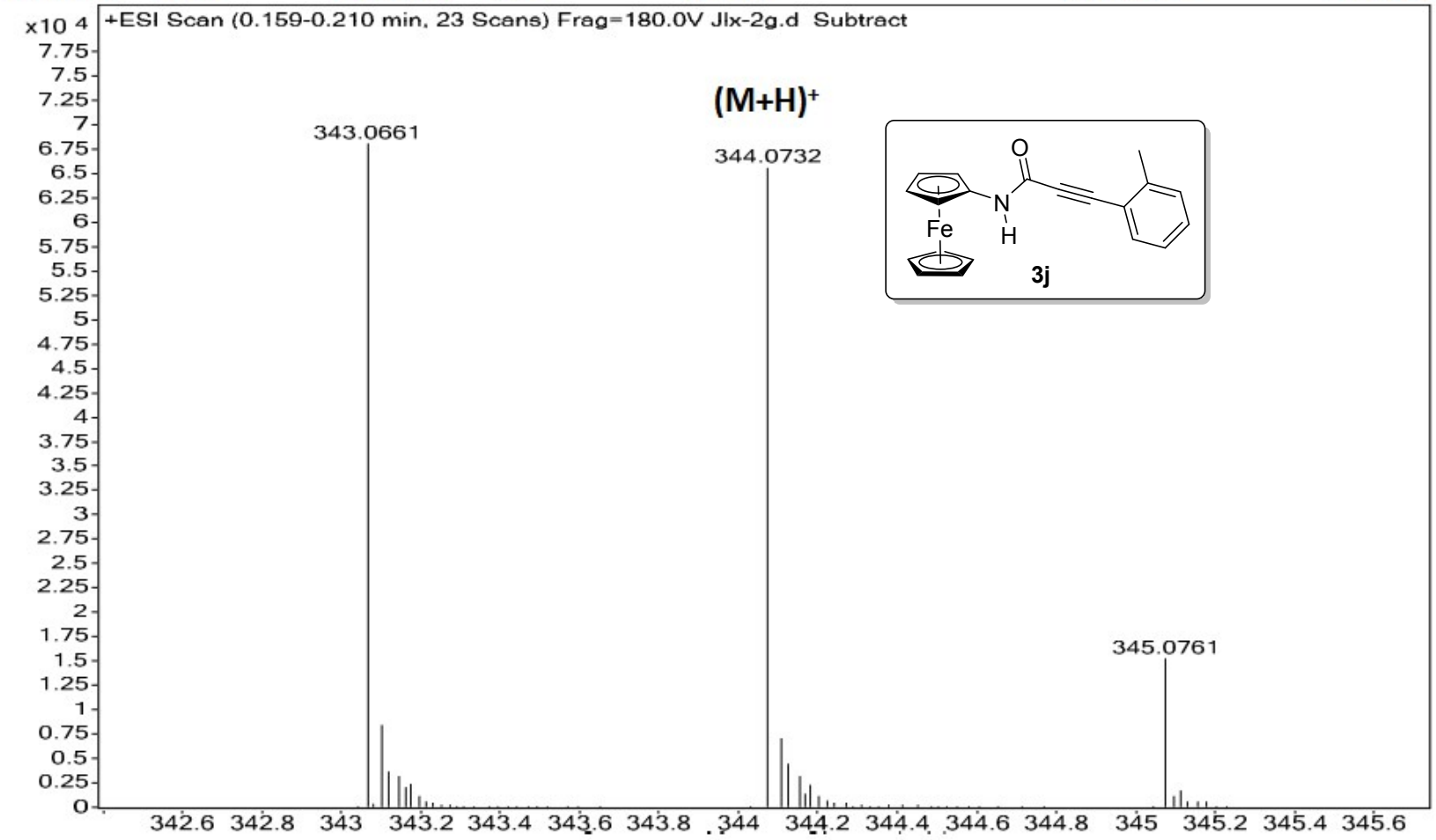


NMR and HMRS Spectra of **3j**

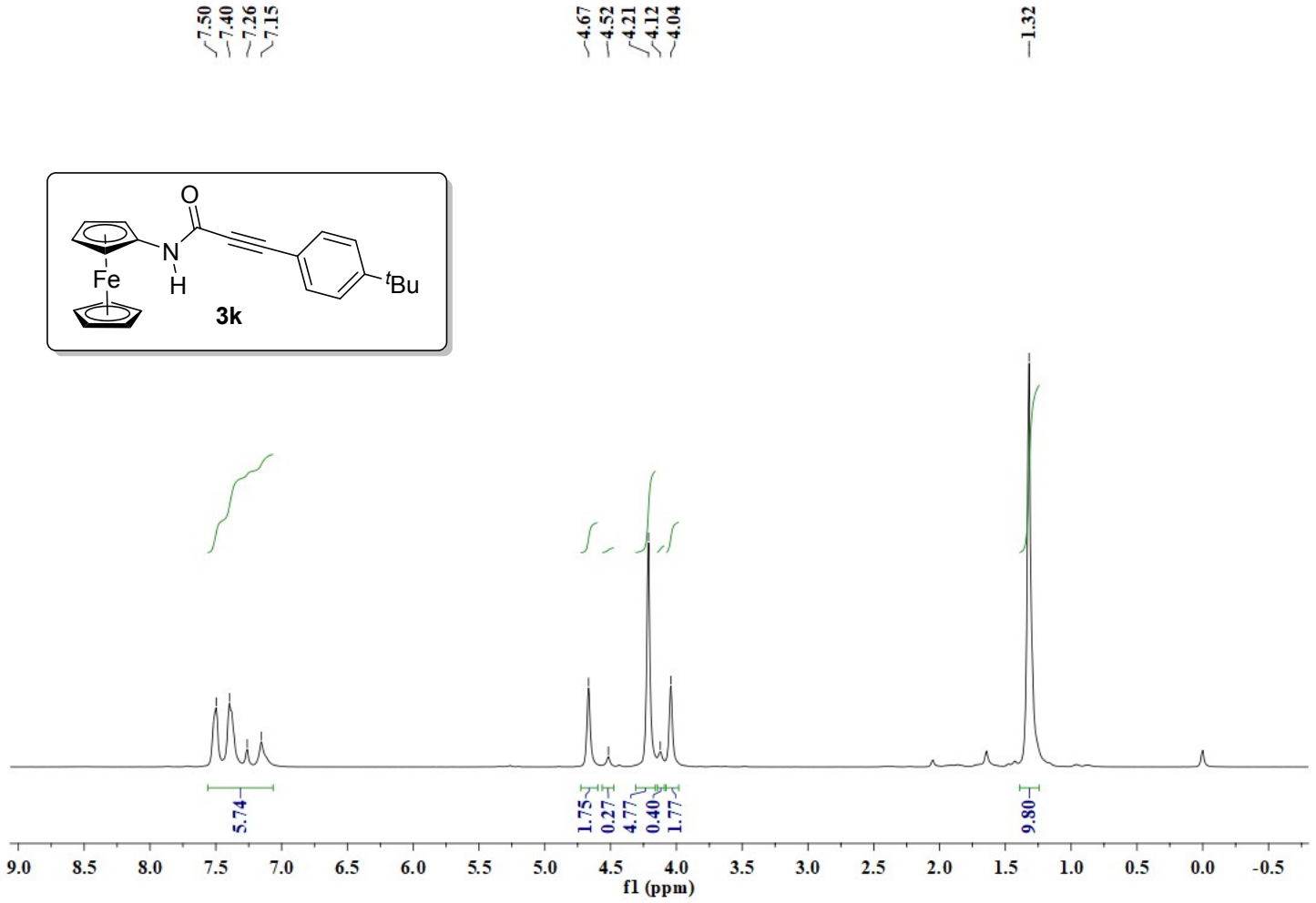


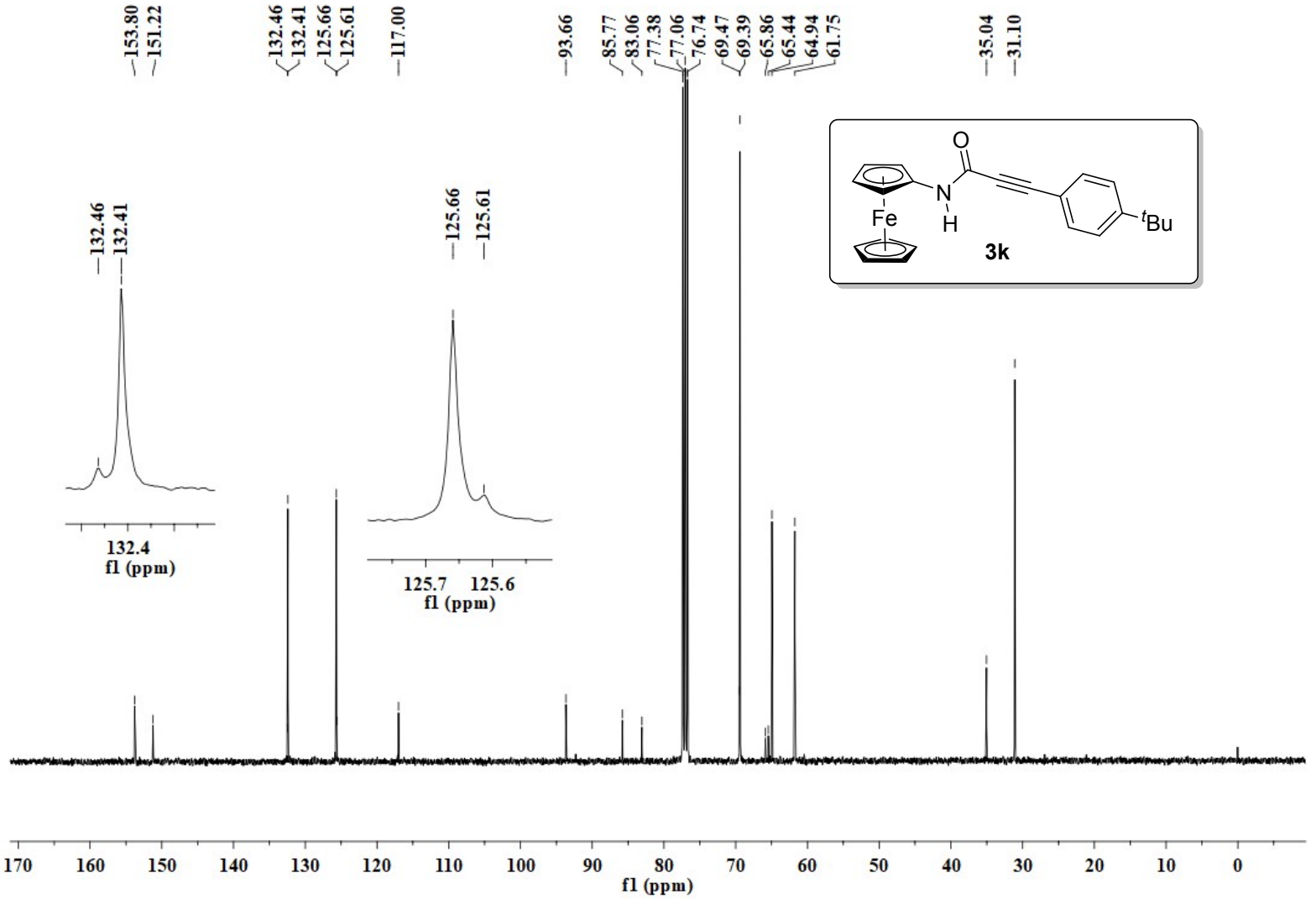

151.15
138.38
133.10
131.34
131.14
129.73
129.68
128.49
128.44
119.98
119.92
93.78
85.67
83.21
69.49
69.45
65.90
65.42
65.00
61.77
21.25
138.38
138.34
131.34
131.14
129.73
129.68
128.49
128.44
f1 (ppm)
131.4
f1 (ppm)
129.8
f1 (ppm)
128.6
f1 (ppm)
O
N
H
Fe
3j
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

Sample Name	Jlx-2g	**Position**	P1-A7	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	Jlx-2g.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	3/20/18 Tue 16:30:34

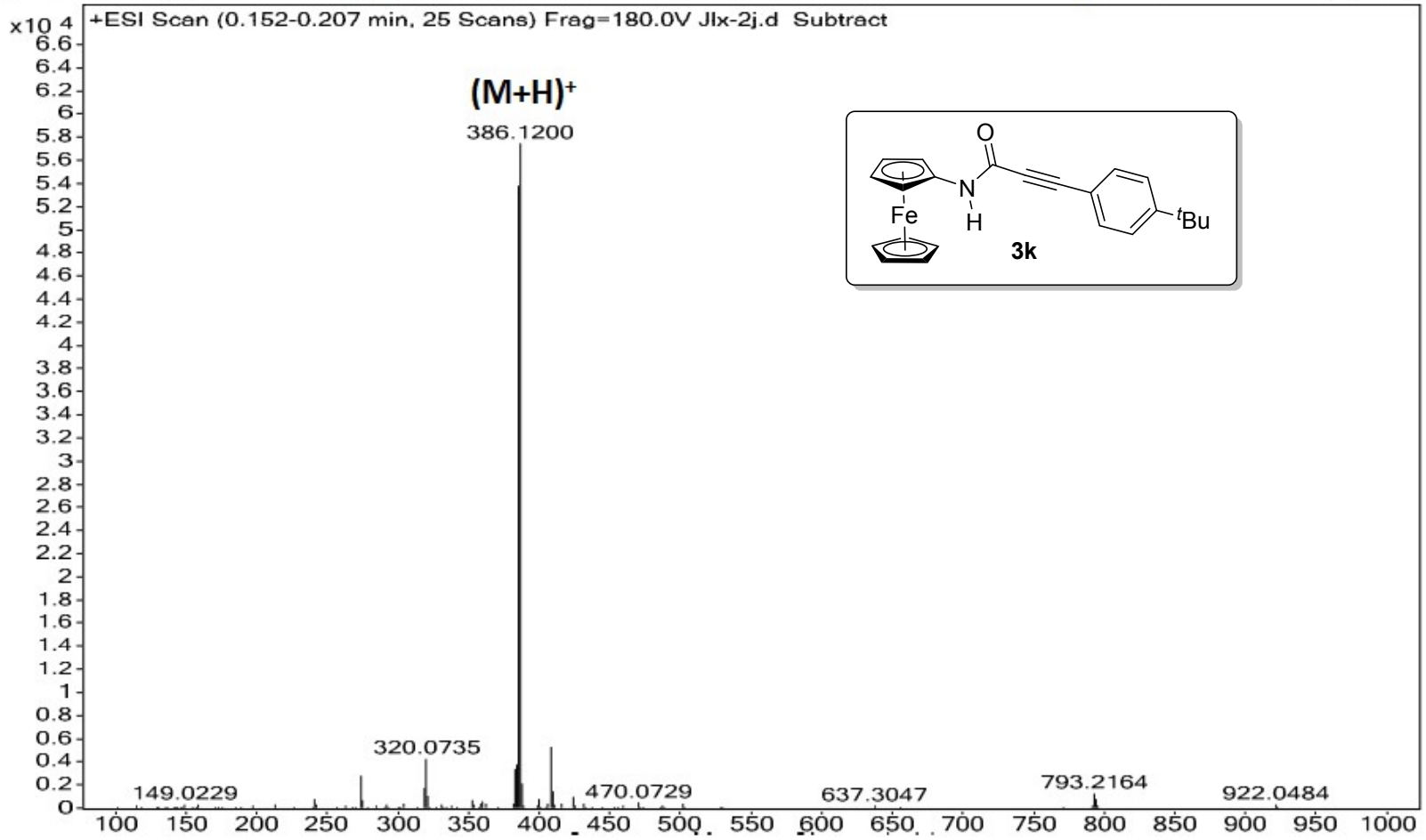


NMR and HMRS Spectra of **3k**

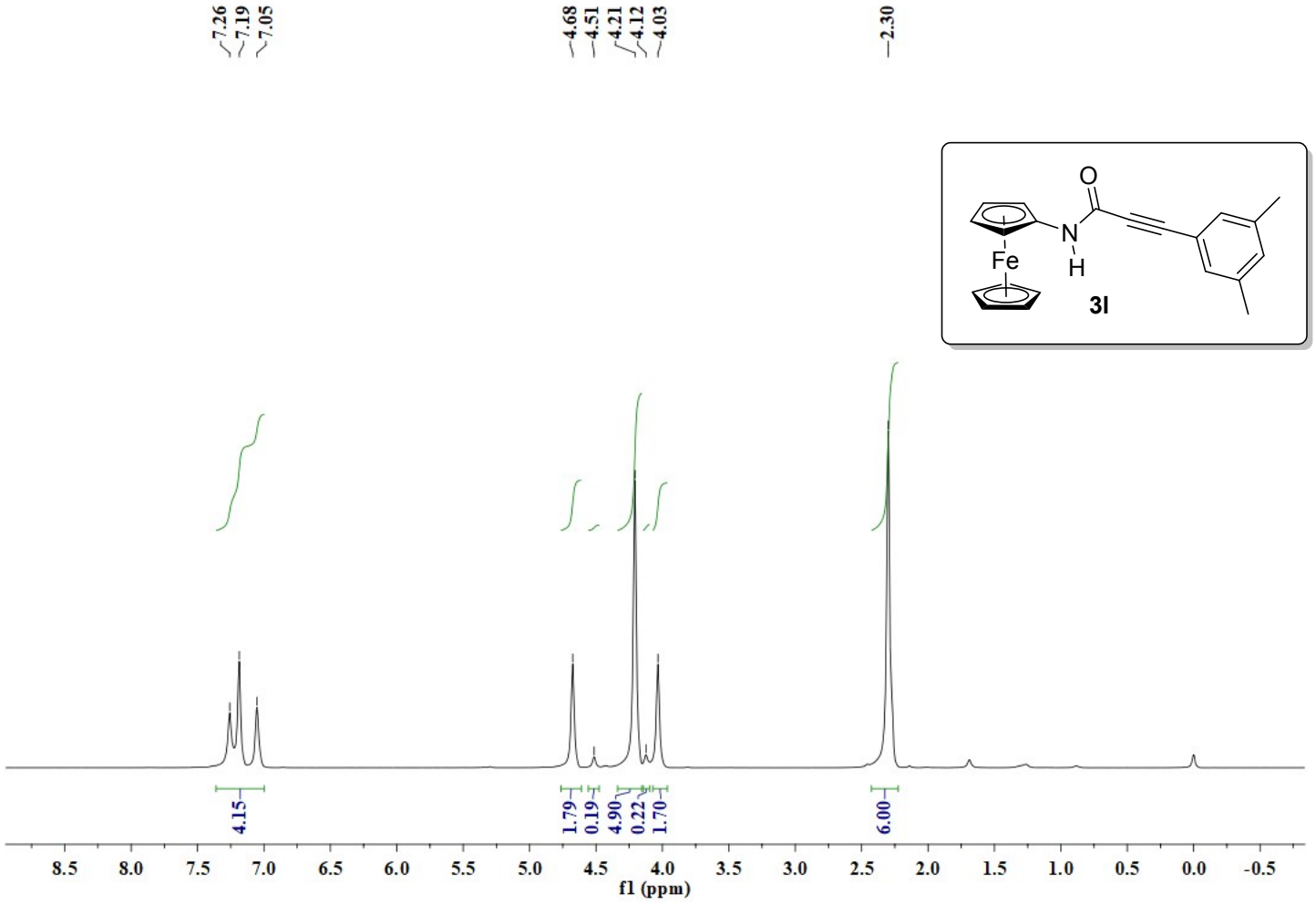


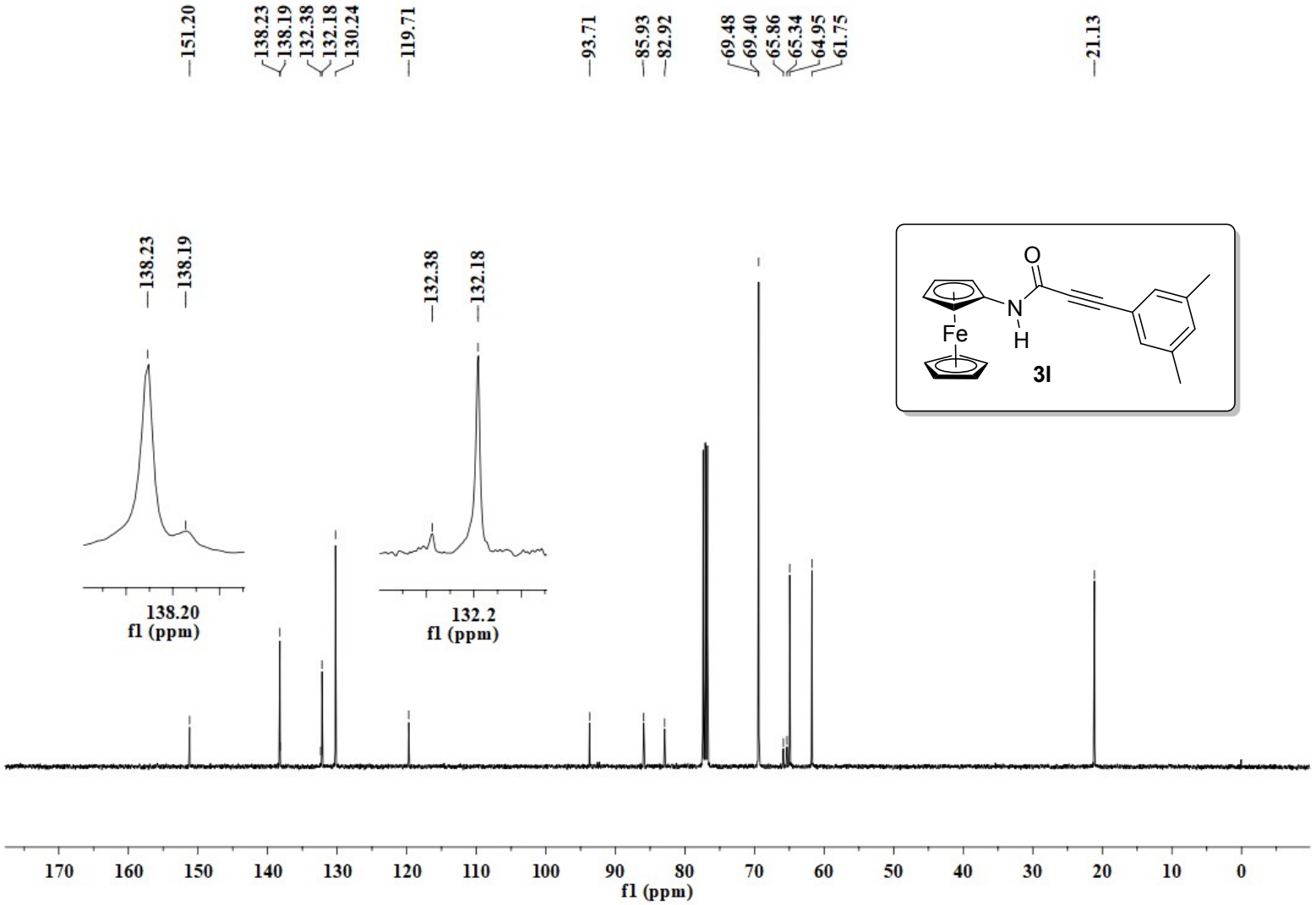

153.80
151.22
132.46
132.41
125.66
125.61
117.00
93.66
85.77
83.06
77.38
77.06
76.74
69.47
69.39
65.86
65.44
64.94
61.75
35.04
31.10
O
N
H
Fe
tBu
3k
132.46
132.41
132.4
f1 (ppm)
125.66
125.61
125.7
125.6
f1 (ppm)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

Sample Name	Jlx-2j	**Position**	P1-B1	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	Jlx-2j.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	3/20/18 Tue 16:34:24

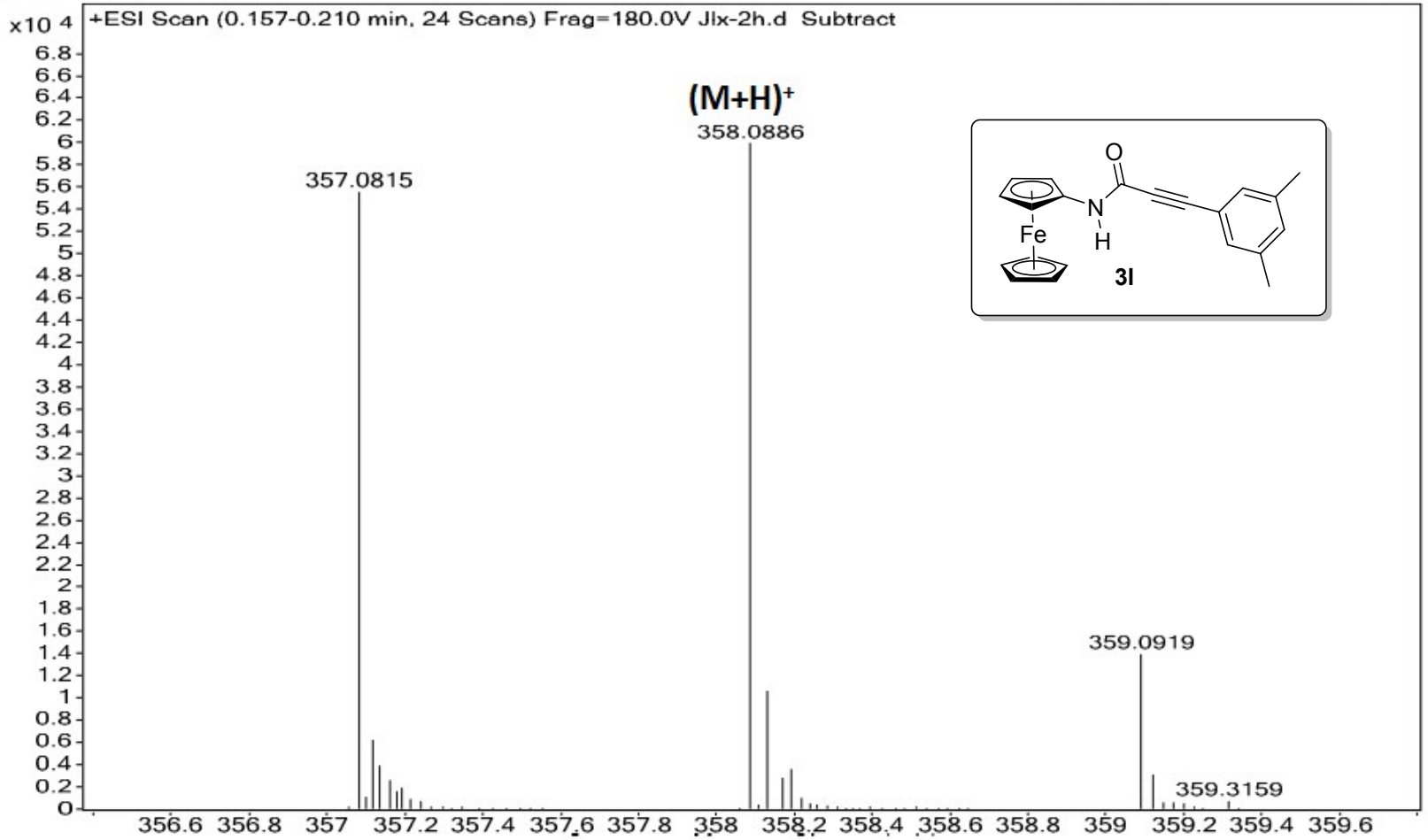


NMR and HMRS Spectra of **3l**

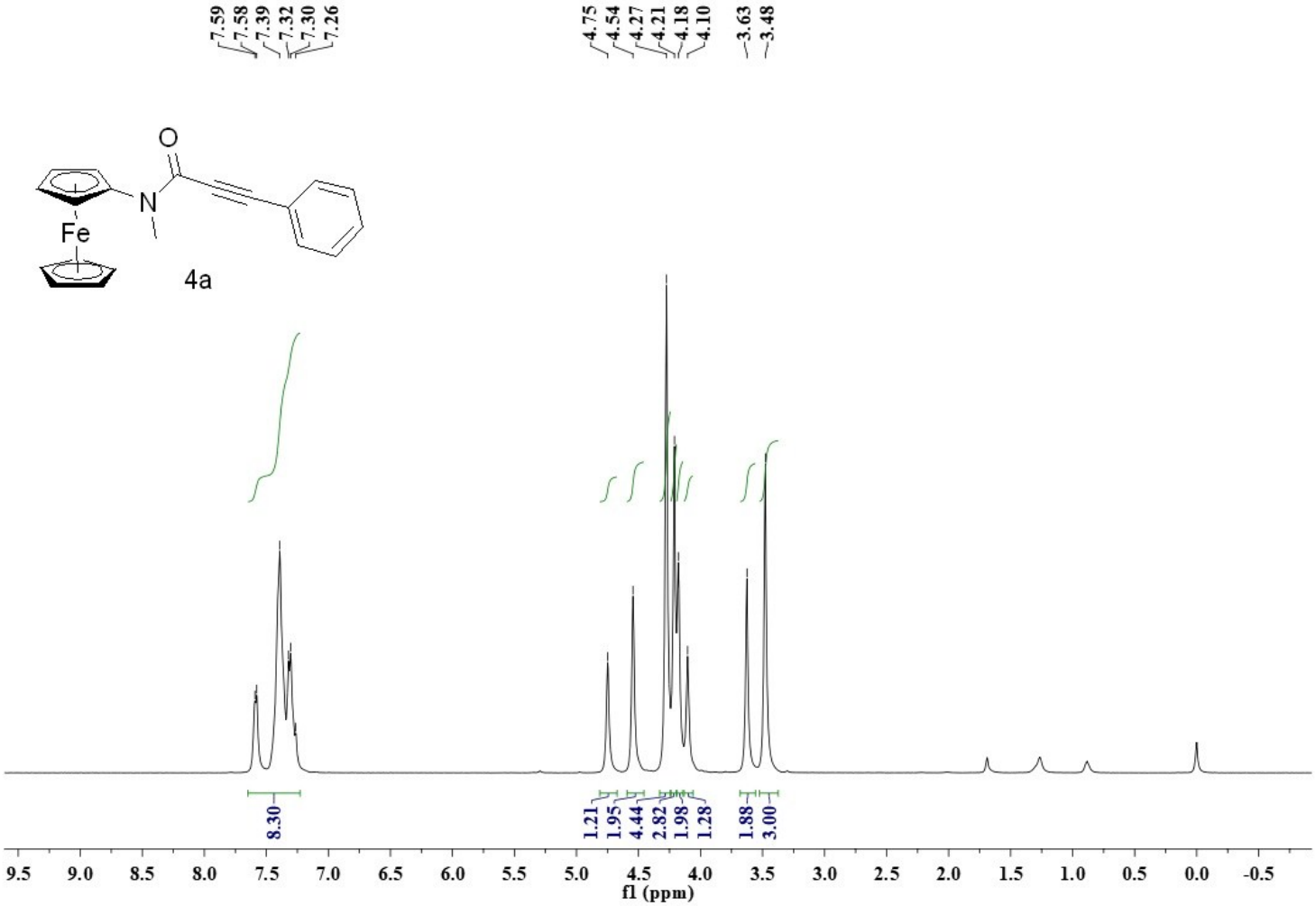


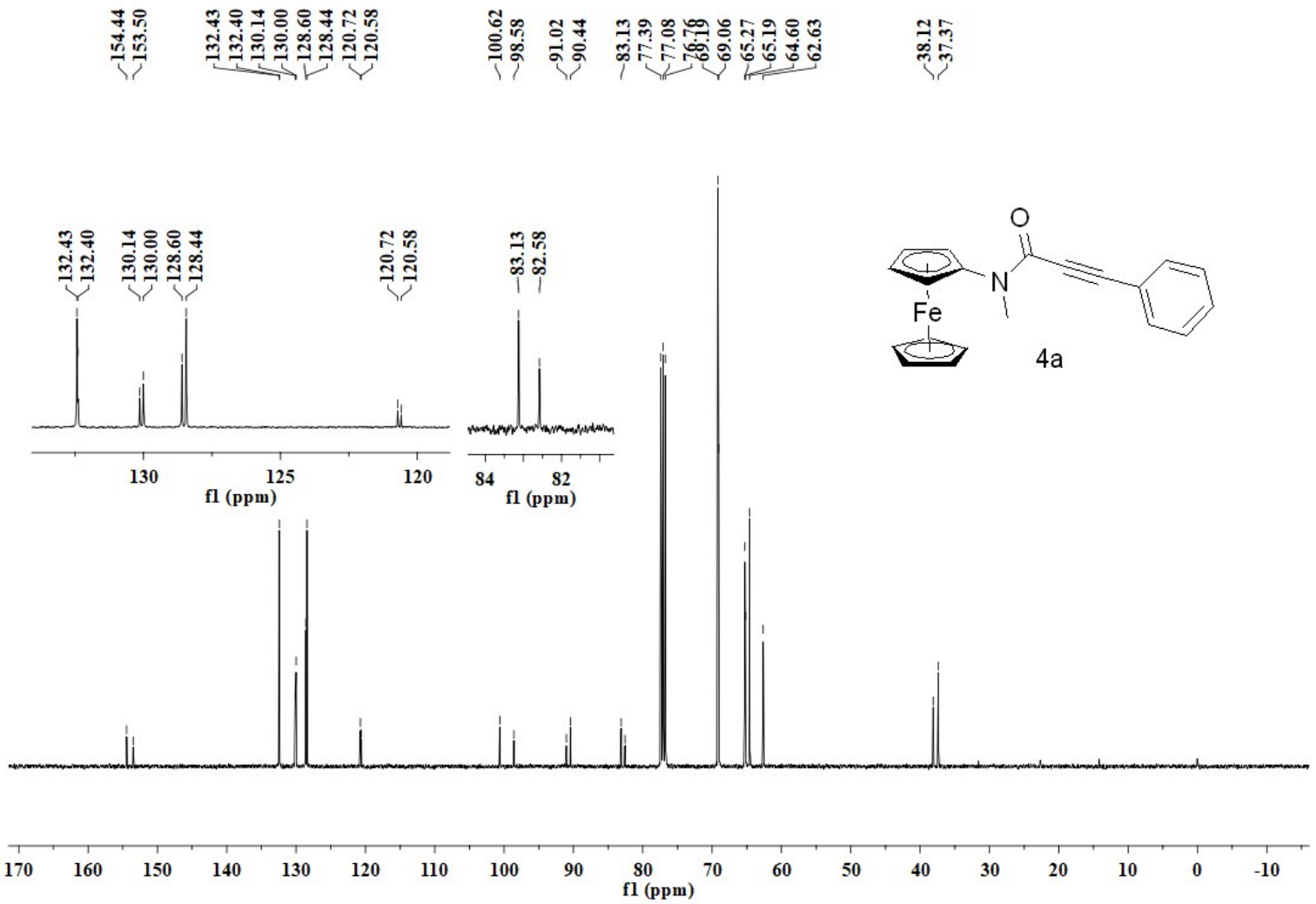

151.20
138.23
138.19
132.38
132.18
130.24
119.71
93.71
85.93
82.92
69.48
69.40
65.86
65.34
64.95
61.75
21.13
138.23
138.19
132.38
132.18
138.20
f1 (ppm)
132.2
f1 (ppm)
O
N
H
Fe
3l
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

Sample Name	Jlx-2h	**Position**	P1-A8	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	Jlx-2h.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	3/20/18 Tue 16:31:52

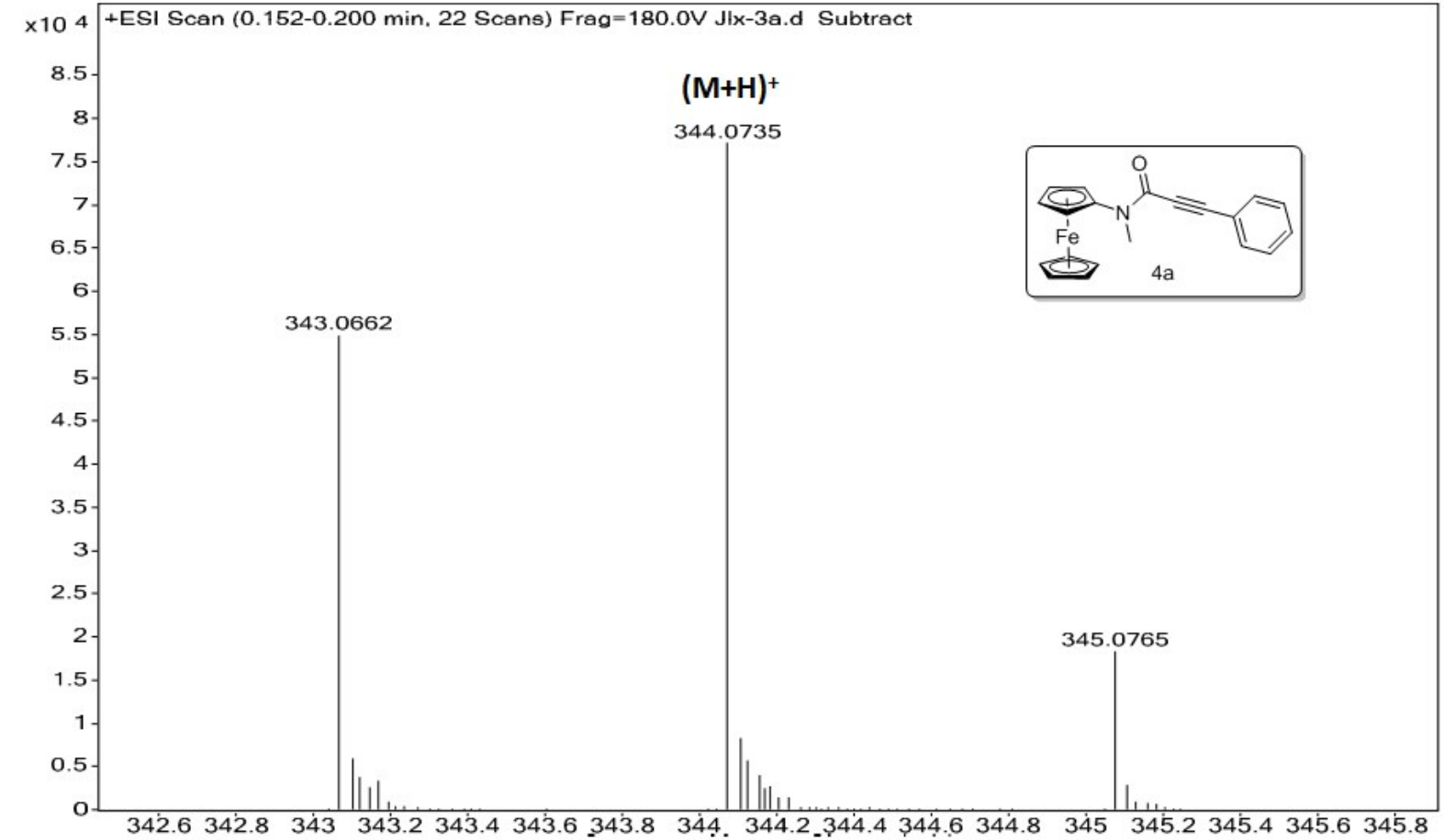


NMR and HMRS Spectra of **4a :**

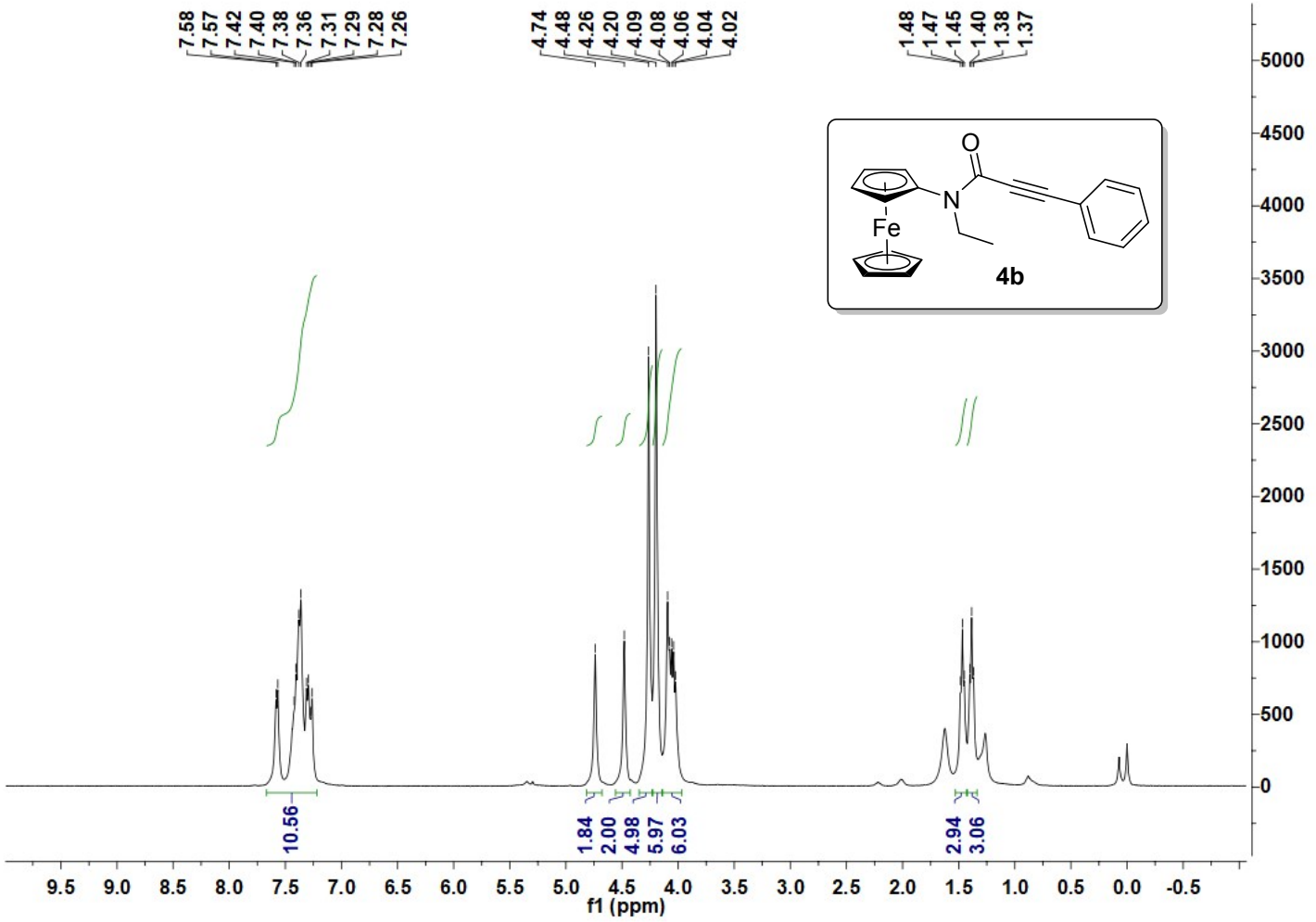


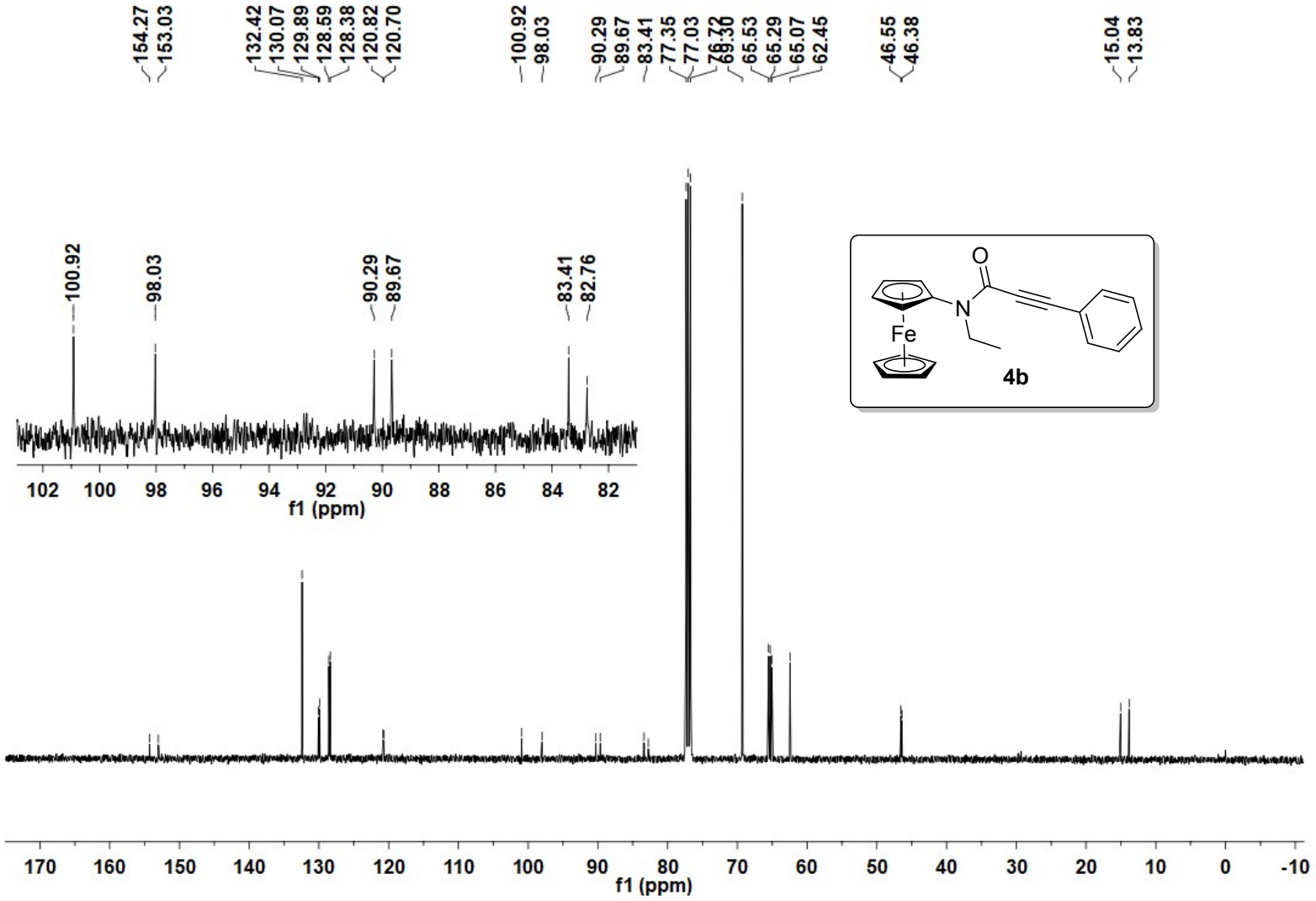

154.44
153.50
132.43
132.40
130.14
130.00
128.60
128.44
120.72
120.58
100.62
98.58
91.02
90.44
83.13
77.39
77.08
76.76
69.19
69.06
65.27
65.19
64.60
62.63
38.12
37.37
O
N
Fe
4a
fl (ppm)
fl (ppm)
fl (ppm)

Sample Name	Jlx-3a	**Position**	P1-A1	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	Jlx-3a.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	3/20/18 Tue 15:44:31

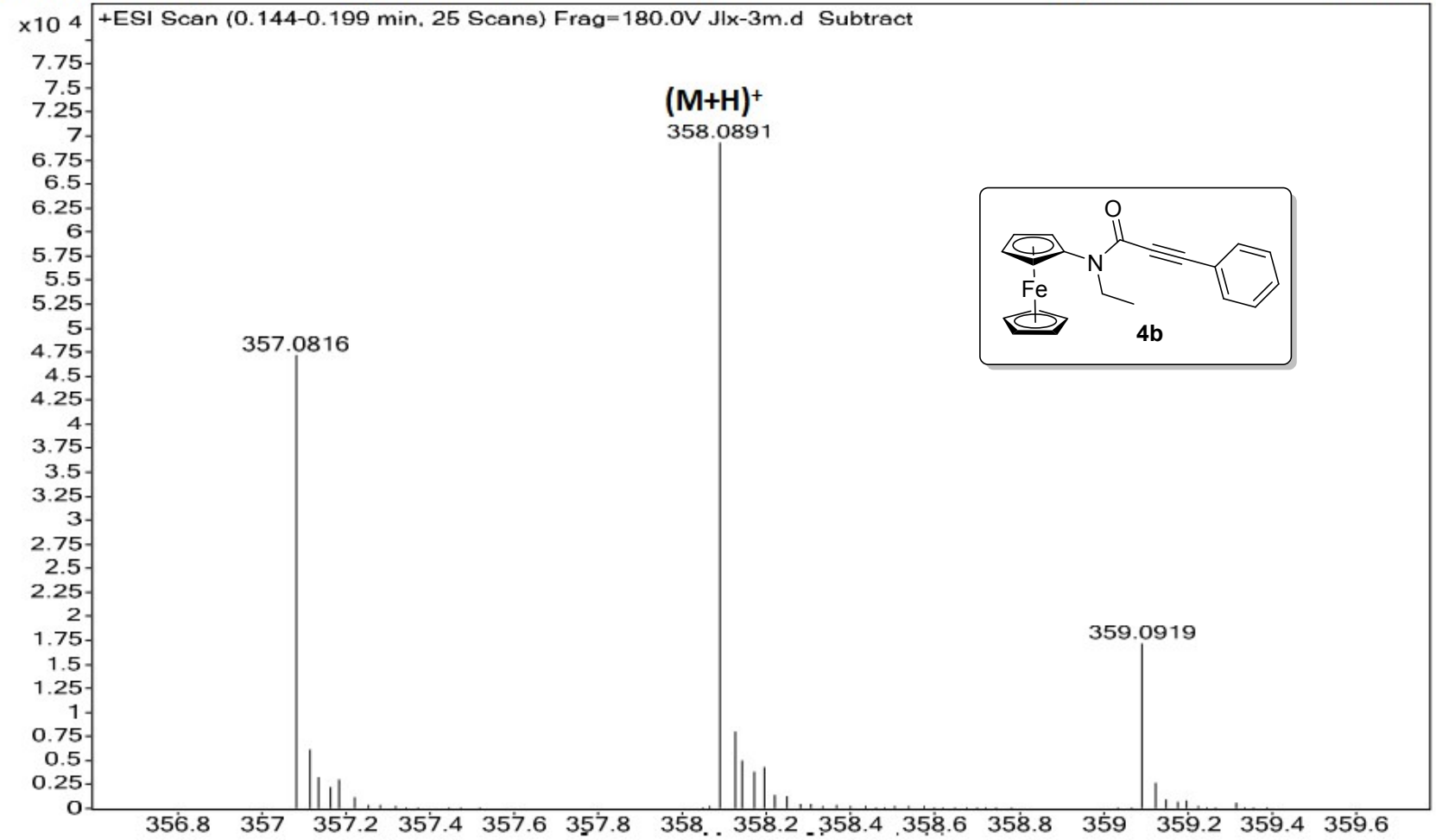


NMR and HMRS Spectra of **4b :**

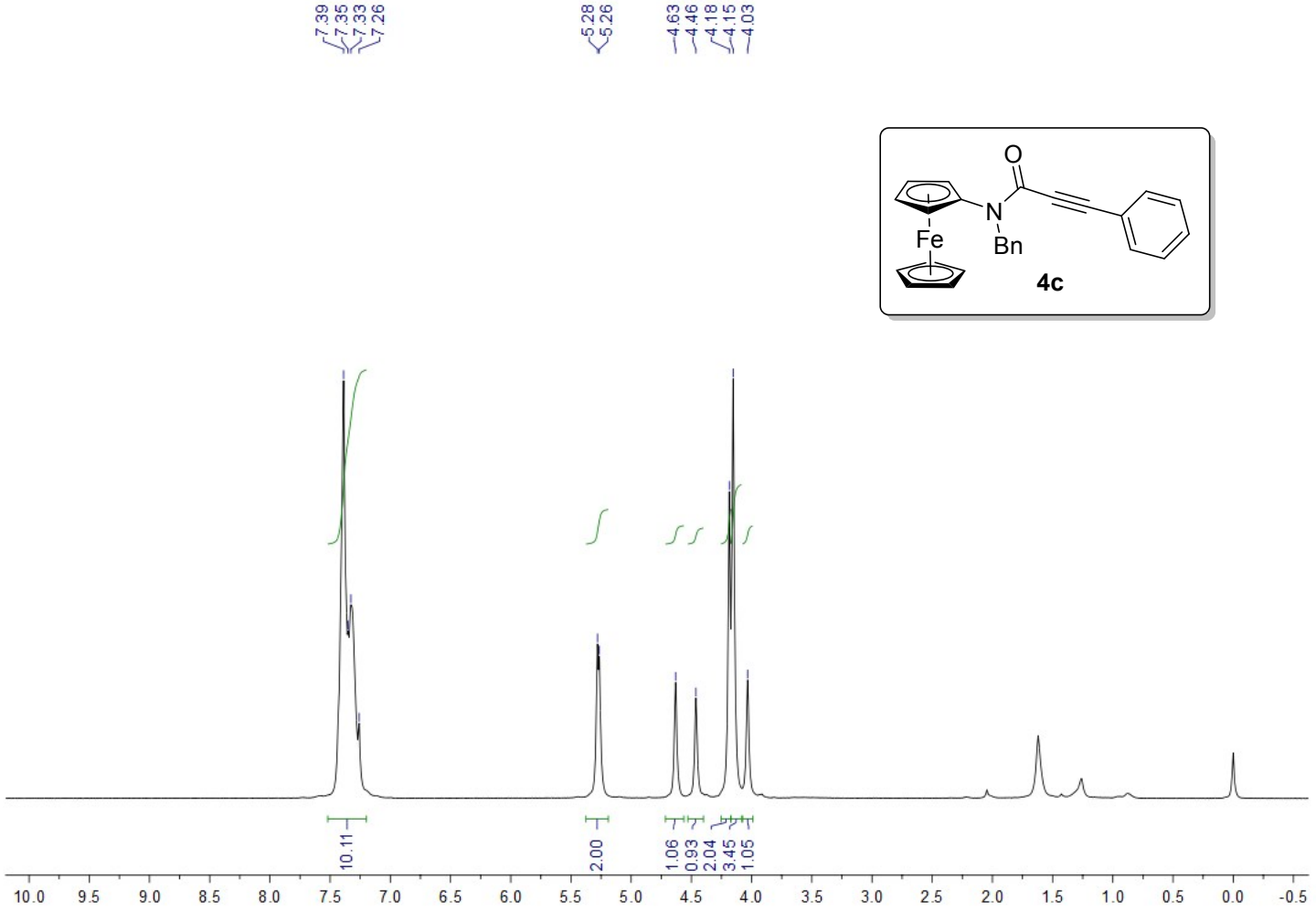


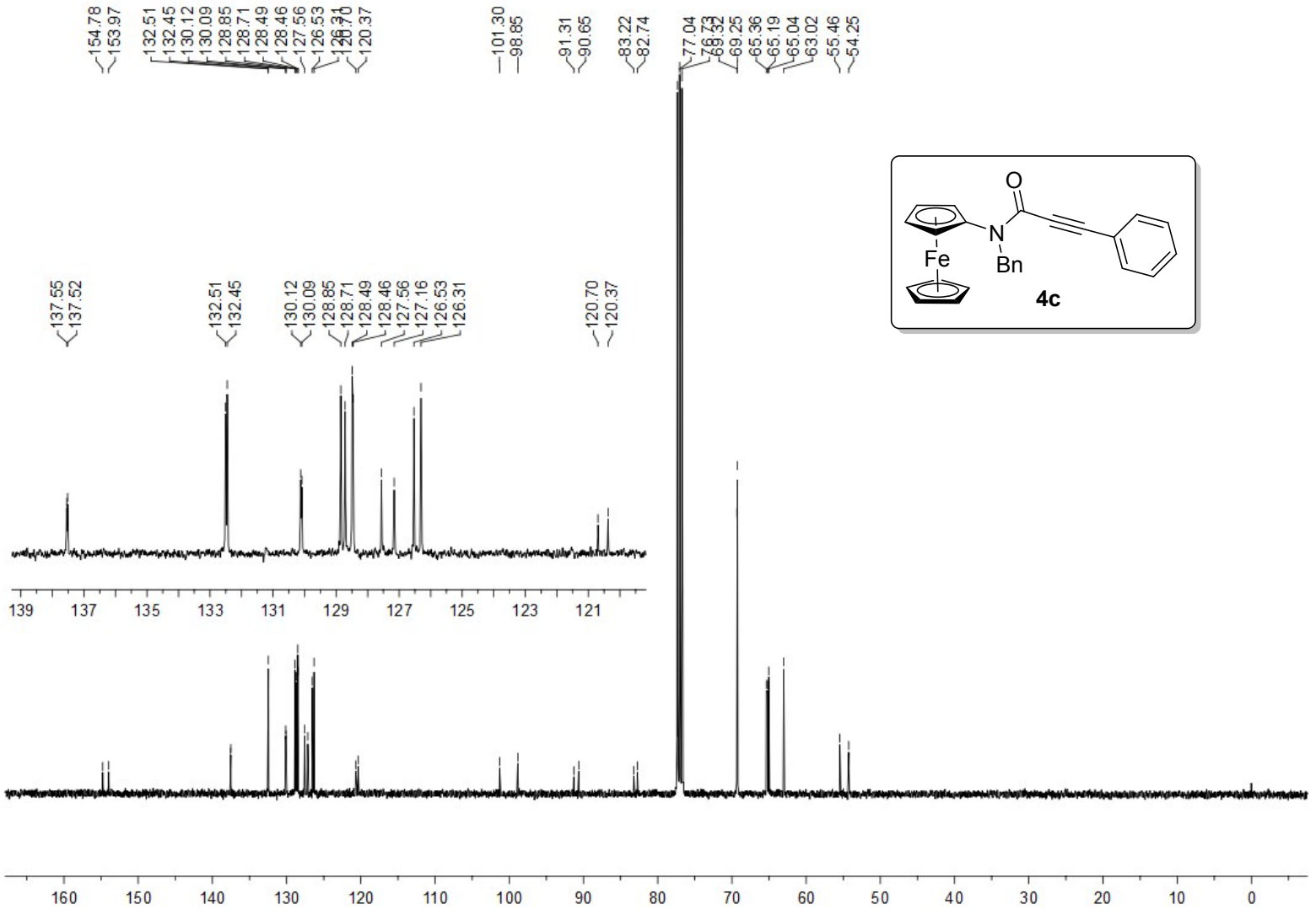

154.27
153.03
132.42
130.07
129.89
128.59
128.38
120.82
120.70
100.92
98.03
90.29
89.67
83.41
77.35
77.03
65.53
65.29
65.07
62.45
46.55
46.38
15.04
13.83
100.92
98.03
90.29
89.67
83.41
82.76
102 100 98 96 94 92 90 88 86 84 82
f1 (ppm)
O
N
Fe
4b
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

Sample Name	Jlx-3m	**Position**	P1-B4	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	Jlx-3m.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	3/20/18 Tue 16:00:24

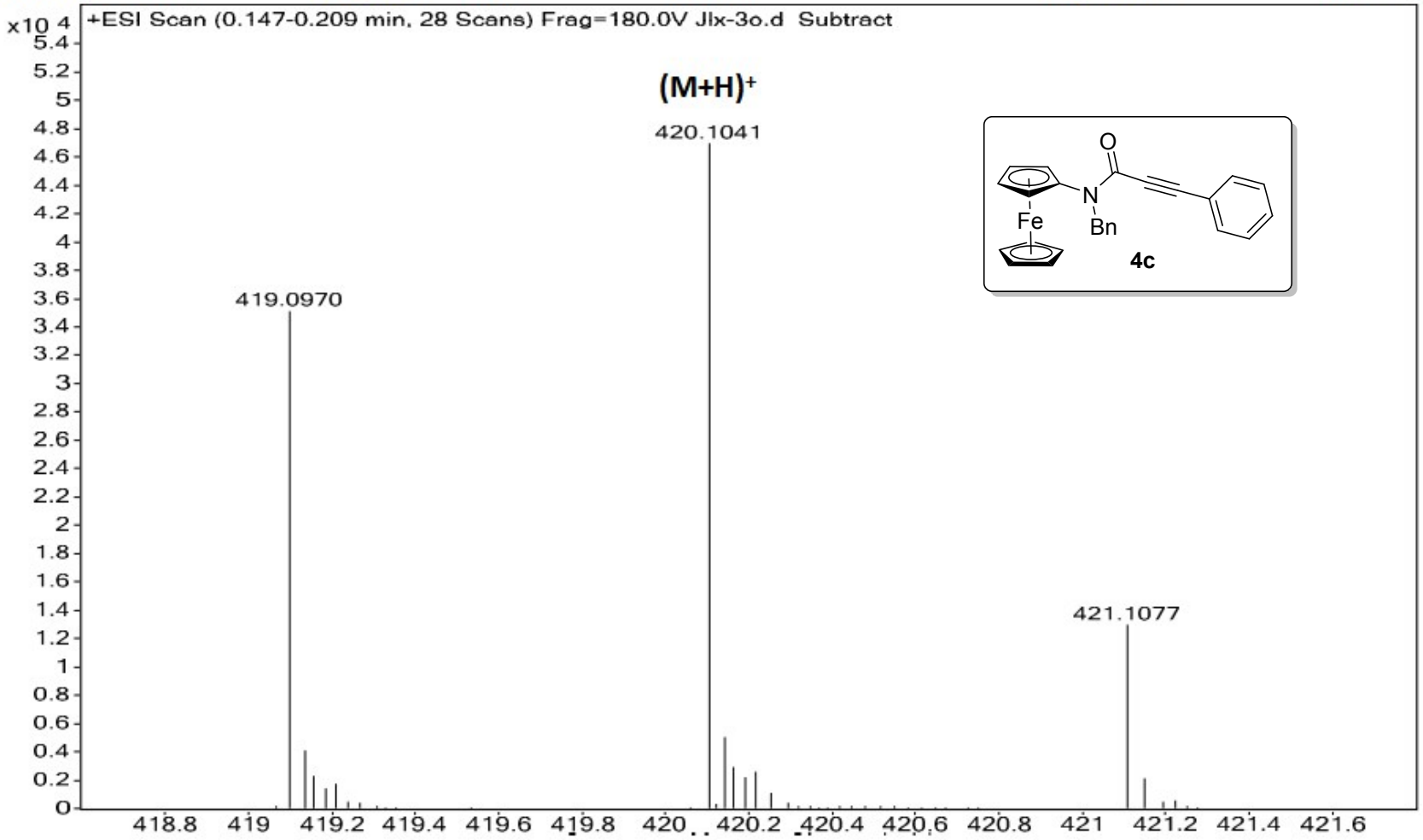


NMR and HMRS Spectra of **4c :**

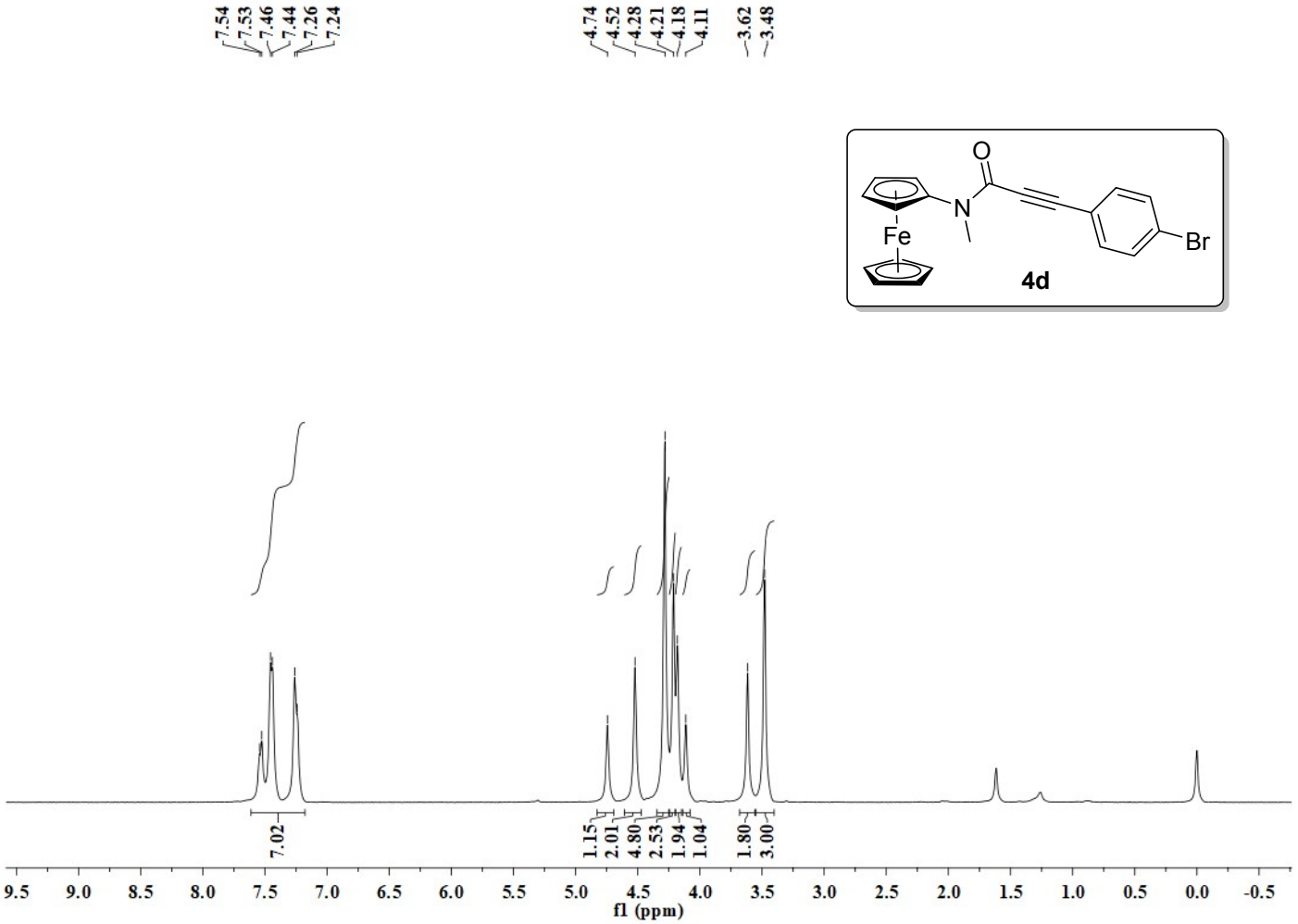


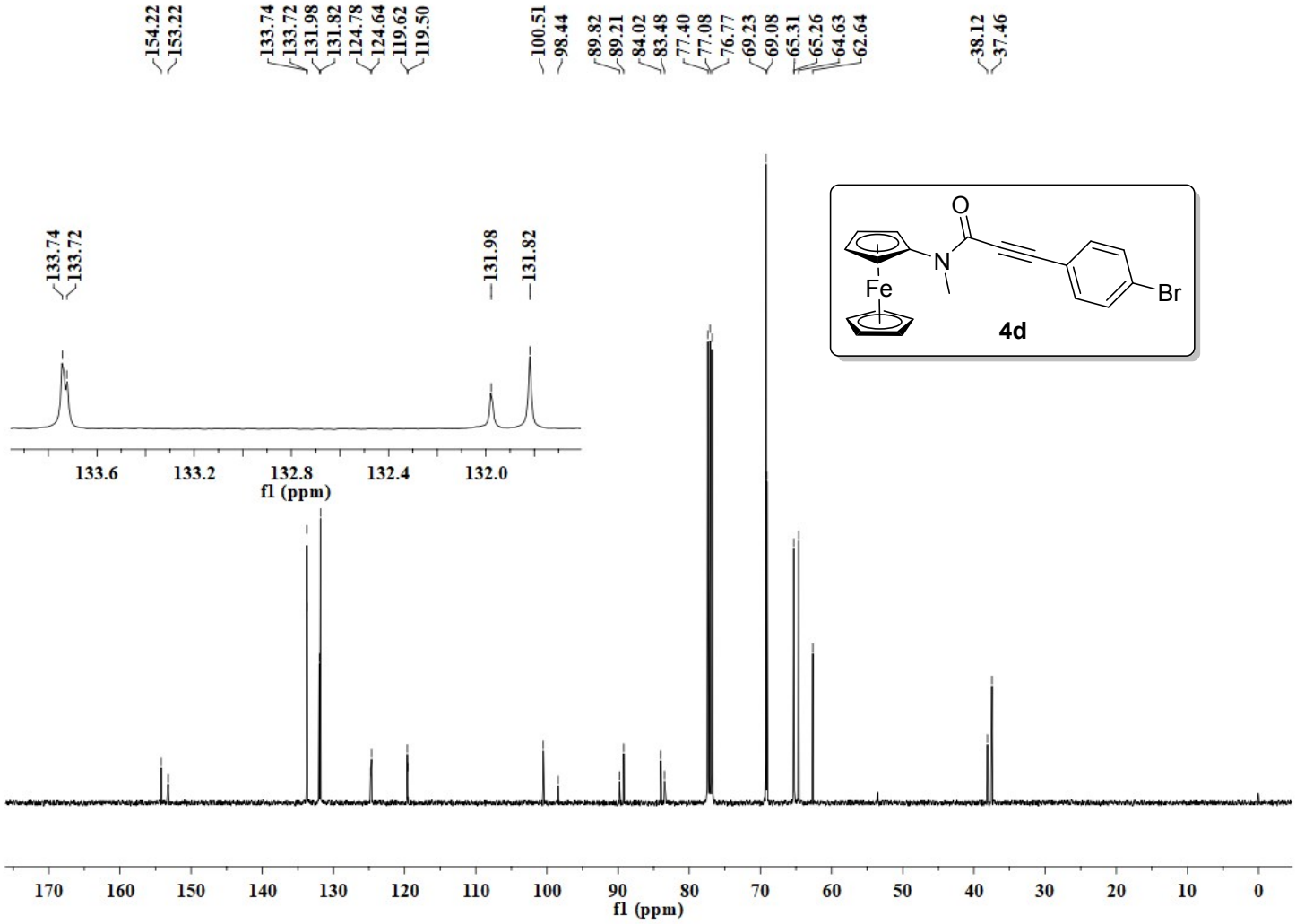

154.78
153.97
132.51
132.45
130.12
130.09
128.85
128.71
128.49
128.46
127.56
126.53
120.37
101.30
98.85
91.31
90.65
83.22
82.74
77.04
69.25
65.36
65.19
65.04
63.02
55.46
54.25
137.55
137.52
132.51
132.45
130.12
130.09
128.85
128.71
128.49
128.46
127.56
127.16
126.53
126.31
120.70
120.37
O
N
Bn
Fe
4c
139
137
135
133
131
129
127
125
123
121
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

Sample Name	Jlx-3o	**Position**	P1-B6	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	Jlx-3o.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	3/20/18 Tue 16:02:56

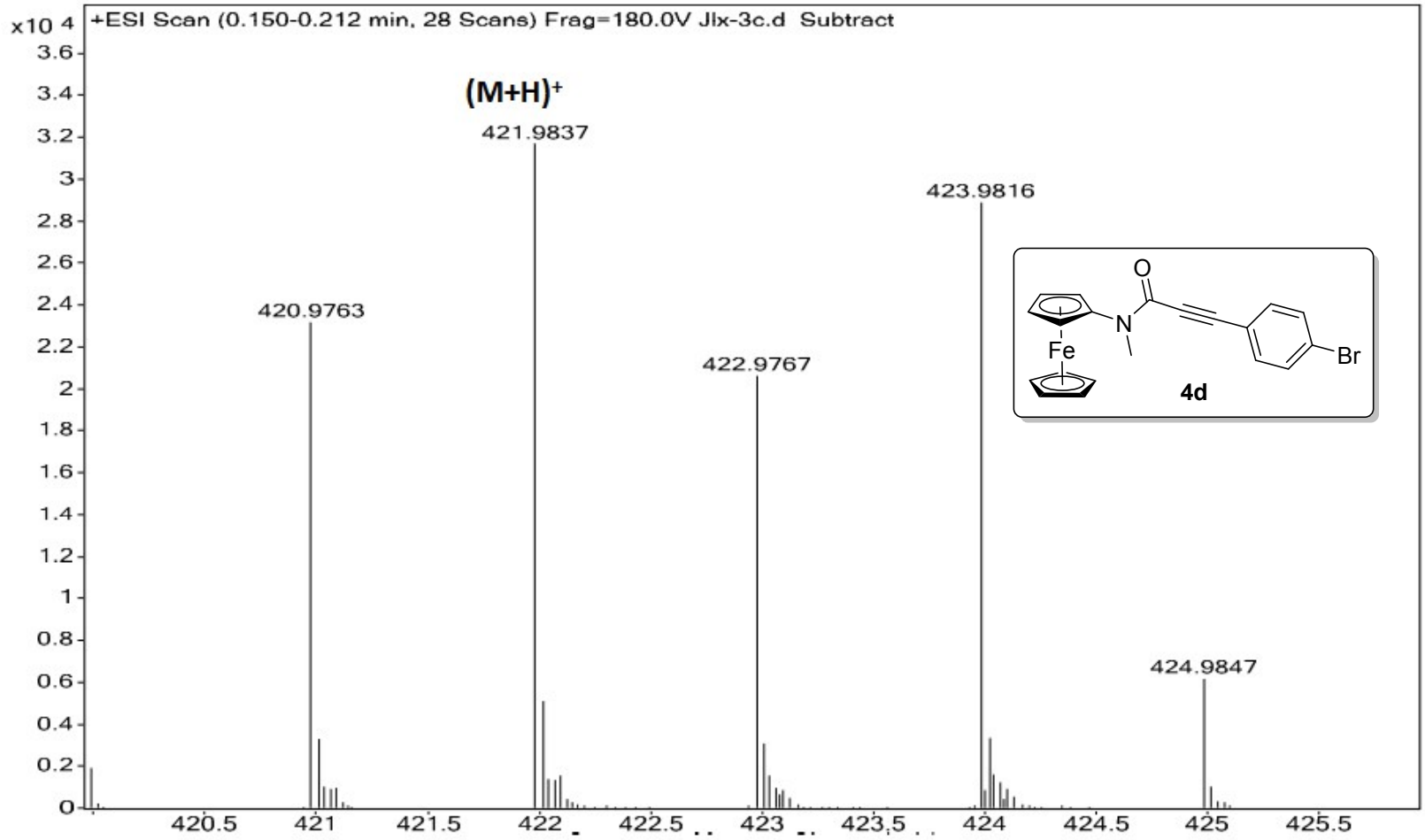


NMR and HMRS Spectra of **4d :**

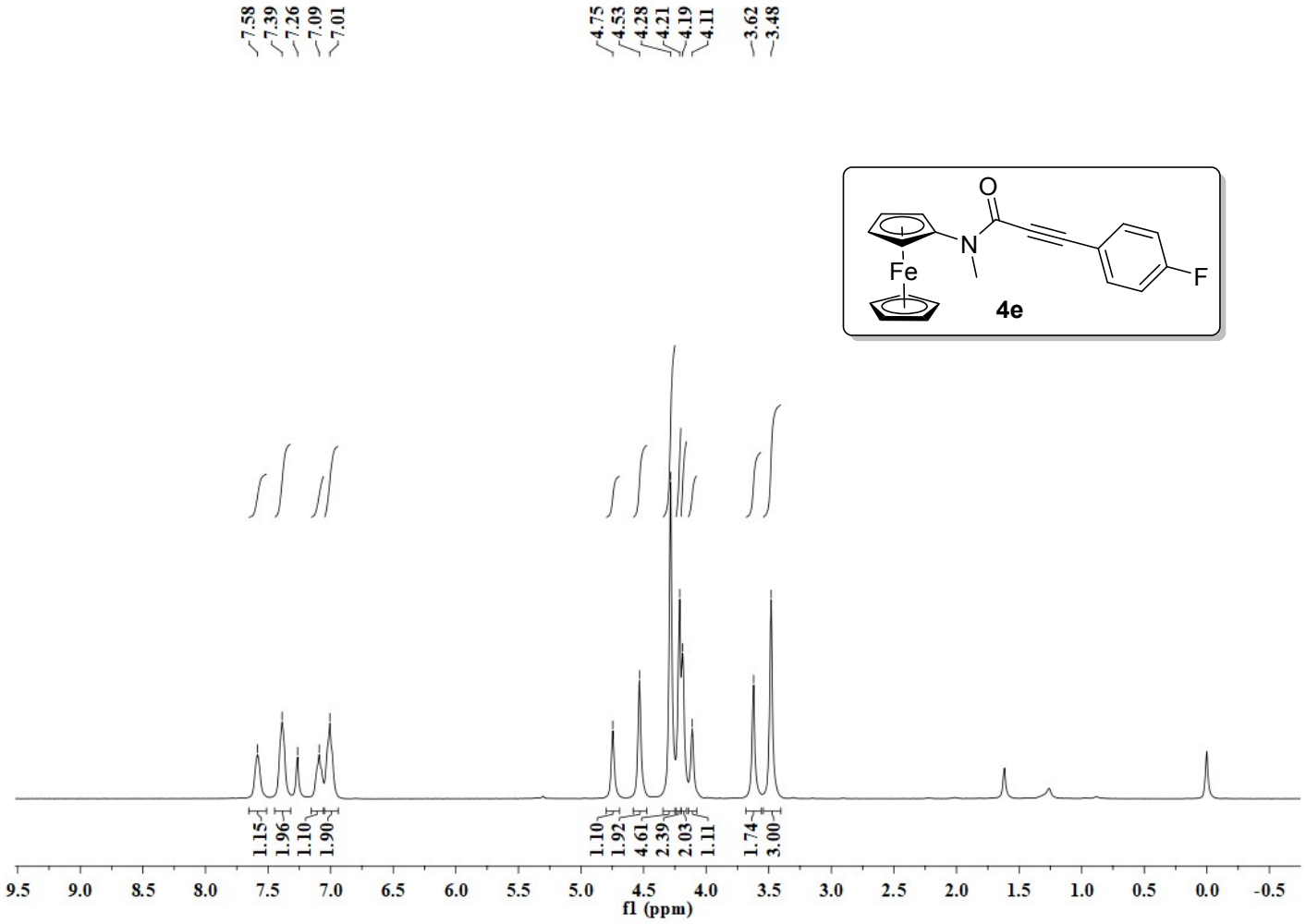


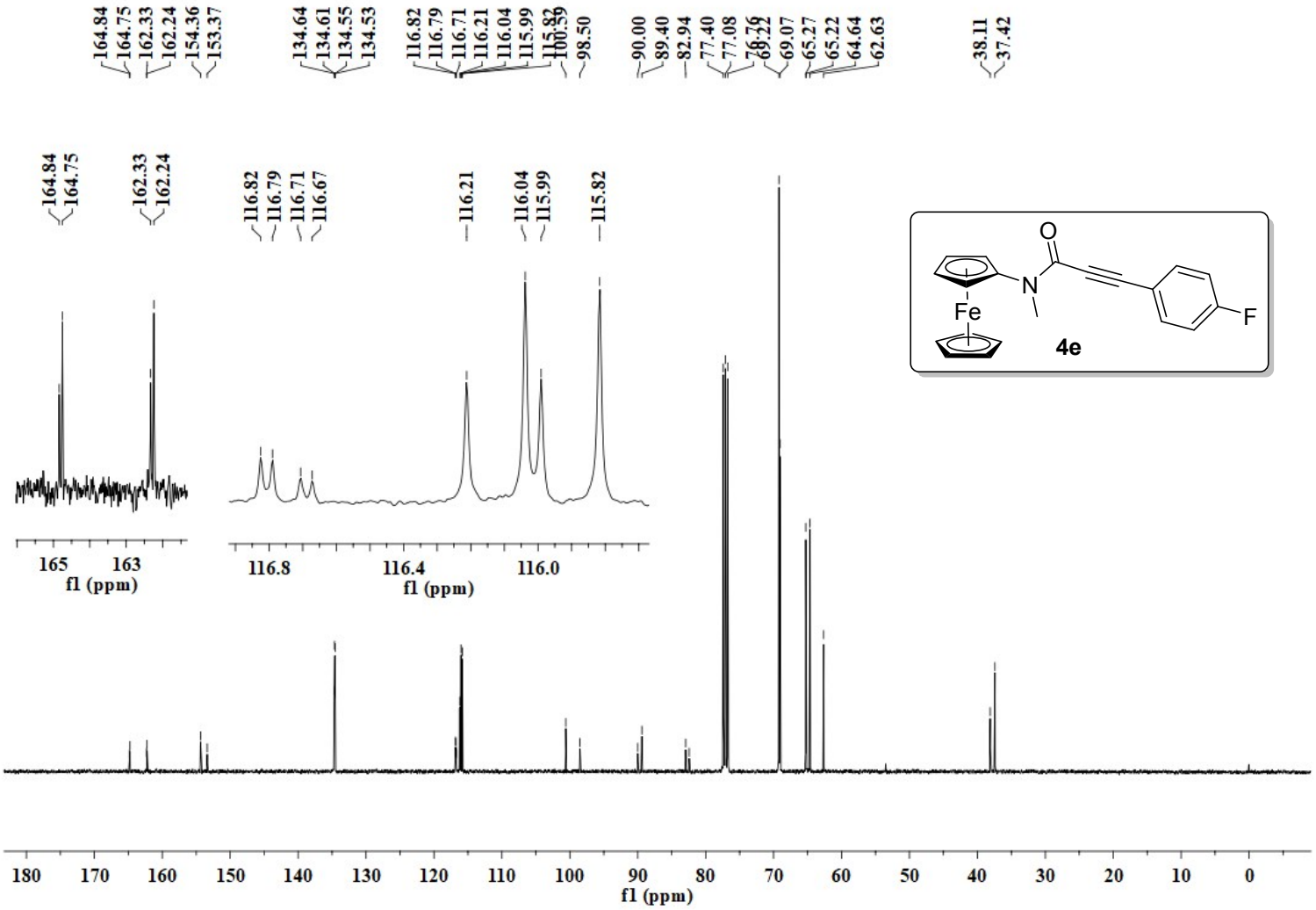

154.22
153.22
133.74
133.72
131.98
131.82
124.78
124.64
119.62
119.50
100.51
98.44
89.82
89.21
84.02
83.48
77.40
77.08
76.77
69.23
69.08
65.31
65.26
64.63
62.64
38.12
37.46
133.74
133.72
131.98
131.82
133.6
133.2
132.8
132.4
132.0
f1 (ppm)
O
N
Fe
Br
4d
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

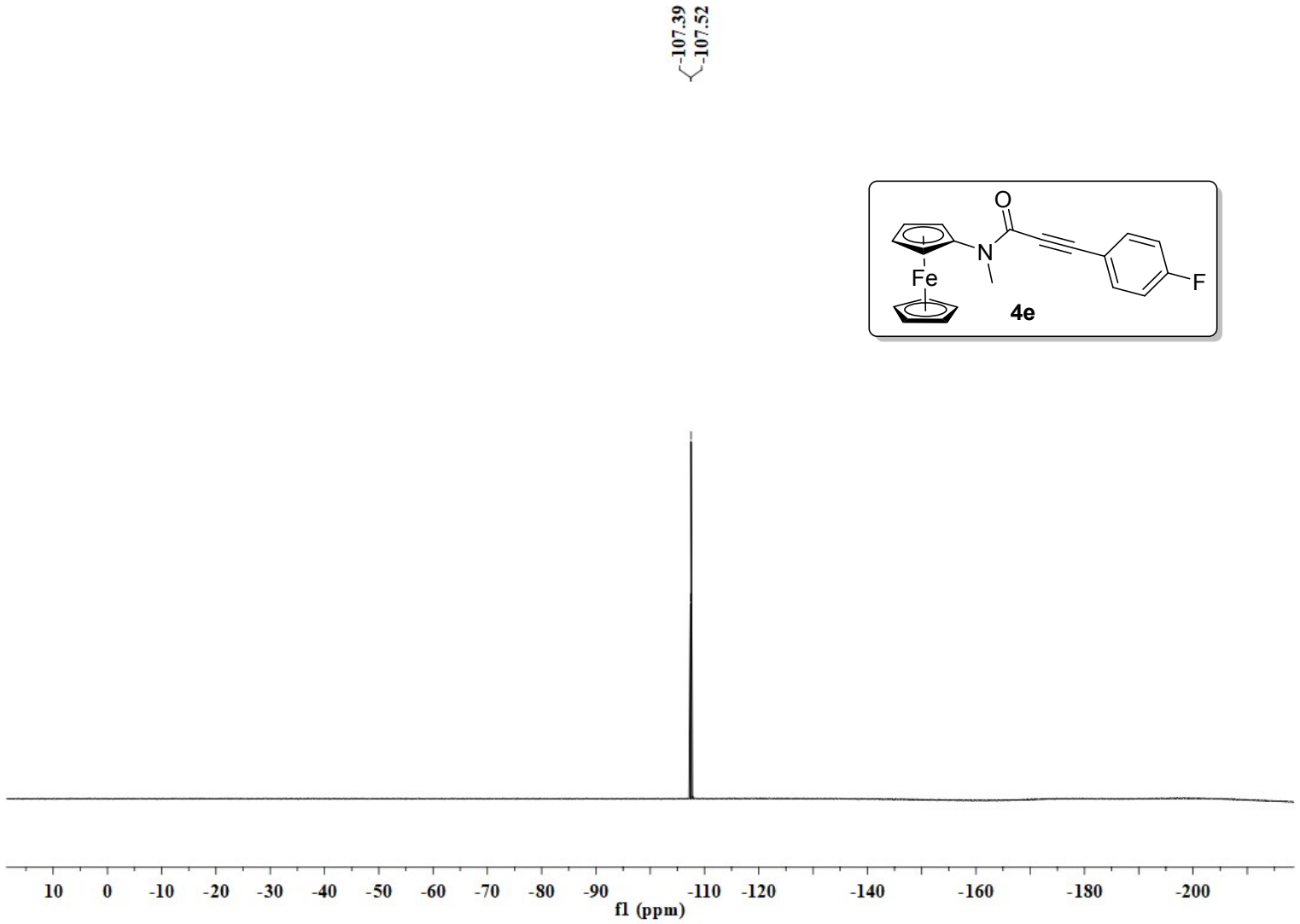
Sample Name	Jlx-3c	**Position**	P1-A3	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	Jlx-3c.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	3/20/18 Tue 15:47:44



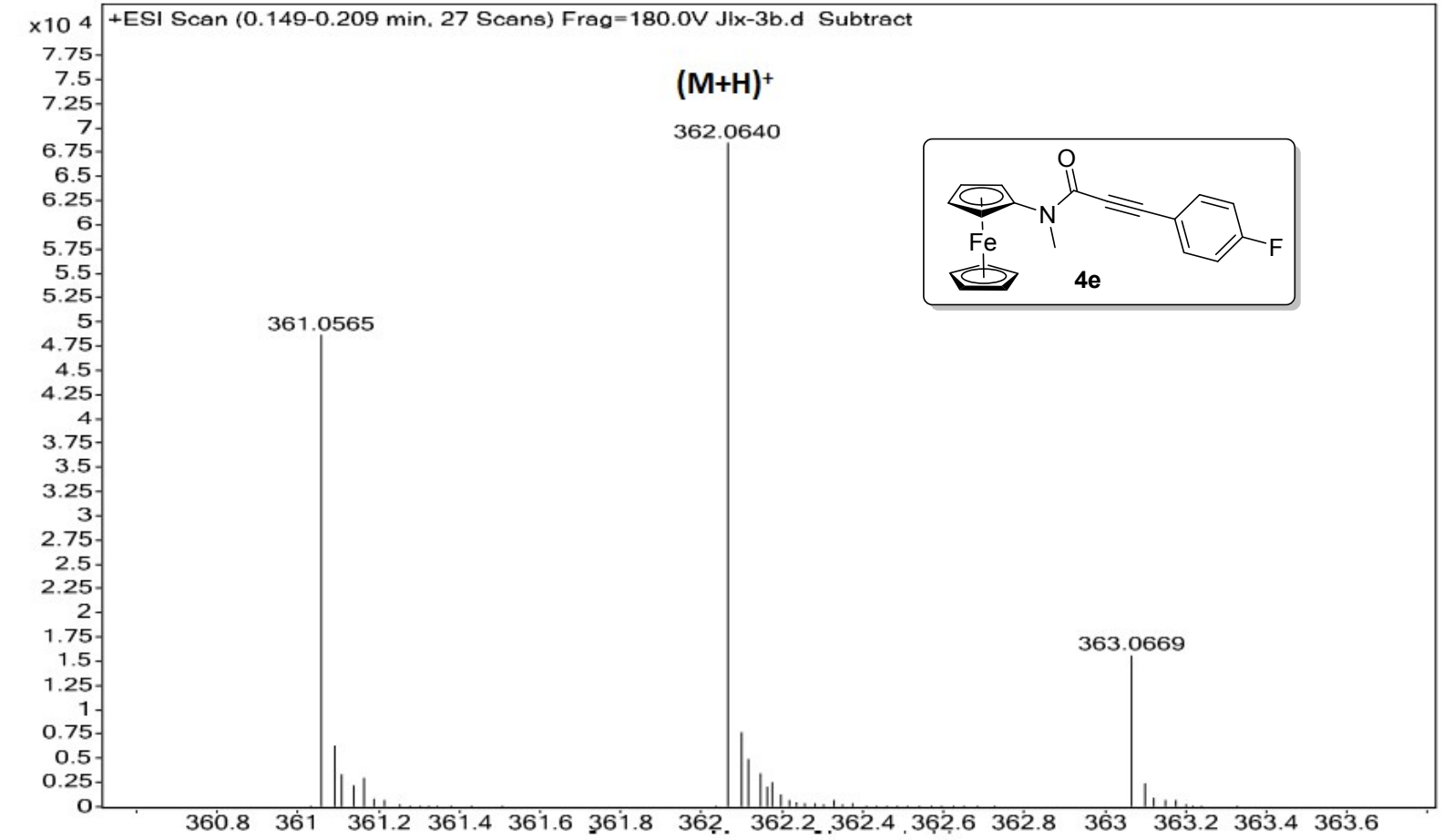
NMR and HMRS Spectra of **4e :**



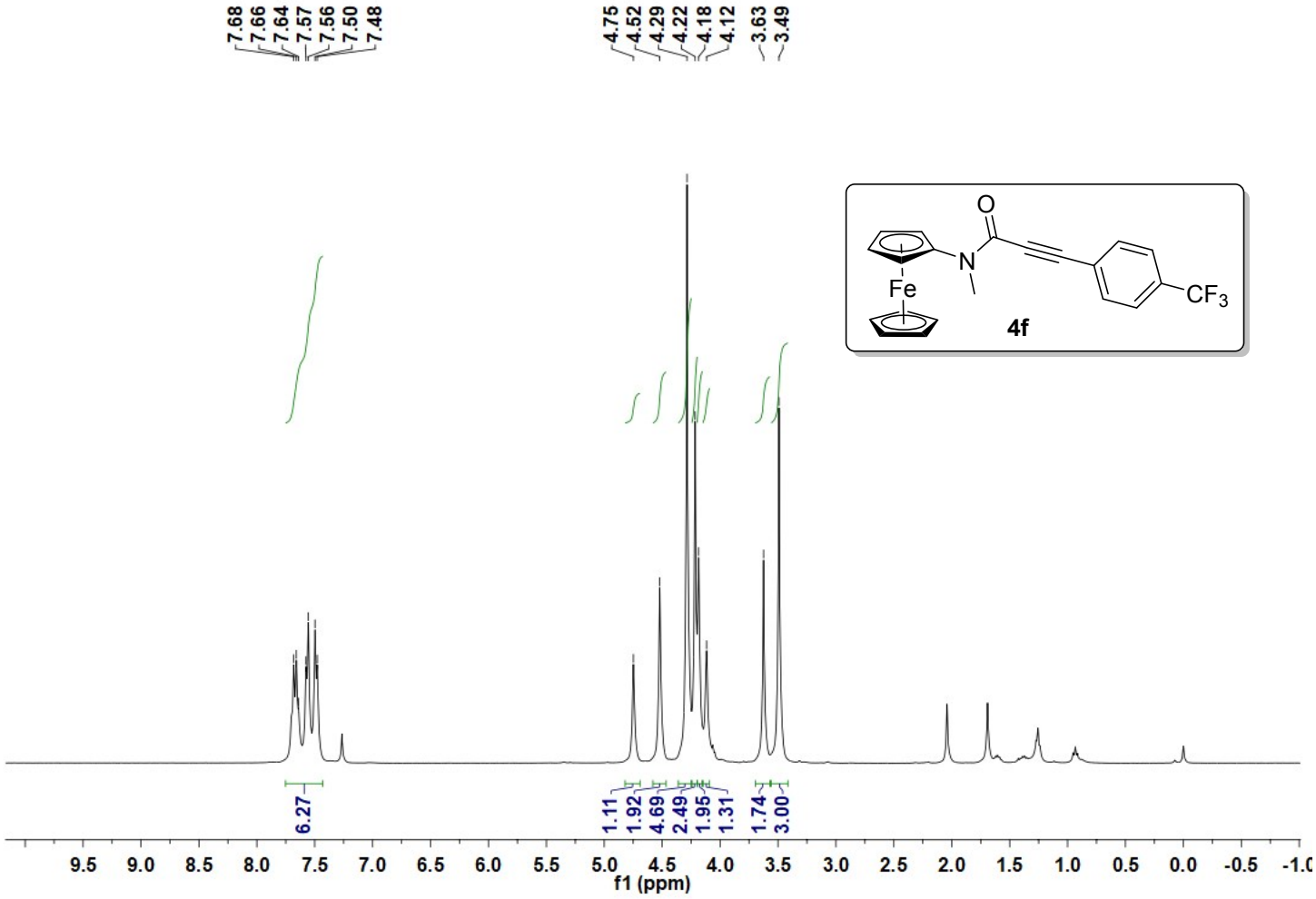

164.84
164.75
162.33
162.24
154.36
153.37
134.64
134.61
134.55
134.53
116.82
116.79
116.71
116.21
116.04
115.99
115.82
98.50
90.00
89.40
82.94
77.40
77.08
69.07
65.27
65.22
64.64
62.63
38.11
37.42
165
163
fl (ppm)
116.8
116.4
116.0
fl (ppm)
O
N
Fe
F
4e
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
fl (ppm)

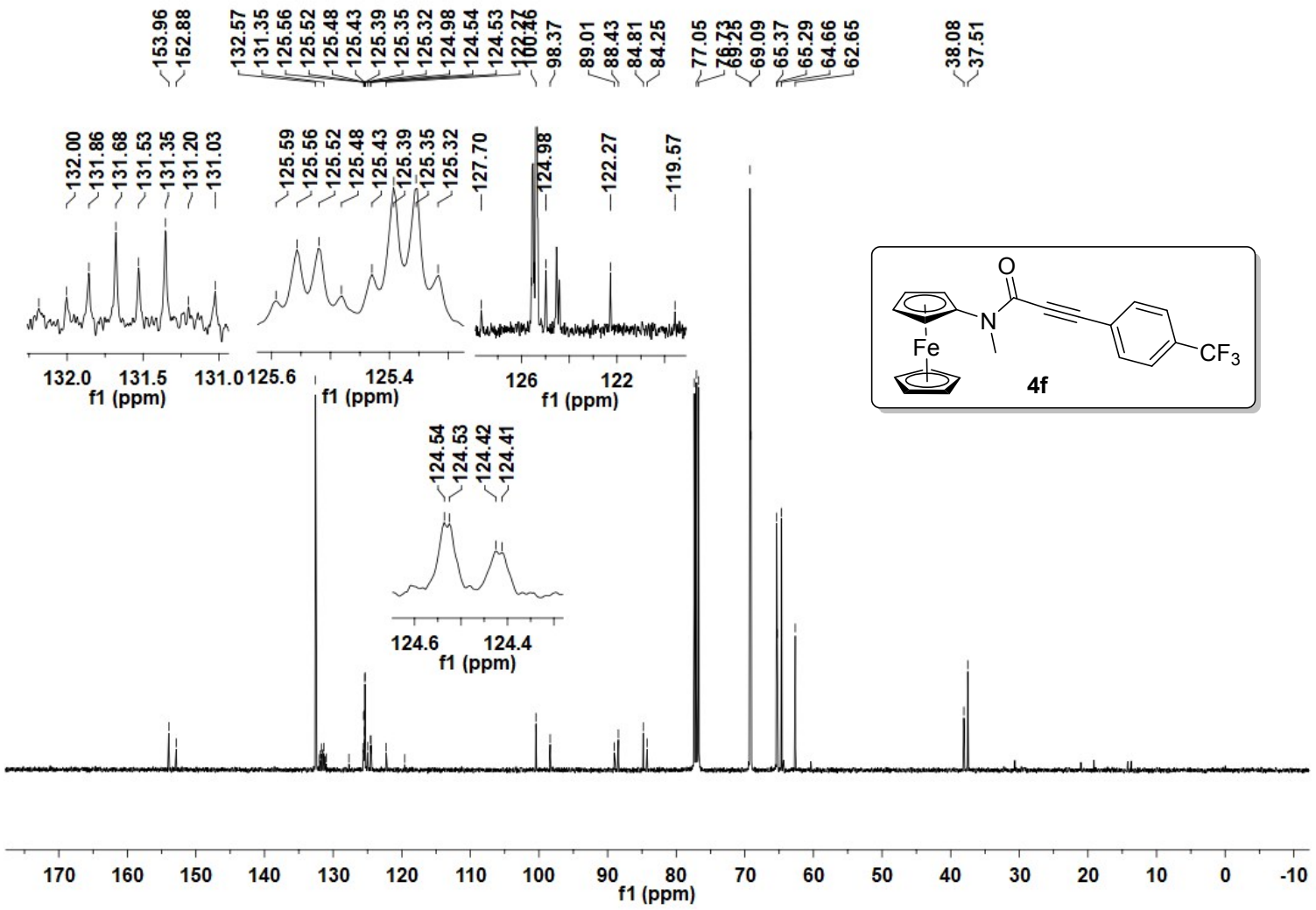

-107.39
-107.52
O
N
Fe
F
4e
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-110
-120
-140
-160
-180
-200
f1 (ppm)

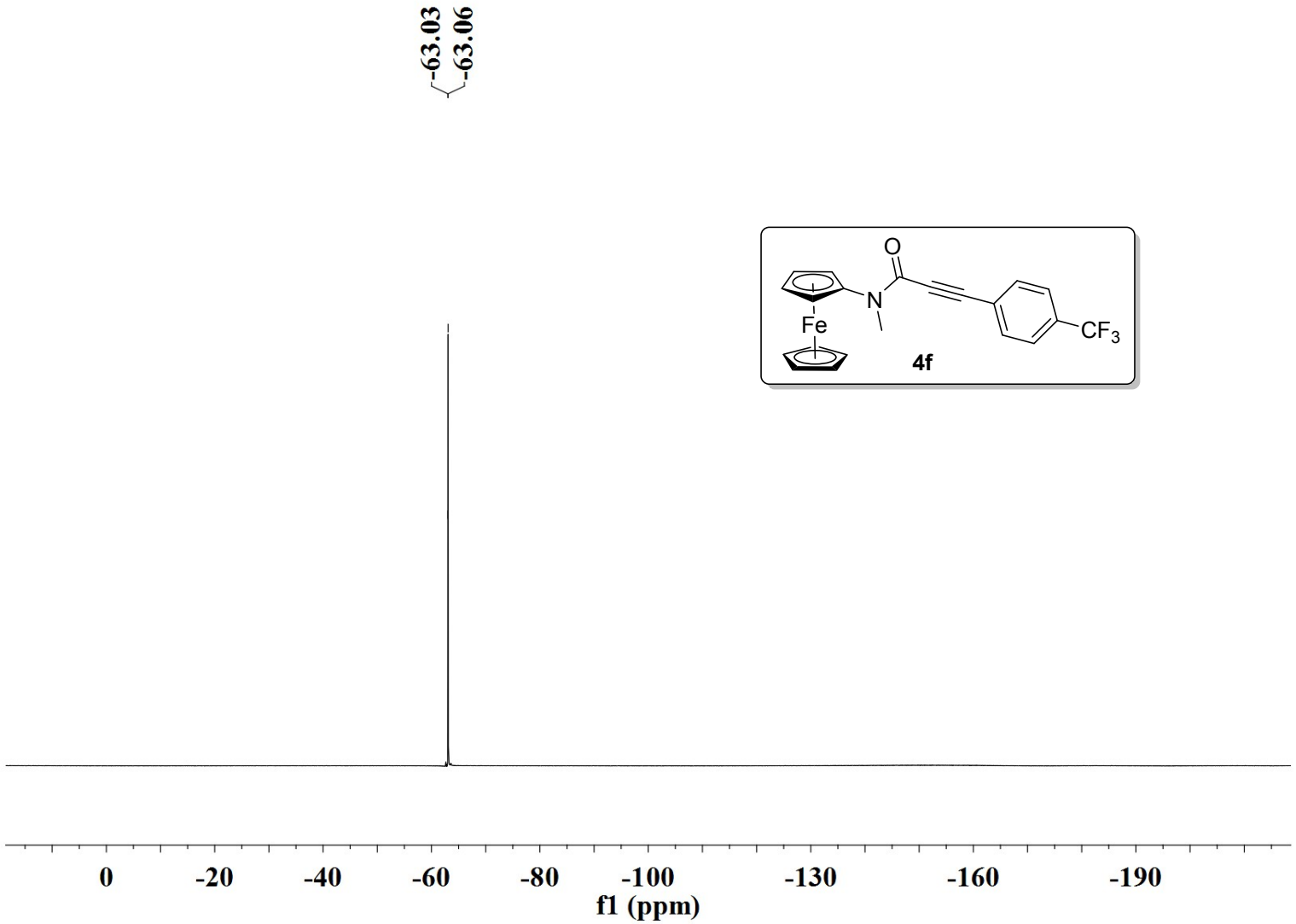
Sample Name	Jlx-3b	**Position**	P1-A2	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	Jlx-3b.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	3/20/18 Tue 15:46:28



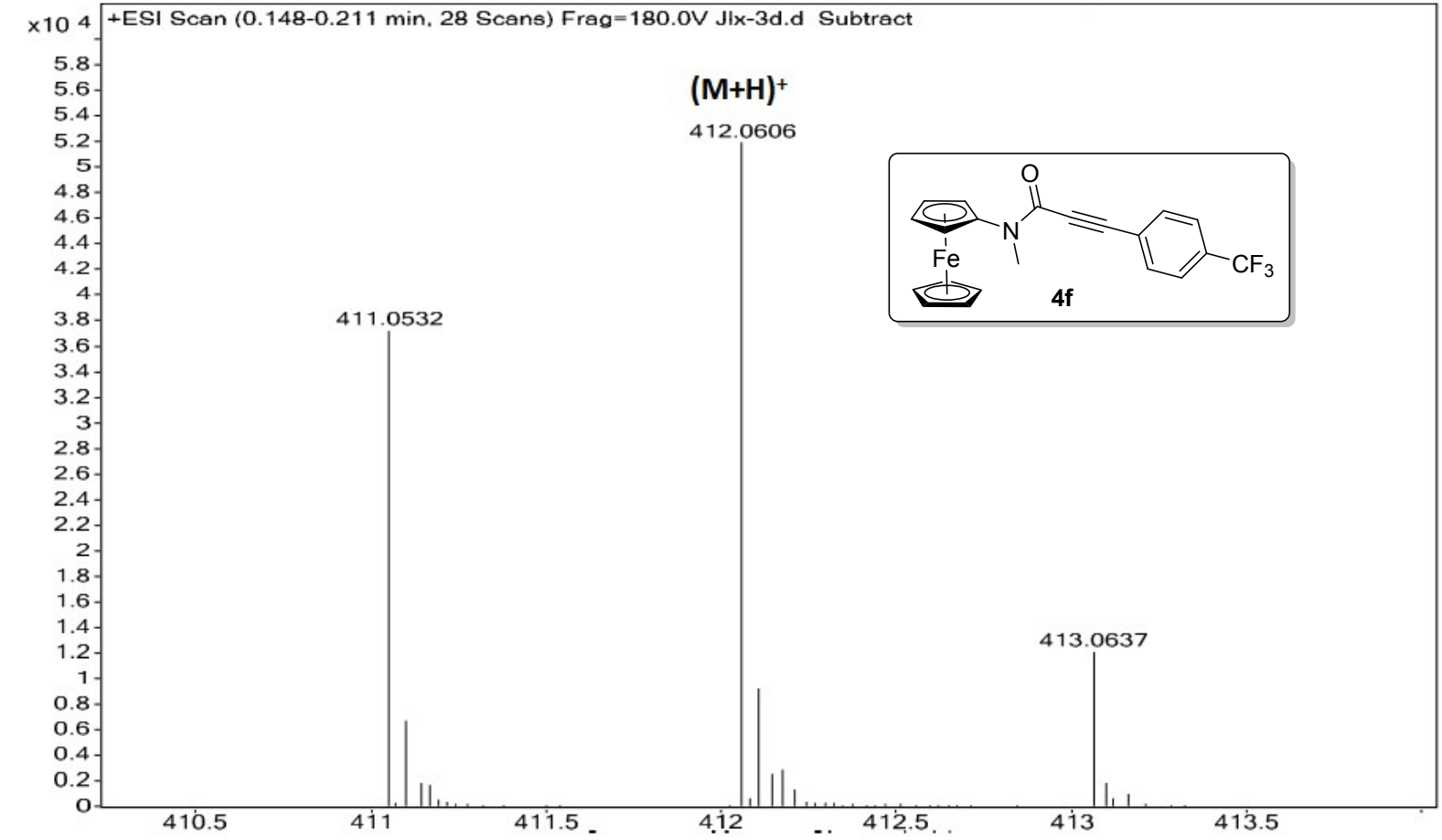
NMR and HMRS Spectra of **4f :**



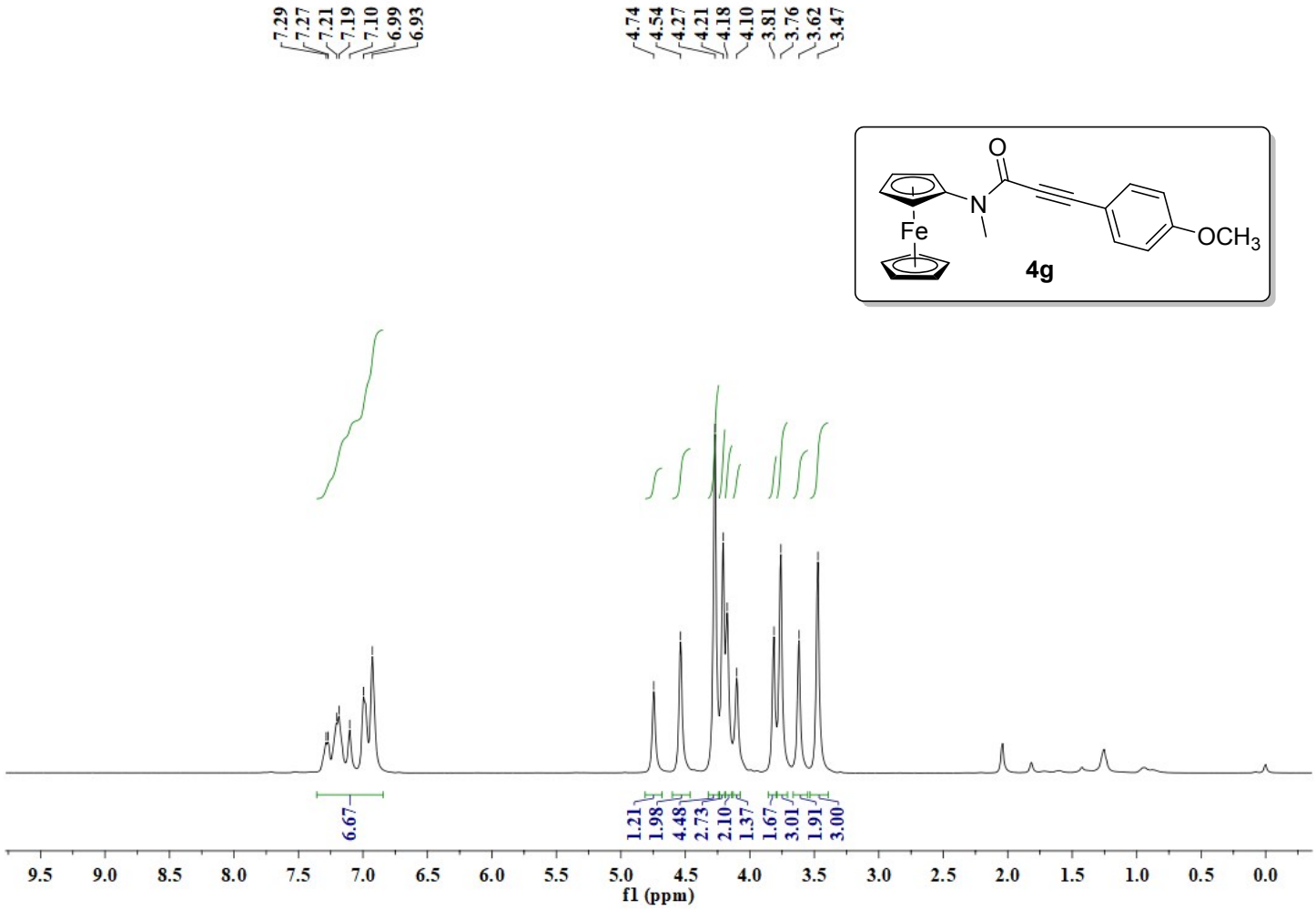

153.96
152.88
132.57
131.35
125.56
125.52
125.48
125.43
125.39
125.35
125.32
124.98
124.54
124.53
122.27
100.46
98.37
89.01
88.43
84.81
84.25
77.05
76.73
69.25
69.09
65.37
65.29
64.66
62.65
38.08
37.51
132.00
131.86
131.68
131.53
131.35
131.20
131.03
125.59
125.56
125.52
125.48
125.43
125.39
125.35
125.32
127.70
124.98
122.27
119.57
124.54
124.53
124.42
124.41
O
N
Fe
CF3
4f
f1 (ppm)

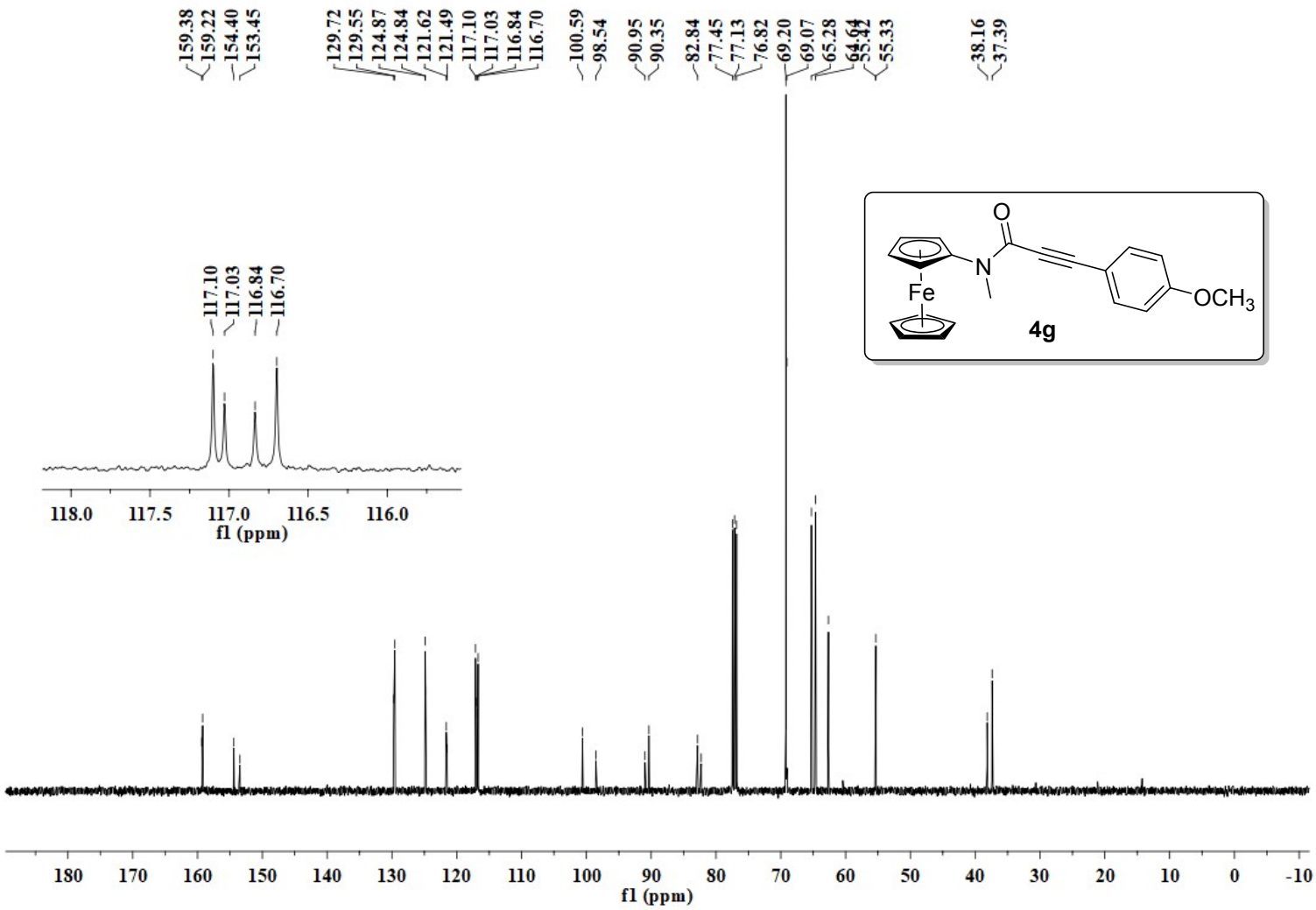

-63.03
-63.06
O
N
Fe
CF3
4f
0
-20
-40
-60
-80
-100
-130
-160
-190
f1 (ppm)

Sample Name	Jlx-3d	**Position**	P1-A4	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	Jlx-3d.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	3/20/18 Tue 15:48:59

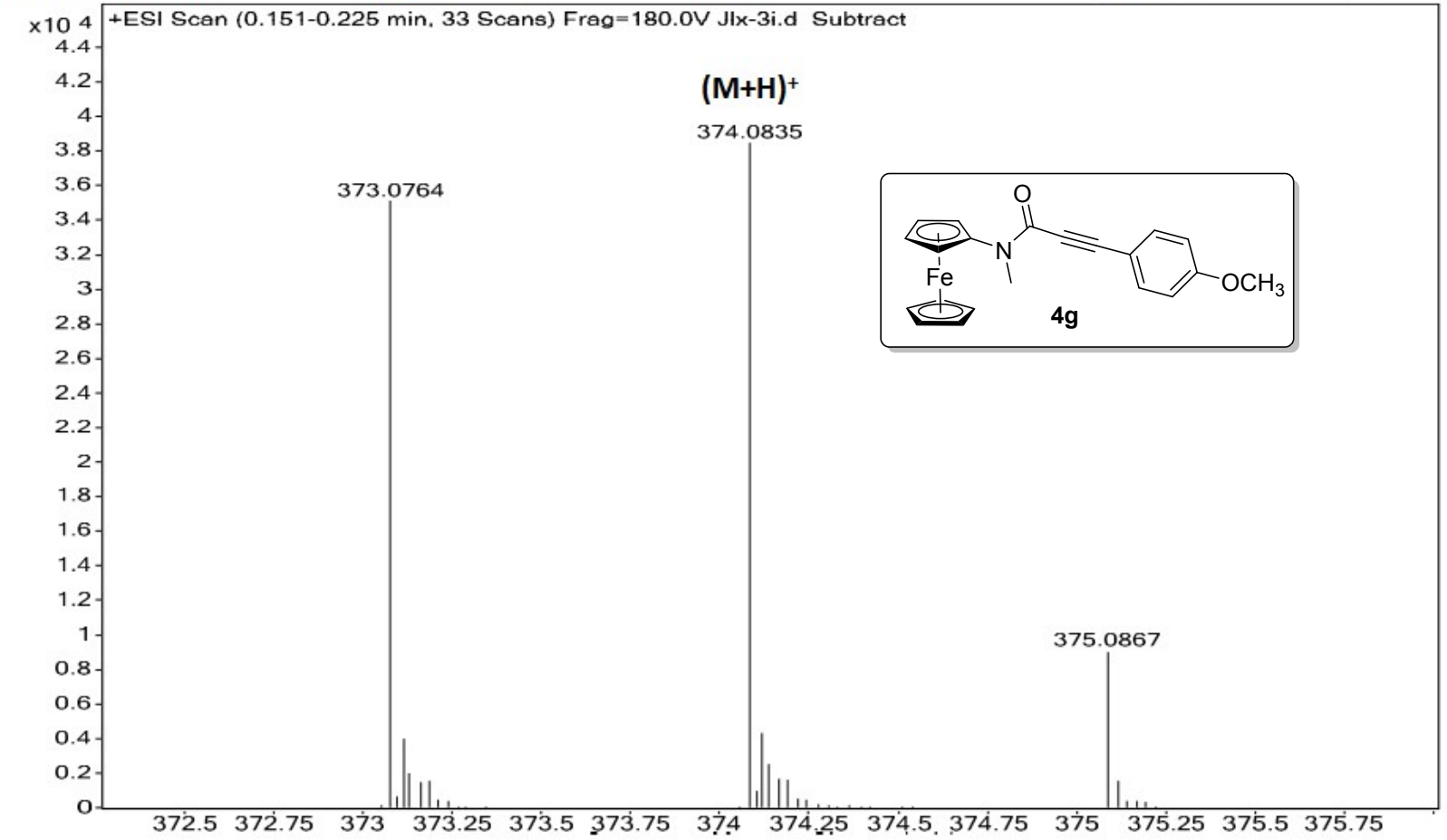


NMR and HMRS Spectra of **4g :**

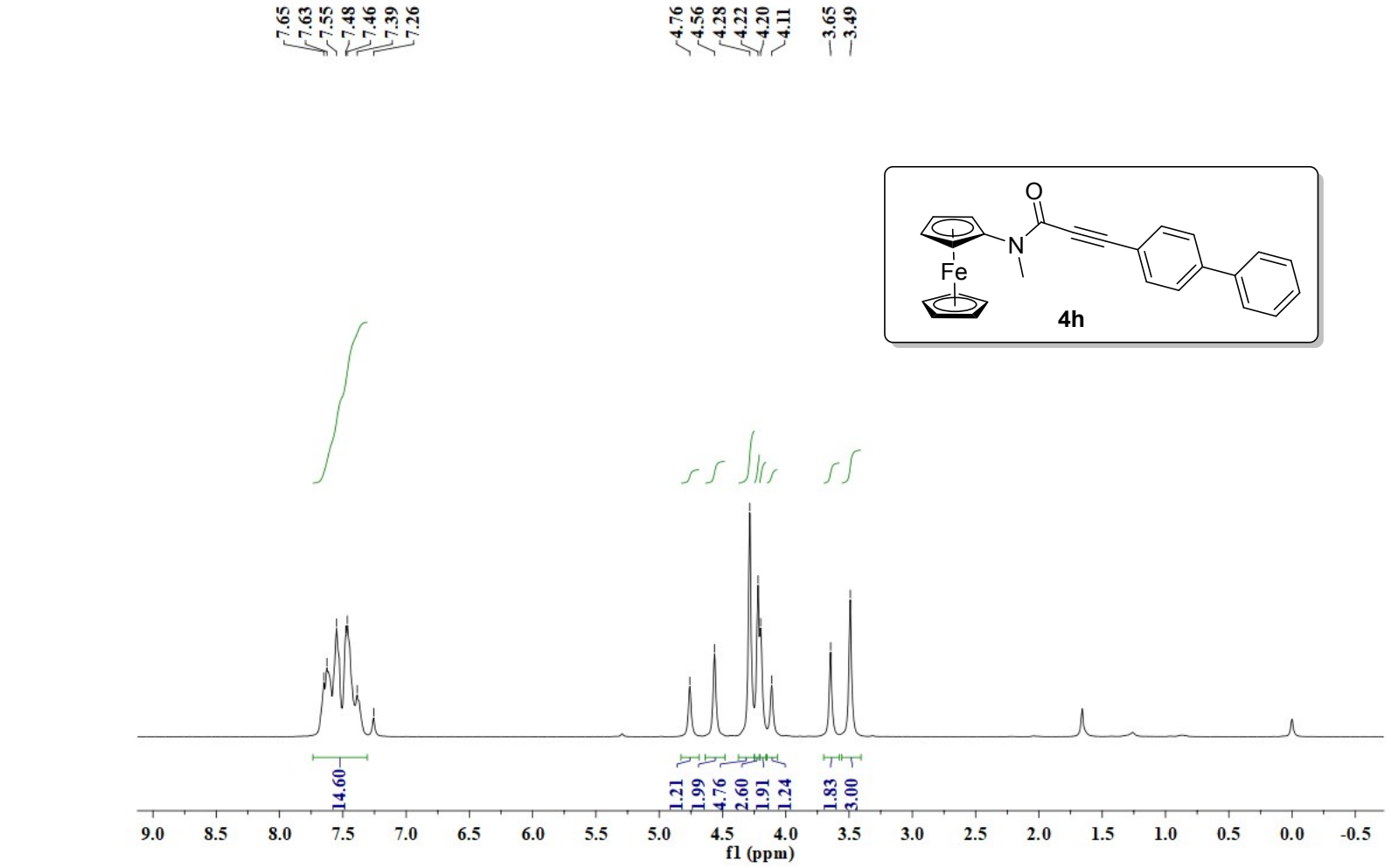


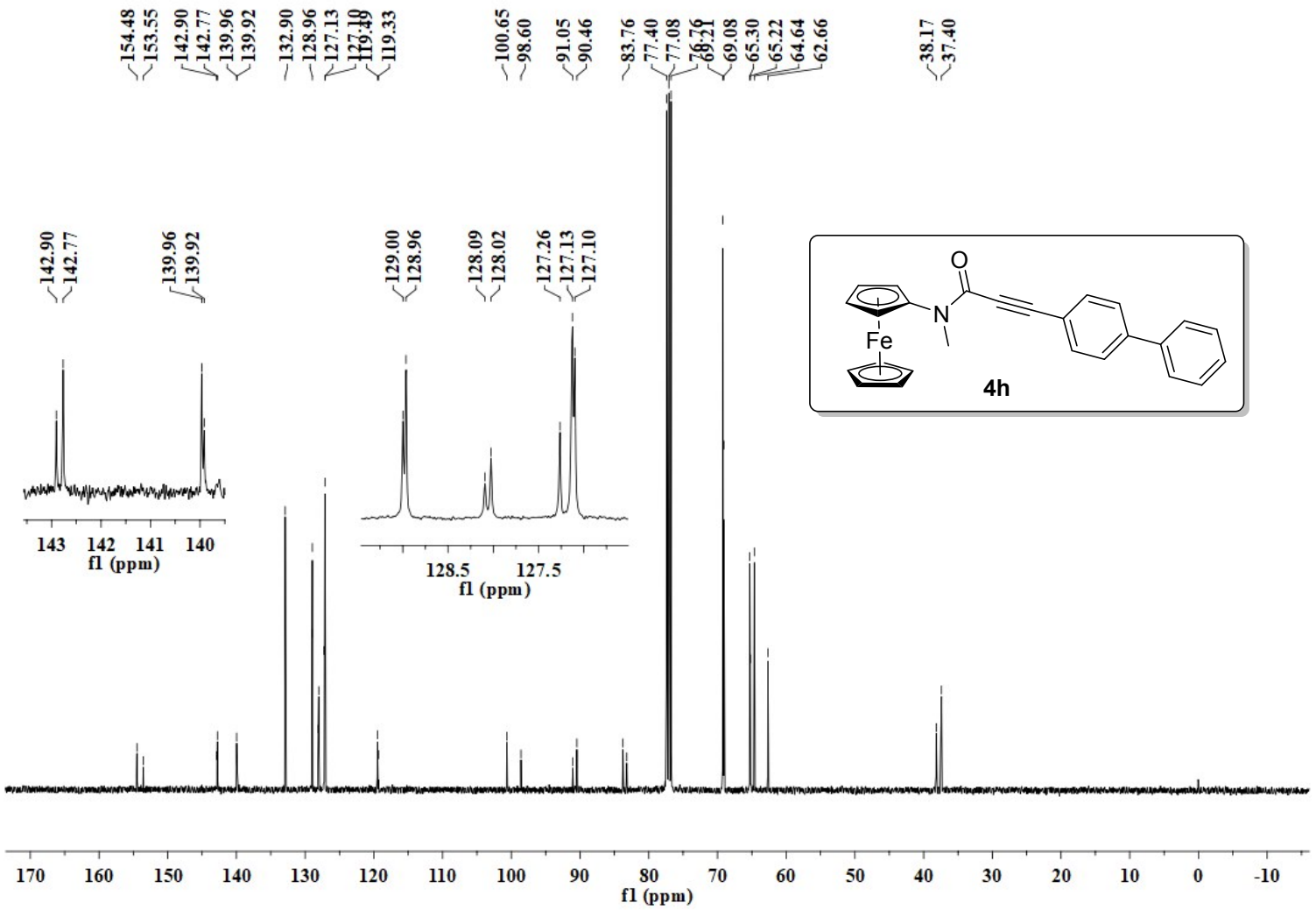

159.38
159.22
154.40
153.45
129.72
129.55
124.87
124.84
121.62
121.49
117.10
117.03
116.84
116.70
100.59
98.54
90.95
90.35
82.84
77.45
77.13
76.82
69.20
69.07
65.28
64.64
55.42
55.33
38.16
37.39
O
N
Fe
OCH3
4g
f1 (ppm)
f1 (ppm)

Sample Name	Jlx-3i	**Position**	P1-A9	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	Jlx-3i.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	3/20/18 Tue 15:55:19

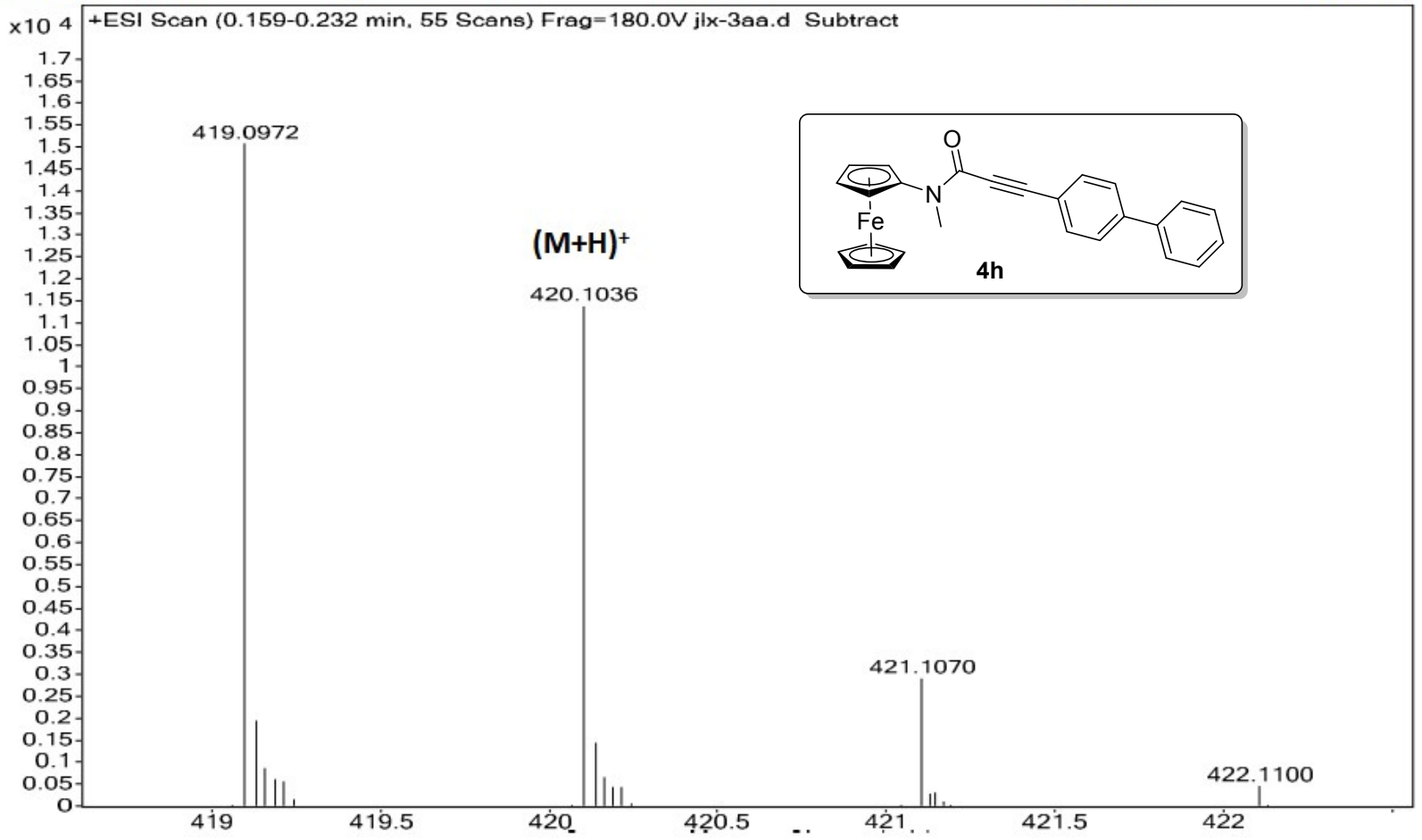


NMR and HMRS Spectra of **4h :**

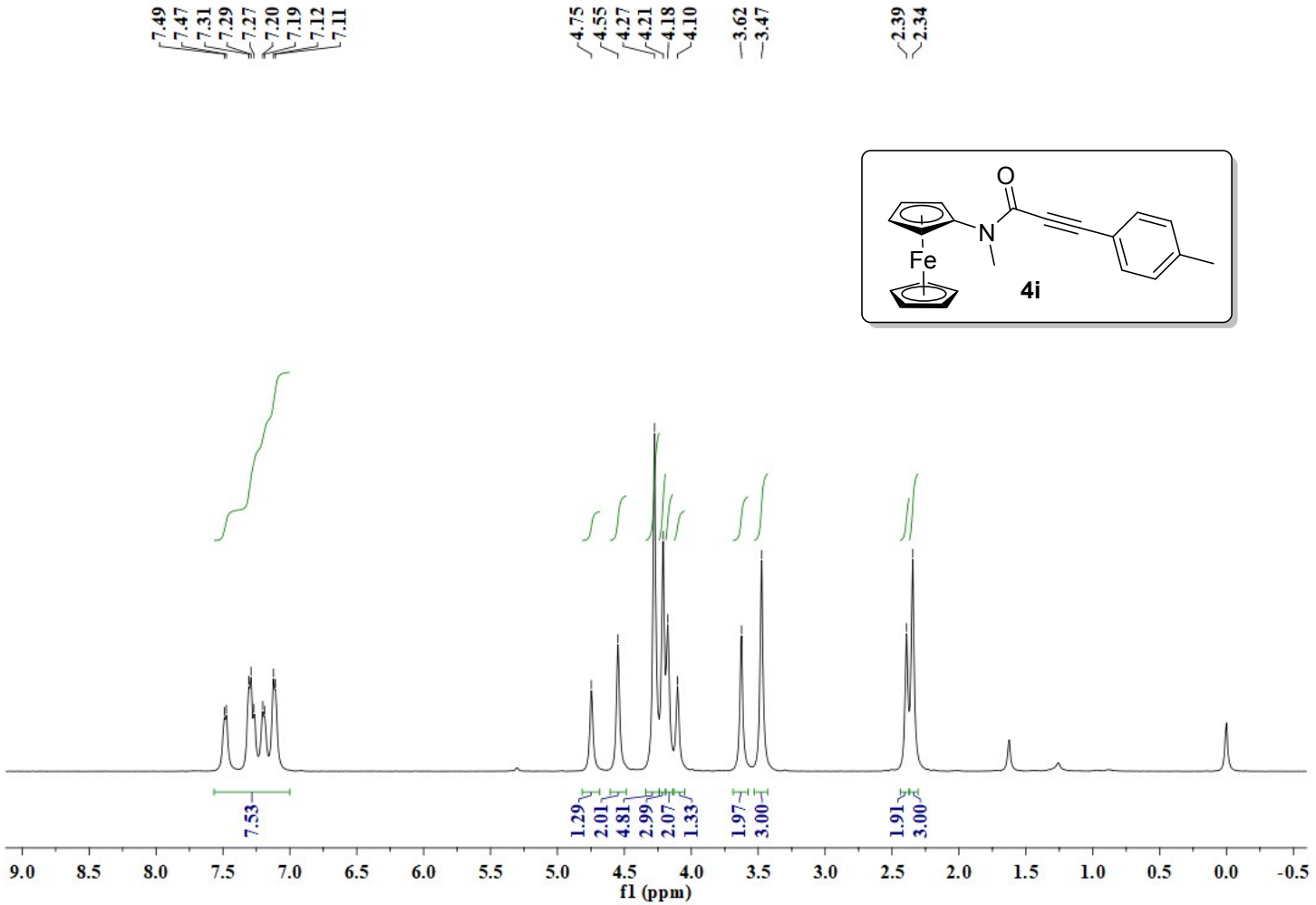


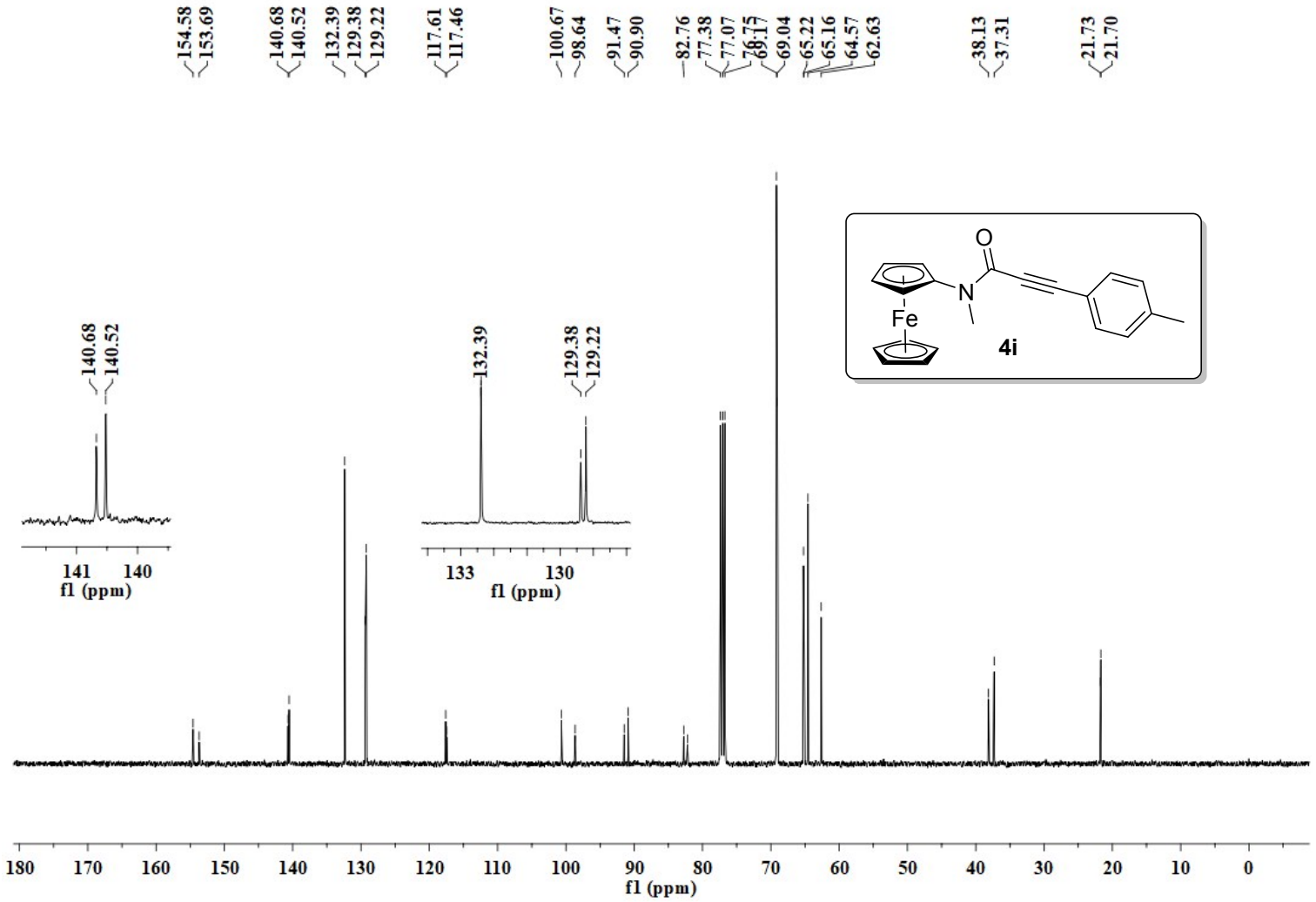

154.48
153.55
142.90
142.77
139.96
139.92
132.90
128.96
127.13
119.33
100.65
98.60
91.05
90.46
83.76
77.40
77.08
69.08
65.30
65.22
64.64
62.66
38.17
37.40
142.90
142.77
139.96
139.92
129.00
128.96
128.09
128.02
127.26
127.13
127.10
143 142 141 140
f1 (ppm)
128.5 127.5
f1 (ppm)
O
N
Fe
4h
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

Sample Name	jlx-3aa	**Position**	P1-A2	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
Data Filename	jlx-3aa.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	5/24/18 Thu 10:33:59

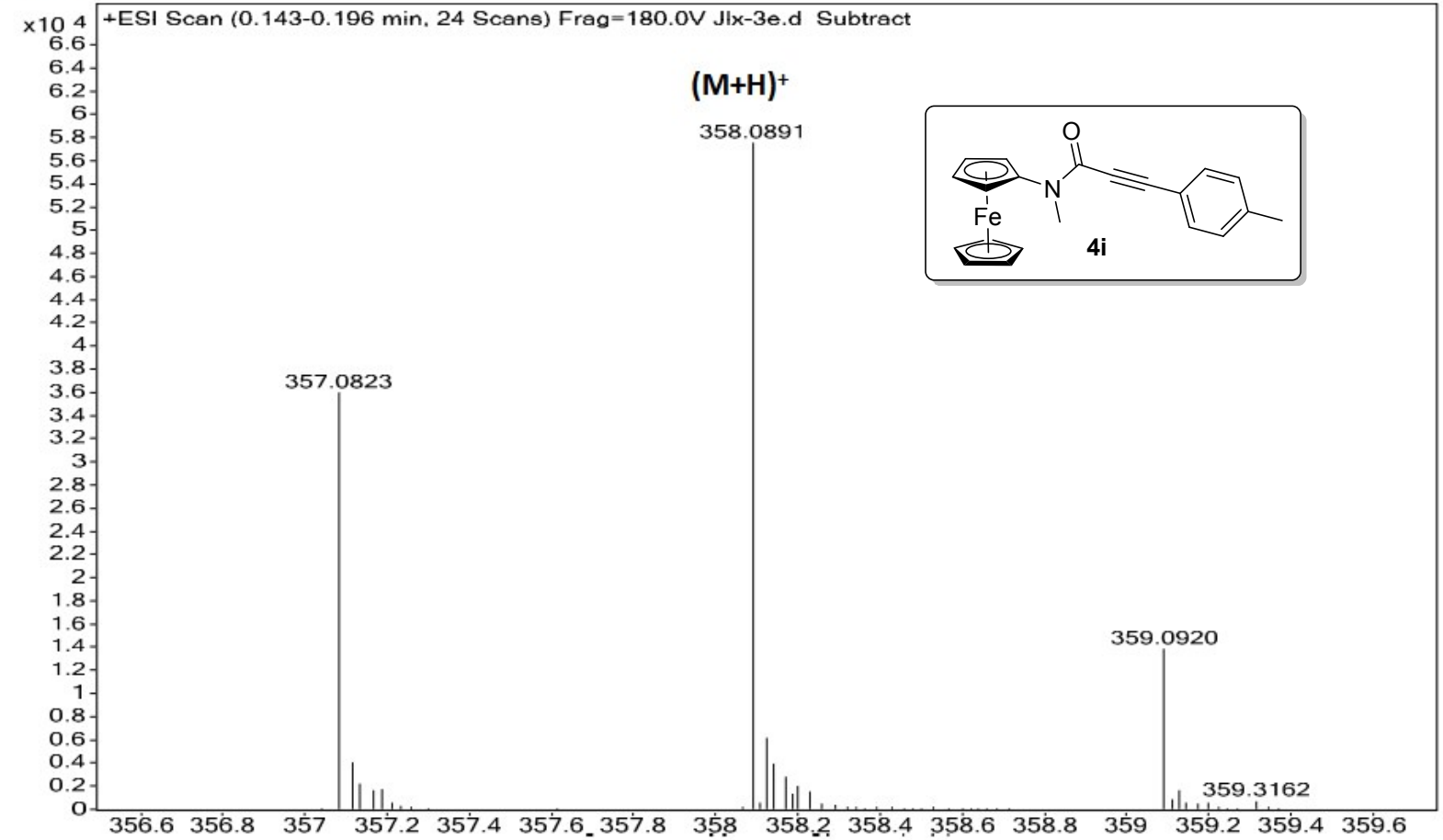


NMR and HMRS Spectra of **4i :**

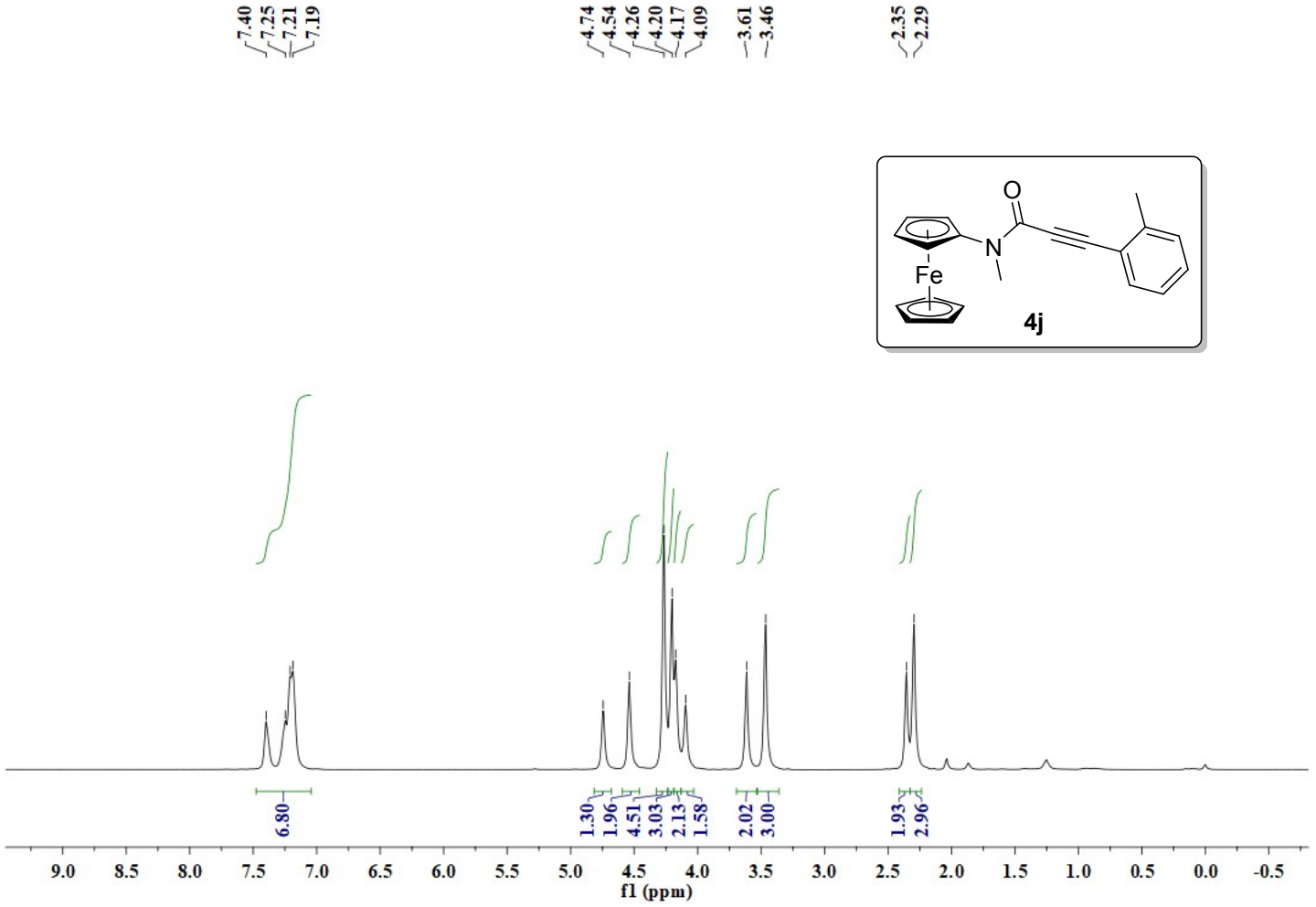


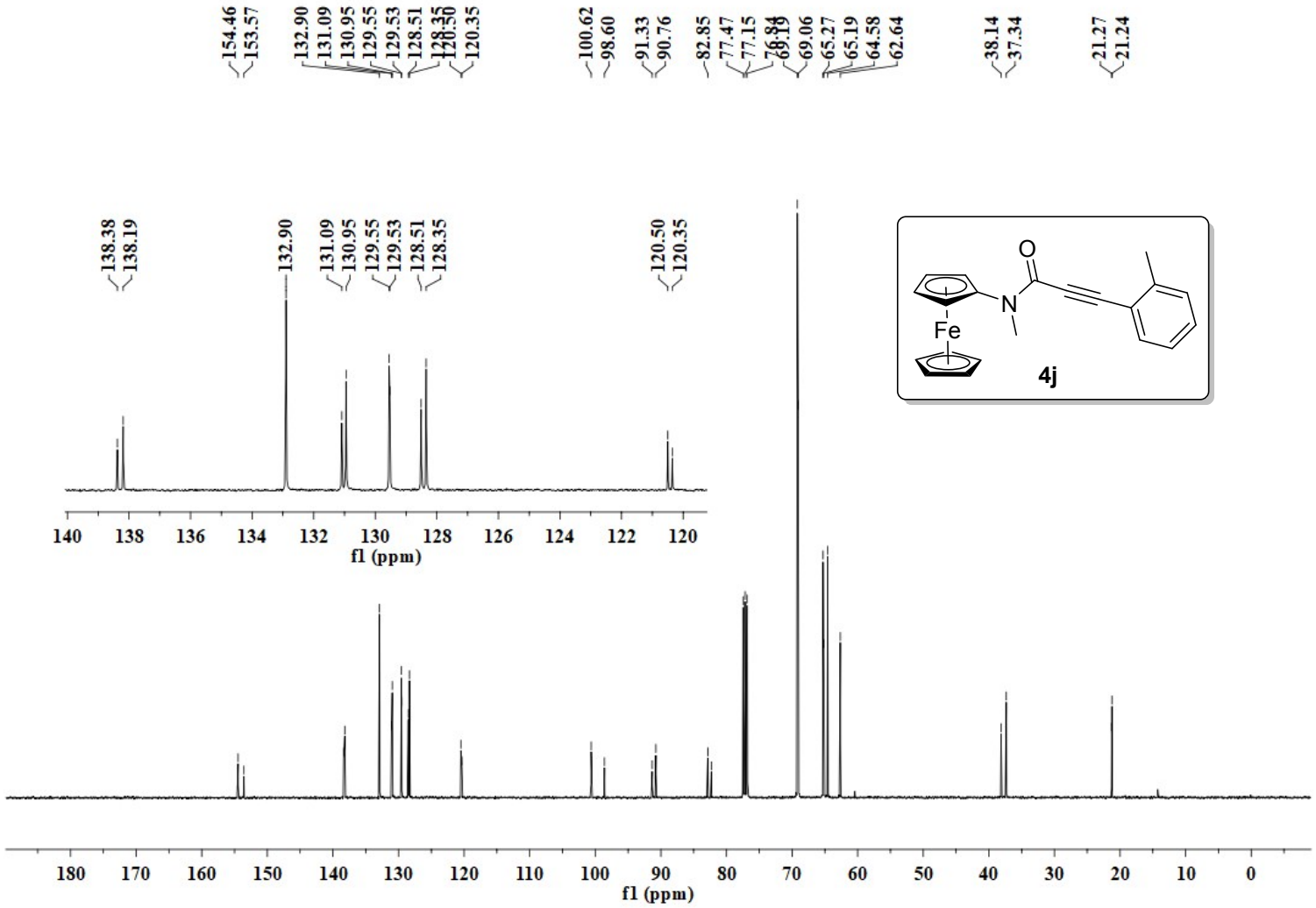

154.58
153.69
140.68
140.52
132.39
129.38
129.22
117.61
117.46
100.67
98.64
91.47
90.90
82.76
77.38
77.07
69.04
65.22
65.16
64.57
62.63
38.13
37.31
21.73
21.70
O
N
Fe
4i
140.68
140.52
141
140
f1 (ppm)
132.39
129.38
129.22
133
130
f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

Sample Name	Jlx-3e	**Position**	P1-A5	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	Jlx-3e.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	3/20/18 Tue 15:50:16

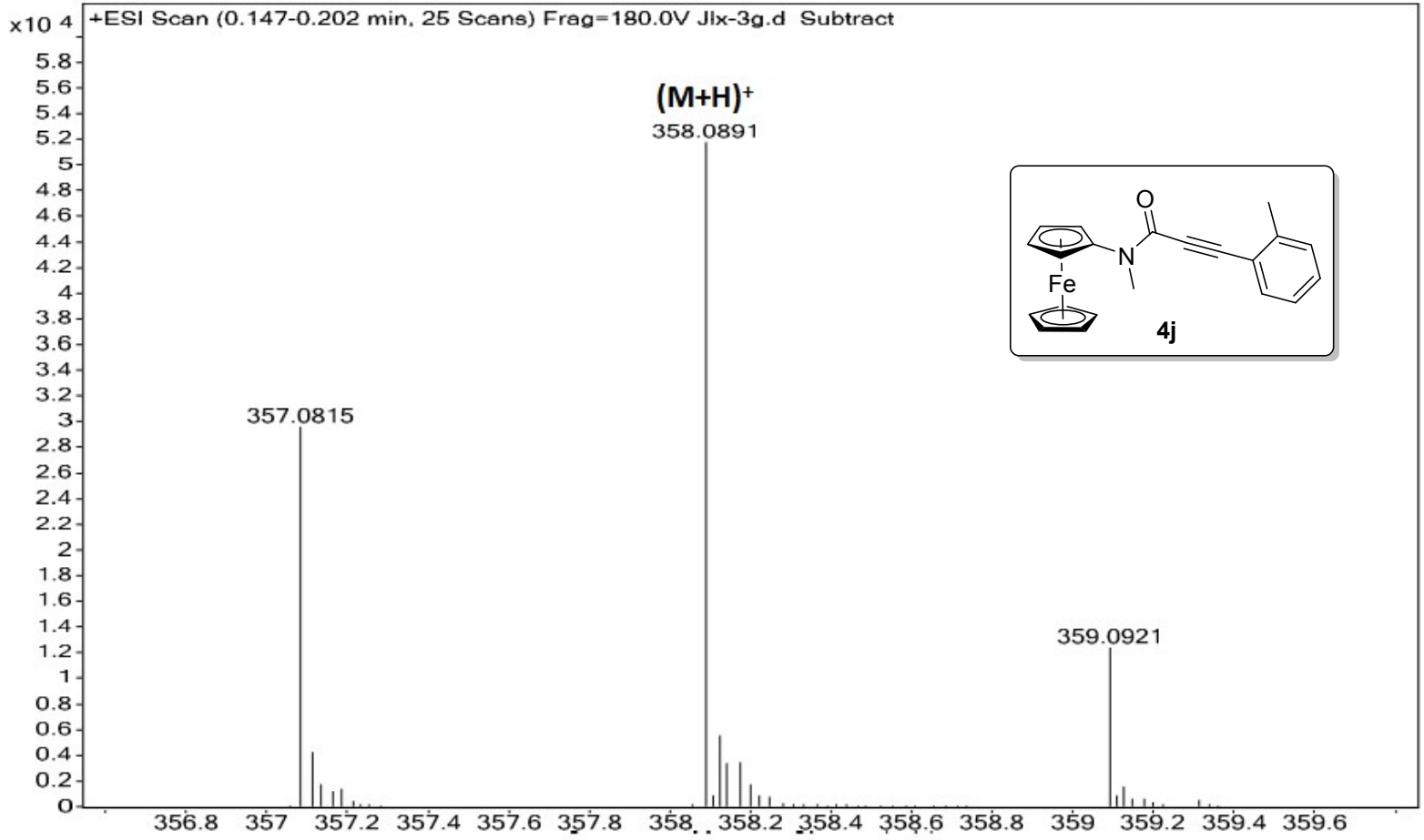


NMR and HMRS Spectra of **4j :**

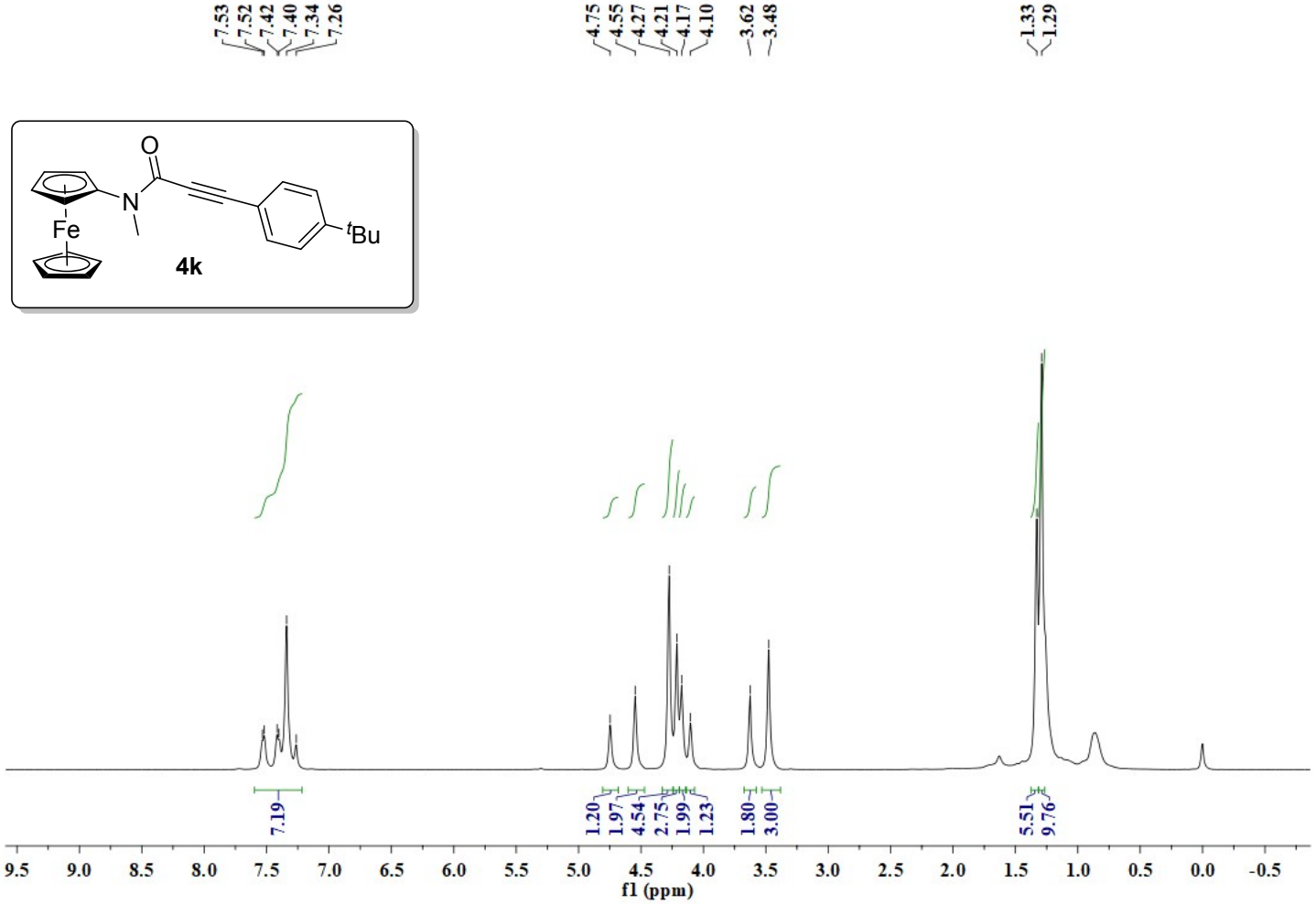


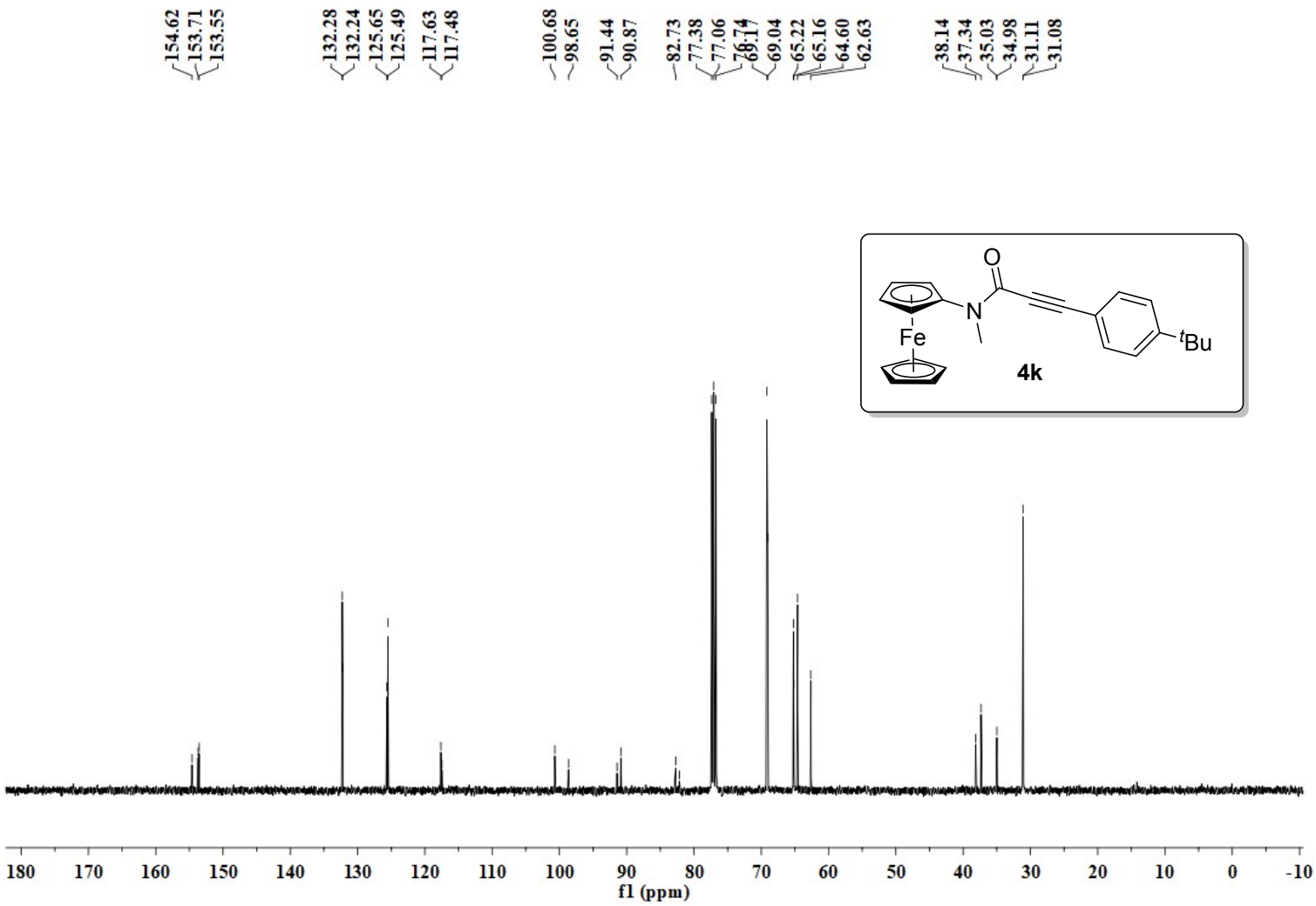

154.46
153.57
132.90
131.09
130.95
129.55
129.53
128.51
128.35
120.50
120.35
100.62
98.60
91.33
90.76
82.85
77.47
77.15
76.84
69.19
69.06
65.27
65.19
64.58
62.64
38.14
37.34
21.27
21.24
138.38
138.19
132.90
131.09
130.95
129.55
129.53
128.51
128.35
120.50
120.35
140 138 136 134 132 130 128 126 124 122 120
f1 (ppm)
O
N
Fe
4j
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

Sample Name	Jlx-3g	**Position**	P1-A7	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	Jlx-3g.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	3/20/18 Tue 15:52:48

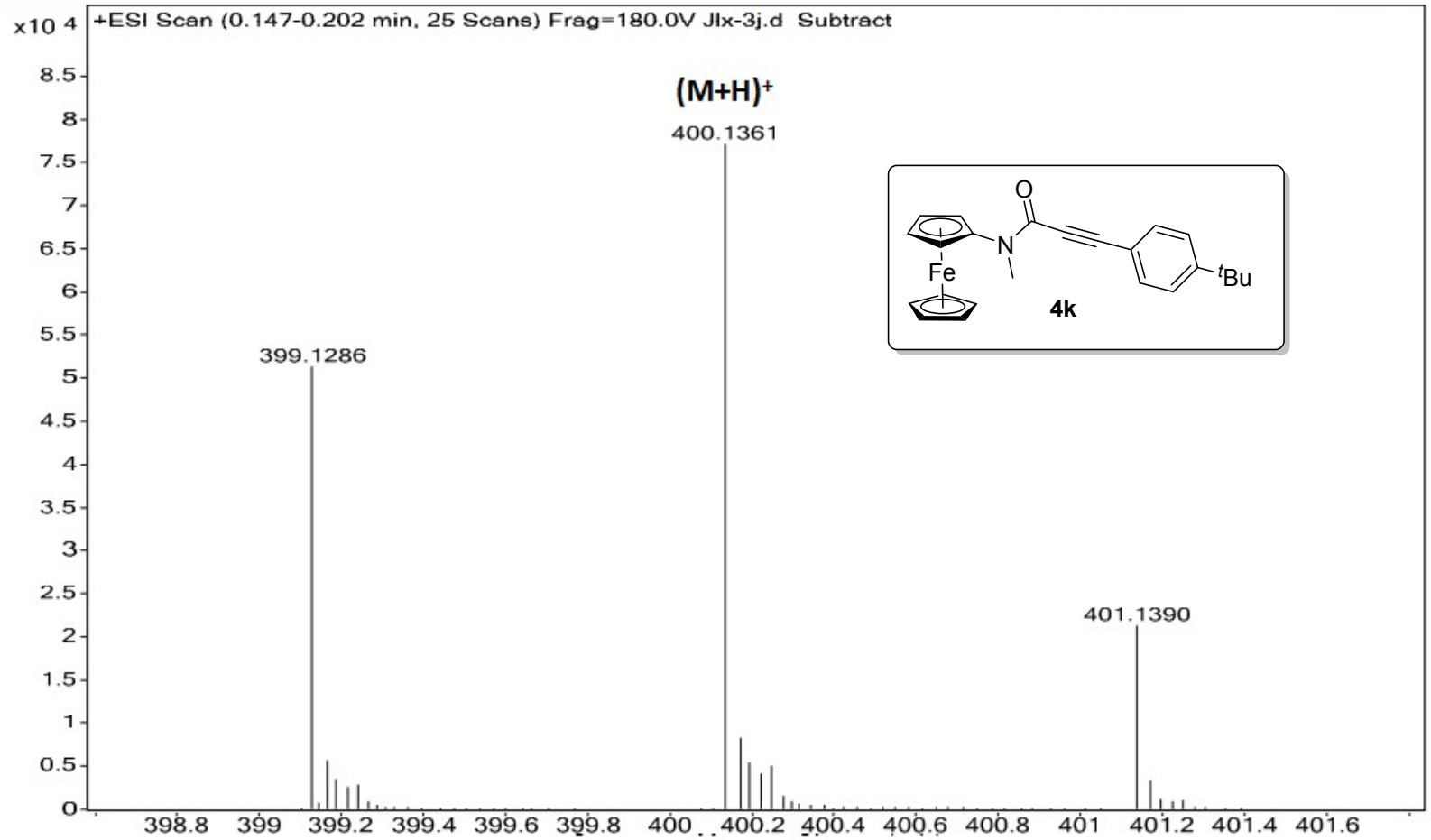


NMR and HMRS Spectra of **4k :**

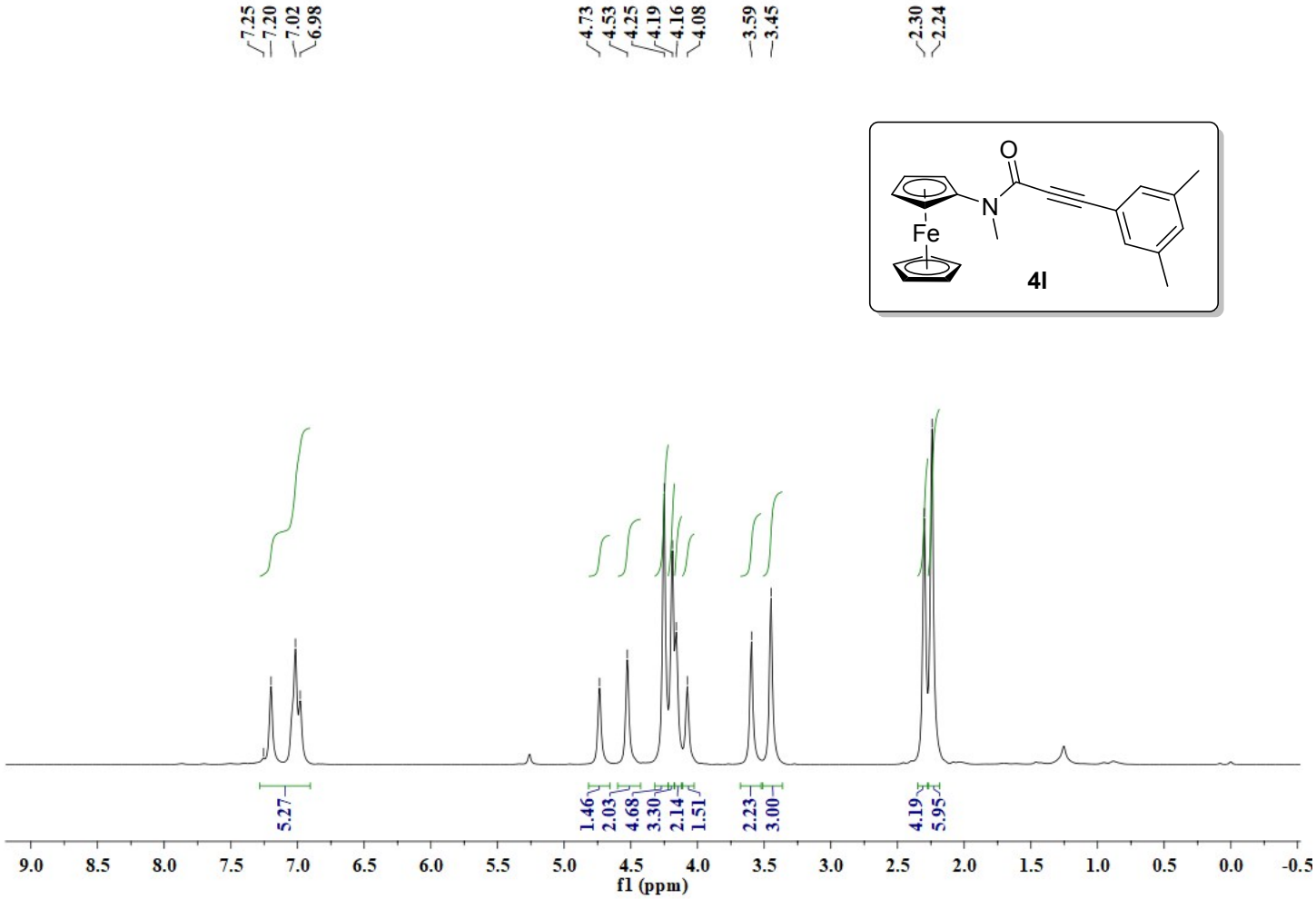


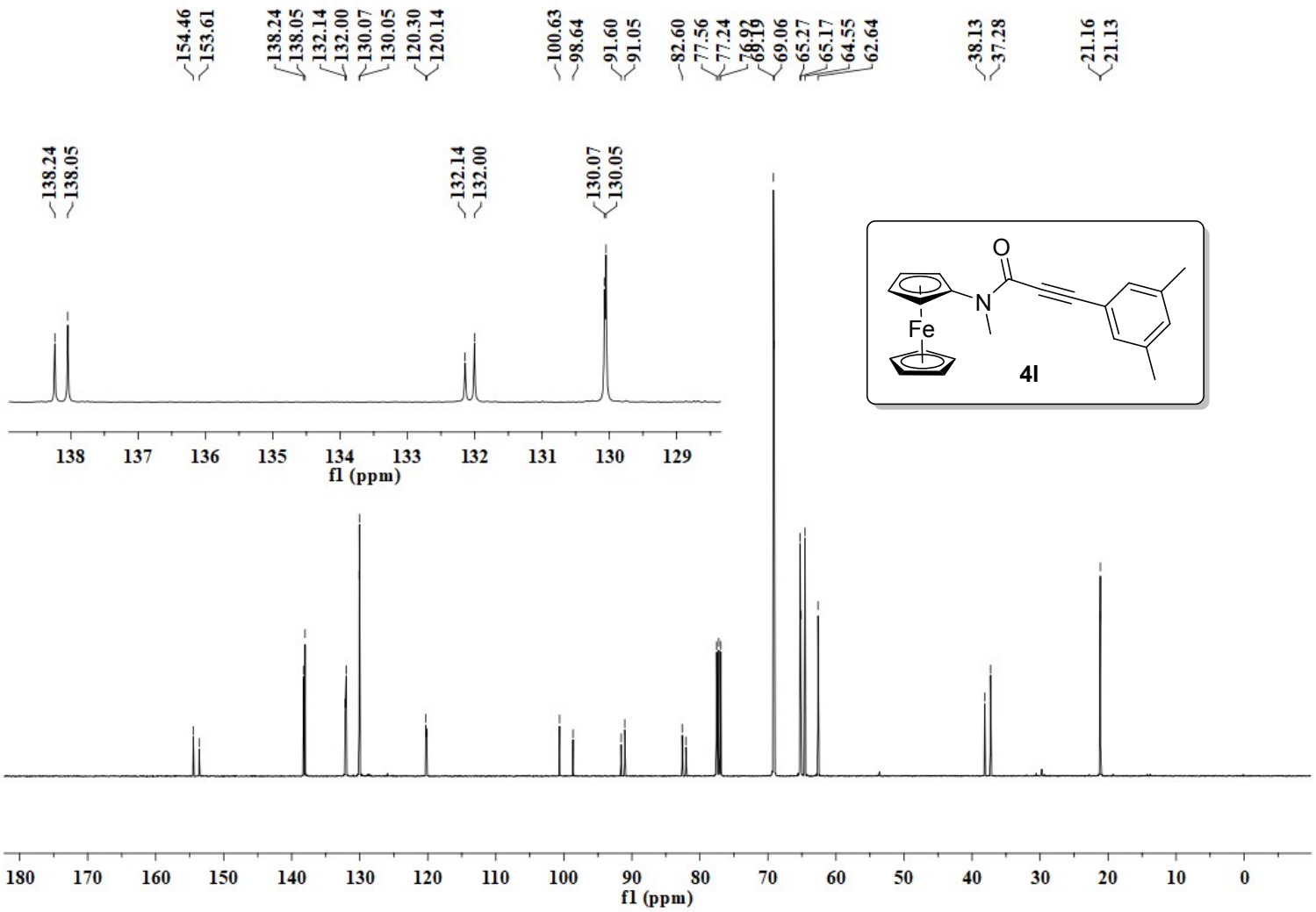

154.62
153.71
153.55
132.28
132.24
125.65
125.49
117.63
117.48
100.68
98.65
91.44
90.87
82.73
77.38
77.06
76.74
69.17
69.04
65.22
65.16
64.60
62.63
38.14
37.34
35.03
34.98
31.11
31.08
O
N
Fe
tBu
4k
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

Sample Name	Jlx-3j	**Position**	P1-B1	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	Jlx-3j.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	3/20/18 Tue 15:56:35

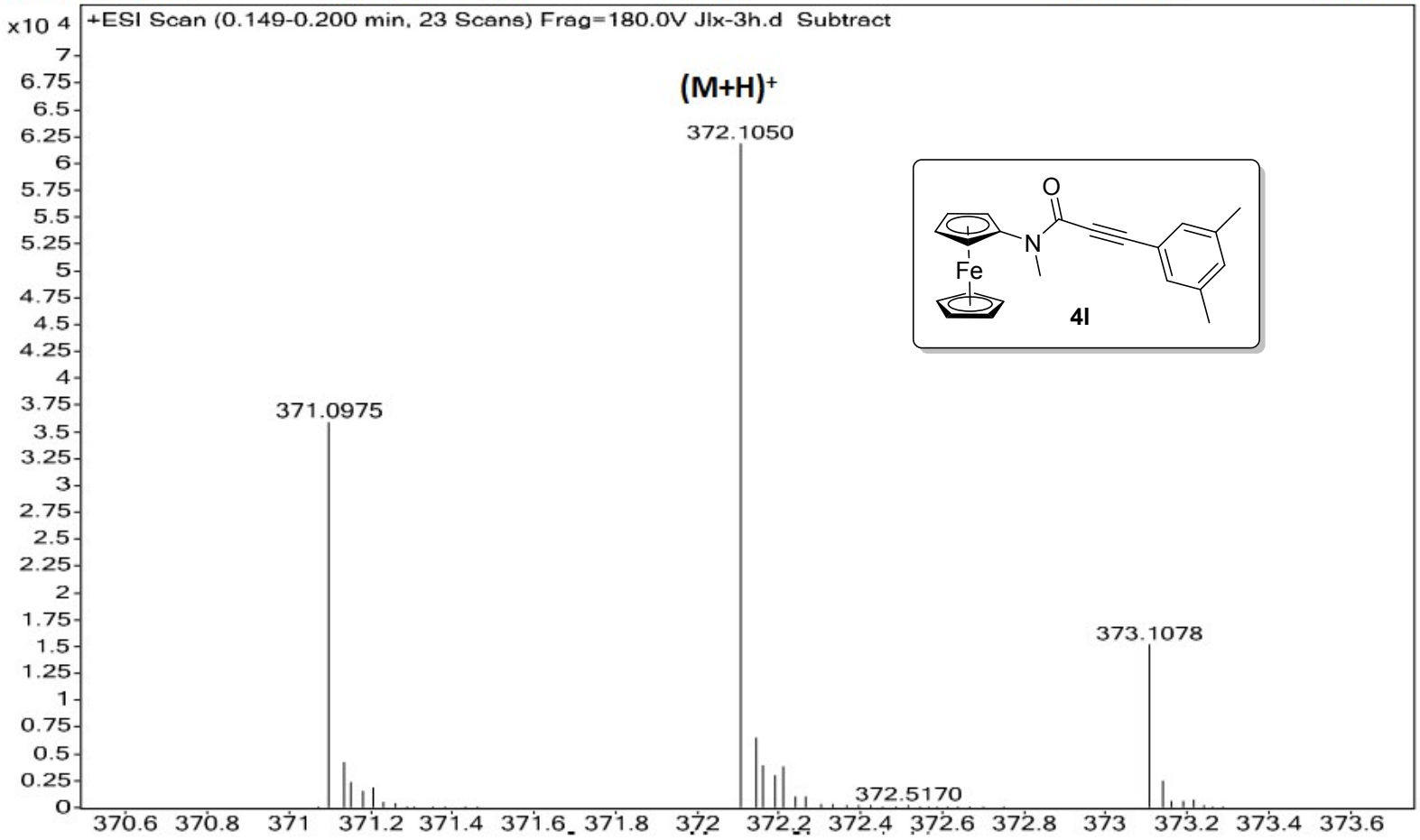


NMR and HMRS Spectra of **4l :**

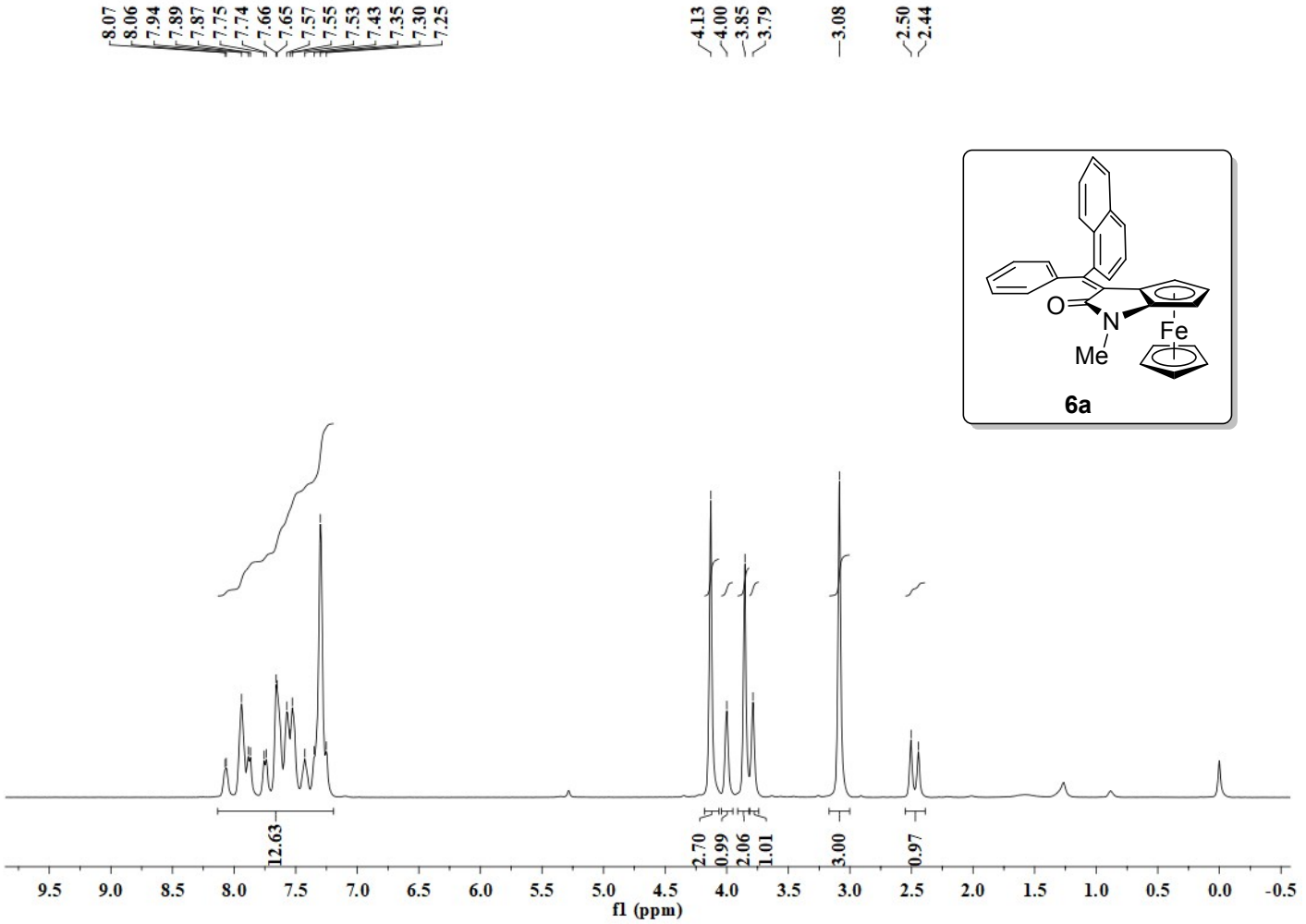


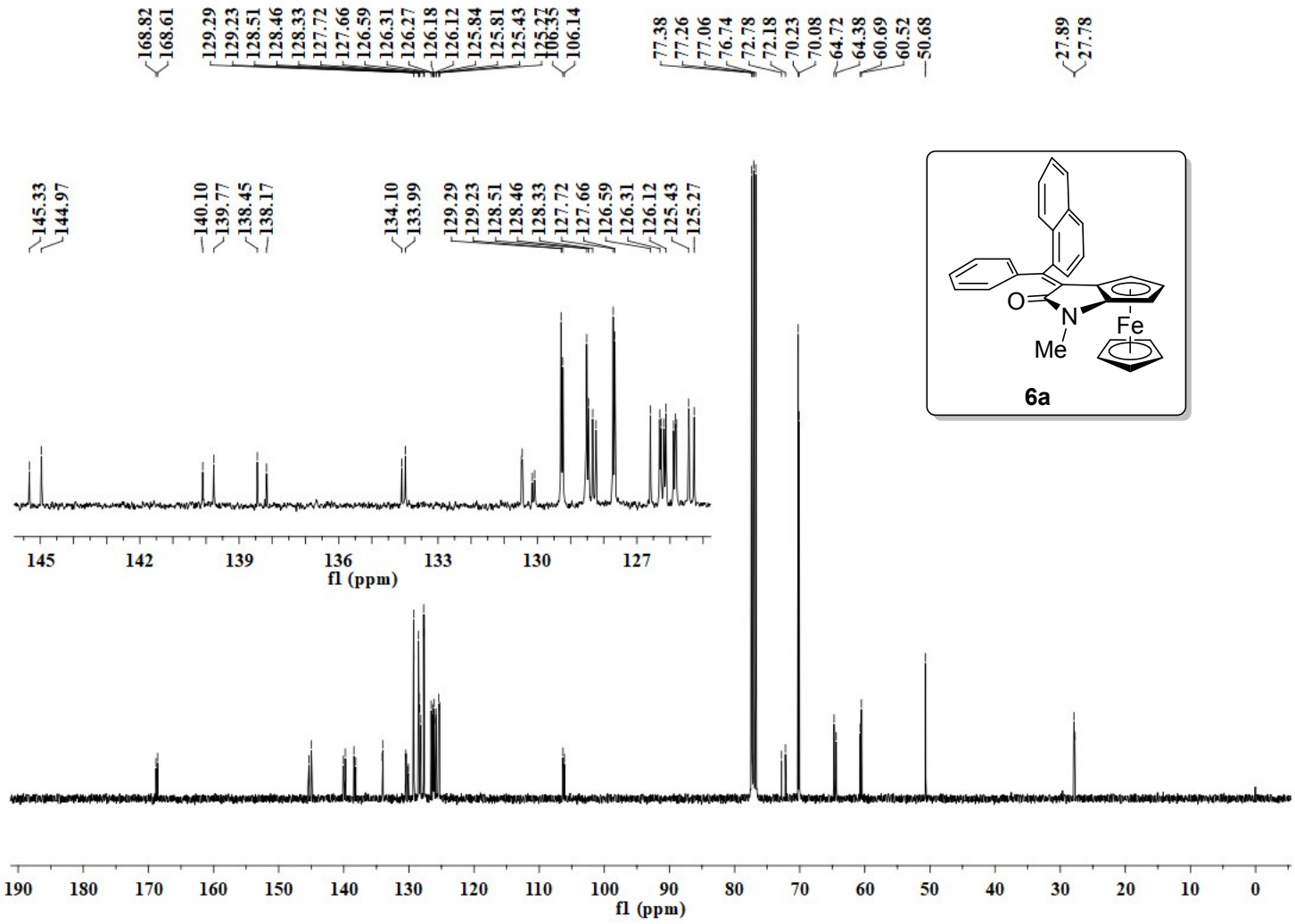

154.46
153.61
138.24
138.05
132.14
132.00
130.07
130.05
120.30
120.14
100.63
98.64
91.60
91.05
82.60
77.56
77.24
76.92
69.19
69.06
65.27
65.17
64.55
62.64
38.13
37.28
21.16
21.13
138.24
138.05
132.14
132.00
130.07
130.05
O
N
Fe
4l
138 137 136 135 134 133 132 131 130 129
f1 (ppm)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

Sample Name	Jlx-3h	**Position**	P1-A8	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	Jlx-3h.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	3/20/18 Tue 15:54:05

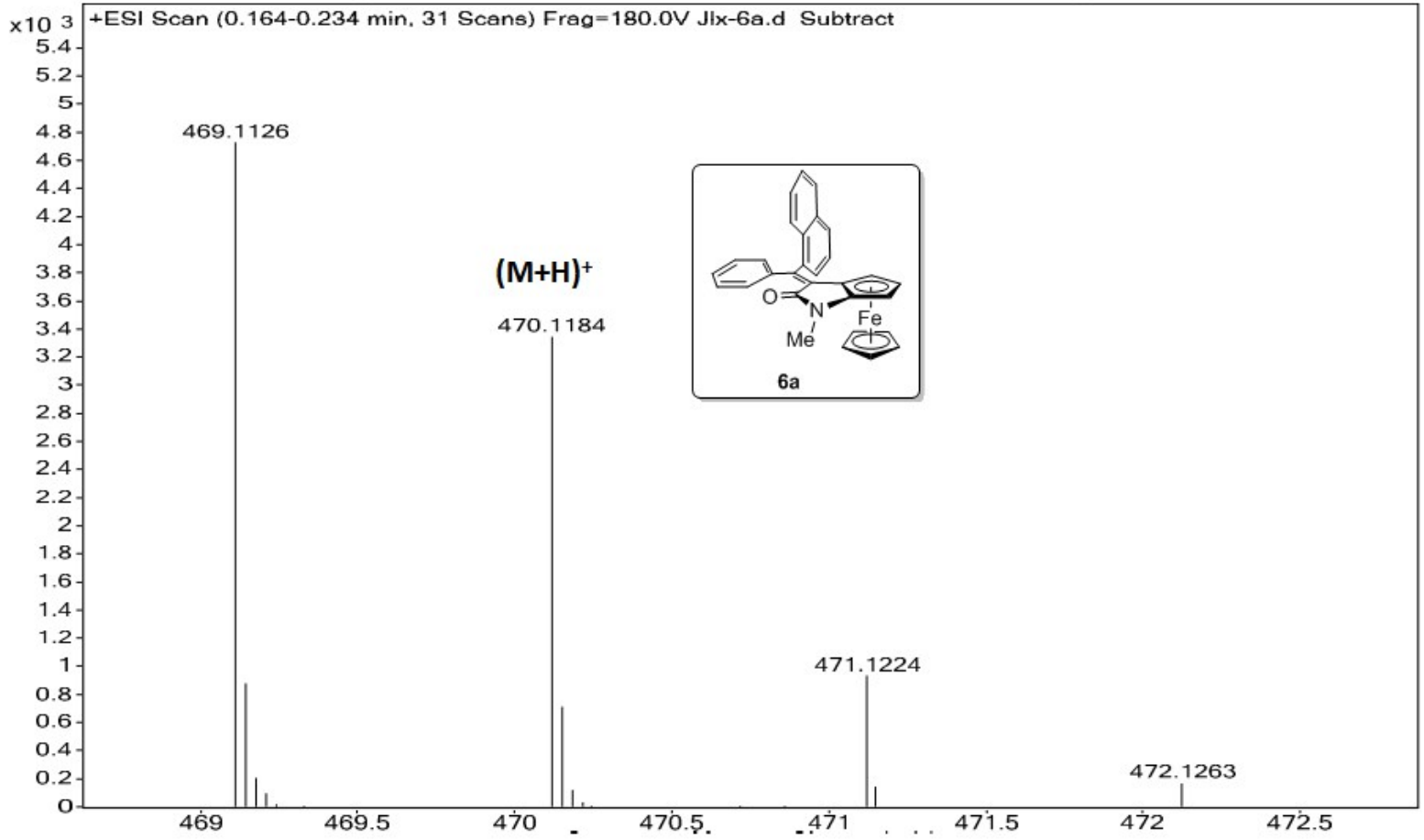


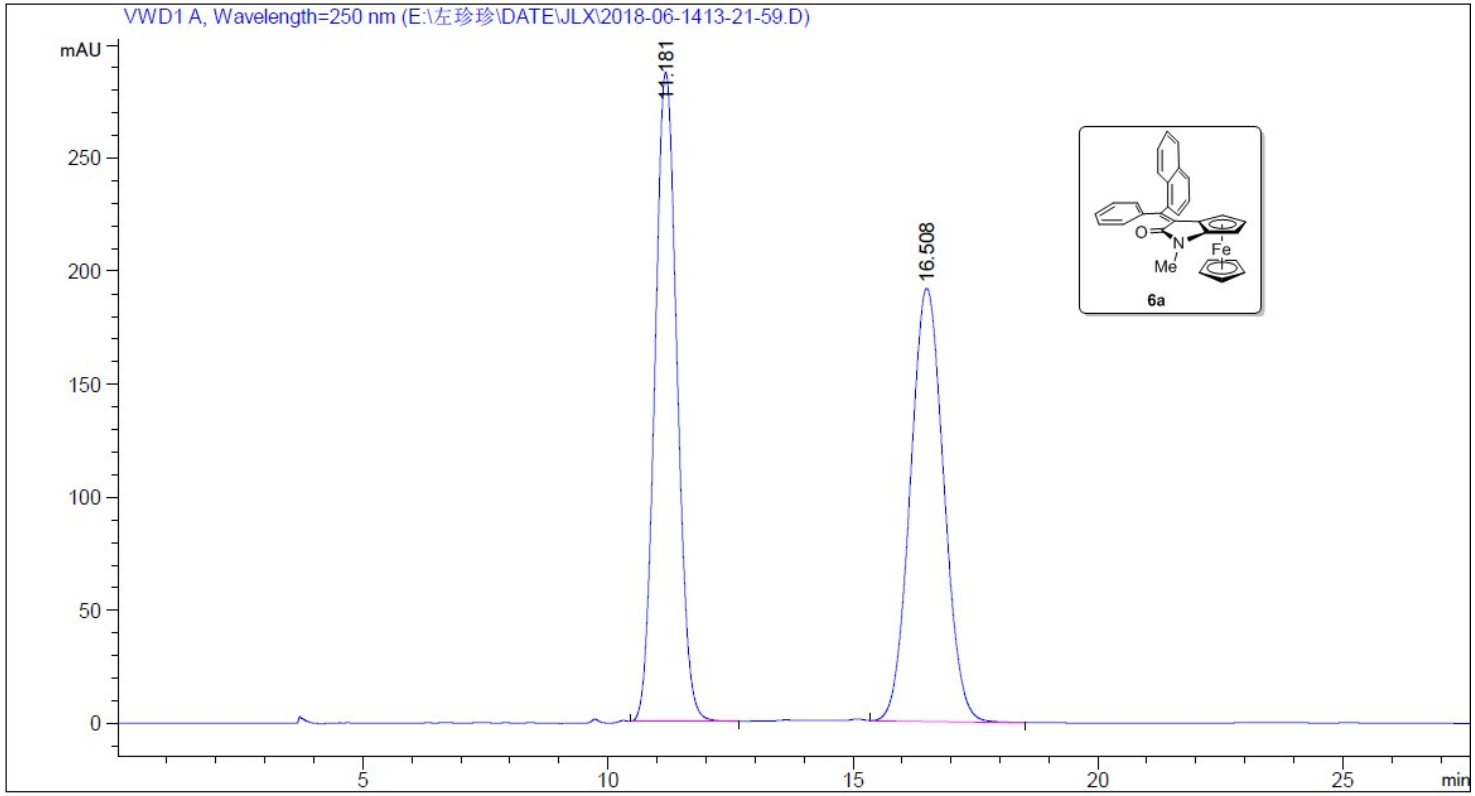
NMR、HMRS Spectra and HPLC Chromatographsof **6a**



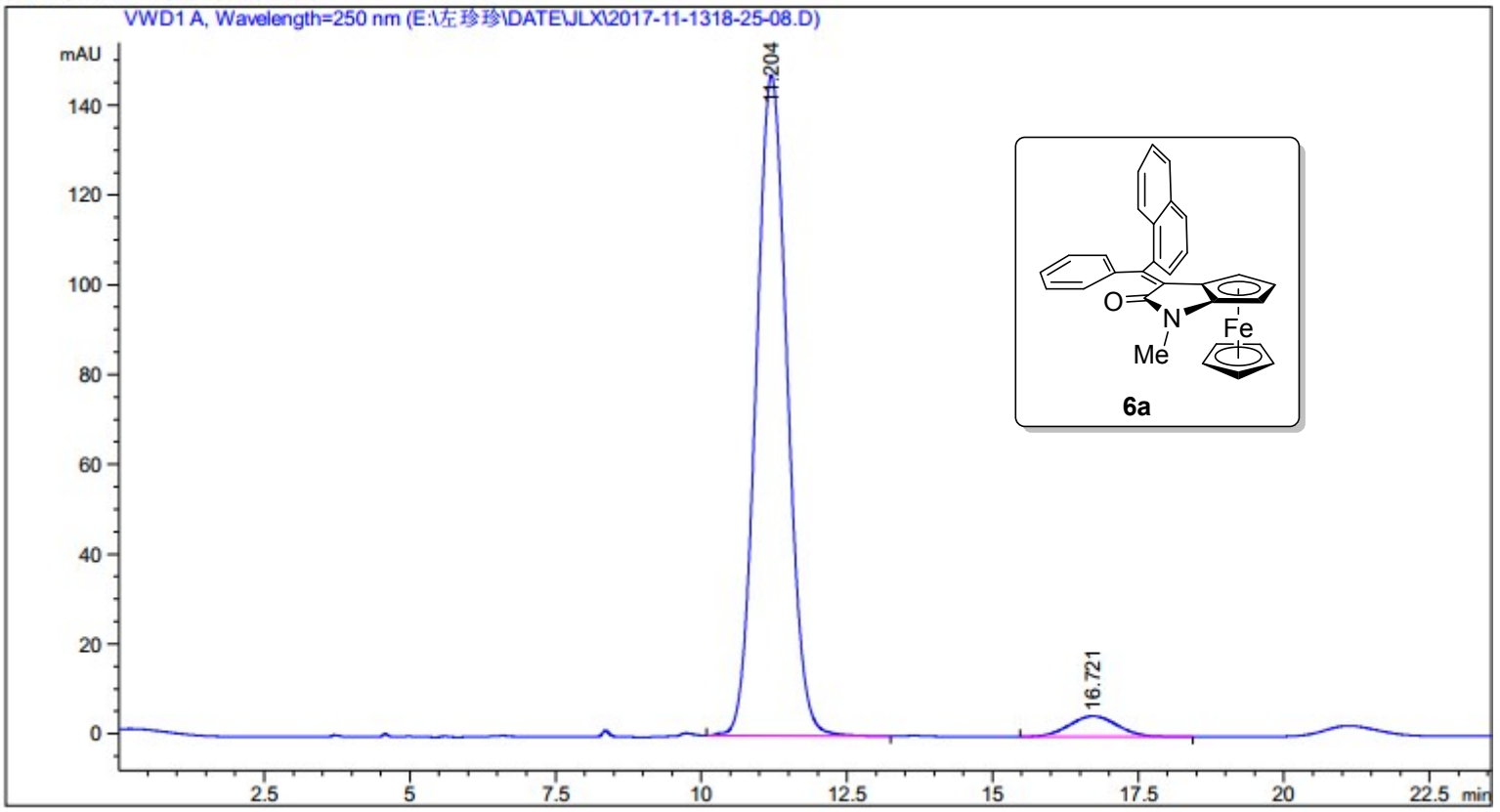

168.82
168.61
129.29
129.23
128.51
128.46
128.33
127.72
127.66
126.59
126.31
126.27
126.18
126.12
125.84
125.81
125.43
125.27
106.35
106.14
77.38
77.26
77.06
76.74
72.78
72.18
70.23
70.08
64.72
64.38
60.69
60.52
50.68
27.89
27.78
145.33
144.97
140.10
139.77
138.45
138.17
134.10
133.99
129.29
129.23
128.51
128.46
128.33
127.72
127.66
126.59
126.31
126.12
125.43
125.27
O
N
Me
Fe
6a
145
142
139
136
133
130
127
f1 (ppm)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

Sample Name	Jlx-6a	**Position**	P1-A1	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	Jlx-6a.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	3/20/18 Tue 14:56:21



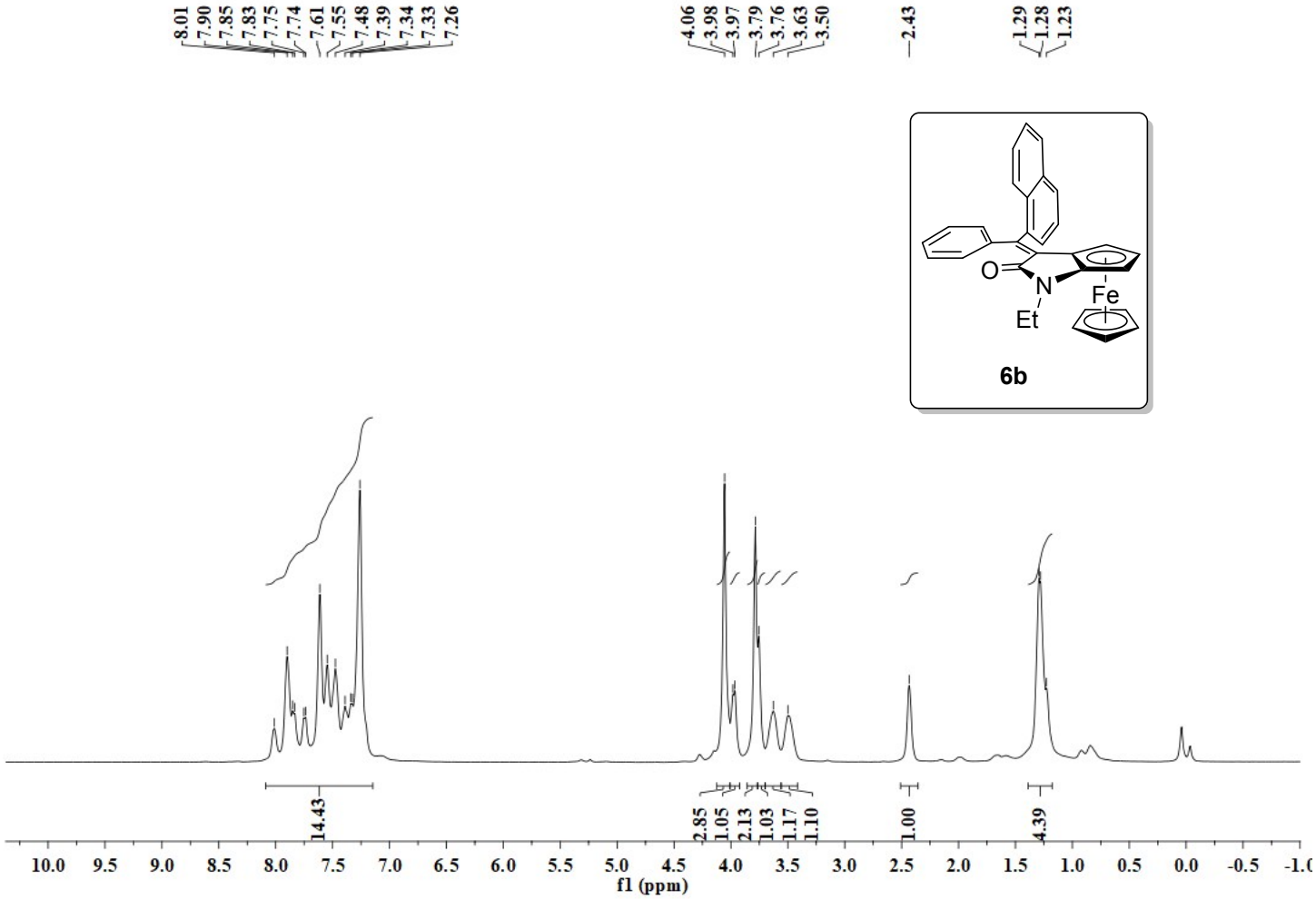


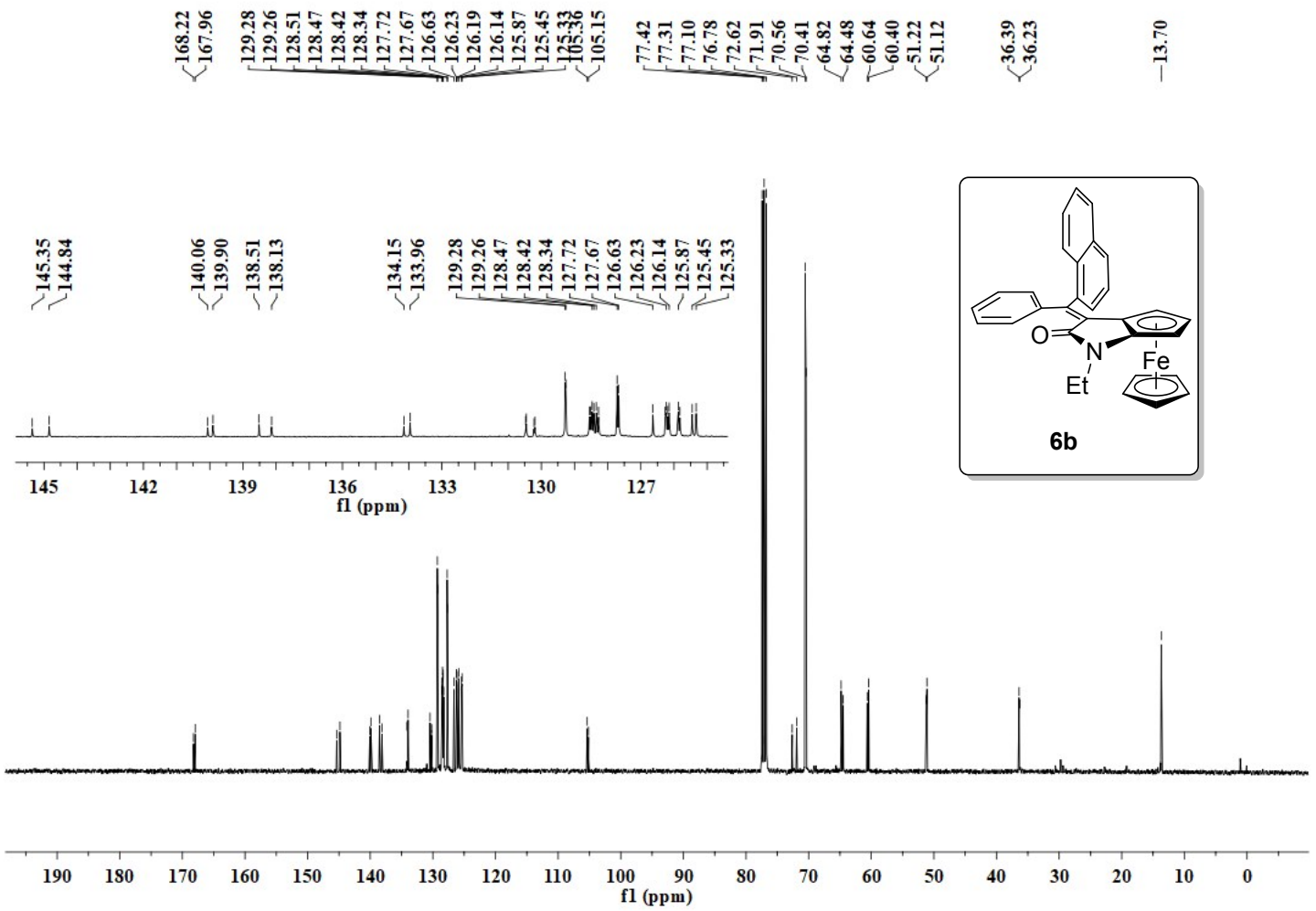
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.181	BB	0.4906	9023.60254	287.13000	49.8444
2	16.508	BB	0.7452	9079.92285	191.48720	50.1556



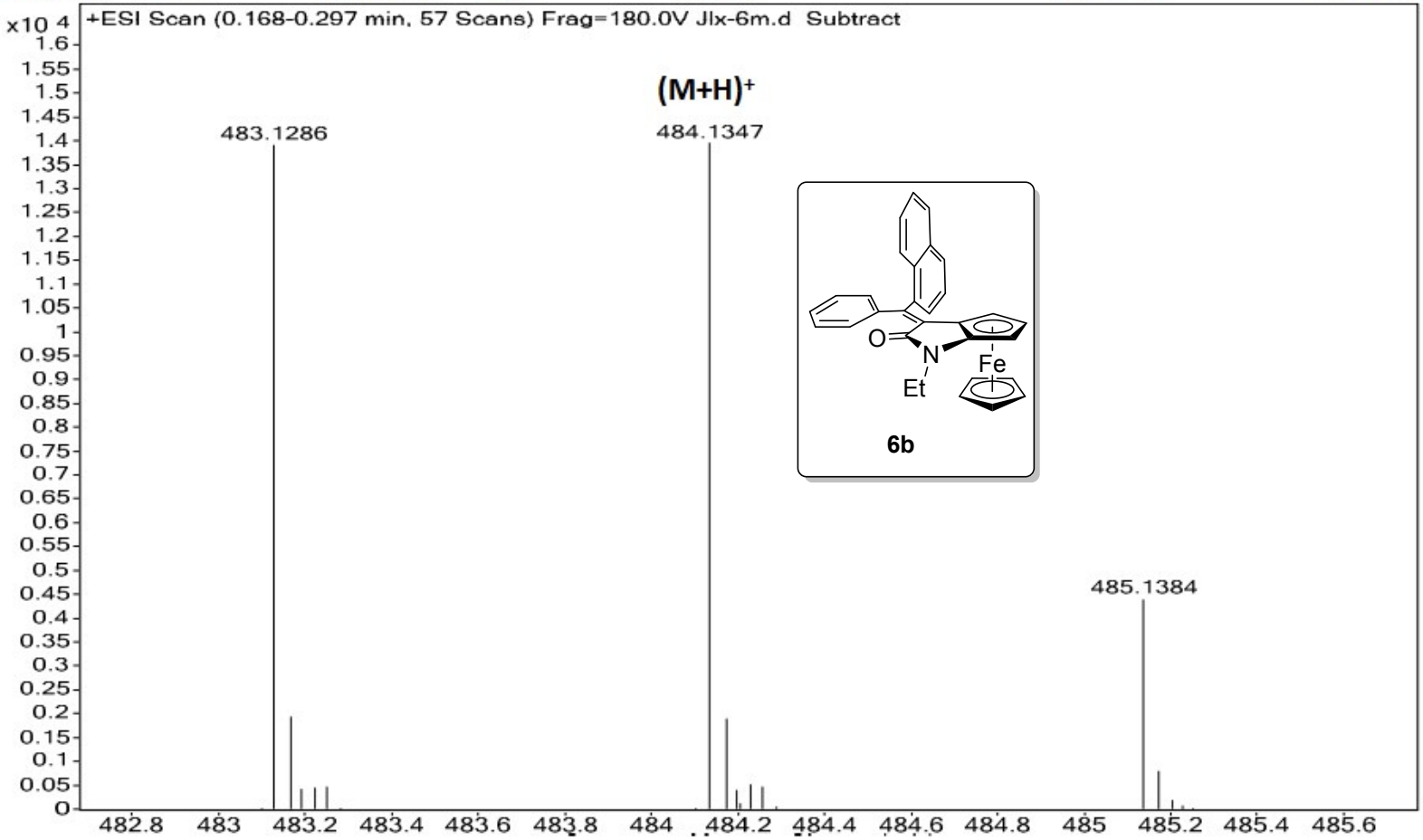
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.204	BB	0.5805	5466.87500	147.12209	95.3802
2	16.721	BB	0.8308	264.78958	4.59136	4.6198

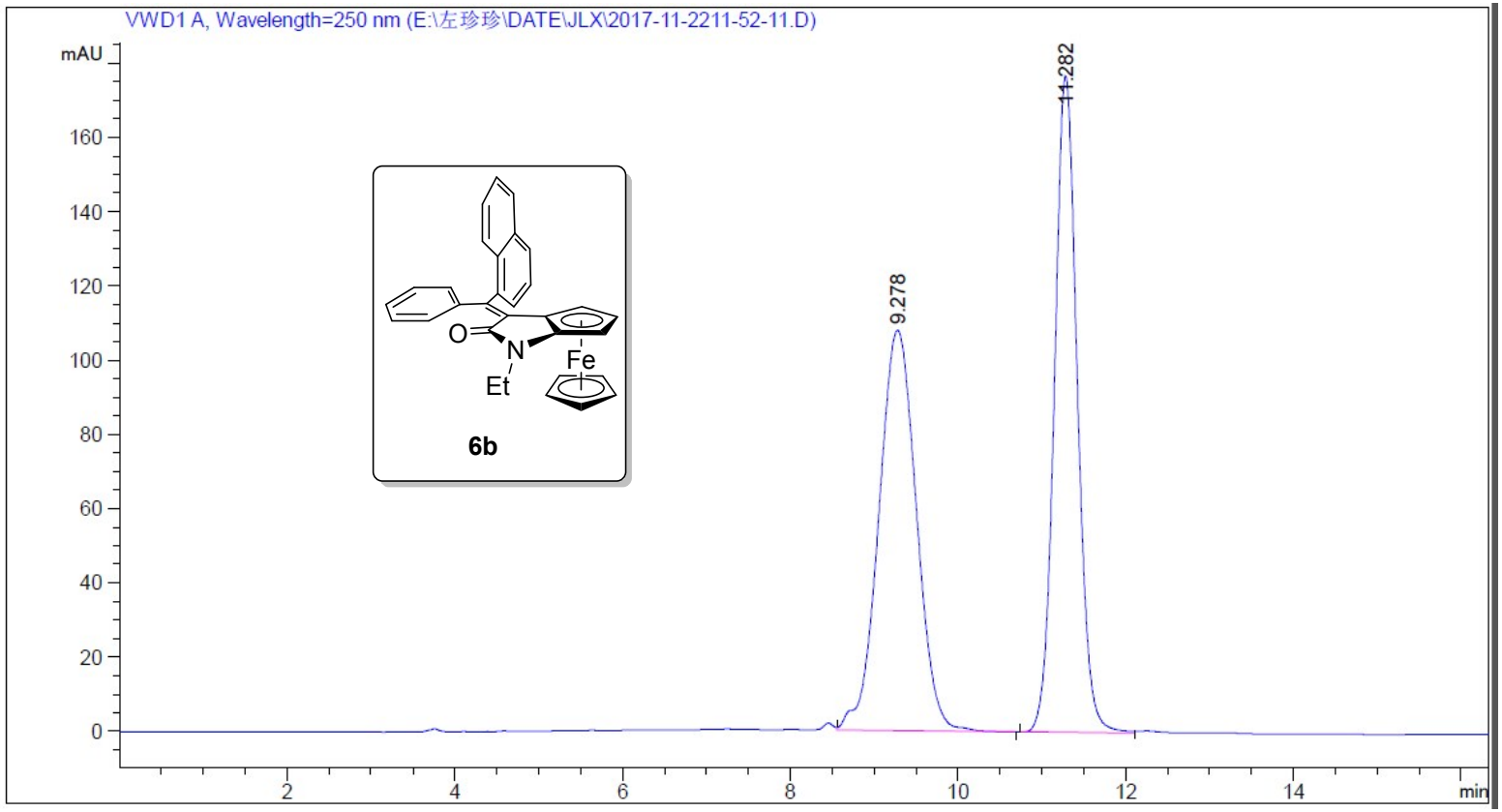
NMR、HMRS Spectra and HPLC Chromatographsof **6b :**



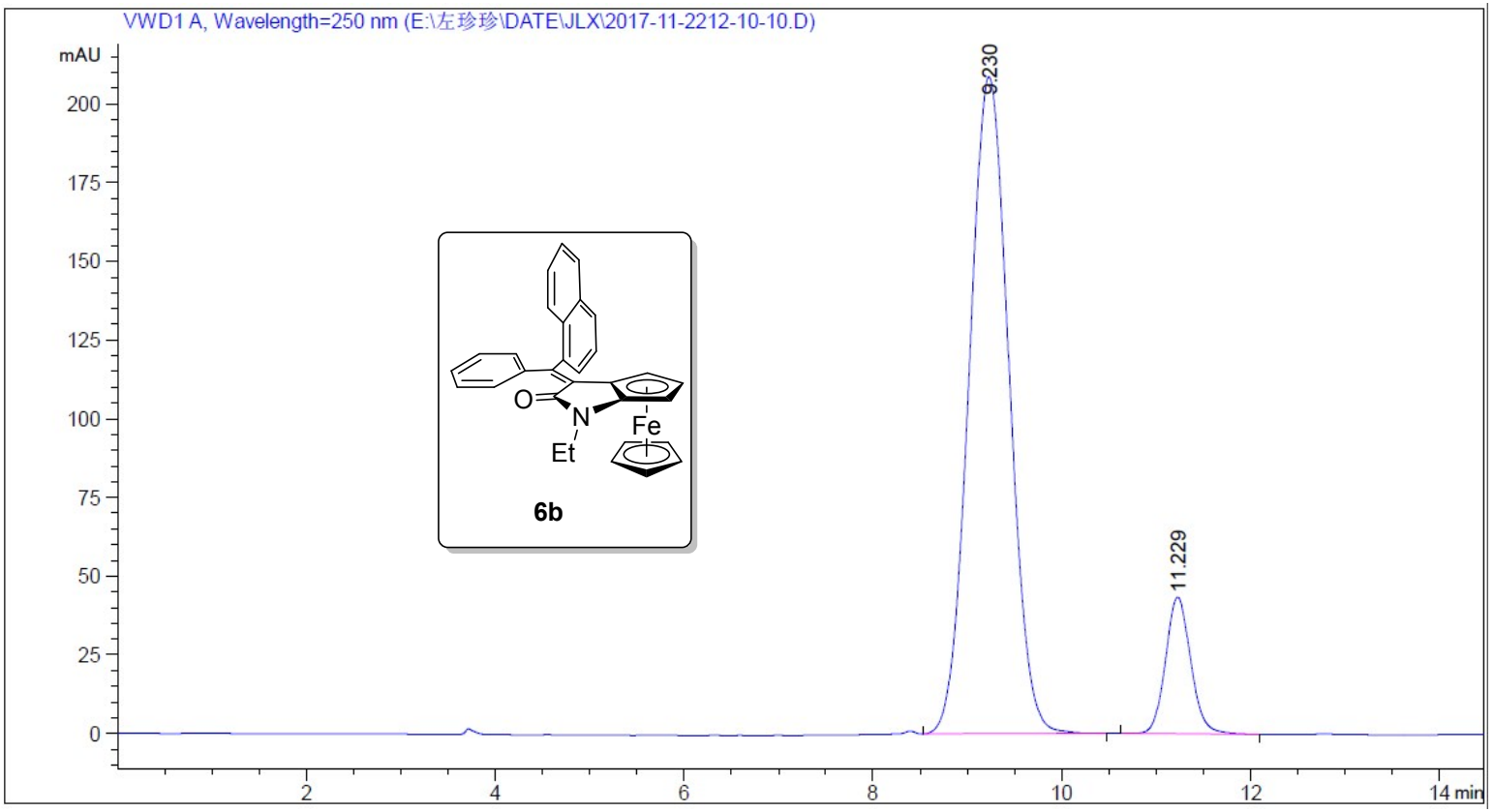

168.22
167.96
129.28
129.26
128.51
128.47
128.42
128.34
127.72
127.67
126.63
126.23
126.19
126.14
125.87
125.45
125.33
105.36
105.15
77.42
77.31
77.10
76.78
72.62
71.91
70.56
70.41
64.82
64.48
60.64
60.40
51.22
51.12
36.39
36.23
13.70
145.35
144.84
140.06
139.90
138.51
138.13
134.15
133.96
129.28
129.26
128.47
128.42
128.34
127.72
127.67
126.63
126.23
126.14
125.87
125.45
125.33
O
N
Et
Fe
6b
145
142
139
136
133
130
127
f1 (ppm)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

Sample Name	Jlx-6m	**Position**	P1-B4	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	Jlx-6m.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	3/20/18 Tue 15:19:40



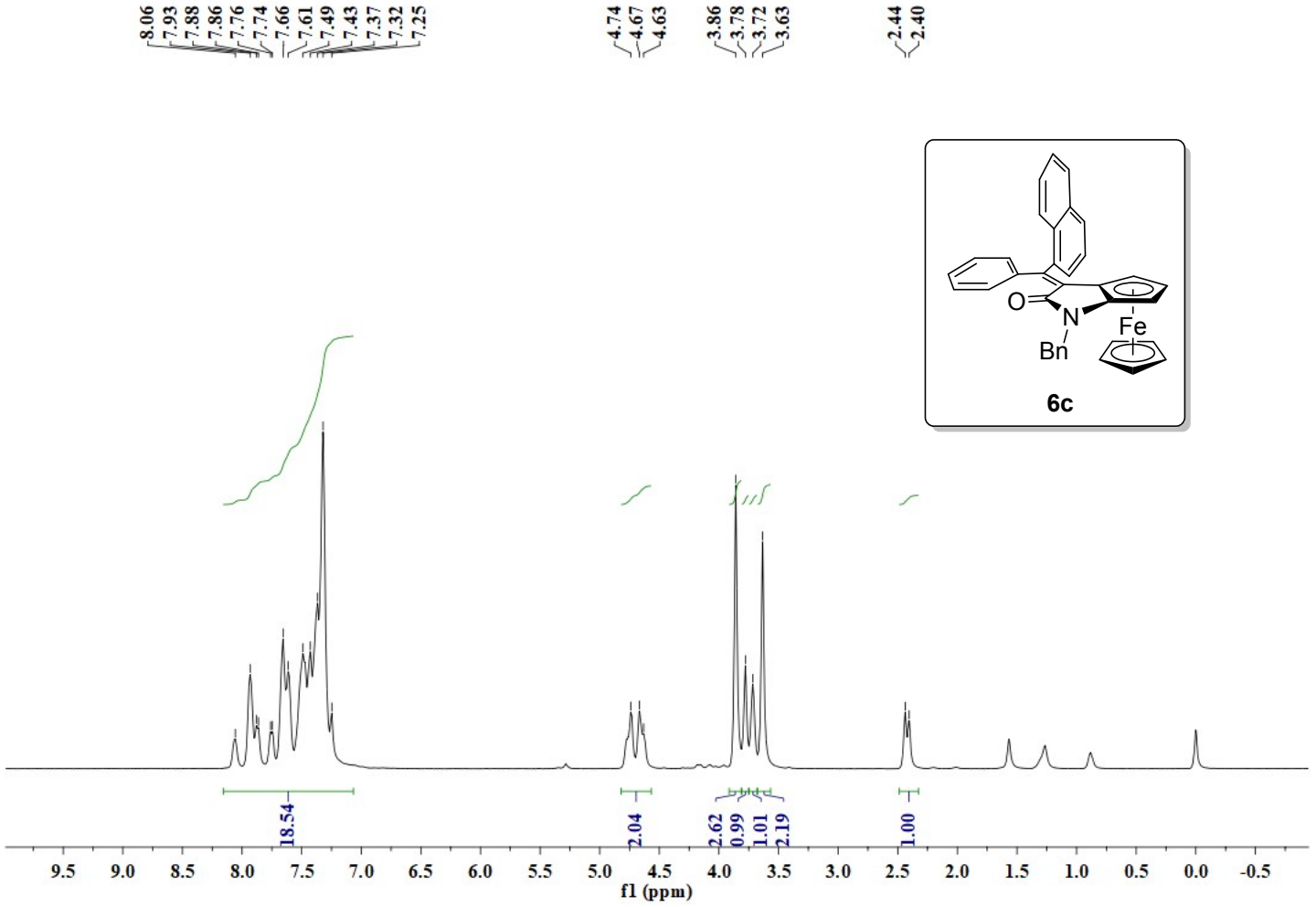


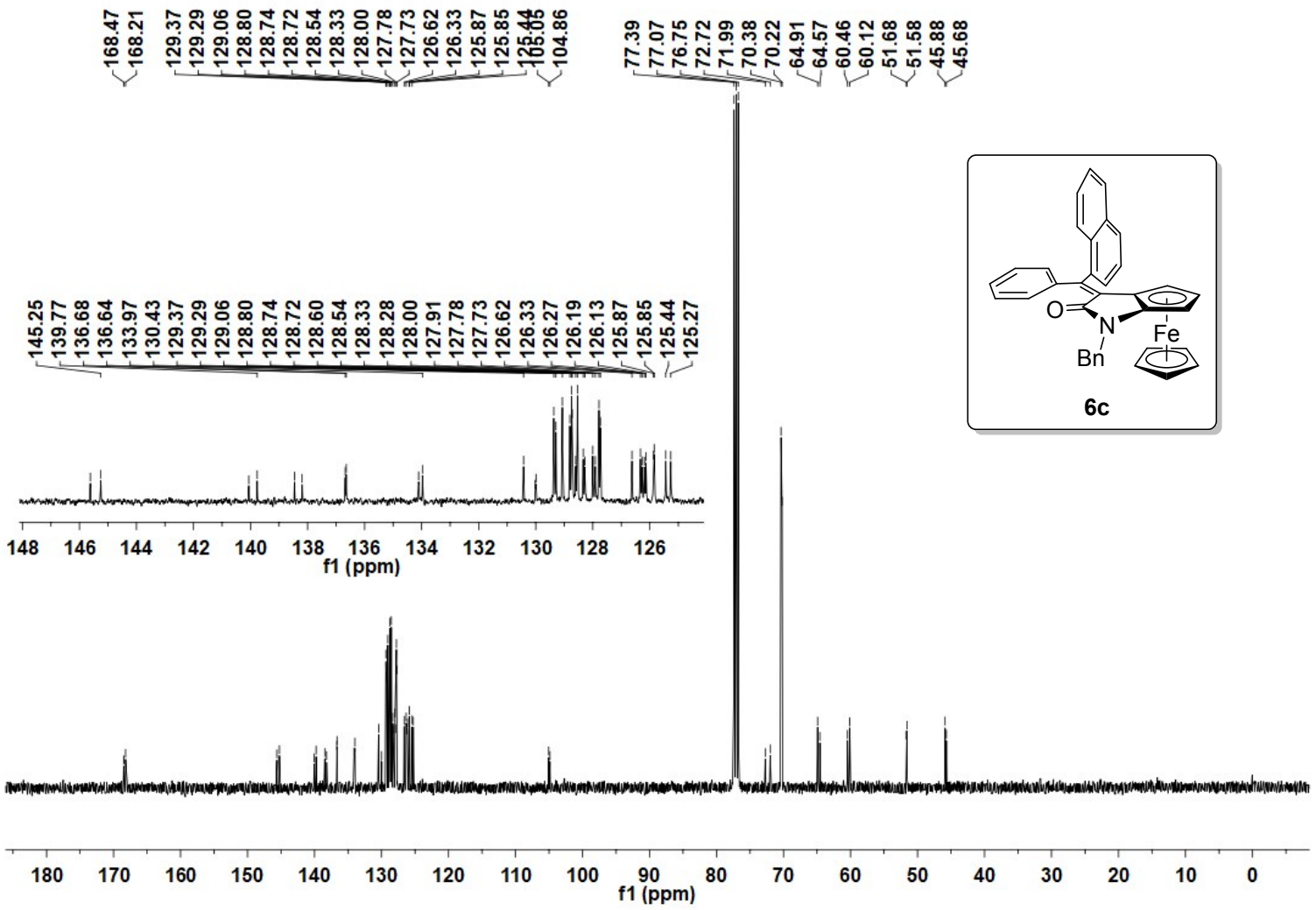
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.278	VB	0.4873	3360.45752	107.92694	50.1569
2	11.282	BV	0.2923	3339.43970	176.88766	49.8431



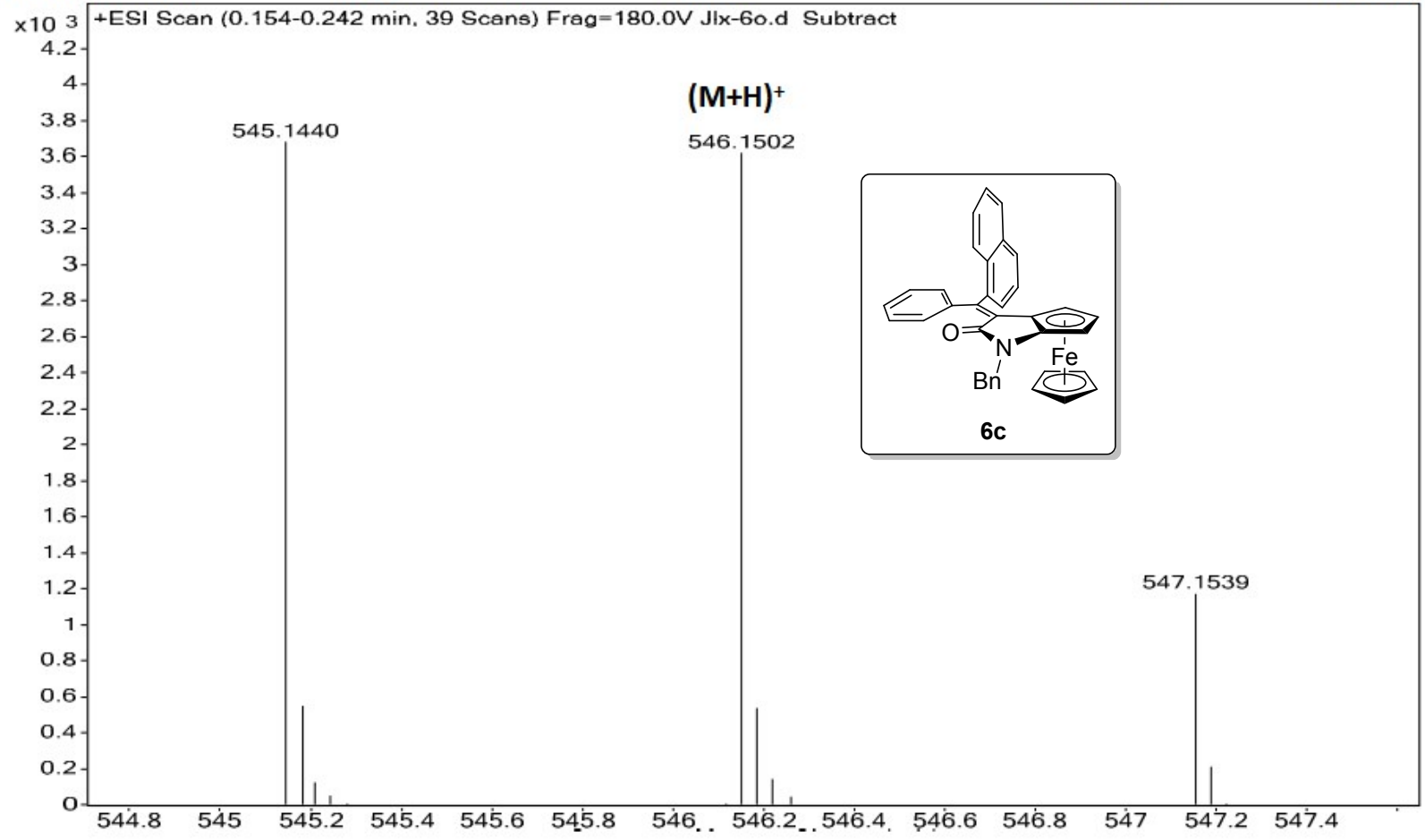
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.230	BB	0.4596	6113.26416	208.77498	88.3150
2	11.229	BB	0.2873	808.84552	43.42768	11.6850

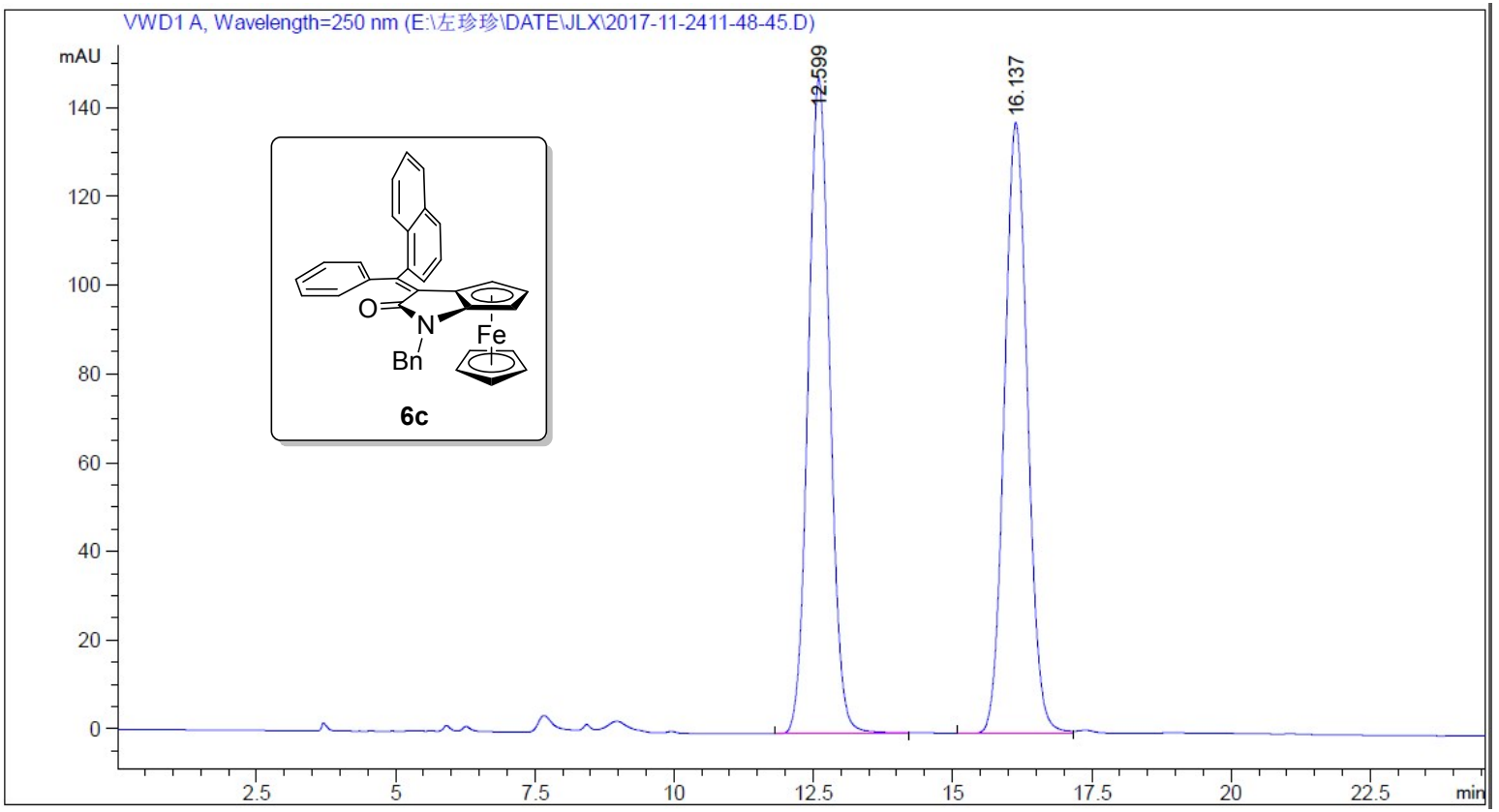
NMR、HMRS Spectra and HPLC Chromatographsof **6e :**



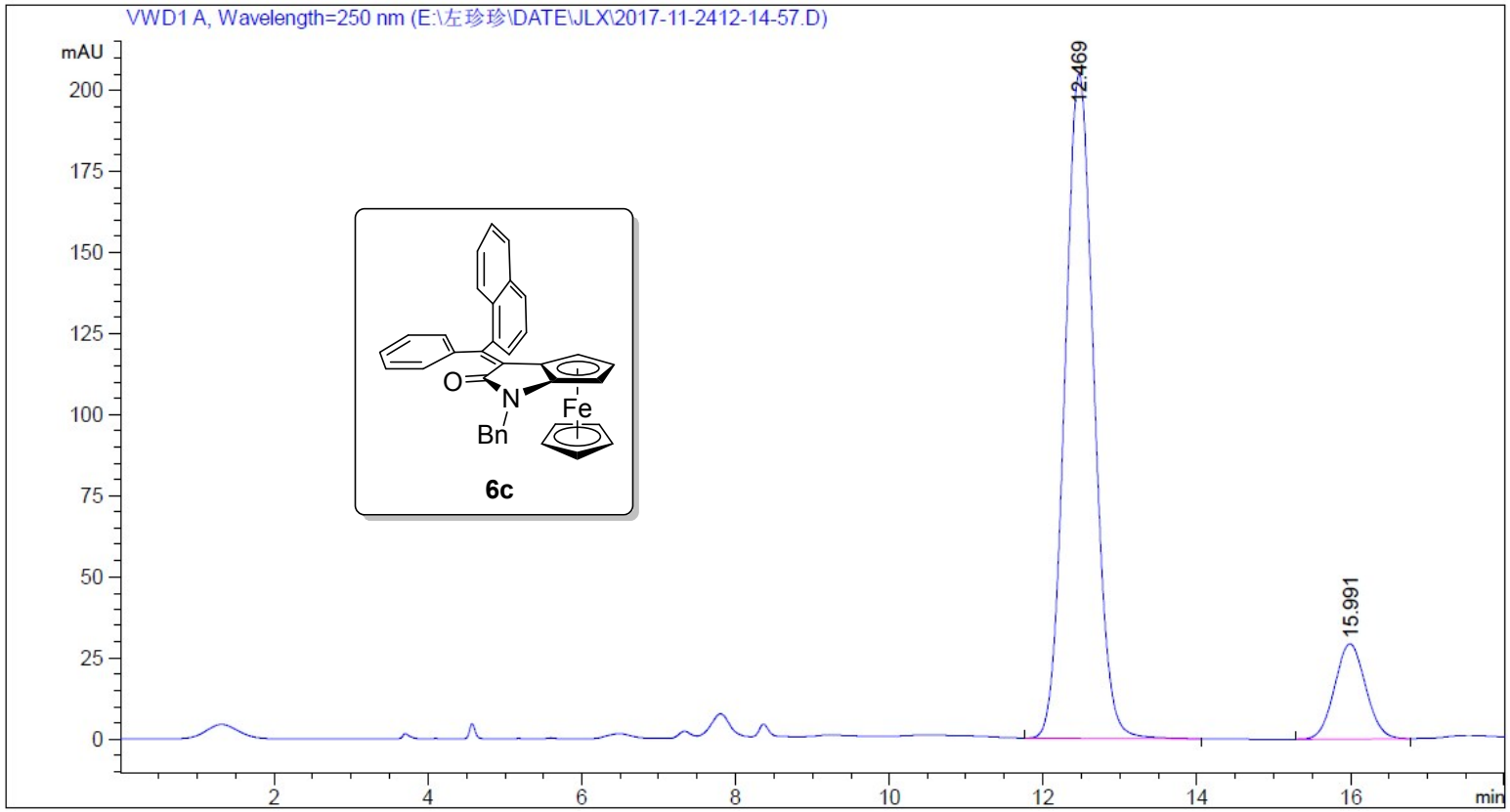

168.47
168.21
129.37
129.29
129.06
128.80
128.74
128.72
128.54
128.33
128.00
127.78
127.73
126.62
126.33
125.87
125.85
125.44
125.05
104.86
77.39
77.07
76.75
72.72
71.99
70.38
70.22
64.91
64.57
60.46
60.12
51.68
51.58
45.88
45.68
145.25
139.77
136.68
136.64
133.97
130.43
129.37
129.29
129.06
128.80
128.74
128.72
128.60
128.54
128.33
128.28
128.00
127.91
127.78
127.73
126.62
126.33
126.27
126.19
126.13
125.87
125.85
125.44
125.27
148 146 144 142 140 138 136 134 132 130 128 126
f1 (ppm)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
O
N
Bn
Fe
6c

Sample Name	Jlx-6o	**Position**	P1-B6	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	Jlx-6o.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	3/20/18 Tue 15:22:12



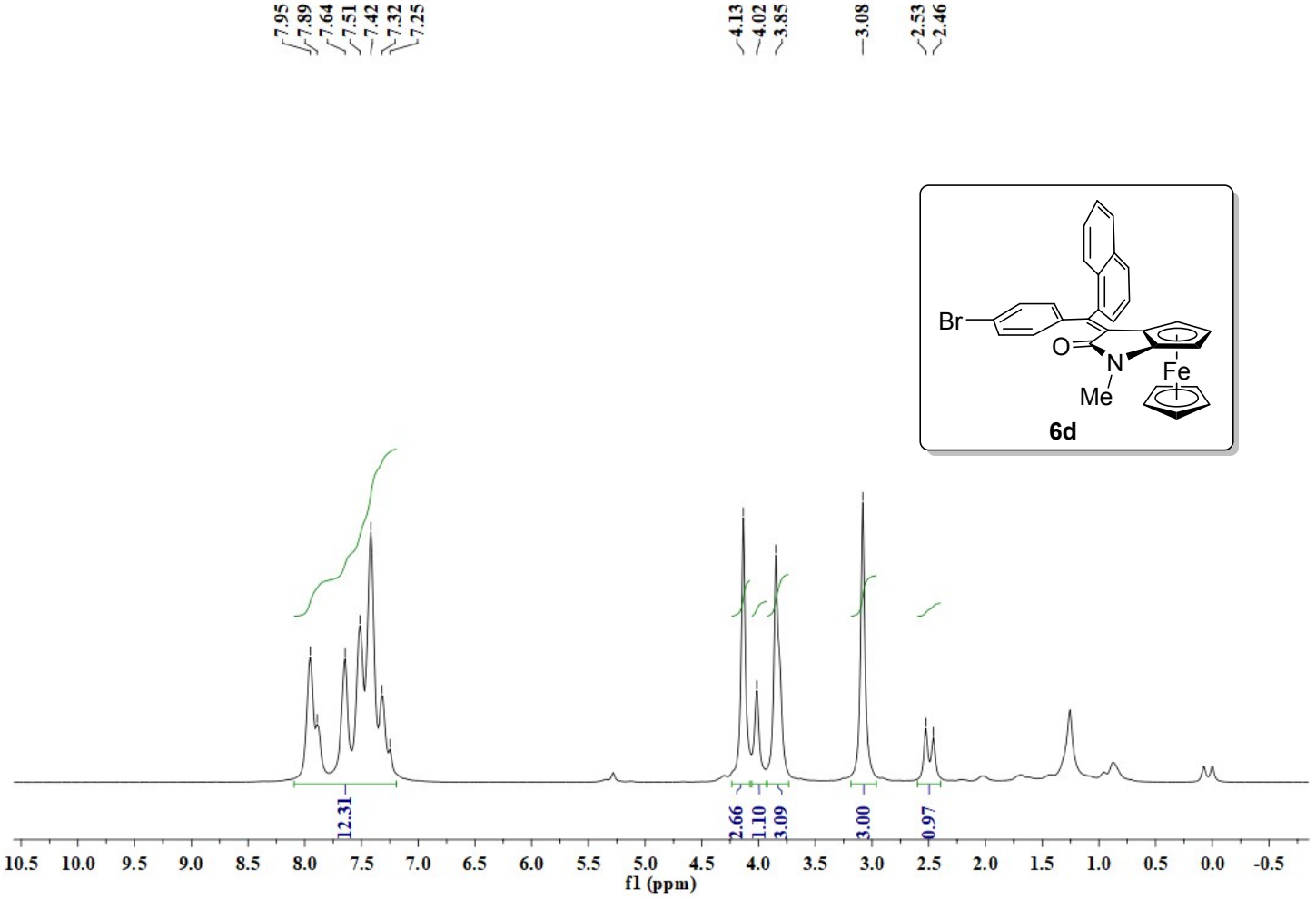


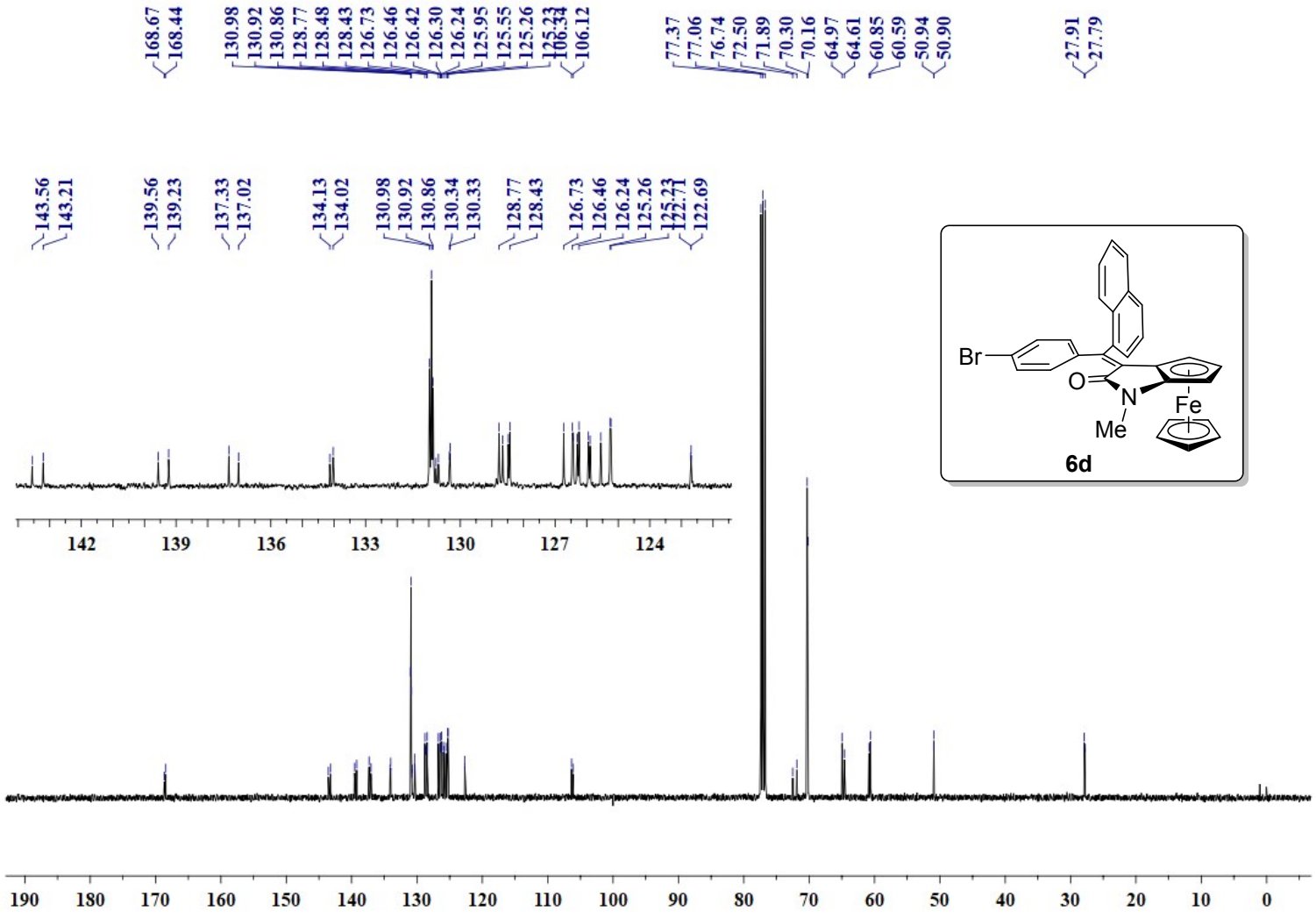
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.599	BV	0.4230	4012.91602	147.69348	50.2145
2	16.137	BV	0.4512	3978.63940	137.67244	49.7855



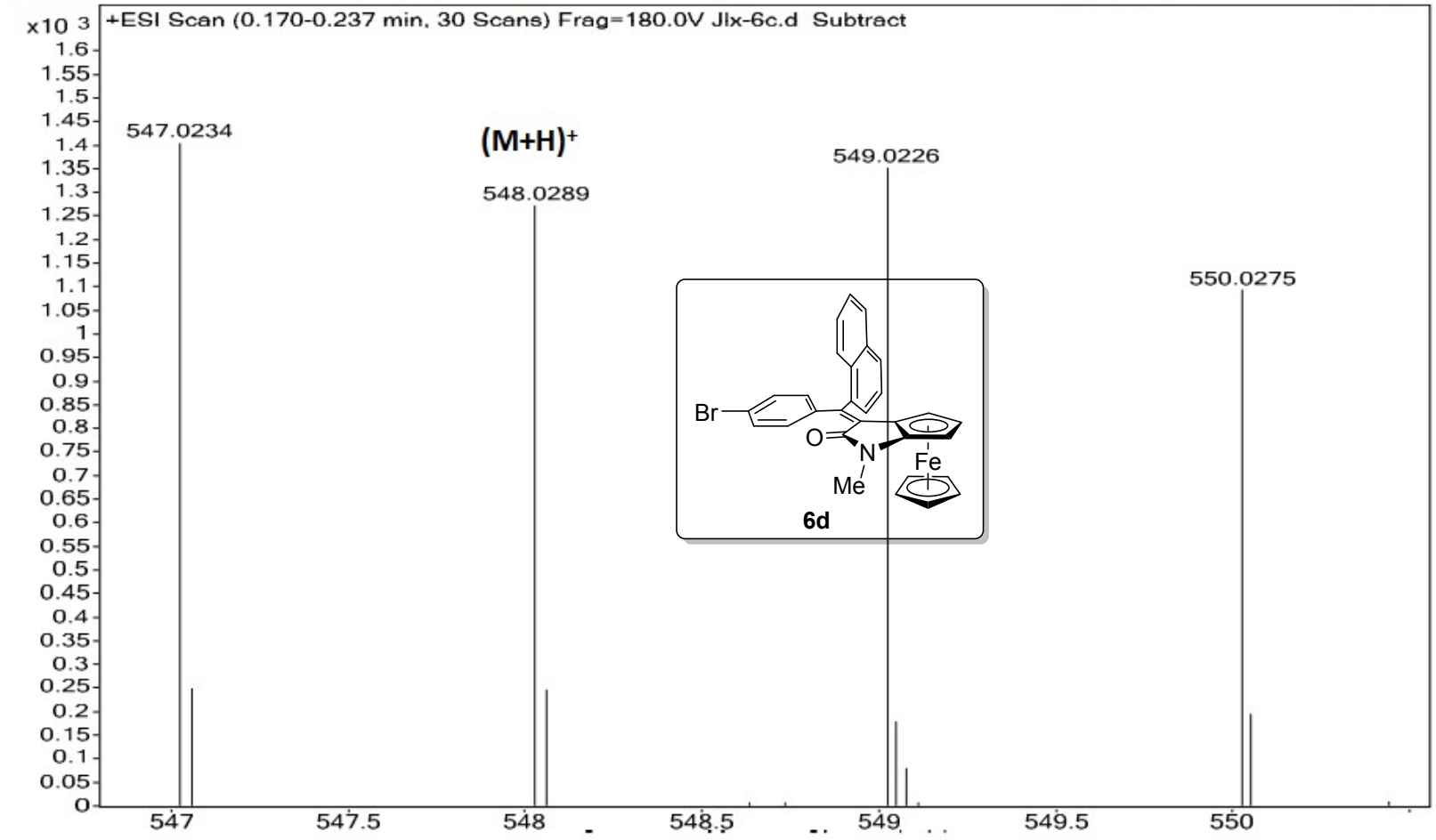
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.469	BB	0.4091	5354.61035	204.75072	86.7314
2	15.991	BB	0.4344	819.17334	29.28166	13.2686

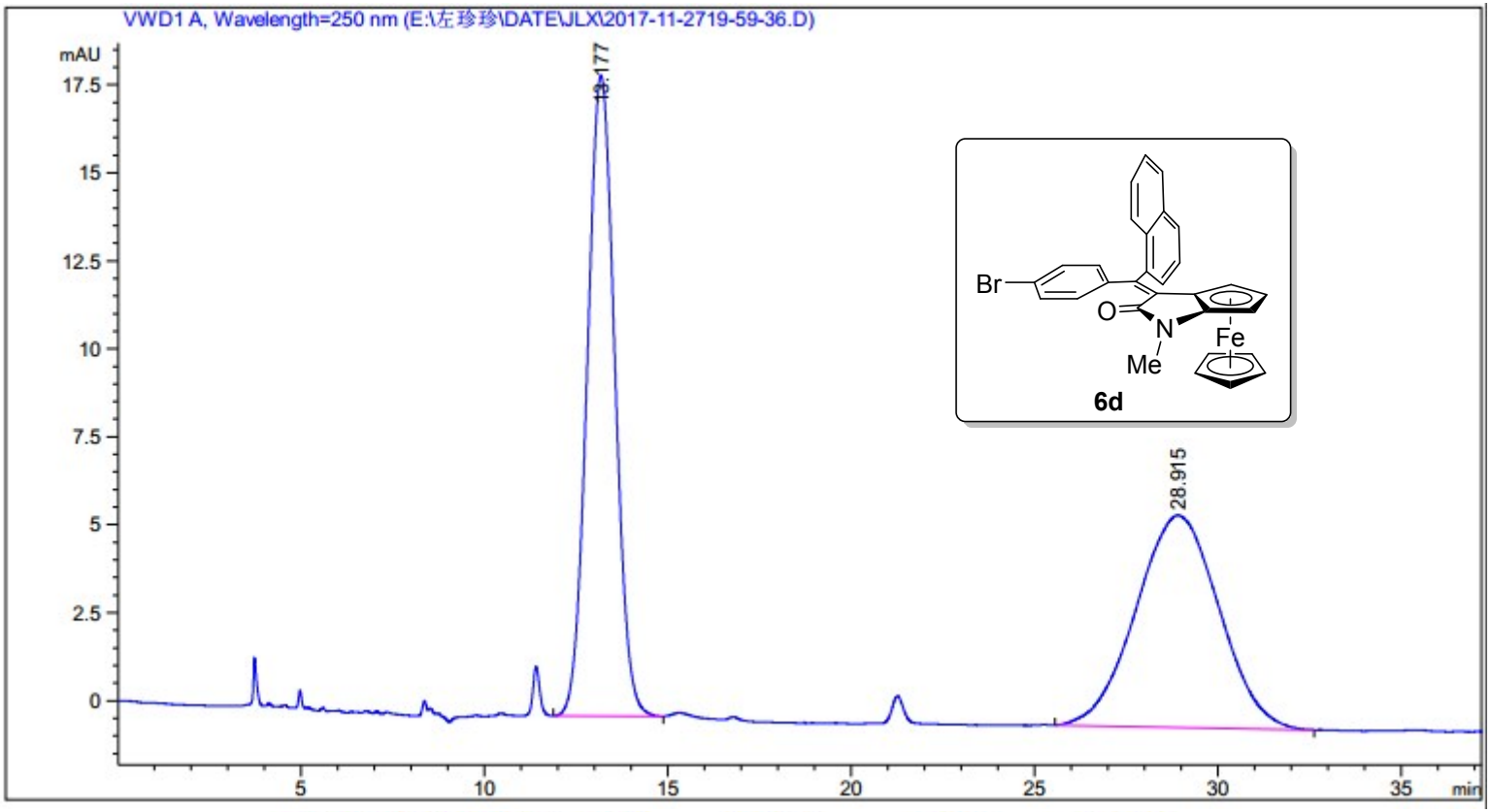
NMR、HMRS Spectra and HPLC Chromatographsof **6d :**



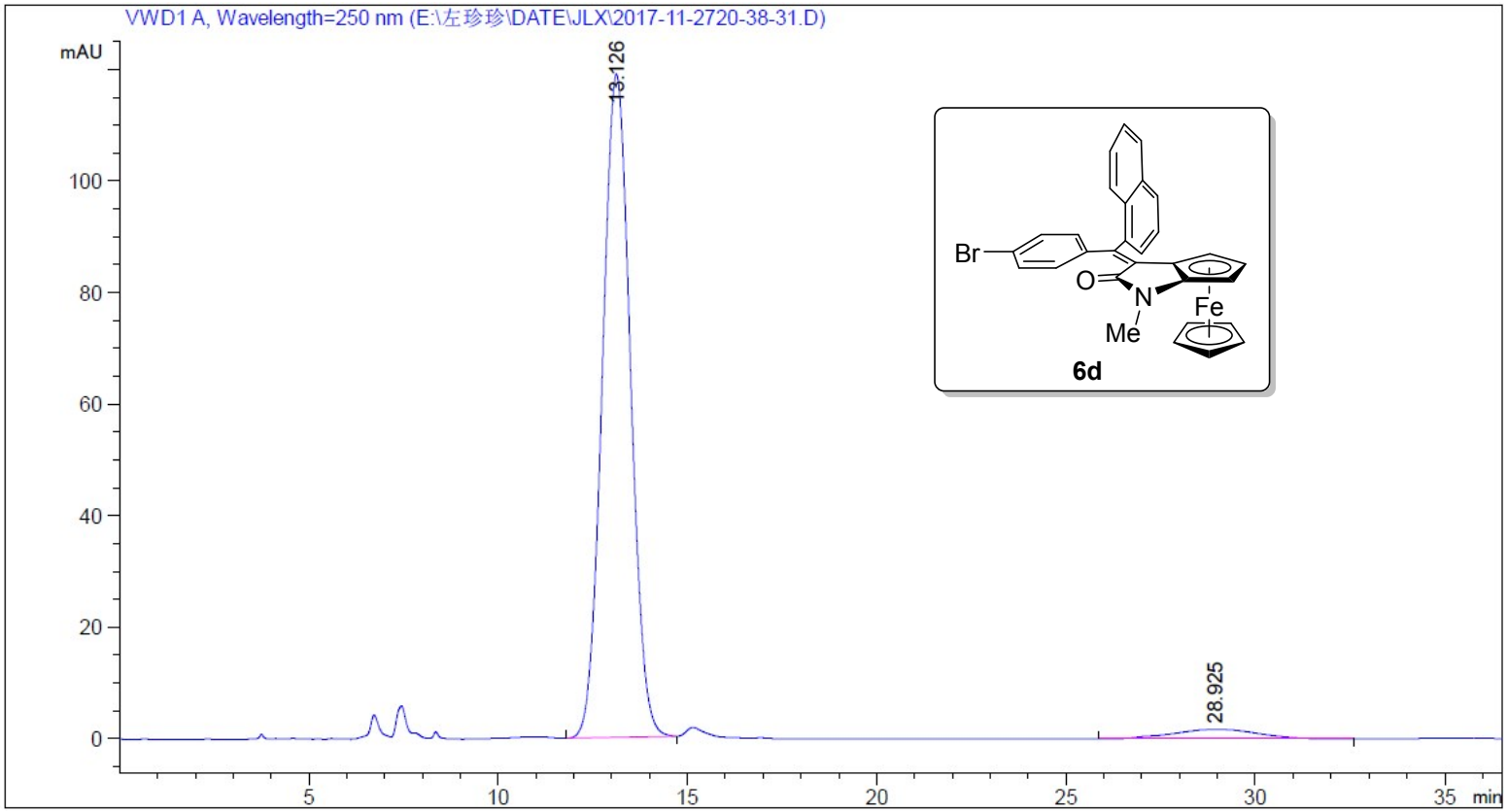

168.67
168.44
130.98
130.92
130.86
128.77
128.48
128.43
126.73
126.46
126.42
126.30
126.24
125.95
125.55
125.26
106.12
77.37
77.06
76.74
72.50
71.89
70.30
70.16
64.97
64.61
60.85
60.59
50.94
50.90
27.91
27.79
143.56
143.21
139.56
139.23
137.33
137.02
134.13
134.02
130.98
130.92
130.86
130.34
130.33
128.77
128.43
126.73
126.46
126.24
125.26
122.69
142
139
136
133
130
127
124
Br
O
N
Me
Fe
6d
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

Sample Name	Jlx-6c	**Position**	P1-A3	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.3	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	Jlx-6c.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	3/20/18 Tue 15:15:53



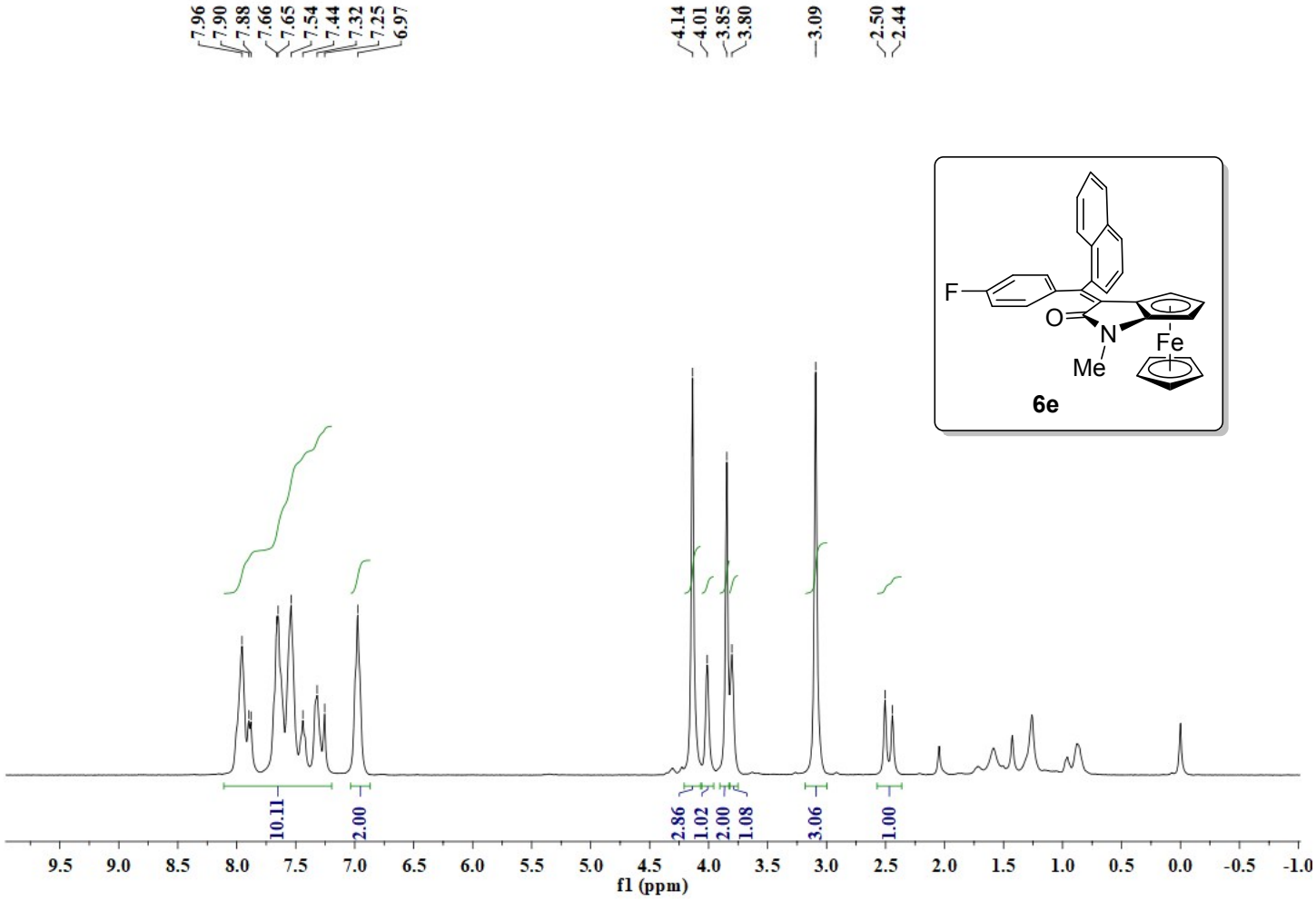


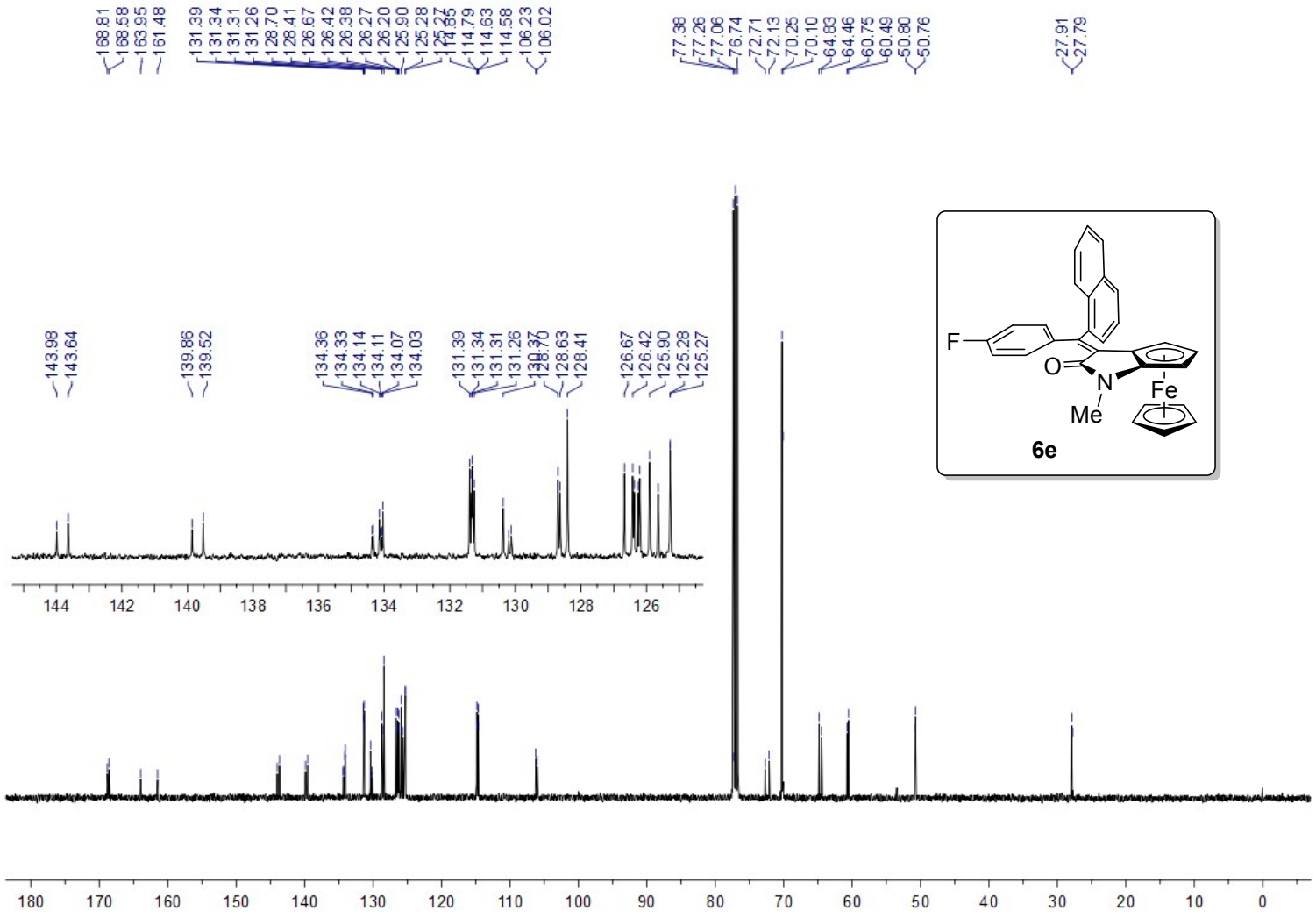
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	13.177	BB	0.8156	948.06305	18.20340	49.9470
2	28.915	BB	2.0535	950.07599	6.02551	50.0530

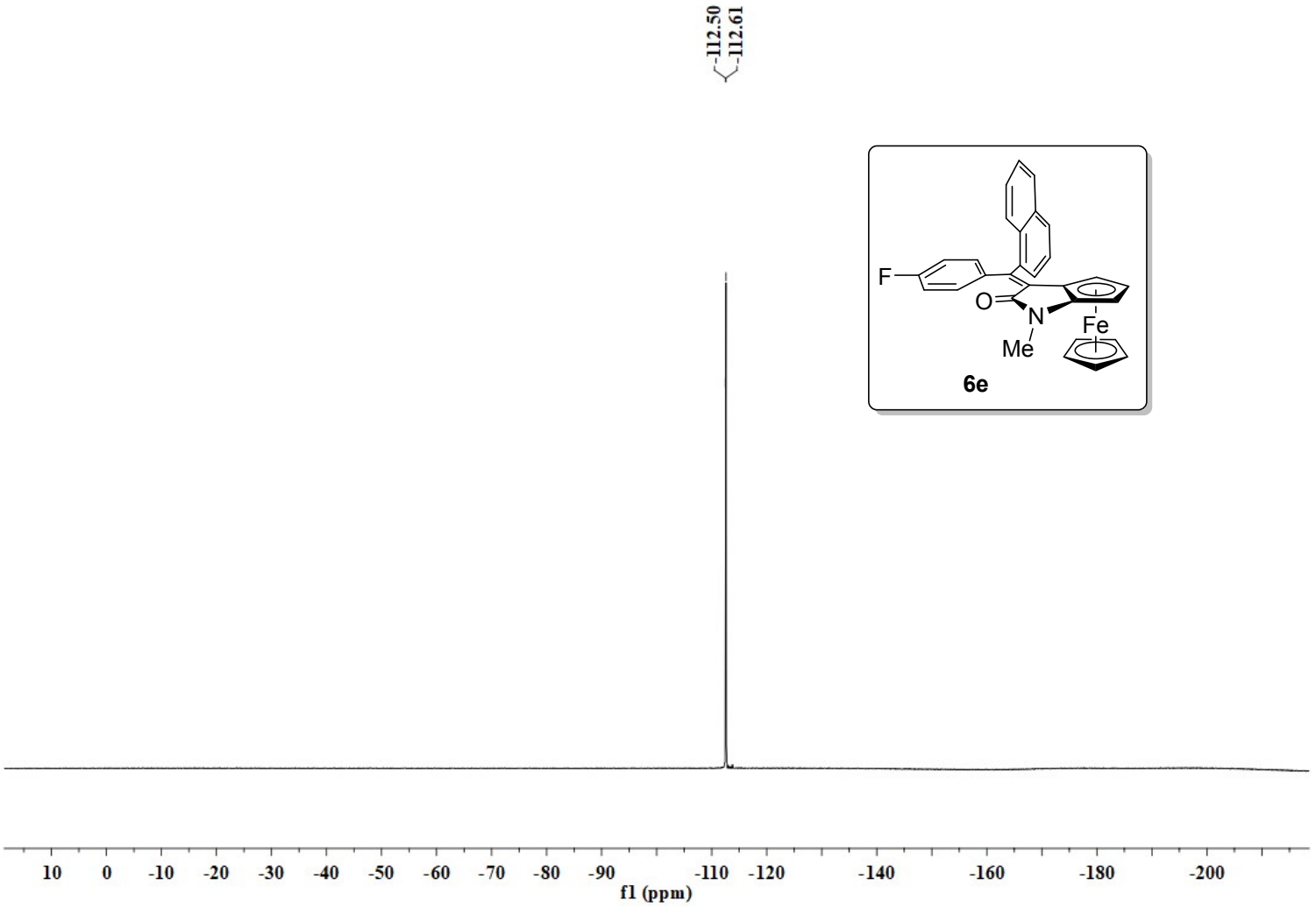


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	13.126	BB	0.8069	6123.85693	118.89569	95.6856
2	28.925	BB	1.8636	276.12231	1.75692	4.3144

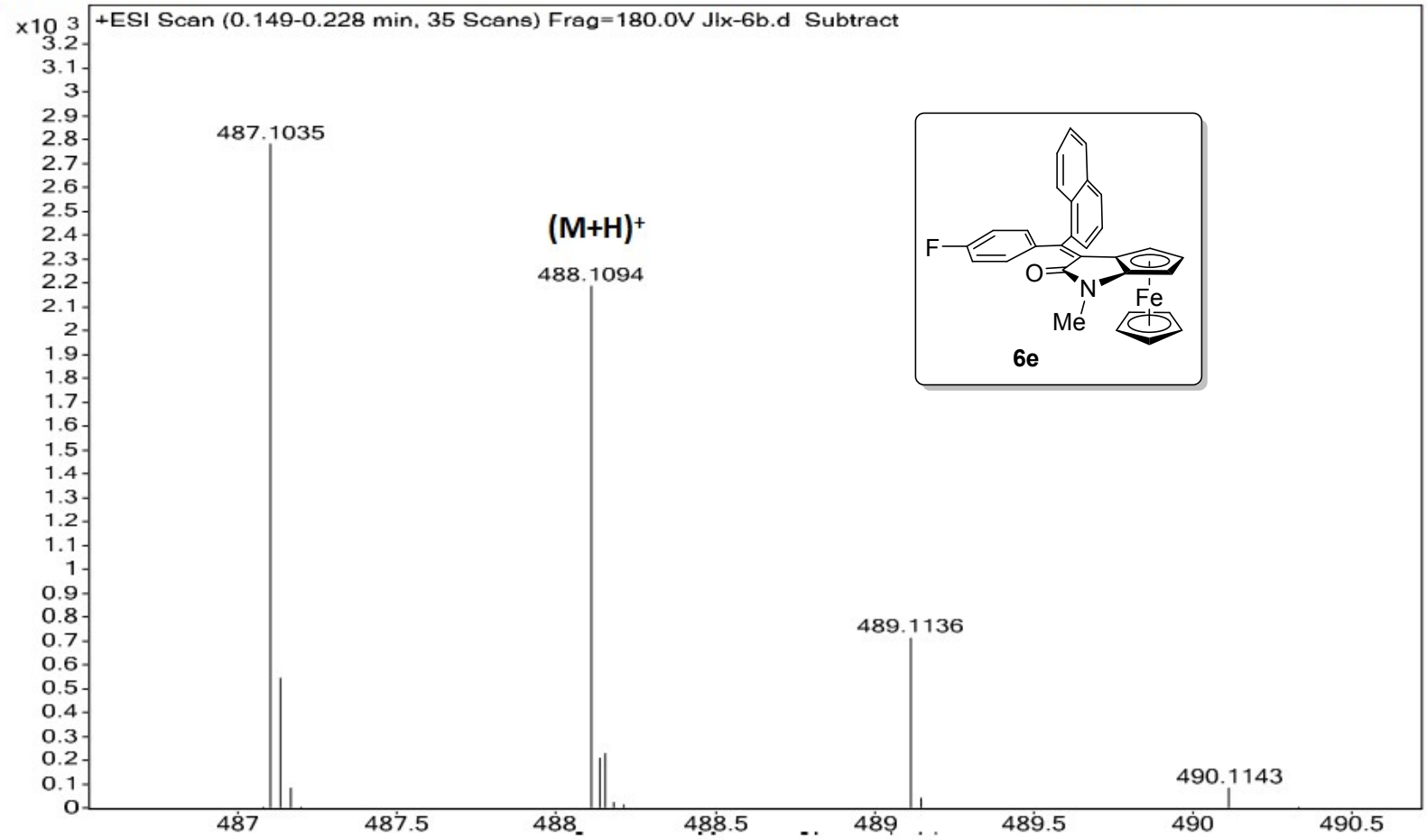
NMR、HMRS Spectra and HPLC Chromatographsof **6e :**

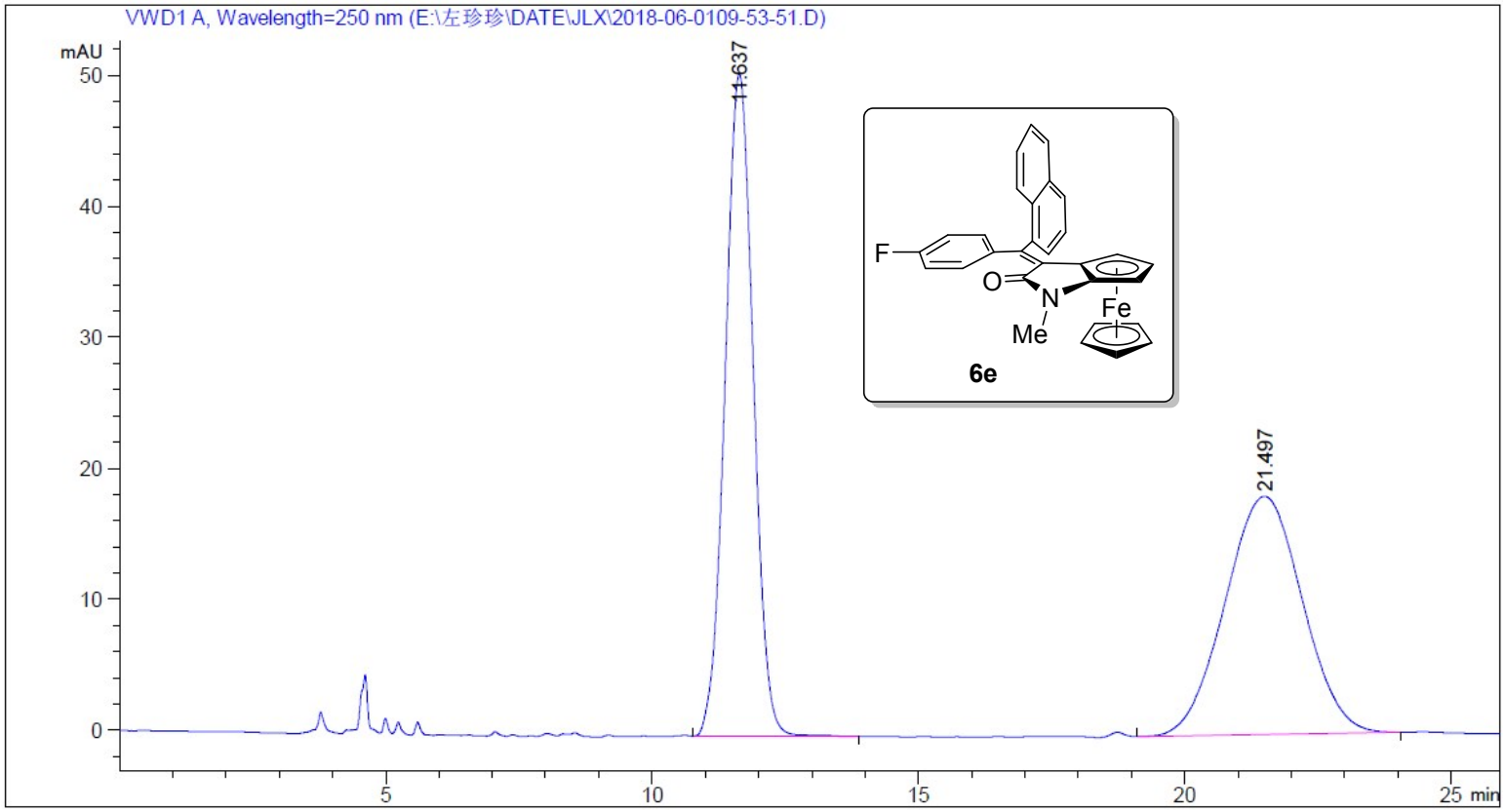



168.81
168.58
163.95
161.48
131.39
131.34
131.31
131.26
128.70
128.41
126.67
126.42
126.38
126.27
126.20
125.90
125.28
114.79
114.63
114.58
106.23
106.02
77.38
77.26
77.06
76.74
72.71
72.13
70.25
70.10
64.83
64.46
60.75
60.49
50.80
50.76
27.91
27.79
143.98
143.64
139.86
139.52
134.36
134.33
134.14
134.11
134.07
134.03
131.39
131.34
131.31
131.26
128.63
128.41
126.67
126.42
125.90
125.28
125.27
F
O
N
Me
Fe
6e

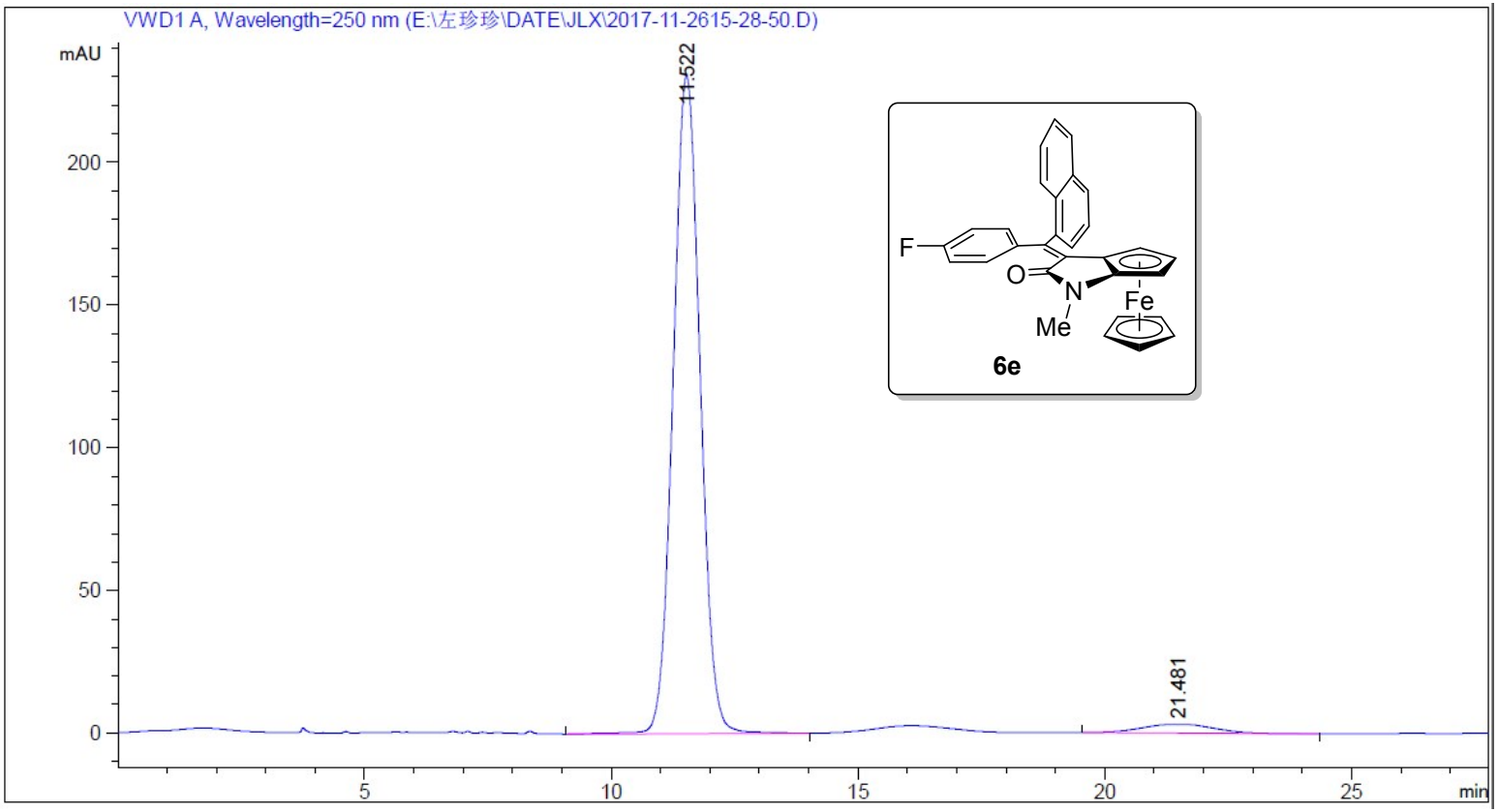

-112.50
-112.61
F
O
N
Me
Fe
6e
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-110
-120
-140
-160
-180
-200
f1 (ppm)

Sample Name	Jlx-6b	**Position**	P1-A2	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	Jlx-6b.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	3/20/18 Tue 14:59:16



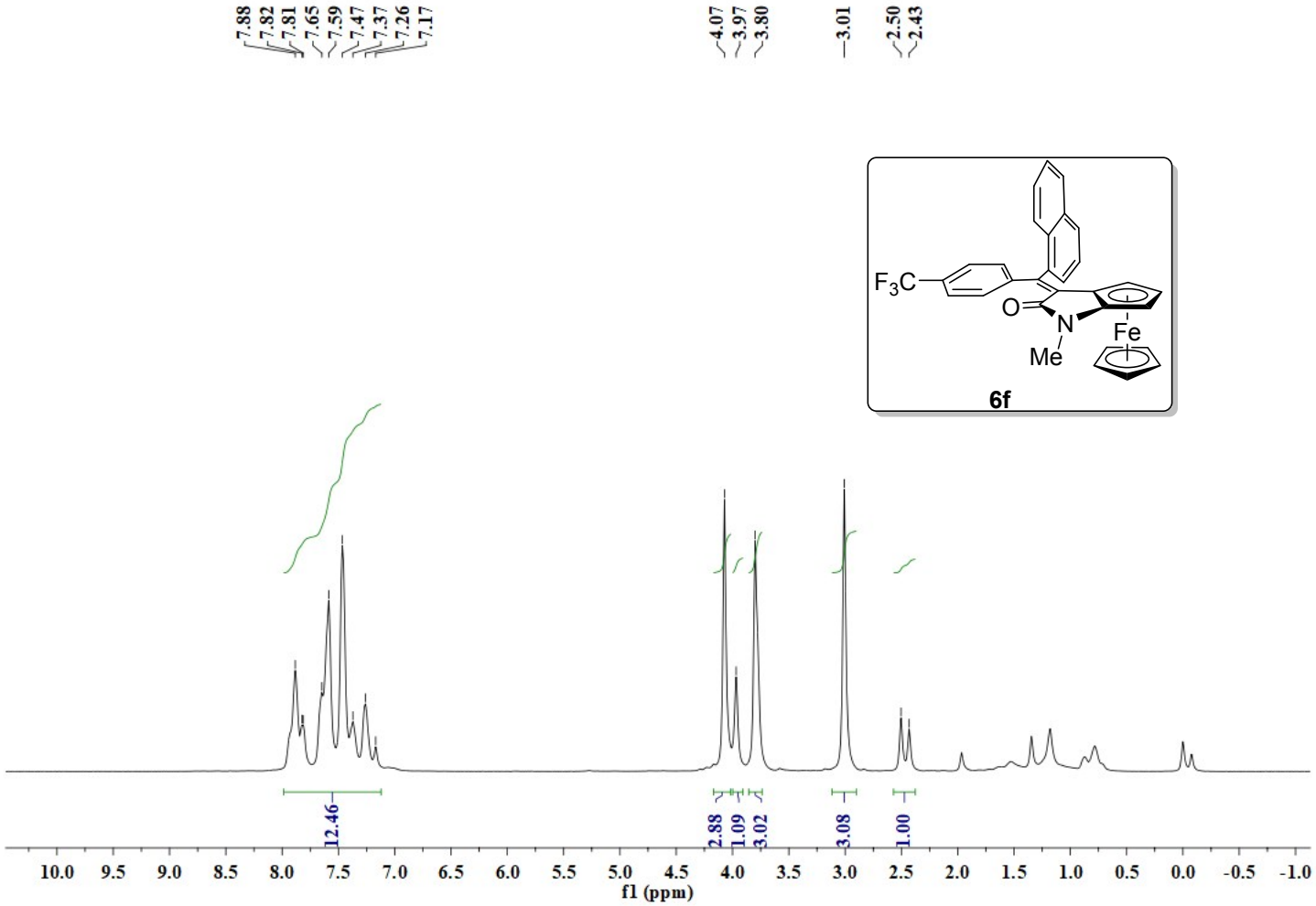


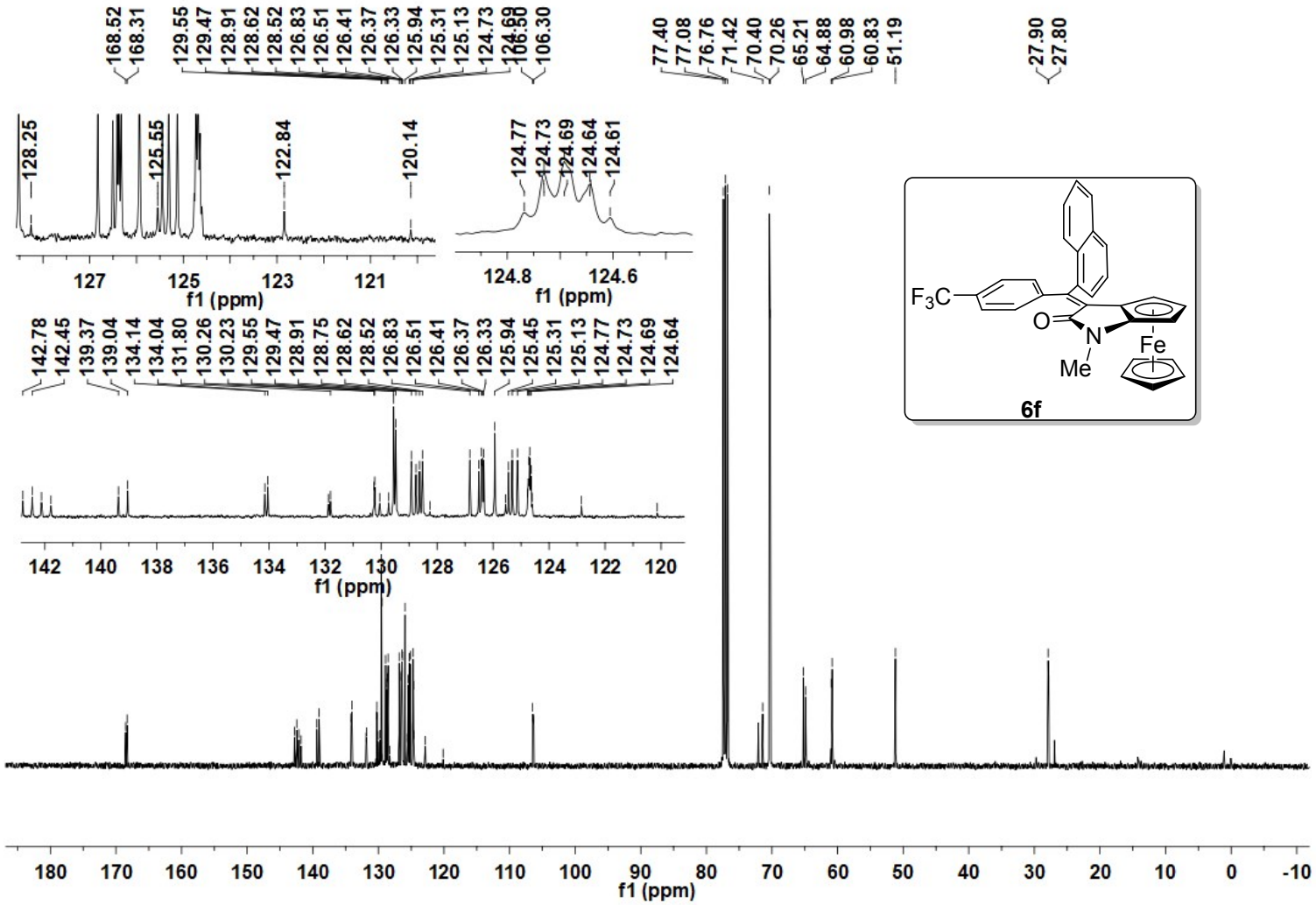
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.637	VB	0.5765	1866.35071	50.58072	50.4458
2	21.497	BB	1.5507	1833.36768	18.17684	49.5542

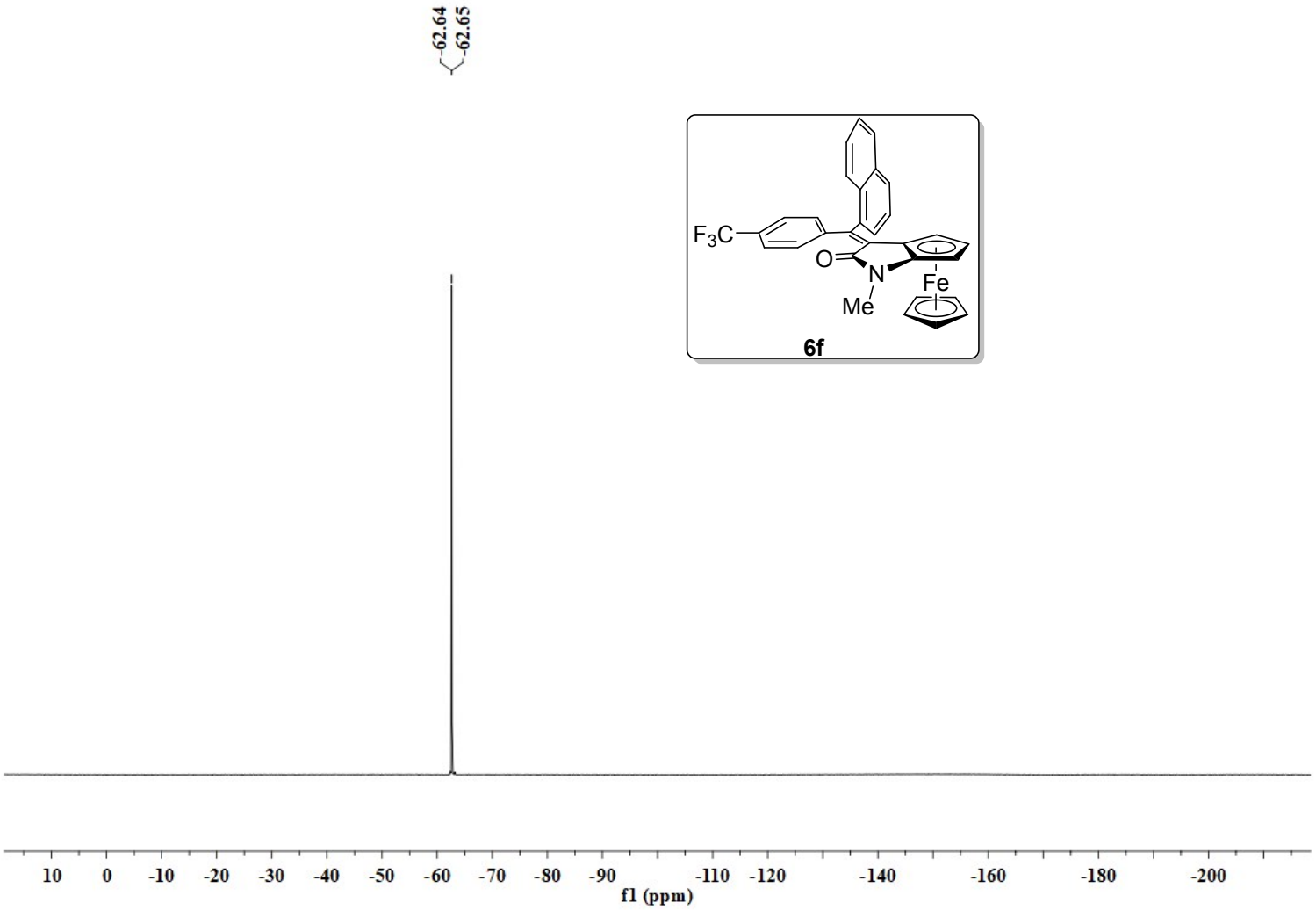


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.522	BB	0.5909	8749.51172	230.45877	96.4724
2	21.480	BB	1.3445	319.93506	3.19435	3.5276

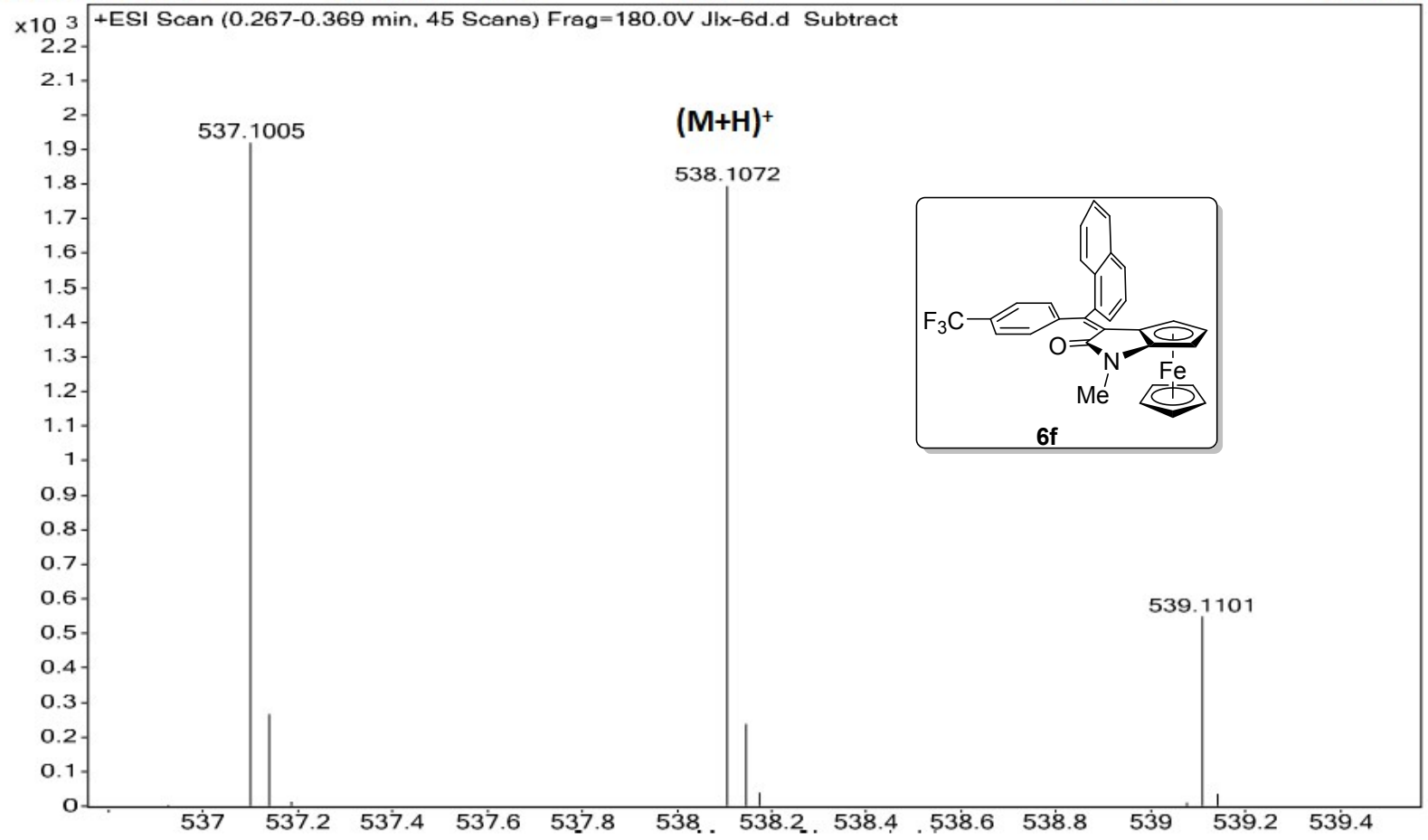
NMR、HMRS Spectra and HPLC Chromatographsof **6f**

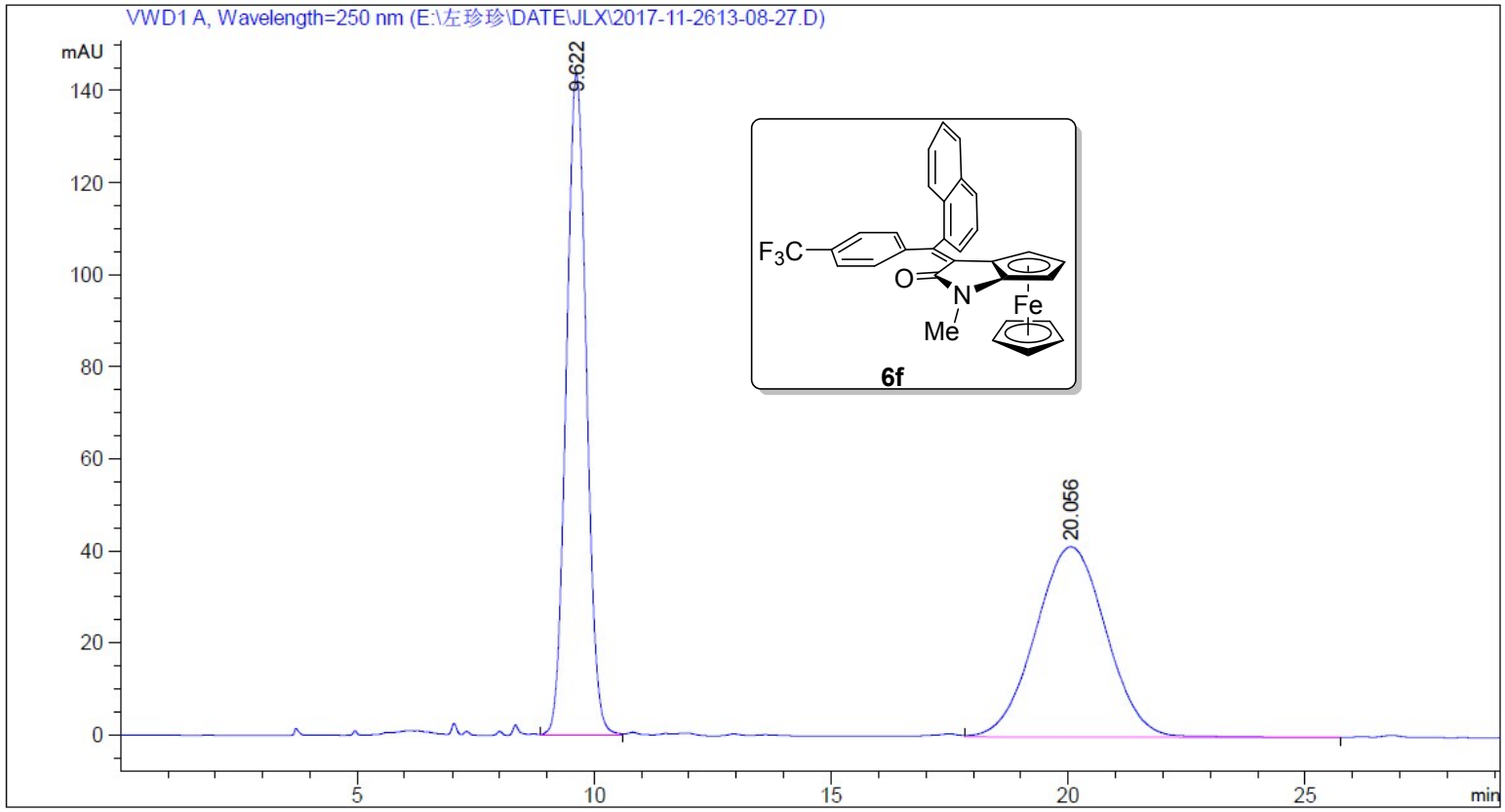



168.52
168.31
129.55
129.47
128.91
128.62
128.52
126.83
126.51
126.41
126.37
126.33
125.94
125.31
125.13
124.73
106.50
106.30
77.40
77.08
76.76
71.42
70.40
70.26
65.21
64.88
60.98
60.83
51.19
27.90
27.80
128.25
125.55
122.84
120.14
124.77
124.73
124.69
124.64
124.61
127
125
123
121
f1 (ppm)
124.8
124.6
f1 (ppm)
142.78
142.45
139.37
139.04
134.14
134.04
131.80
130.26
130.23
129.55
129.47
128.91
128.75
128.62
128.52
126.83
126.51
126.41
126.37
126.33
125.94
125.45
125.31
125.13
124.77
124.73
124.69
124.64
142
140
138
136
134
132
130
128
126
124
122
120
f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)
F3C
O
N
Me
Fe
6f

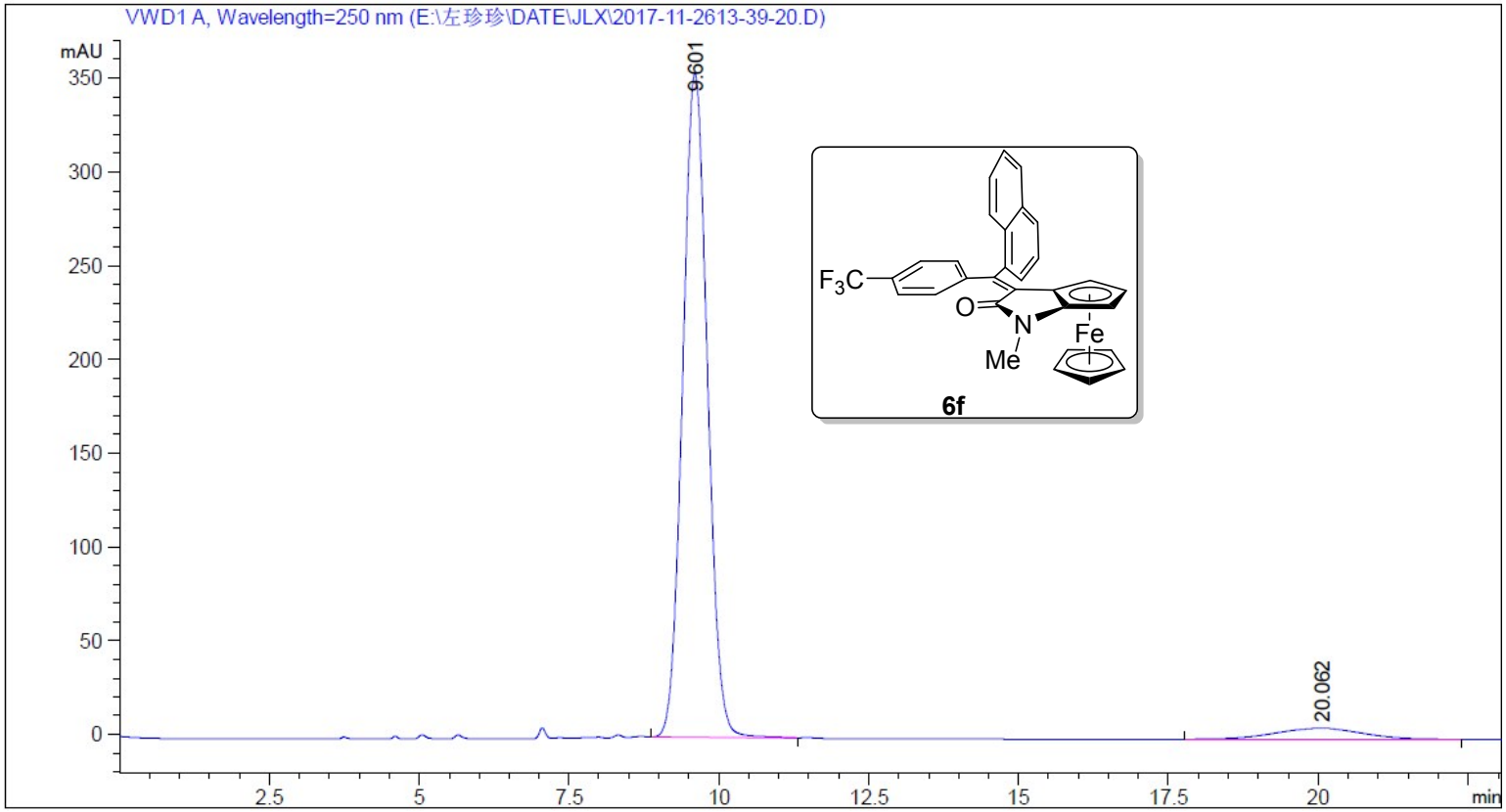

-62.64
-62.65
F3C
O
N
Me
Fe
6f
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-110
-120
-140
-160
-180
-200
f1 (ppm)

Sample Name	Jlx-6d	**Position**	P1-A4	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	Jlx-6d.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	3/20/18 Tue 15:01:48



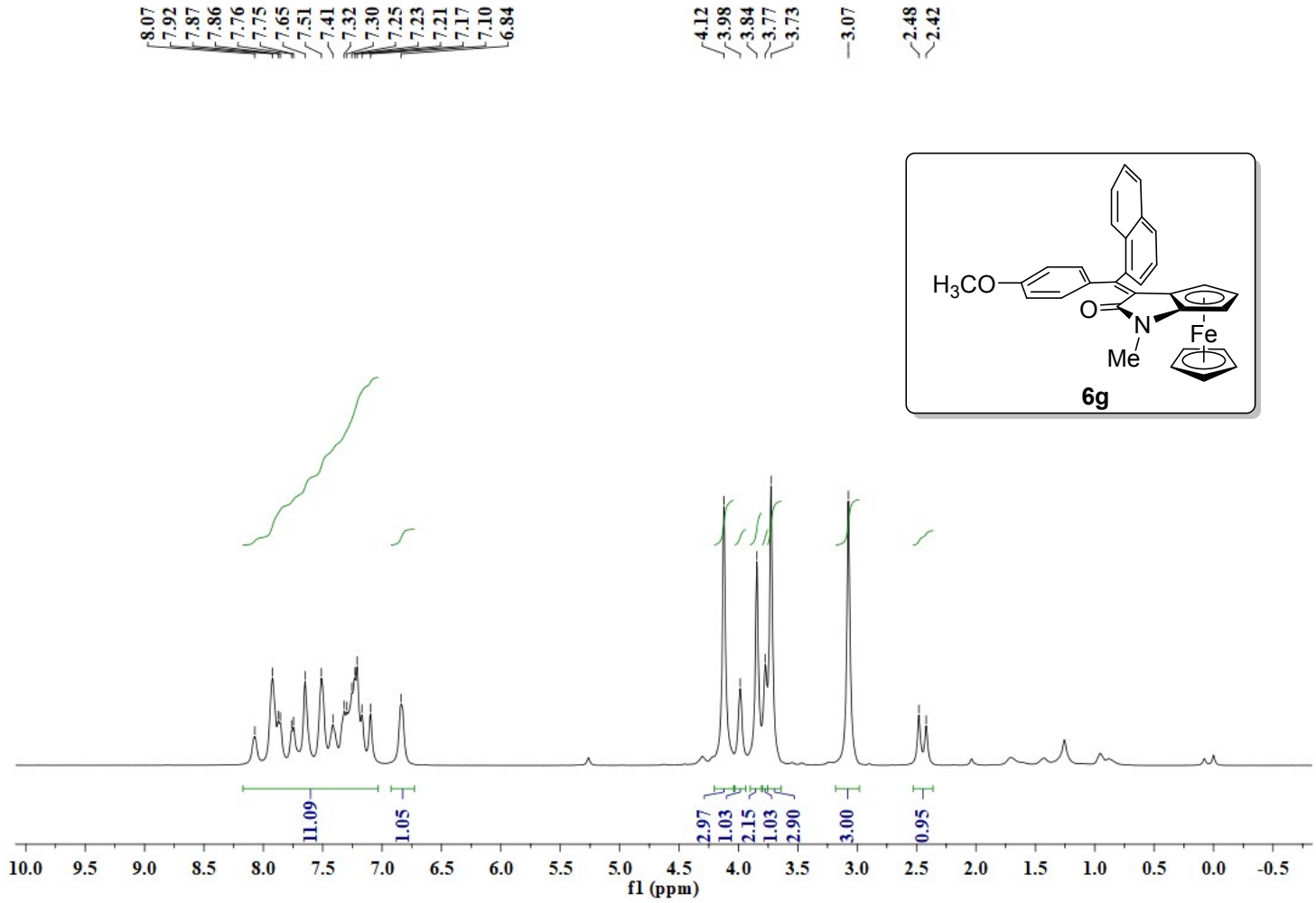


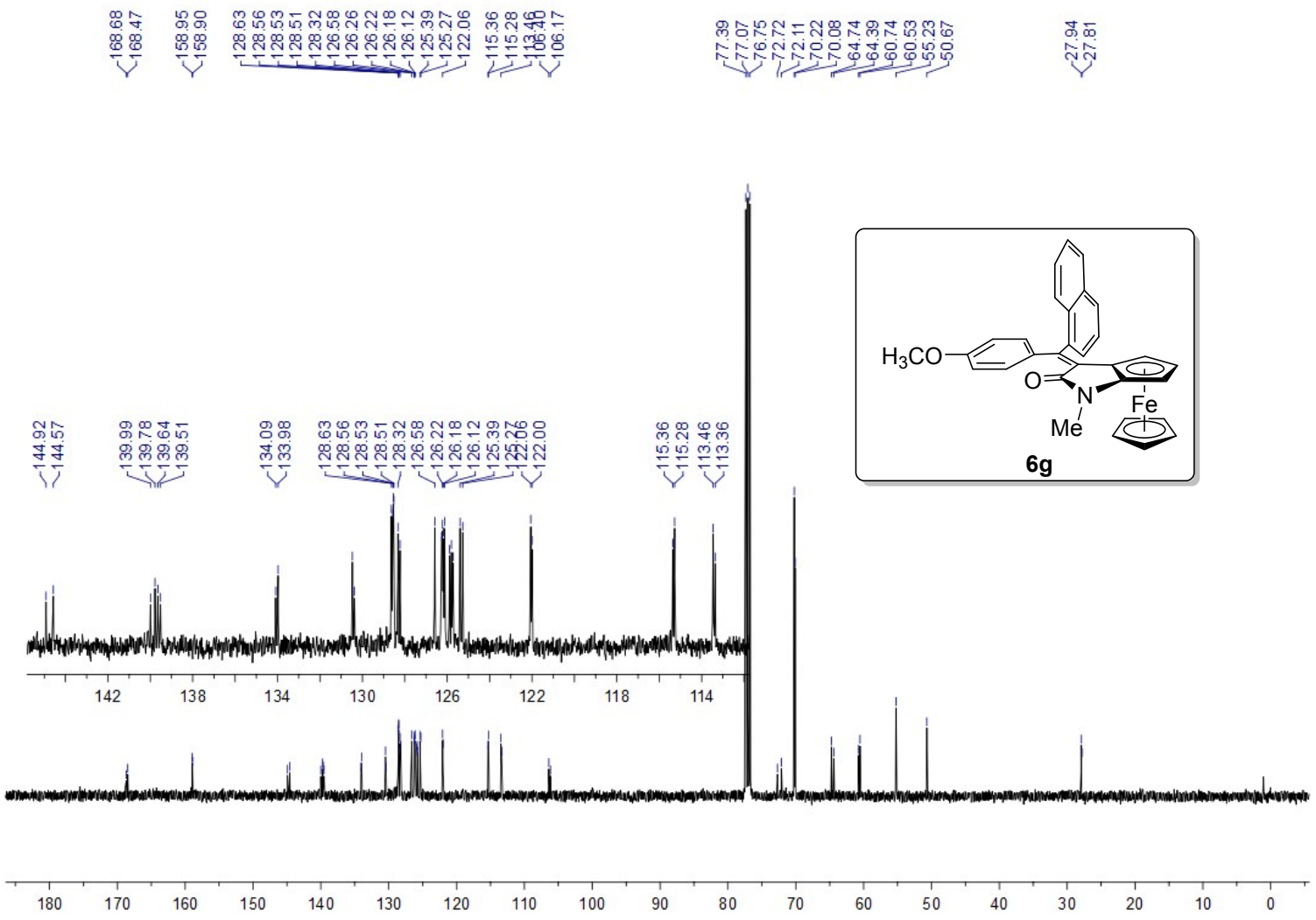
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.622	VV	0.4603	4236.86035	143.58069	49.7192
2	20.056	VB	1.6298	4284.71582	41.31823	50.2808



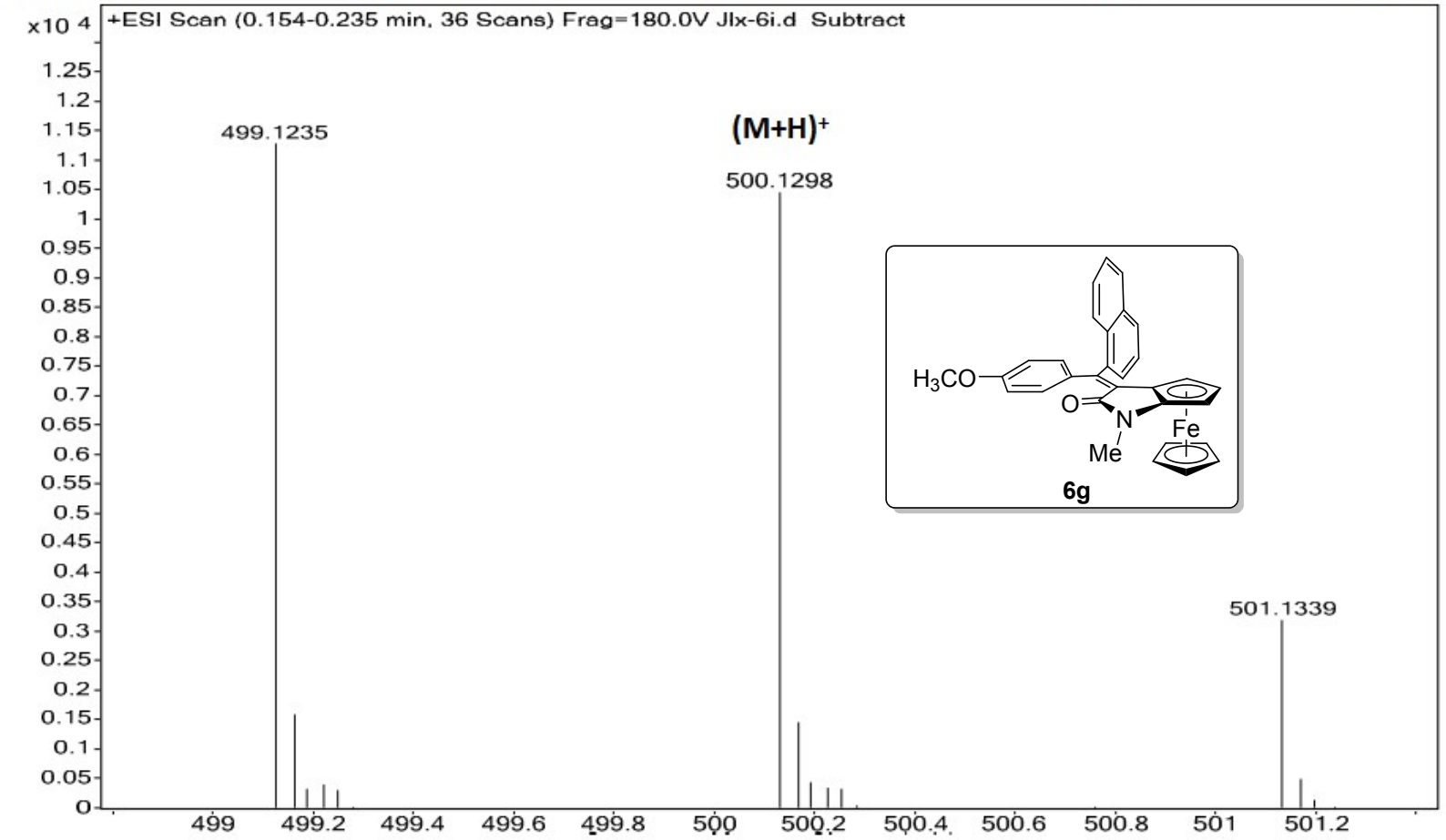
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.601	BB	0.4464	1.01495e4	354.13367	94.6445
2	20.062	BB	1.2416	574.32019	6.02788	5.3555

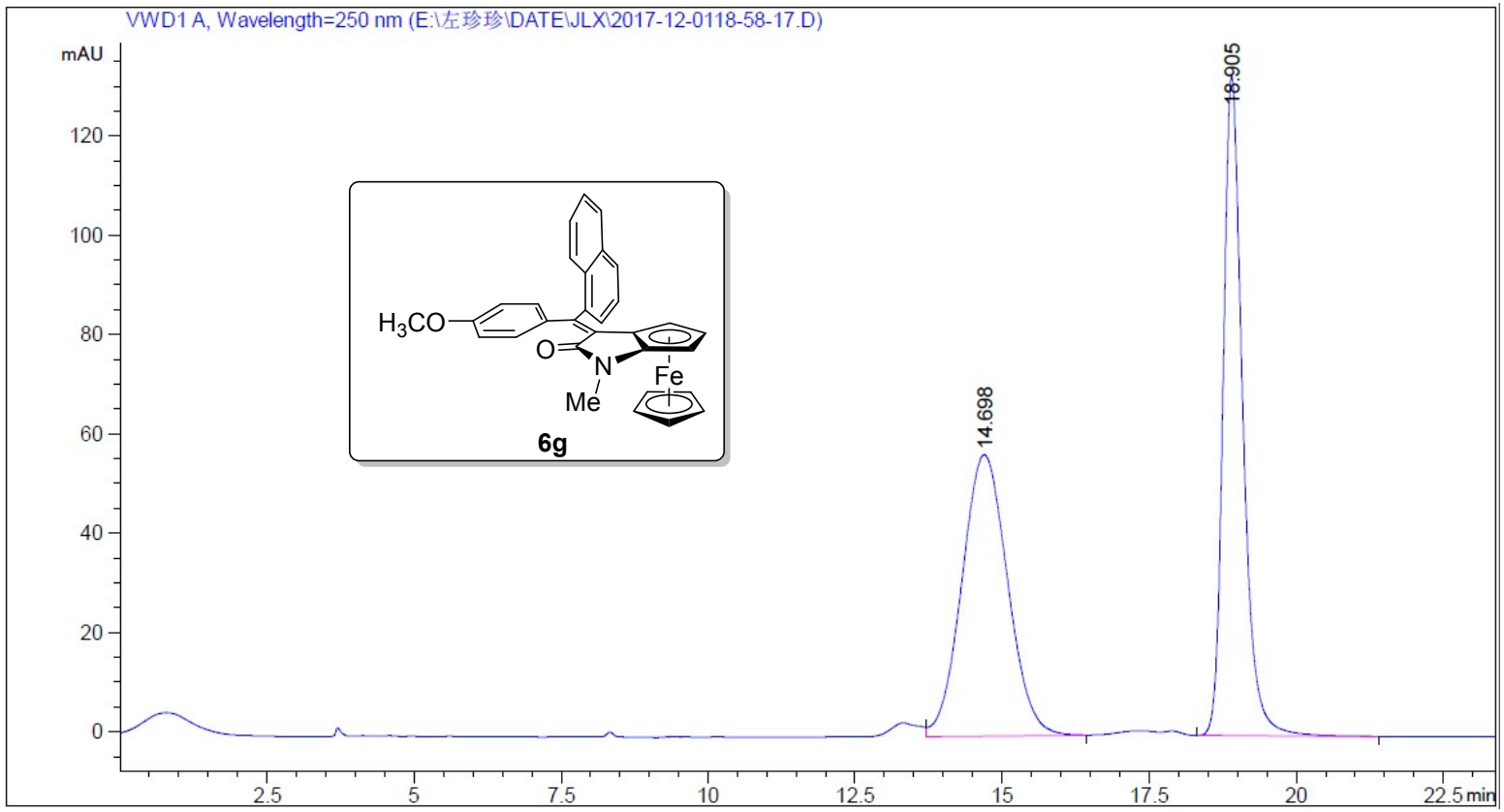
NMR、HMRS Spectra and HPLC Chromatographs of **6g :**



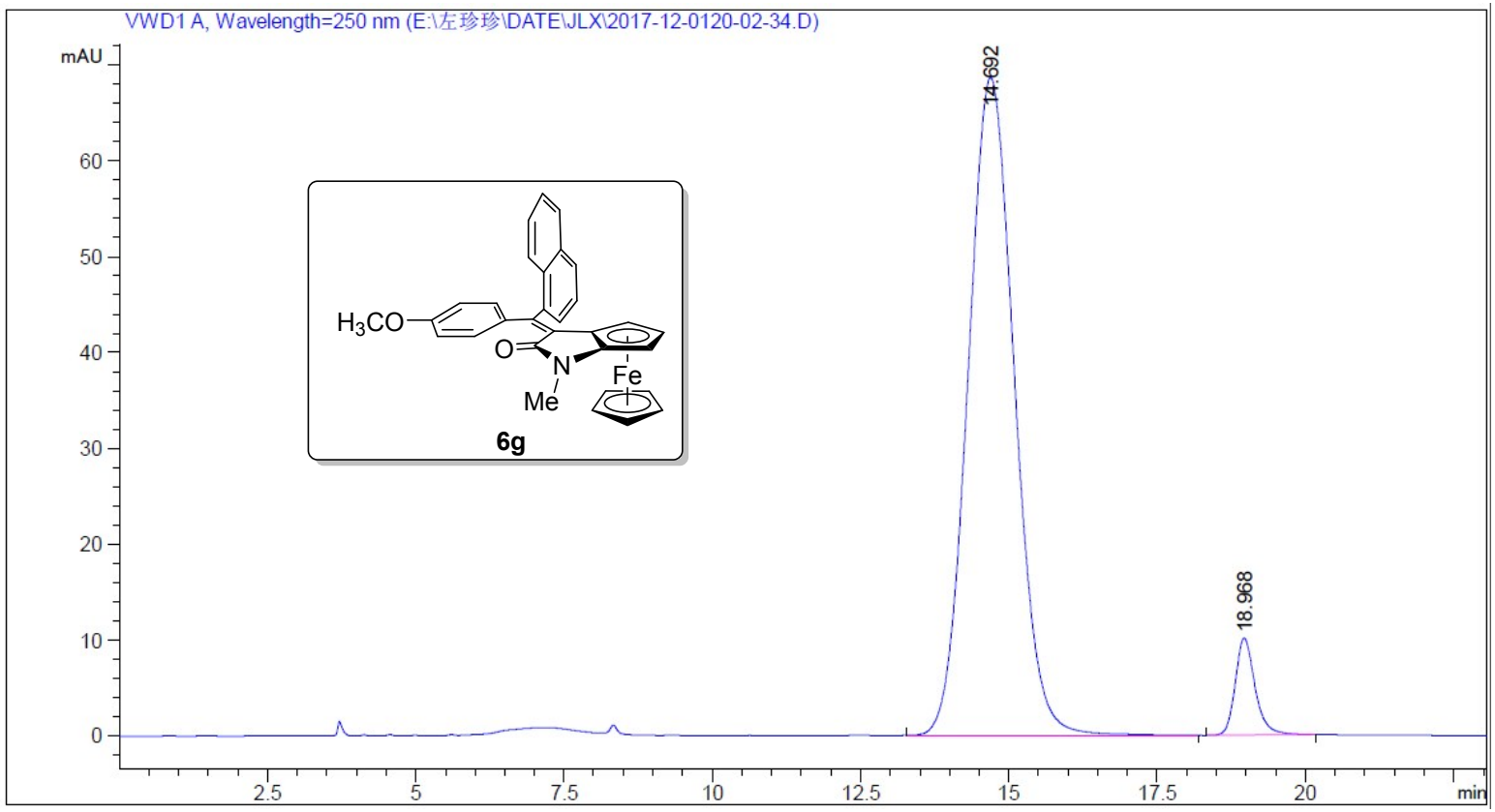

168.68
168.47
158.95
158.90
128.63
128.56
128.53
128.51
128.32
126.58
126.26
126.22
126.18
126.12
125.39
125.27
122.06
115.36
115.28
113.46
113.40
106.17
77.39
77.07
76.75
72.72
72.11
70.22
70.08
64.74
64.39
60.74
60.53
55.23
50.67
27.94
27.81
144.92
144.57
139.99
139.78
139.64
139.51
134.09
133.98
128.63
128.56
128.53
128.51
128.32
126.58
126.22
126.18
126.12
125.39
122.06
122.00
115.36
115.28
113.46
113.36
H3CO
O
N
Me
Fe
6g
142
138
134
130
126
122
118
114
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

Sample Name	Jlx-6i	**Position**	P1-A9	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	Jlx-6i.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	3/20/18 Tue 15:08:08



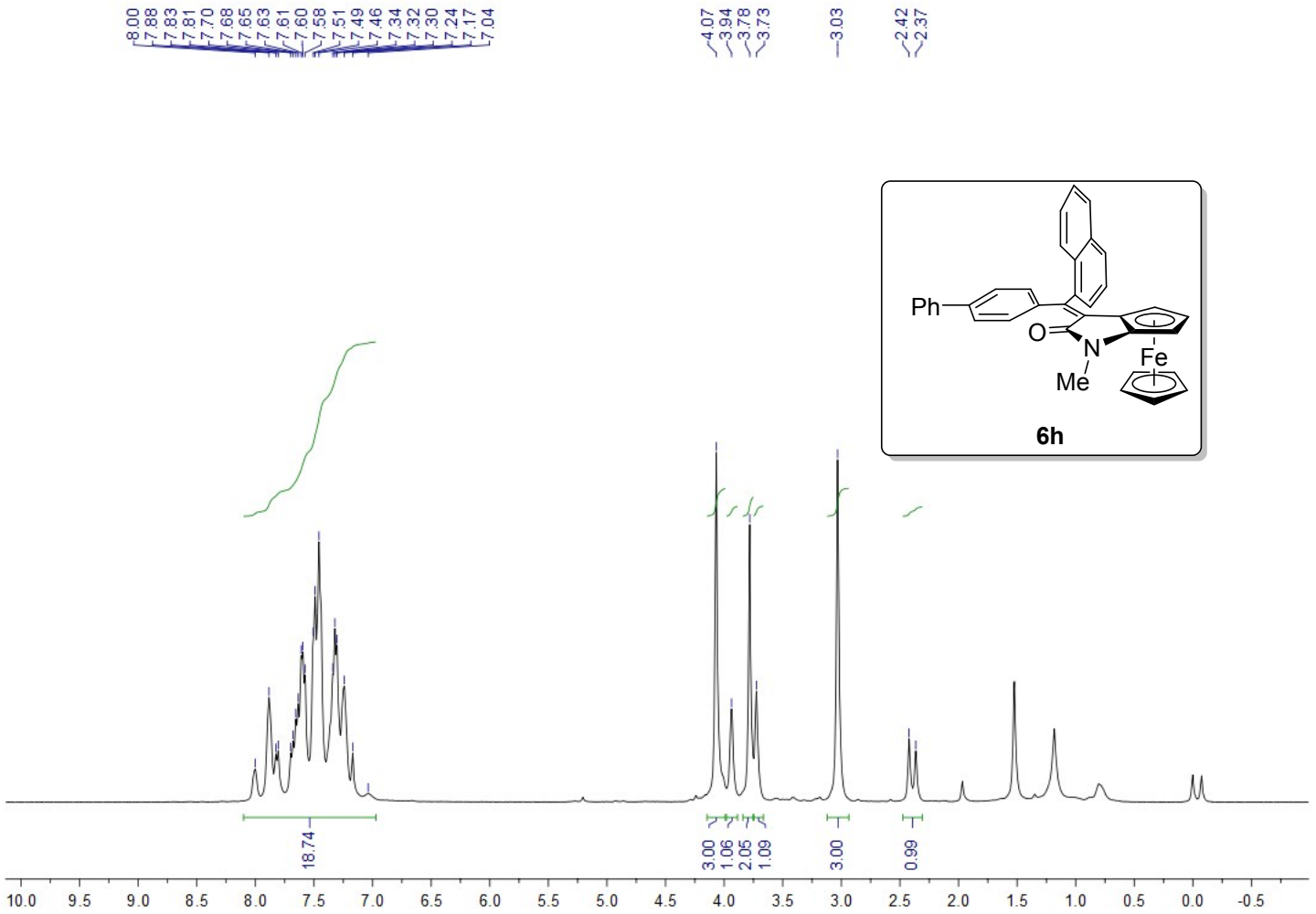


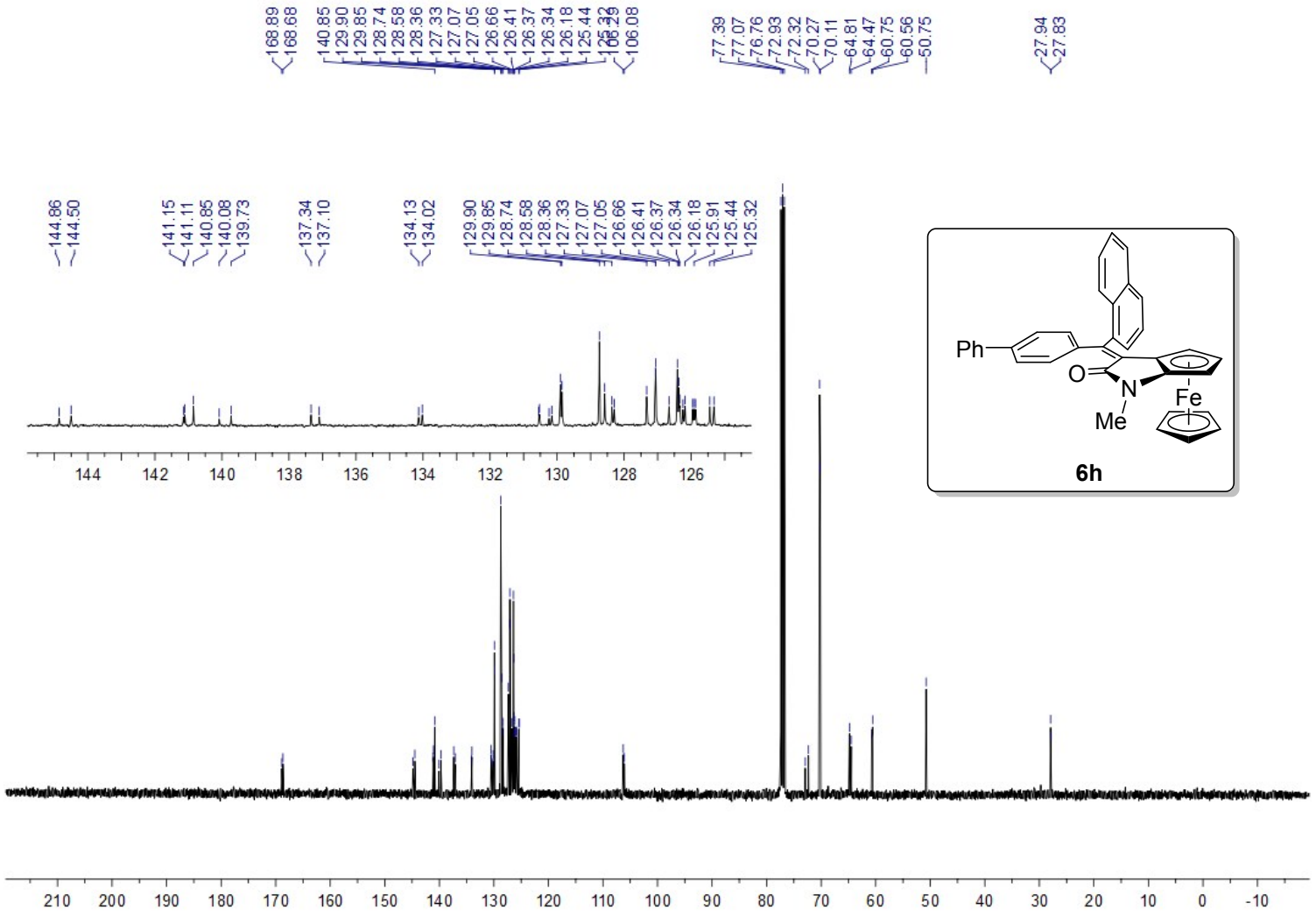
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	14.698	VB	0.8441	3057.01392	56.60234	49.9143
2	18.905	BB	0.3504	3067.51514	132.86098	50.0857



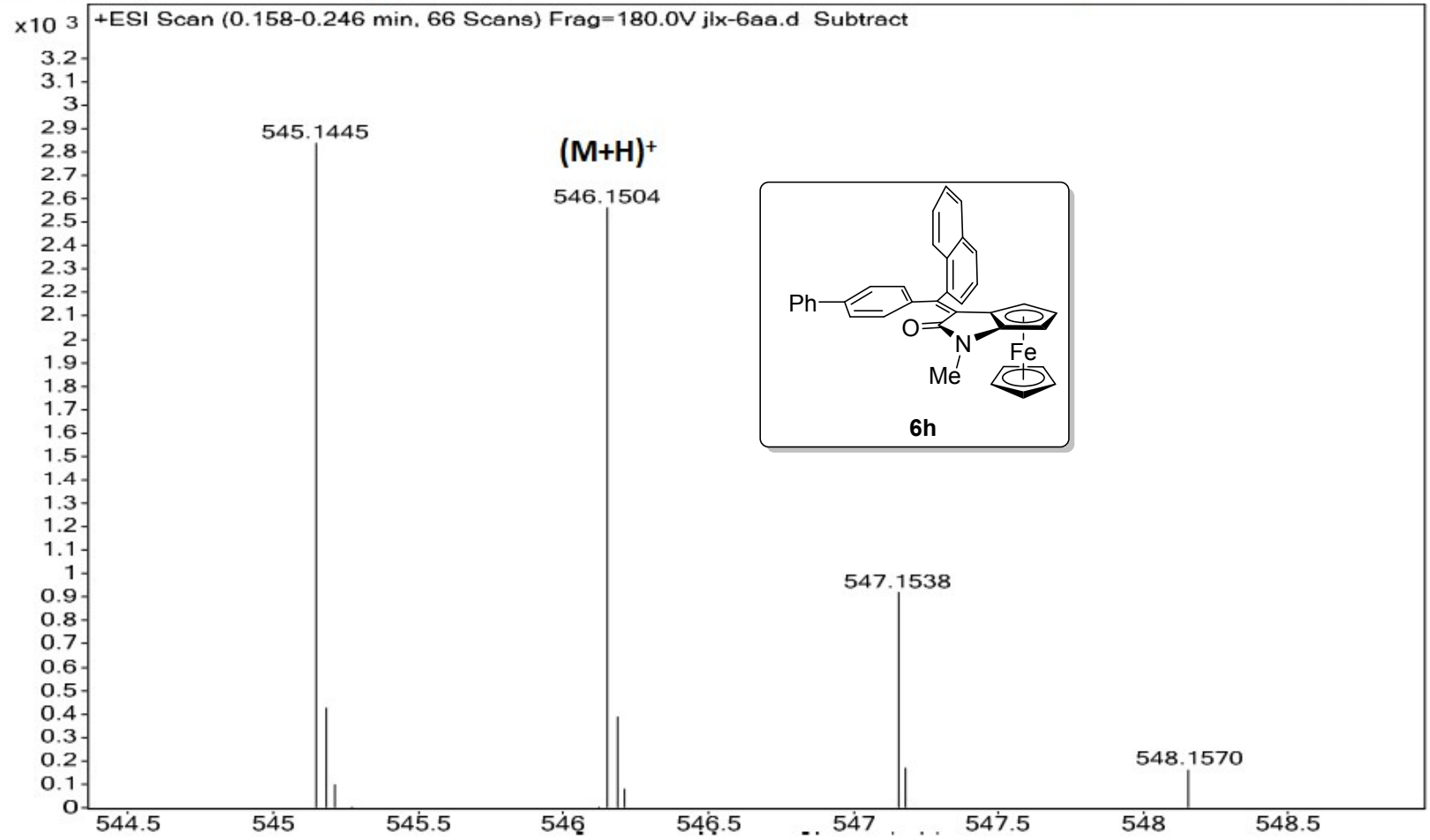
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	14.692	BB	0.8462	3730.11890	68.62302	94.0243
2	18.968	BB	0.3540	237.06908	10.12994	5.9757

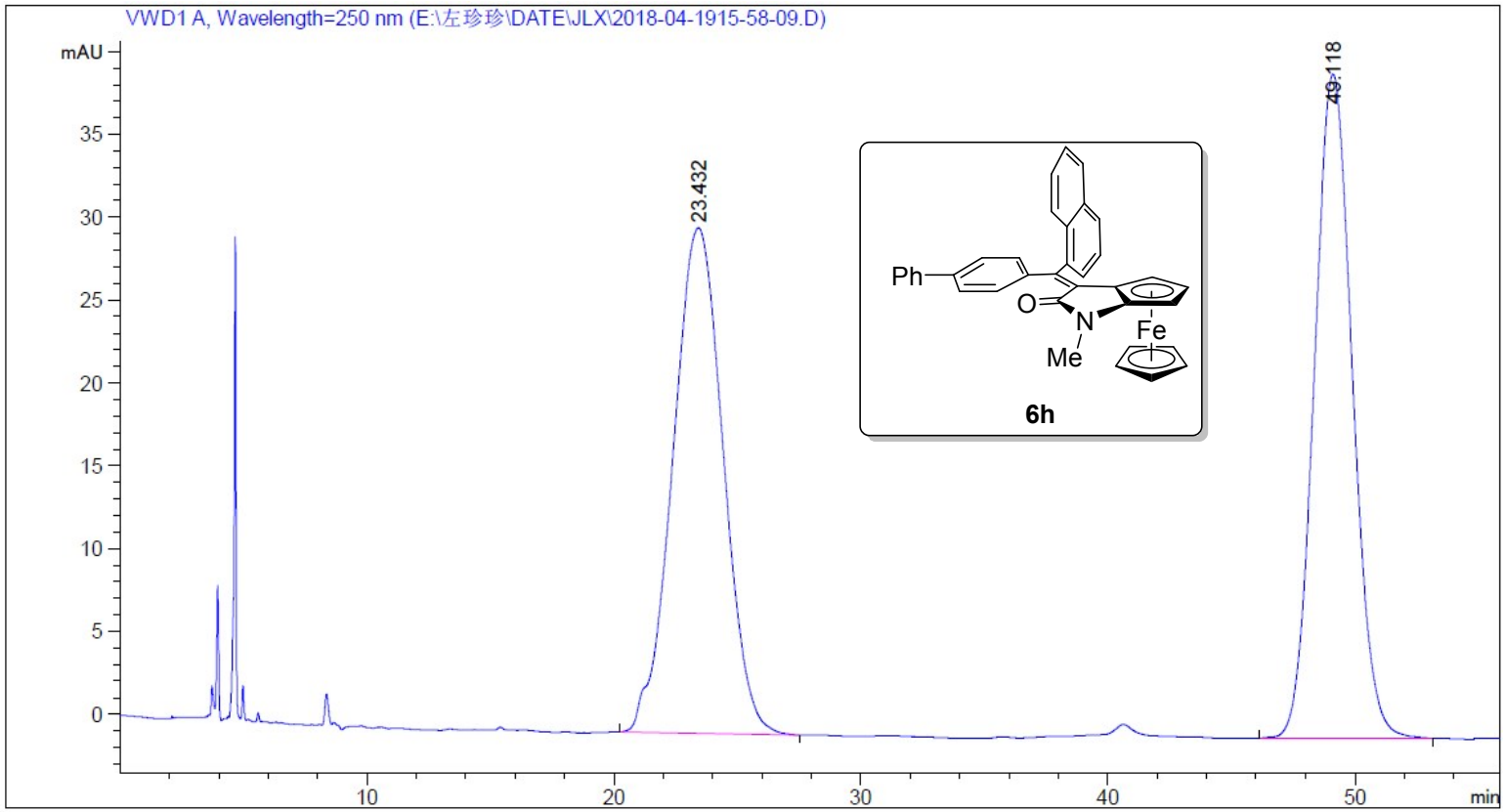
NMR、HMRS Spectra and HPLC Chromatographs of **6h :**



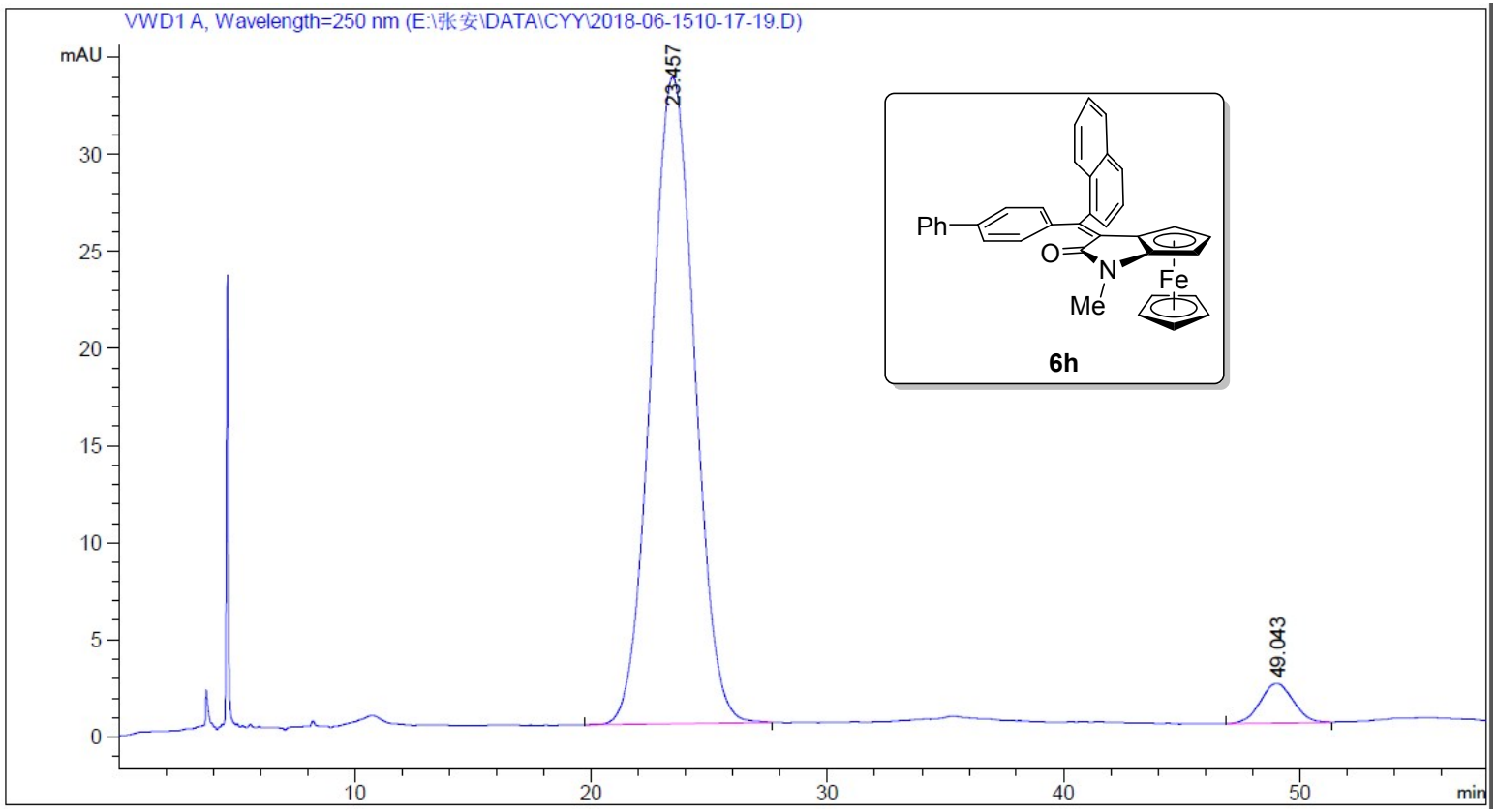

168.89
168.68
140.85
129.90
129.85
128.74
128.58
128.36
127.33
127.07
127.05
126.66
126.41
126.37
126.34
126.18
125.44
106.08
77.39
77.07
76.76
72.93
72.32
70.27
70.11
64.81
64.47
60.75
60.56
50.75
27.94
27.83
144.86
144.50
141.15
141.11
140.85
140.08
139.73
137.34
137.10
134.13
134.02
129.90
129.85
128.74
128.58
128.36
127.33
127.07
127.05
126.66
126.41
126.37
126.34
126.18
125.91
125.44
125.32
144
142
140
138
136
134
132
130
128
126
Ph
O
N
Me
Fe
6h
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

Sample Name	jlx-6aa	**Position**	P1-A3	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
Data Filename	jlx-6aa.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	5/24/18 Thu 10:35:16



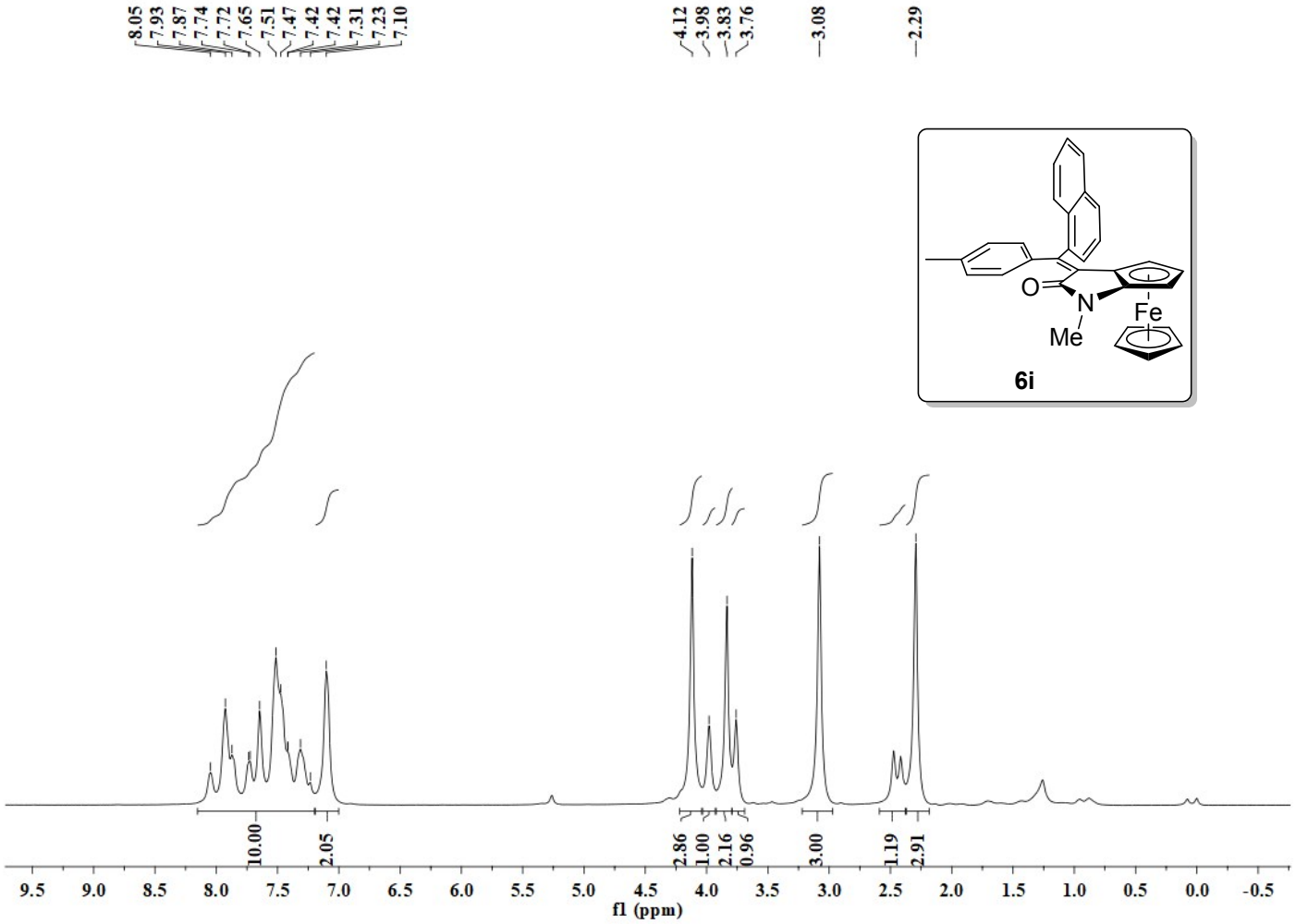


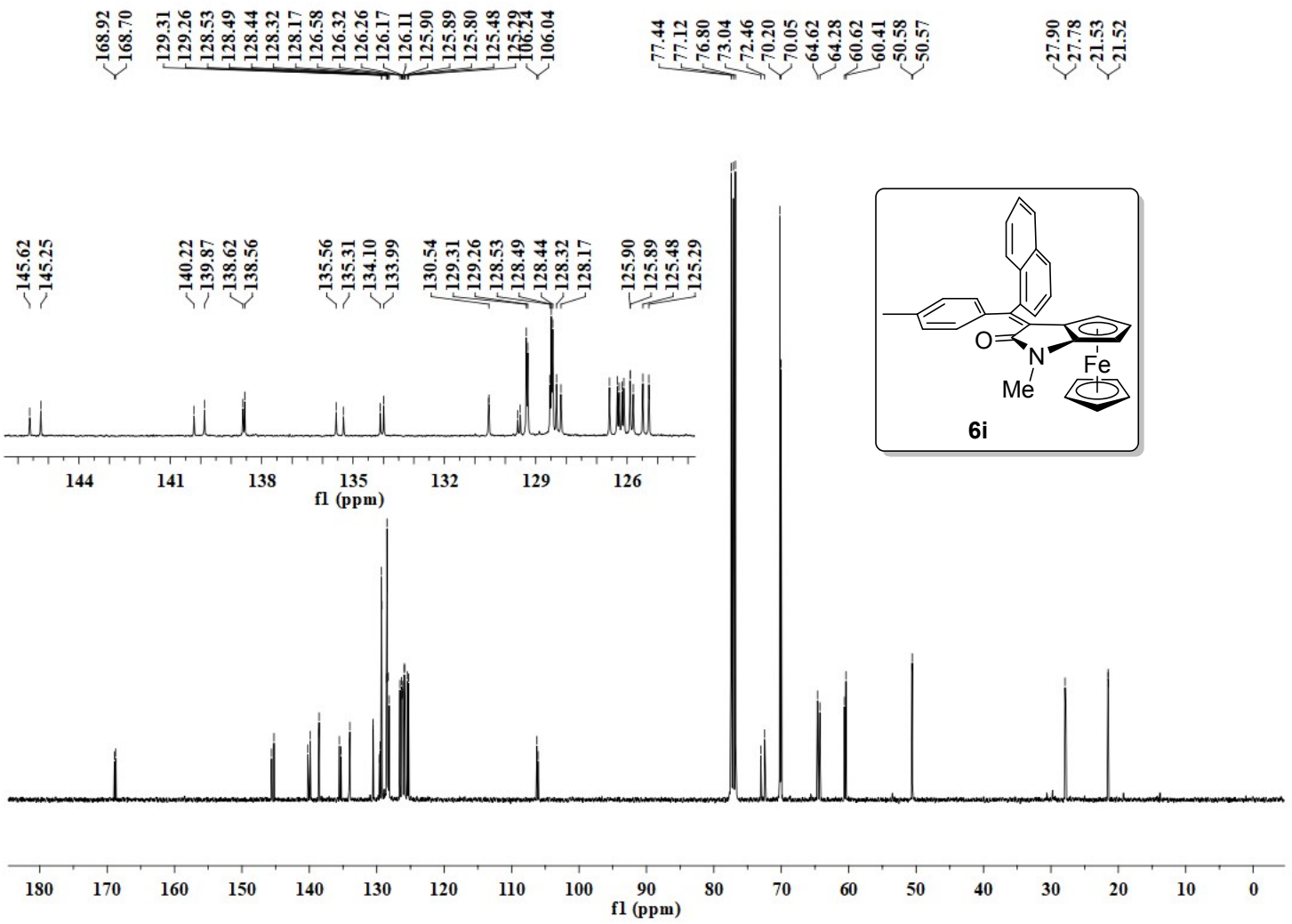
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	23.432	BB	2.1306	4314.40137	30.51306	50.0782
2	49.118	BB	1.6451	4300.92529	40.07438	49.9218



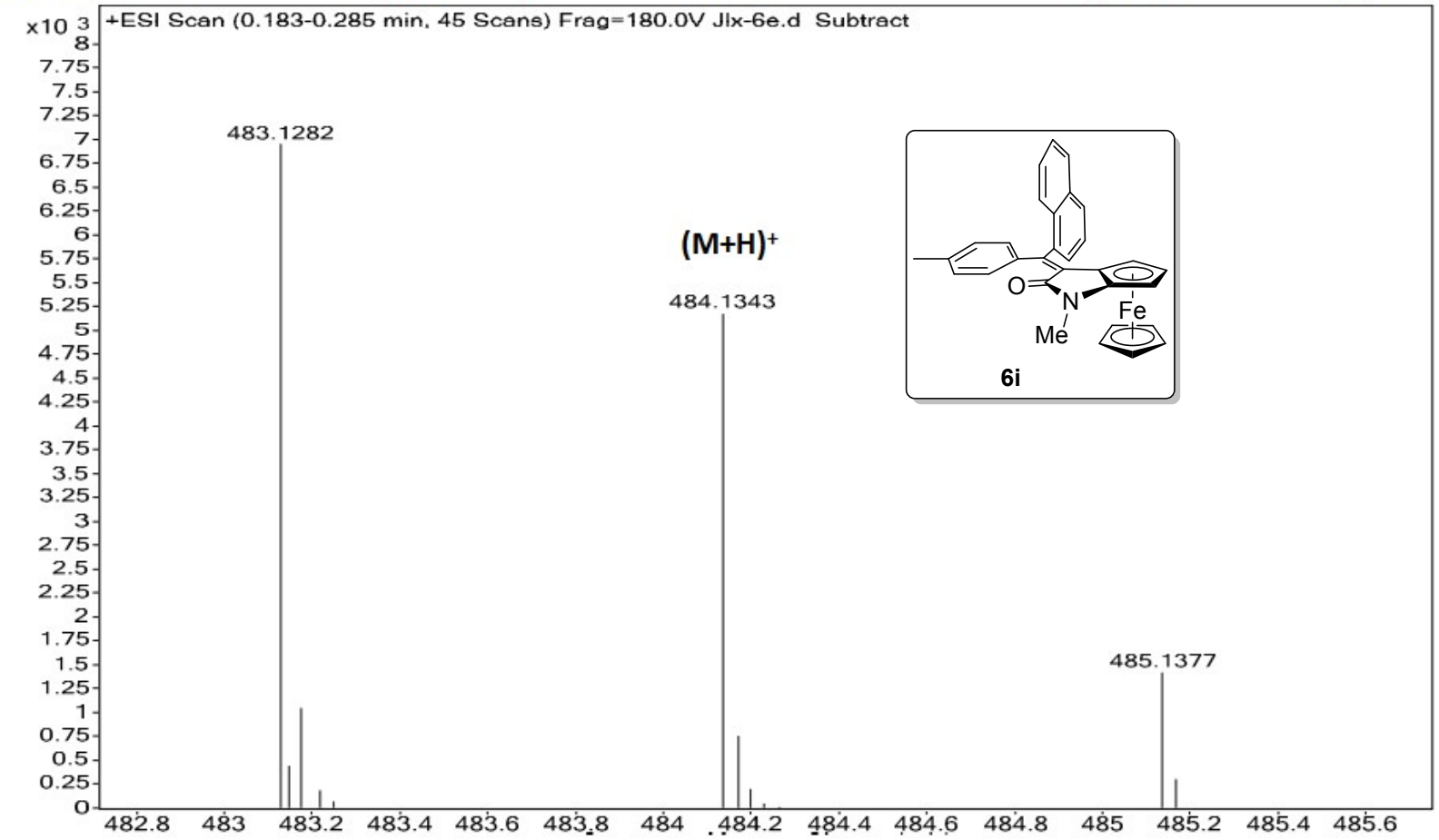
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	23.457	BB	1.9714	4293.48438	33.31906	95.5871
2	49.043	BB	1.2244	198.21378	2.03489	4.4129

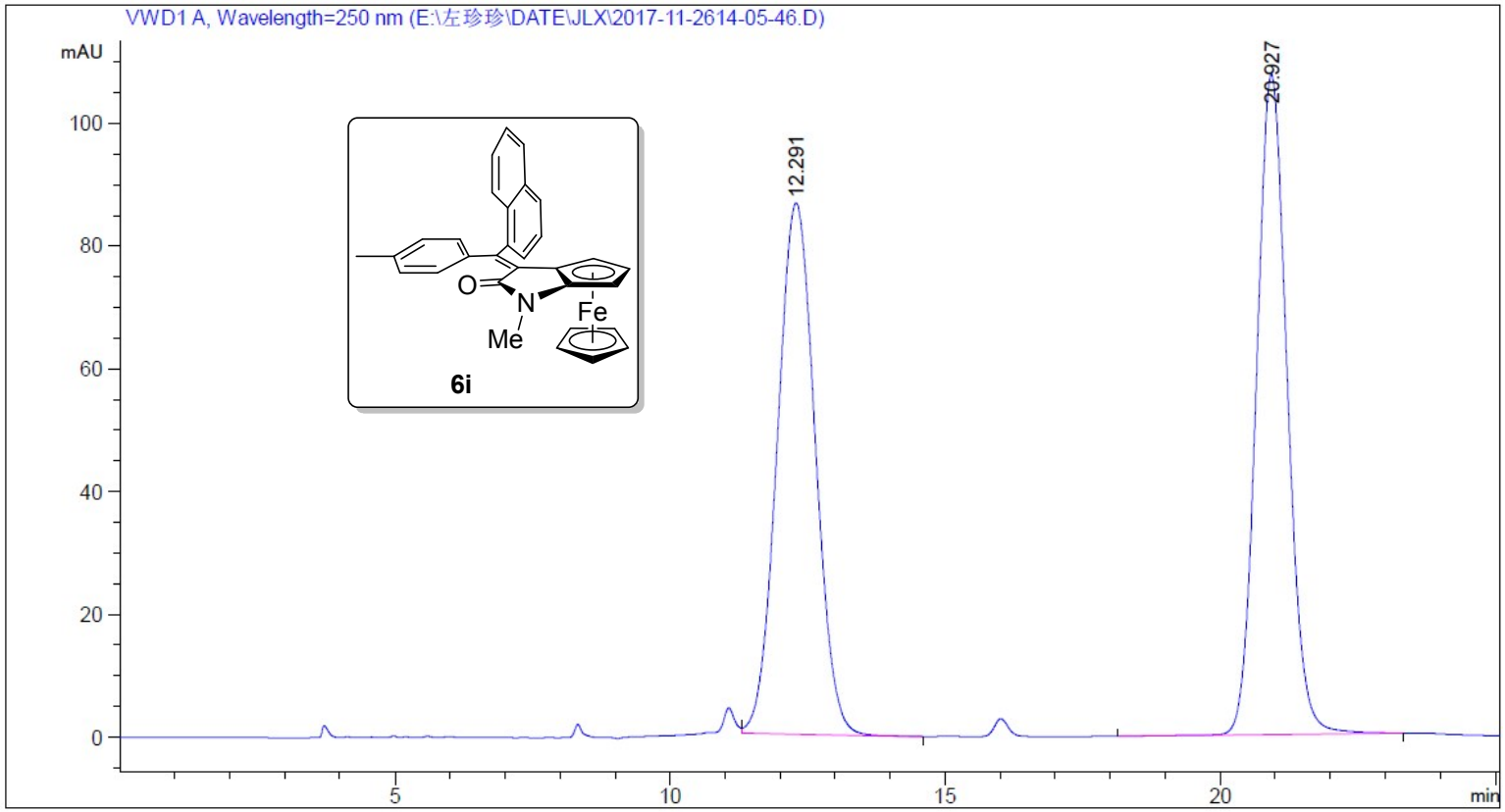
NMR、HMRS Spectra and HPLC Chromatographs of **6i :**



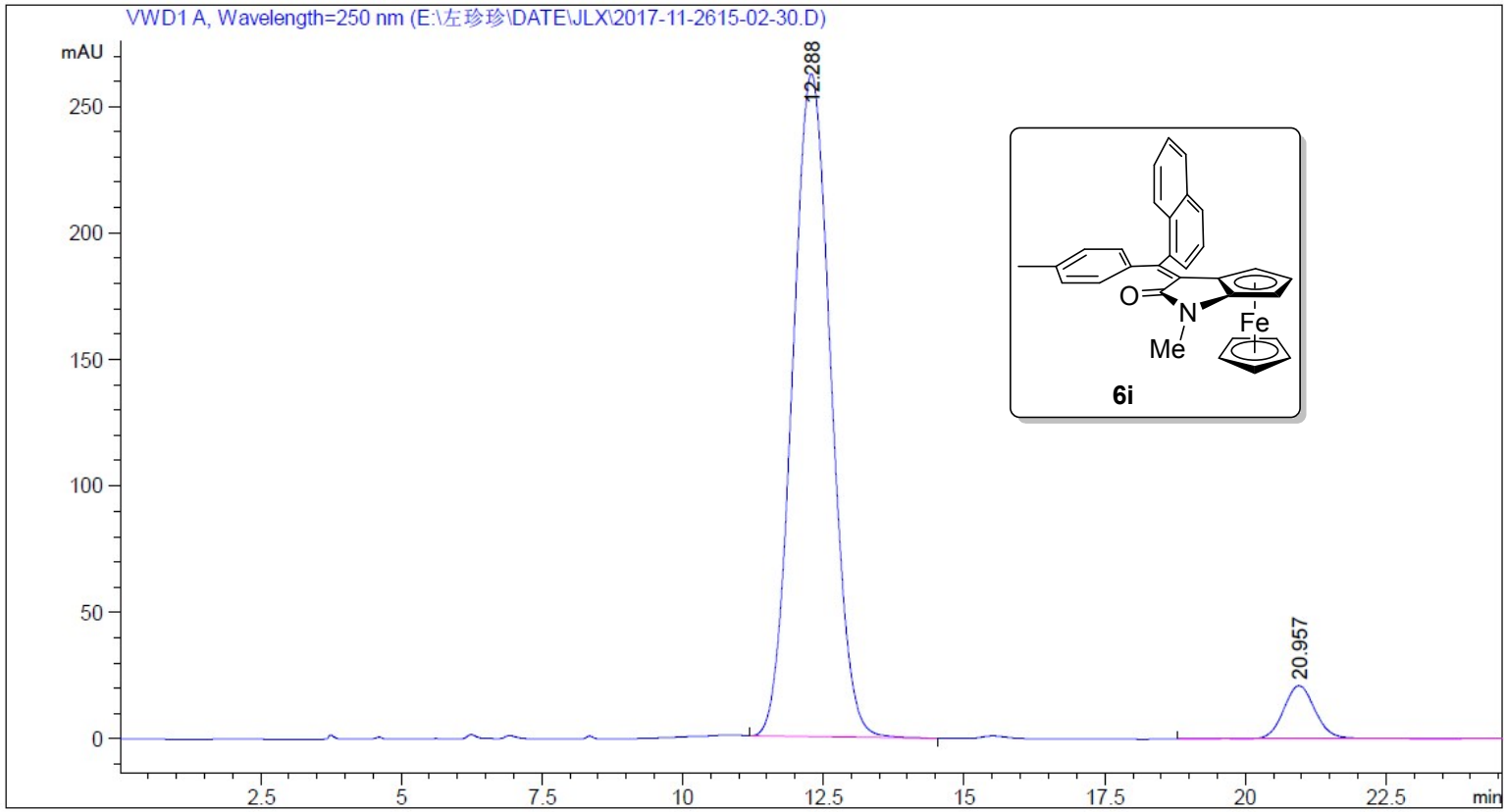

168.92
168.70
129.31
129.26
128.53
128.49
128.44
128.32
128.17
126.58
126.32
126.26
126.17
126.11
125.90
125.89
125.80
125.48
125.29
106.24
106.04
77.44
77.12
76.80
73.04
72.46
70.20
70.05
64.62
64.28
60.62
60.41
50.58
50.57
27.90
27.78
21.53
21.52
145.62
145.25
140.22
139.87
138.62
138.56
135.56
135.31
134.10
133.99
130.54
129.31
129.26
128.53
128.49
128.44
128.32
128.17
125.90
125.89
125.48
125.29
144
141
138
135
132
129
126
f1 (ppm)
O
N
Me
Fe
6i
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

Sample Name	Jlx-6e	**Position**	P1-A5	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	Jlx-6e.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	3/20/18 Tue 15:03:04



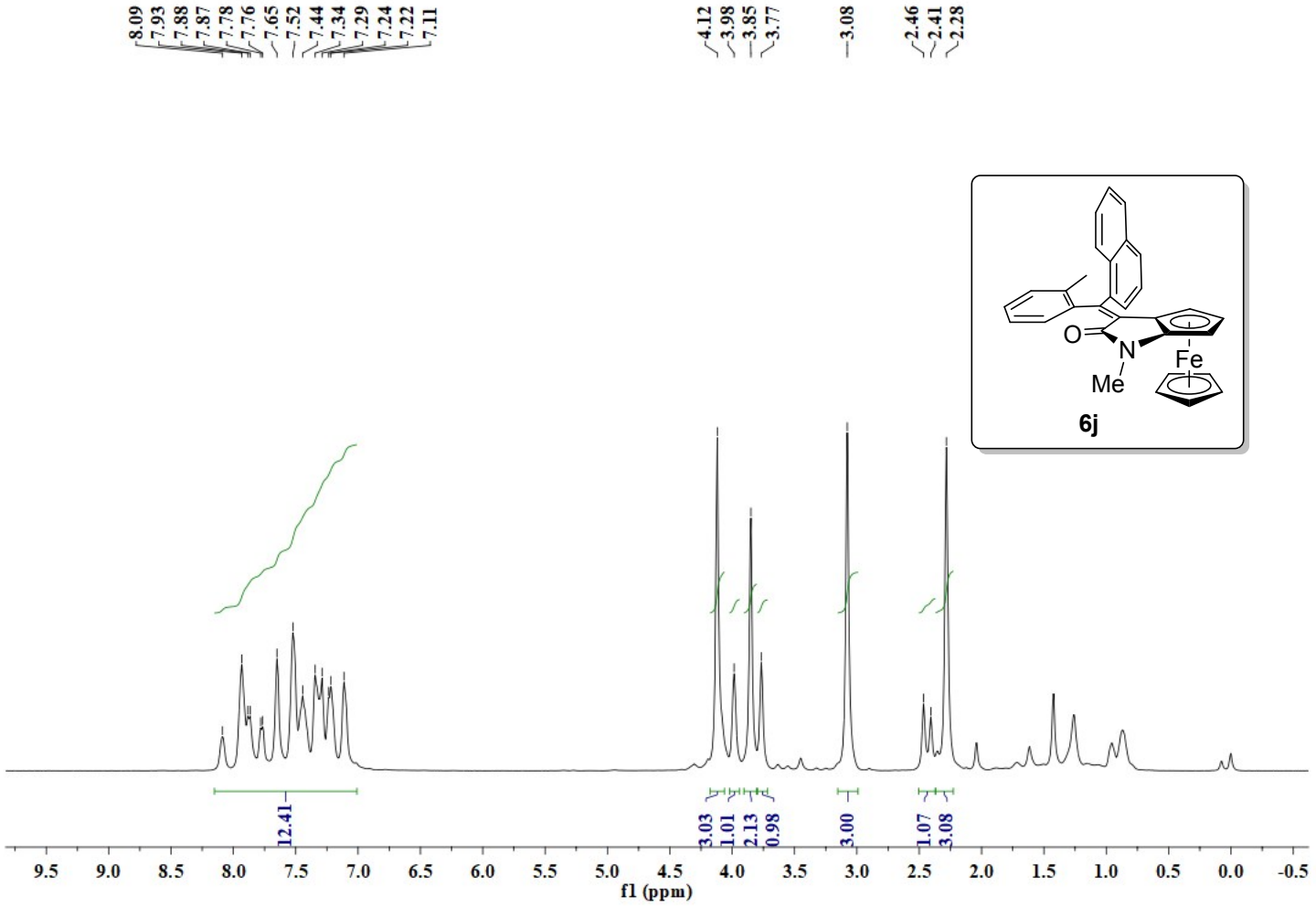


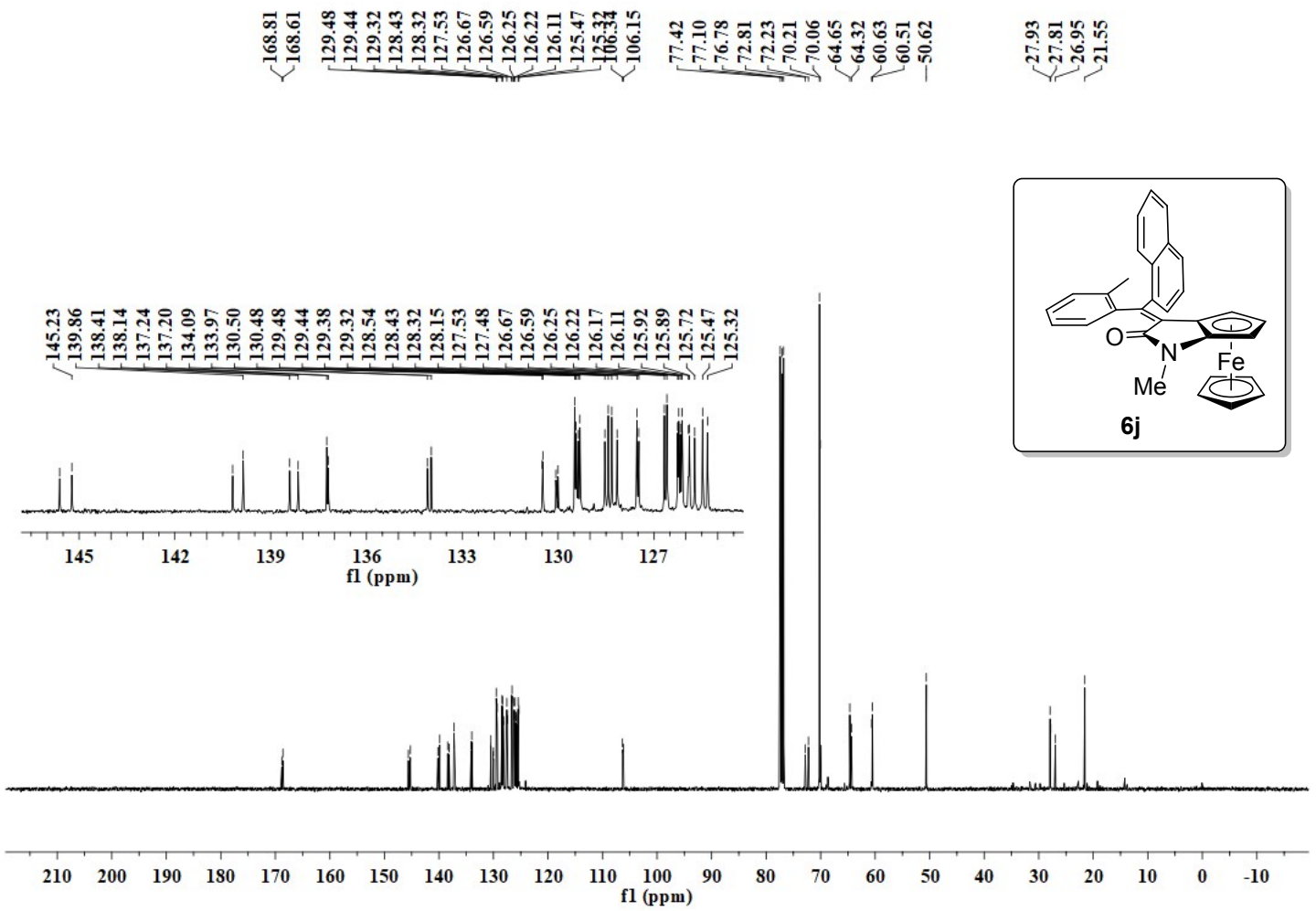
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.291	VB	0.7480	4133.82617	86.43540	49.7682
2	20.927	BB	0.6009	4172.34180	107.47616	50.2318



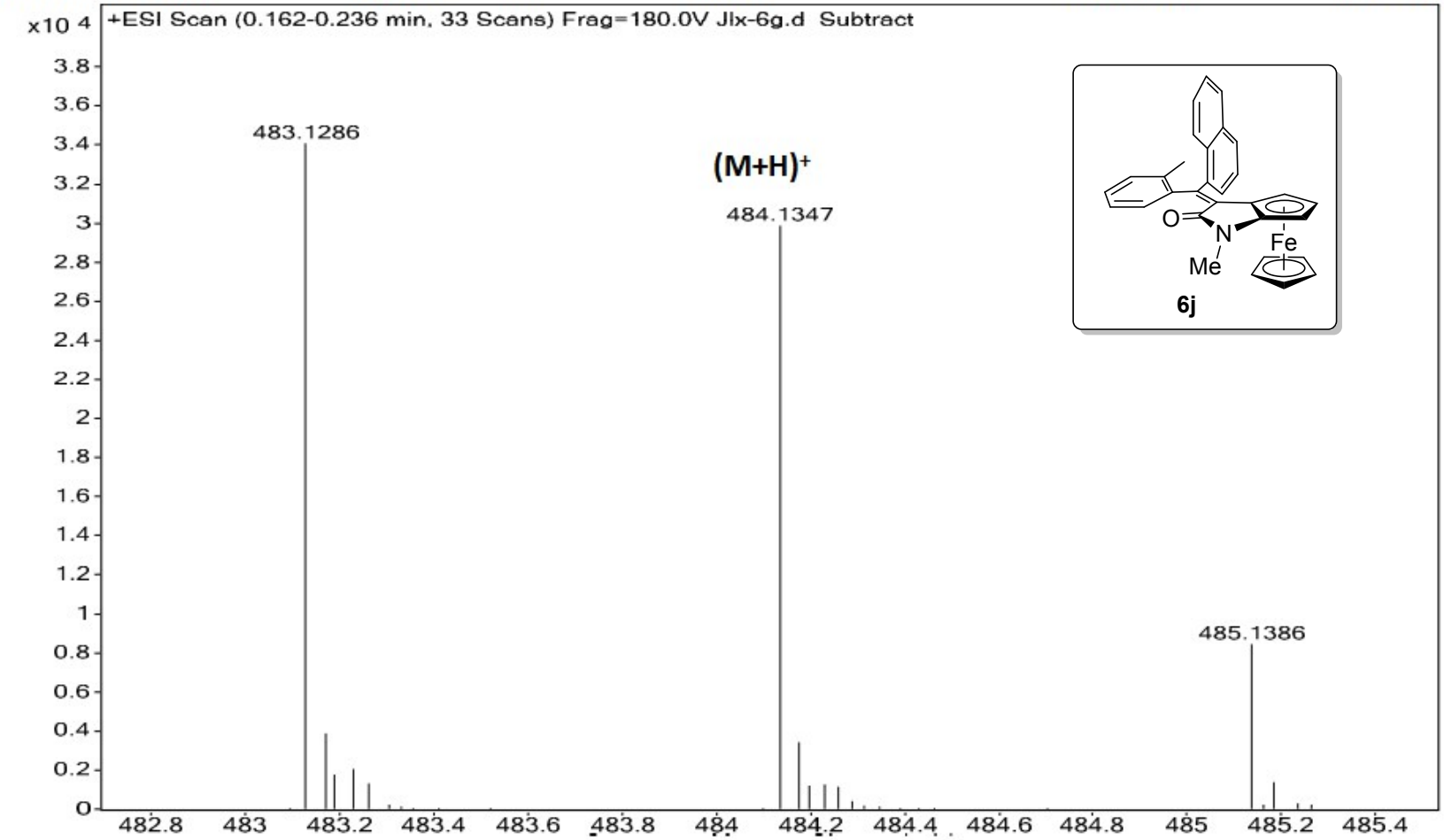
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.288	BB	0.7414	1.23790e4	261.92545	93.5001
2	20.957	BBA	0.6251	860.56354	21.13221	6.4999

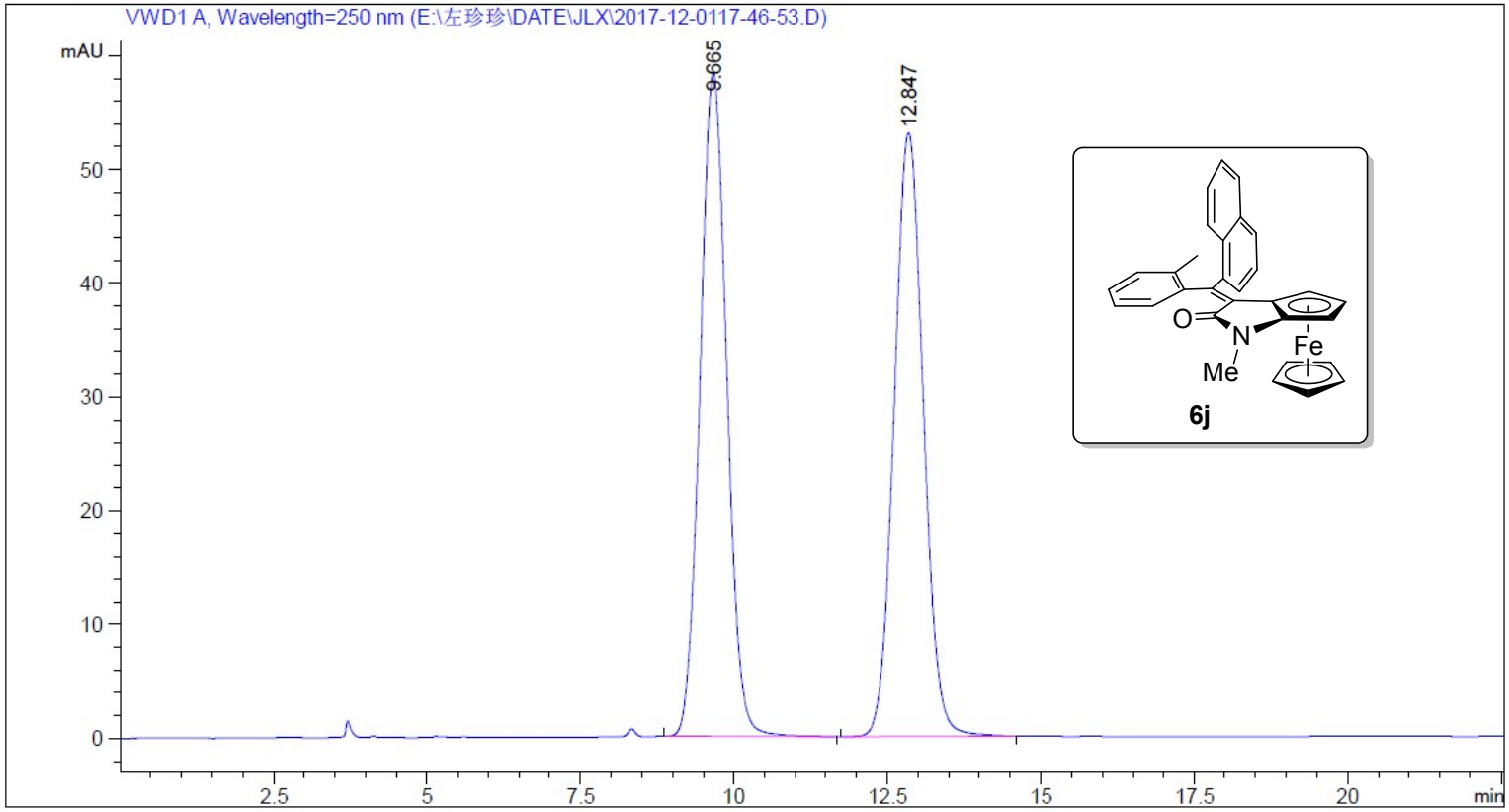
NMR、HMRS Spectra and HPLC Chromatographs of **6j :**



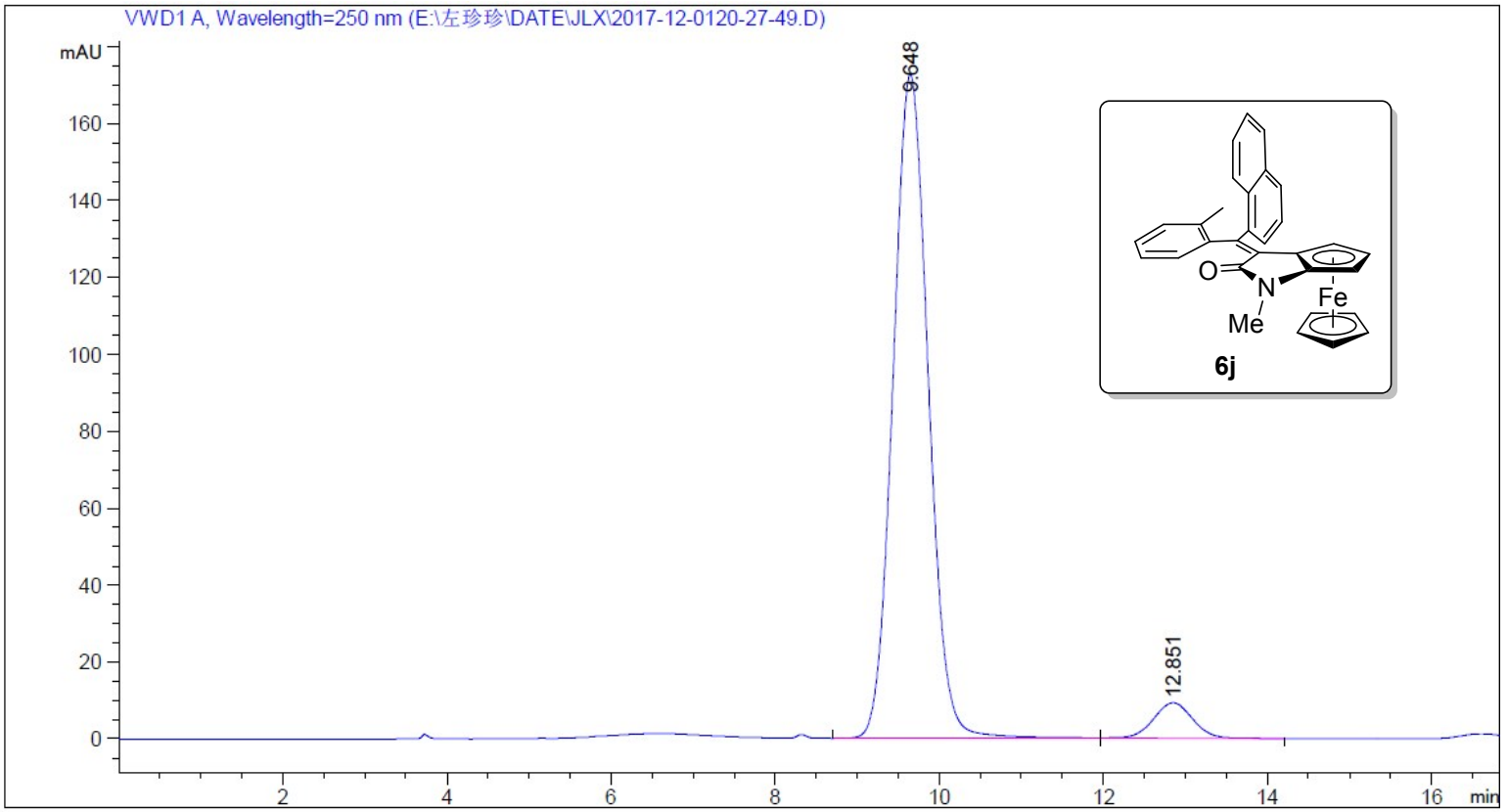

168.81
168.61
129.48
129.44
129.32
128.43
128.32
127.53
126.67
126.59
126.25
126.22
126.11
125.47
125.32
106.34
106.15
77.42
77.10
76.78
72.81
72.23
70.21
70.06
64.65
64.32
60.63
60.51
50.62
27.93
27.81
26.95
21.55
145.23
139.86
138.41
138.14
137.24
137.20
134.09
133.97
130.50
130.48
129.48
129.44
129.38
129.32
128.54
128.43
128.32
128.15
127.53
127.48
126.67
126.59
126.25
126.22
126.17
126.11
125.92
125.89
125.72
125.47
125.32
145
142
139
136
133
130
127
f1 (ppm)
O
N
Me
Fe
6j
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

Sample Name	Jlx-6g	**Position**	P1-A7	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	Jlx-6g.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	3/20/18 Tue 15:05:37



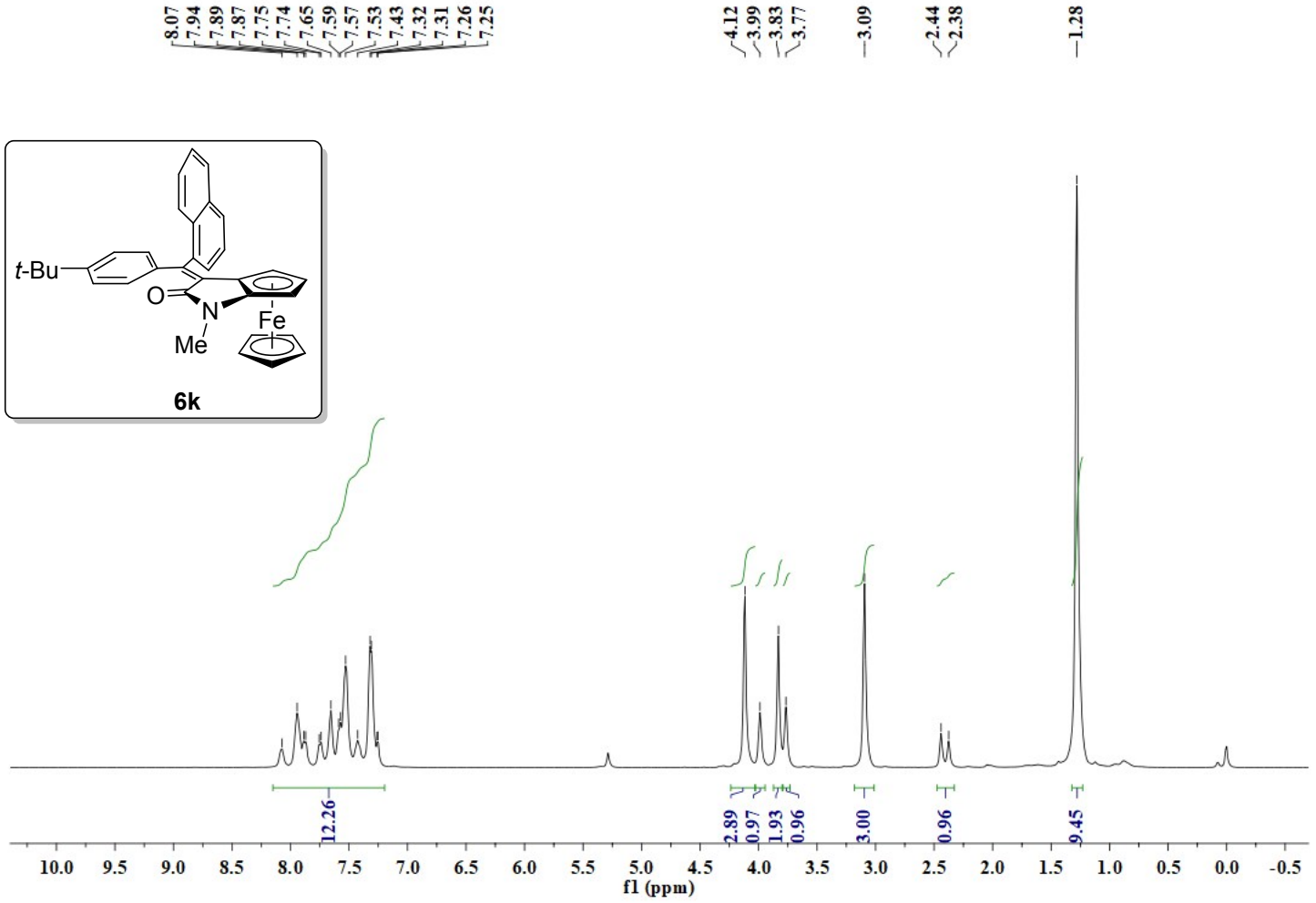


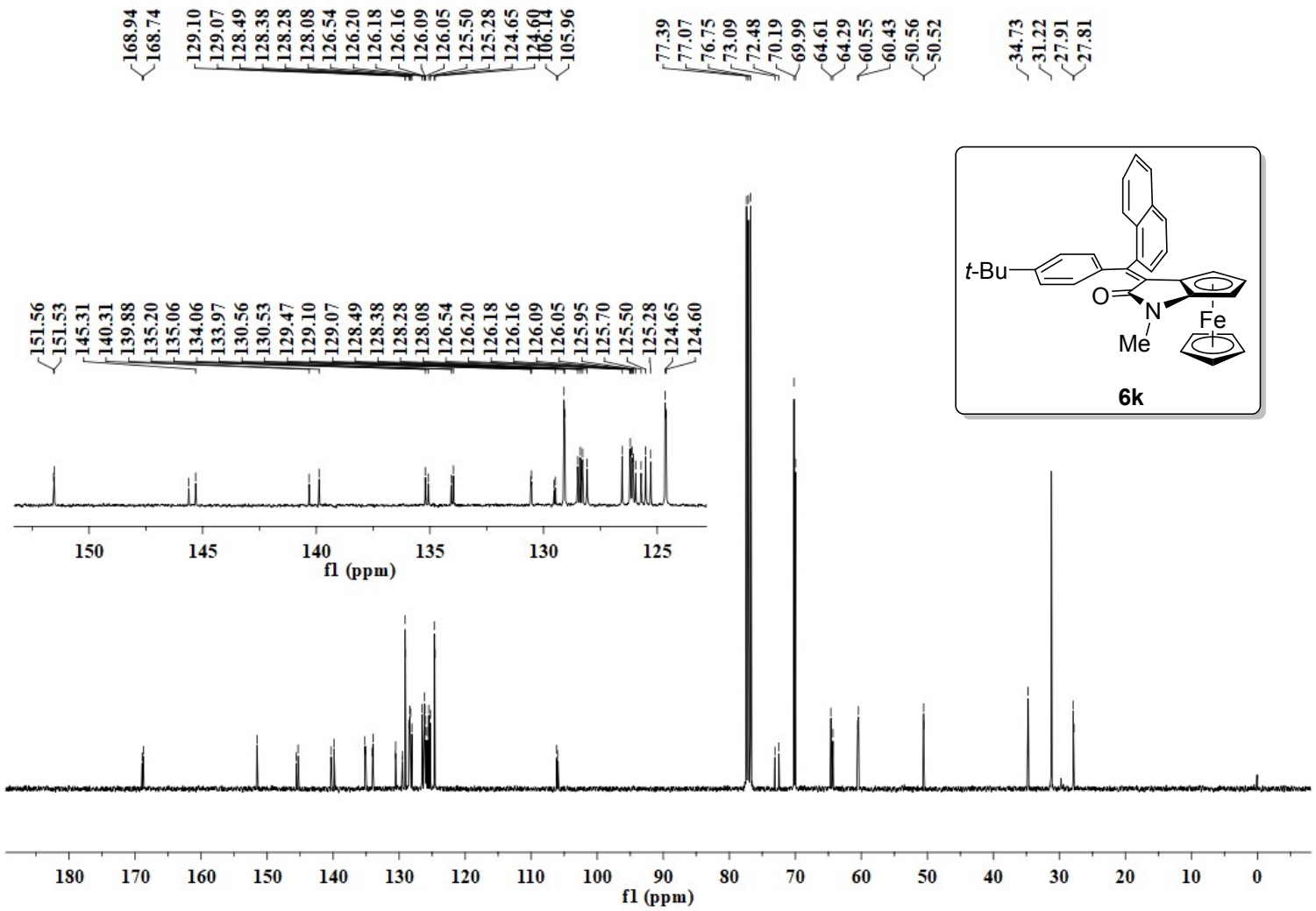
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.665	BB	0.4699	1758.64221	58.31021	49.9976
2	12.847	BB	0.5147	1758.81213	53.05725	50.0024



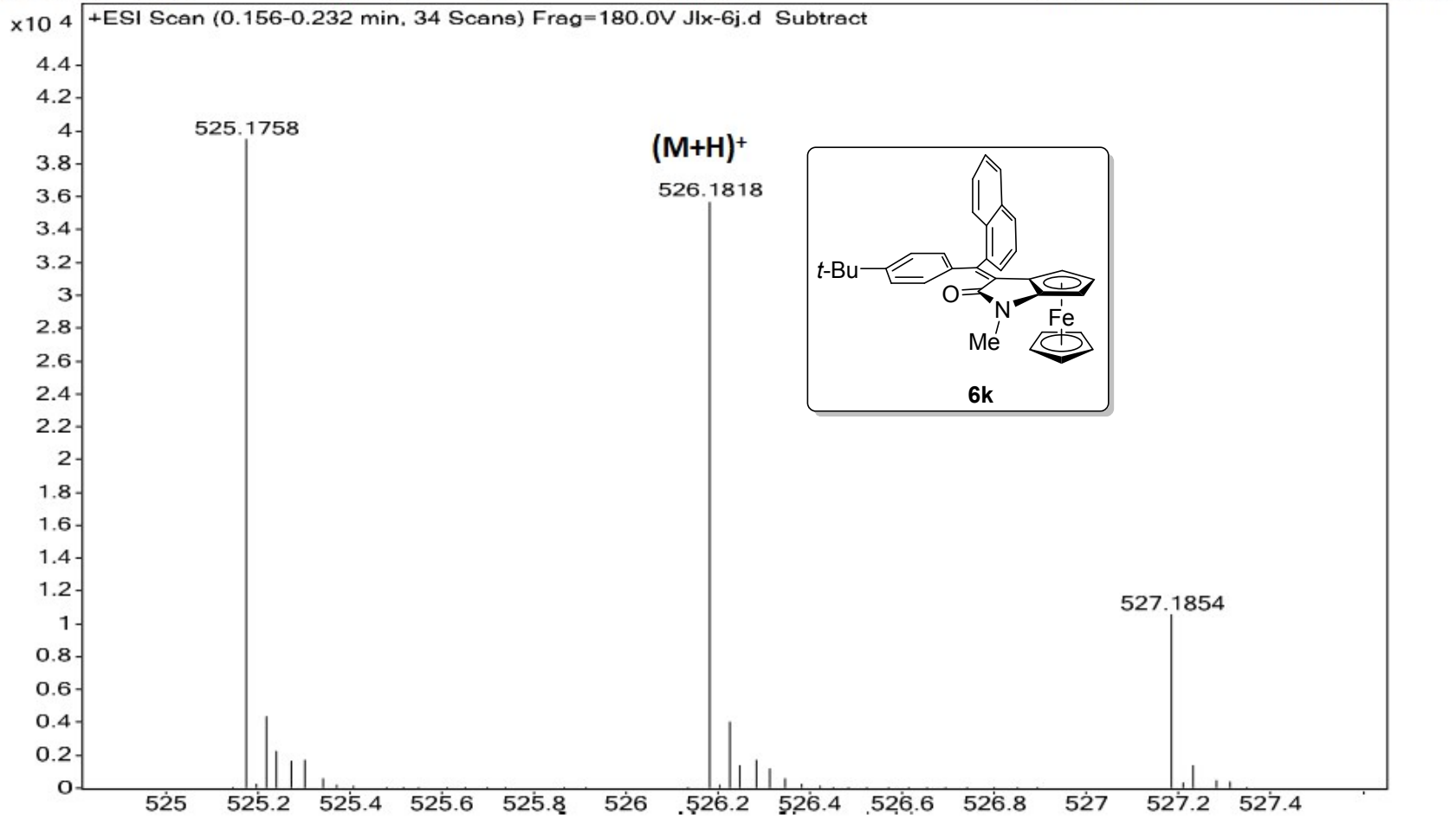
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.648	BB	0.4630	5136.25977	172.68881	94.4959
2	12.851	BB	0.5125	299.17340	9.12583	5.5041

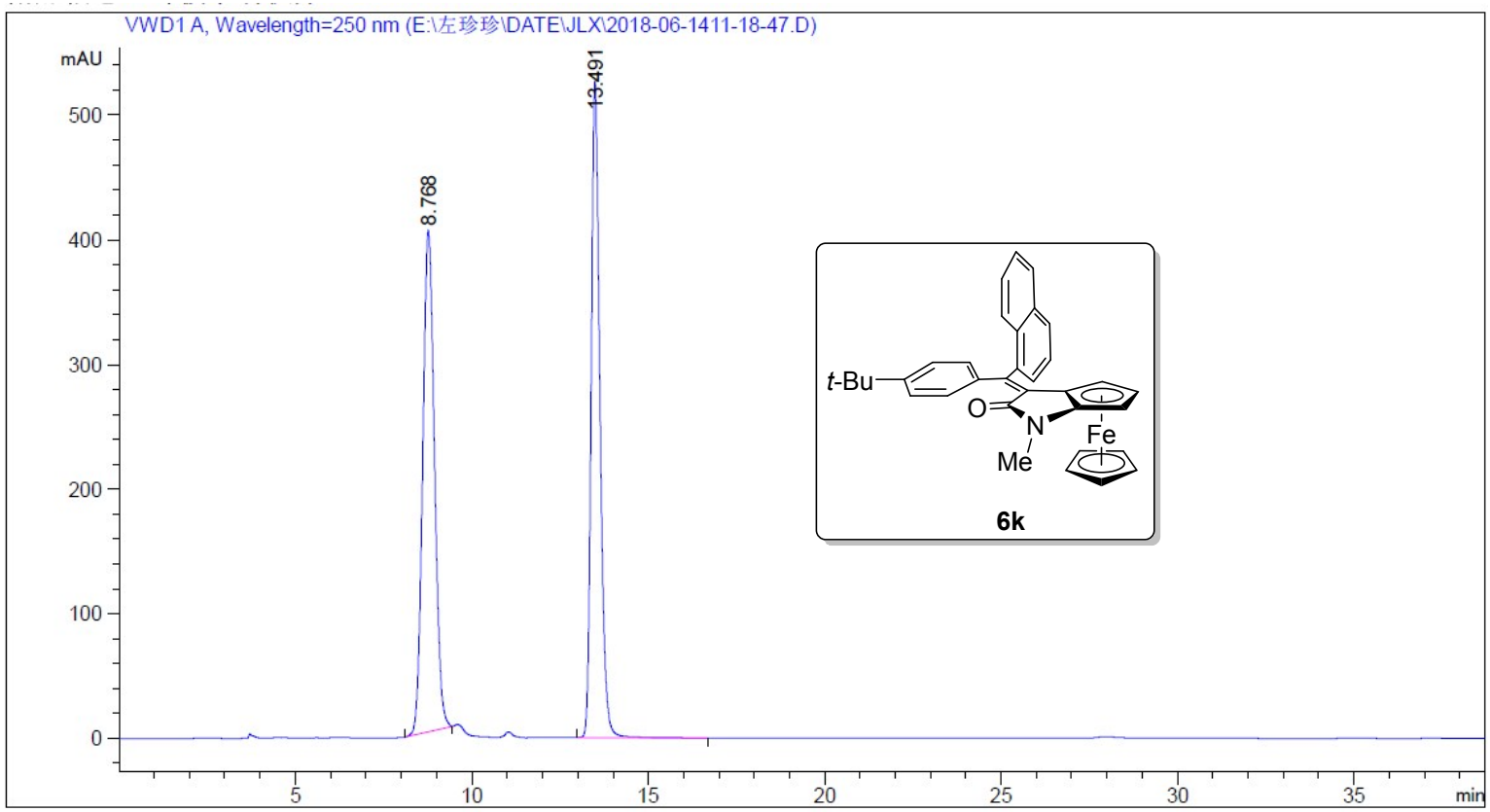
NMR、HMRS Spectra and HPLC Chromatographsof **6k :**



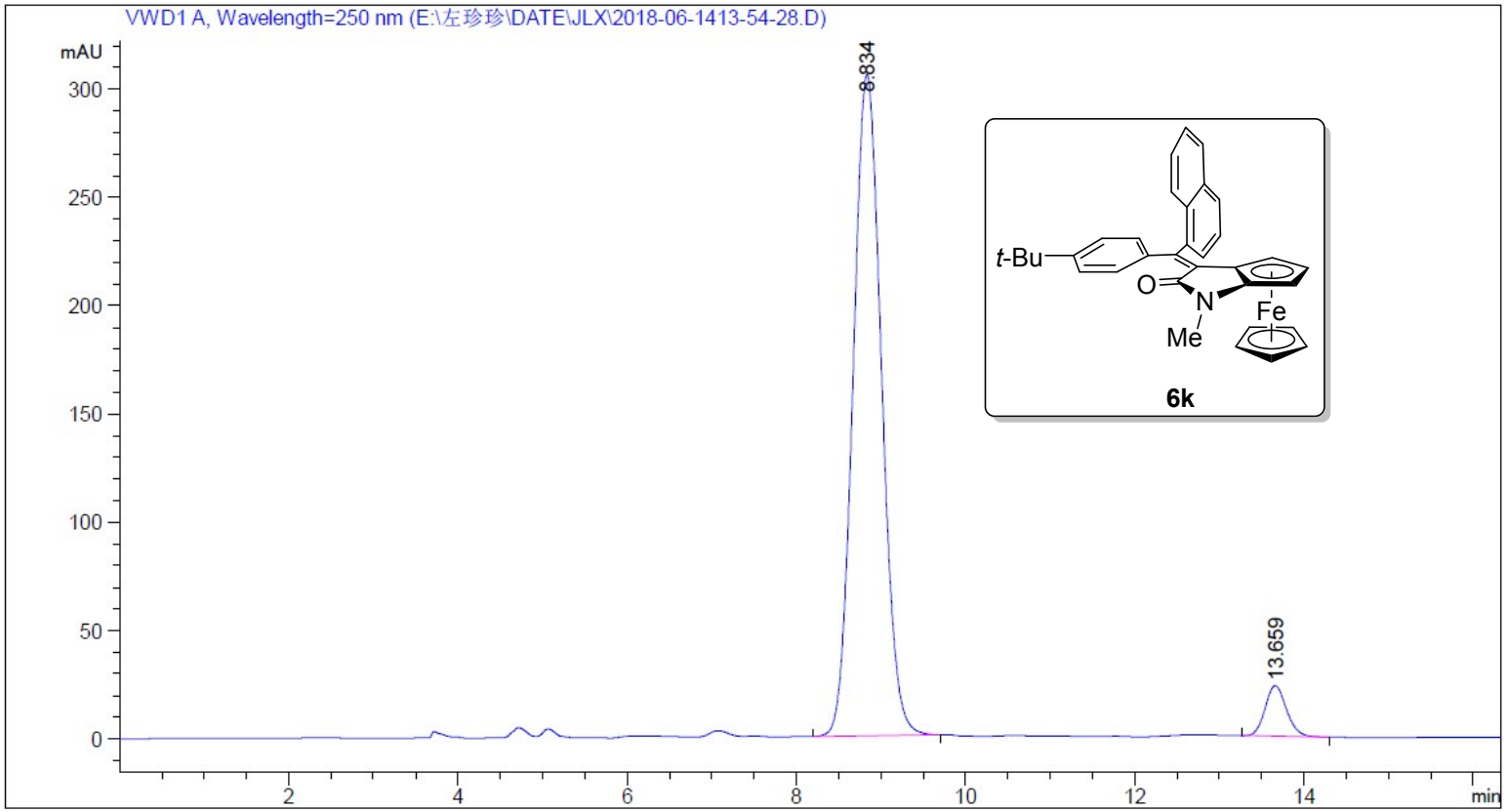

168.94
168.74
129.10
129.07
128.49
128.38
128.28
128.08
126.54
126.20
126.18
126.16
126.09
126.05
125.50
125.28
124.65
124.60
106.14
105.96
77.39
77.07
76.75
73.09
72.48
70.19
69.99
64.61
64.29
60.55
60.43
50.56
50.52
34.73
31.22
27.91
27.81
151.56
151.53
145.31
140.31
139.88
135.20
135.06
134.06
133.97
130.56
130.53
129.47
129.10
129.07
128.49
128.38
128.28
128.08
126.54
126.20
126.18
126.16
126.09
126.05
125.95
125.70
125.50
125.28
124.65
124.60
150
145
140
135
130
125
f1 (ppm)
t-Bu
O
N
Me
Fe
6k
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

Sample Name	Jlx-6j	**Position**	P1-B1	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	Jlx-6j.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	3/20/18 Tue 15:09:24



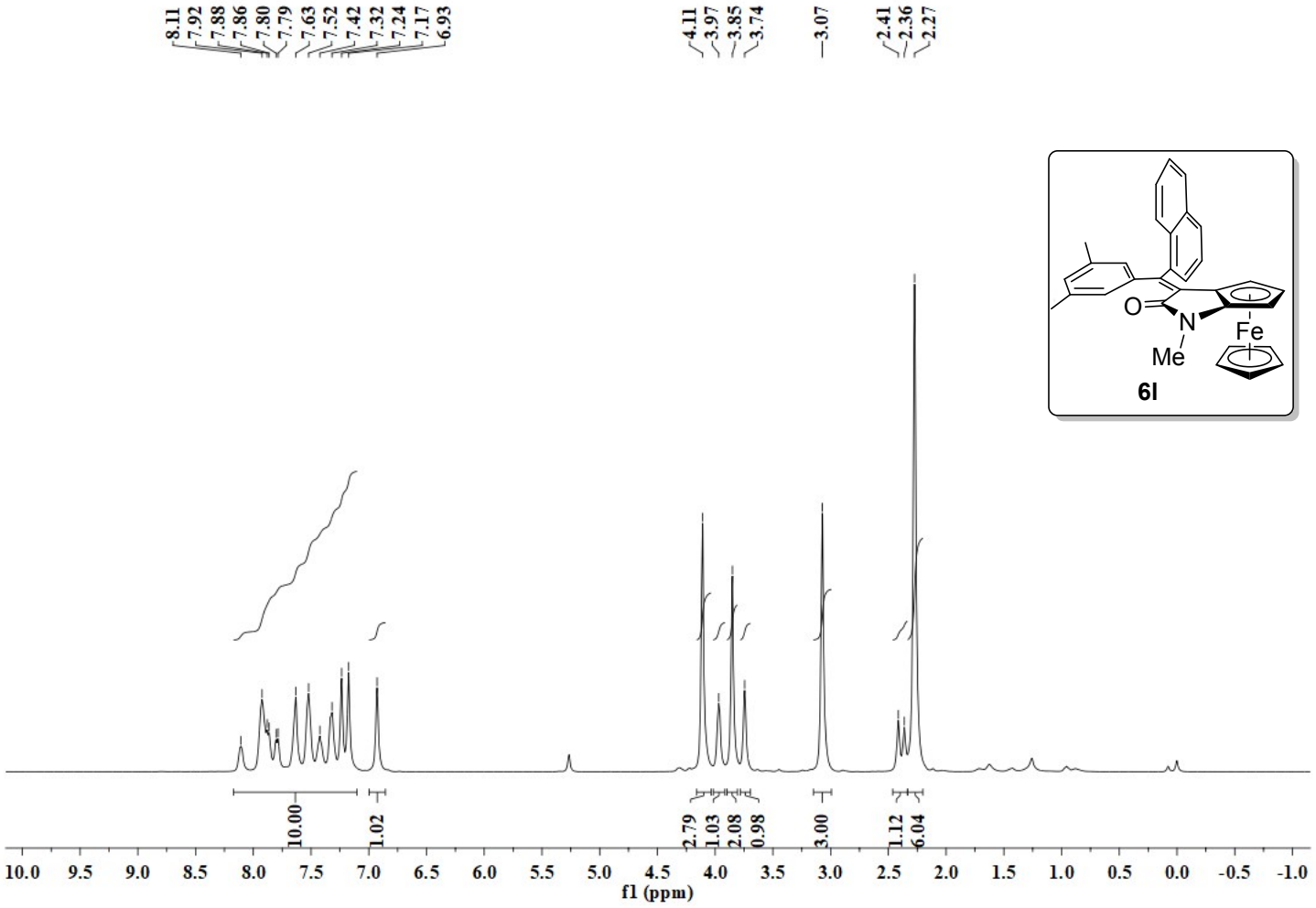


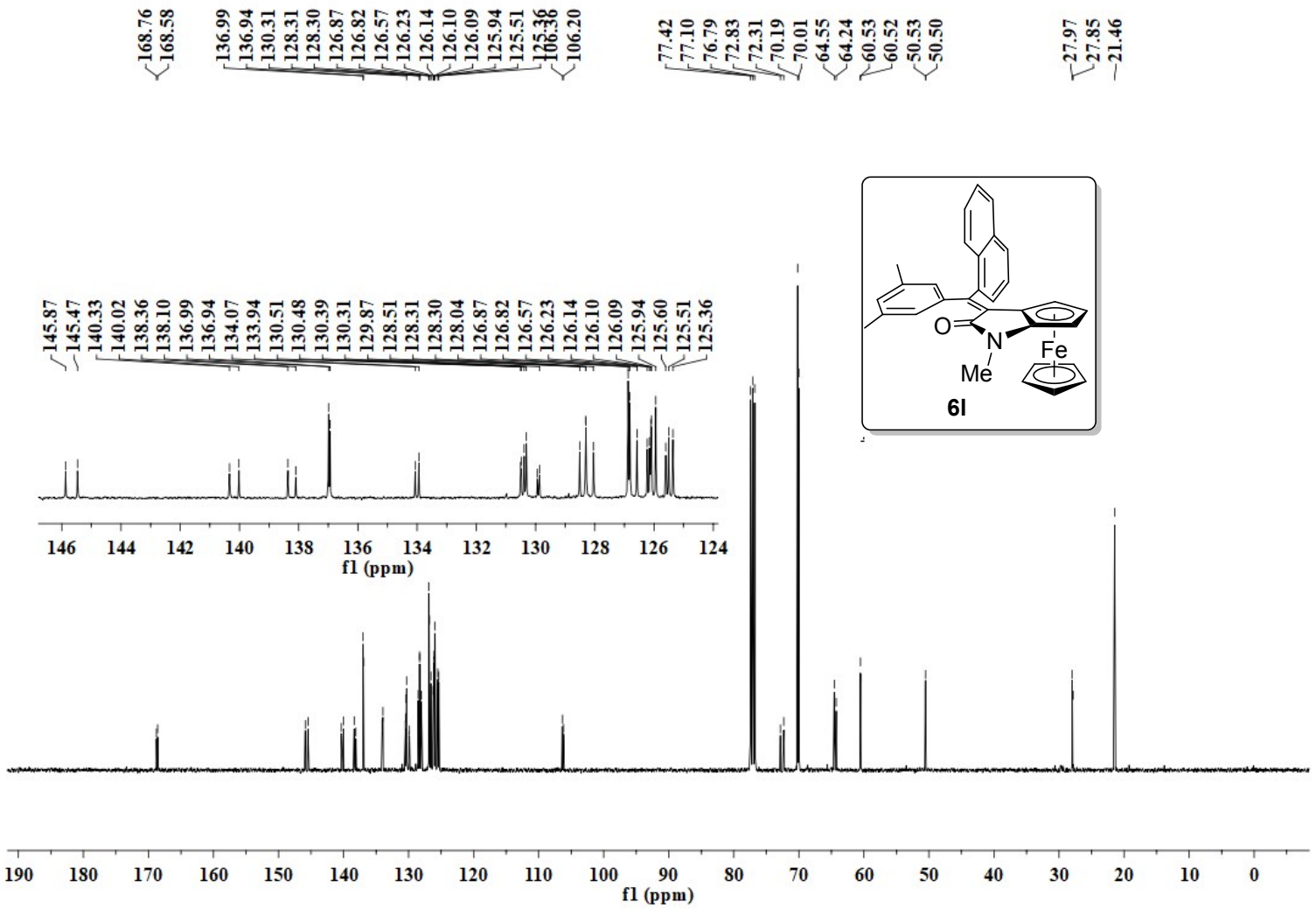
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	8.768	BB	0.3581	9306.51172	401.93668	50.4335
2	13.491	BB	0.2669	9146.52734	526.01135	49.5665



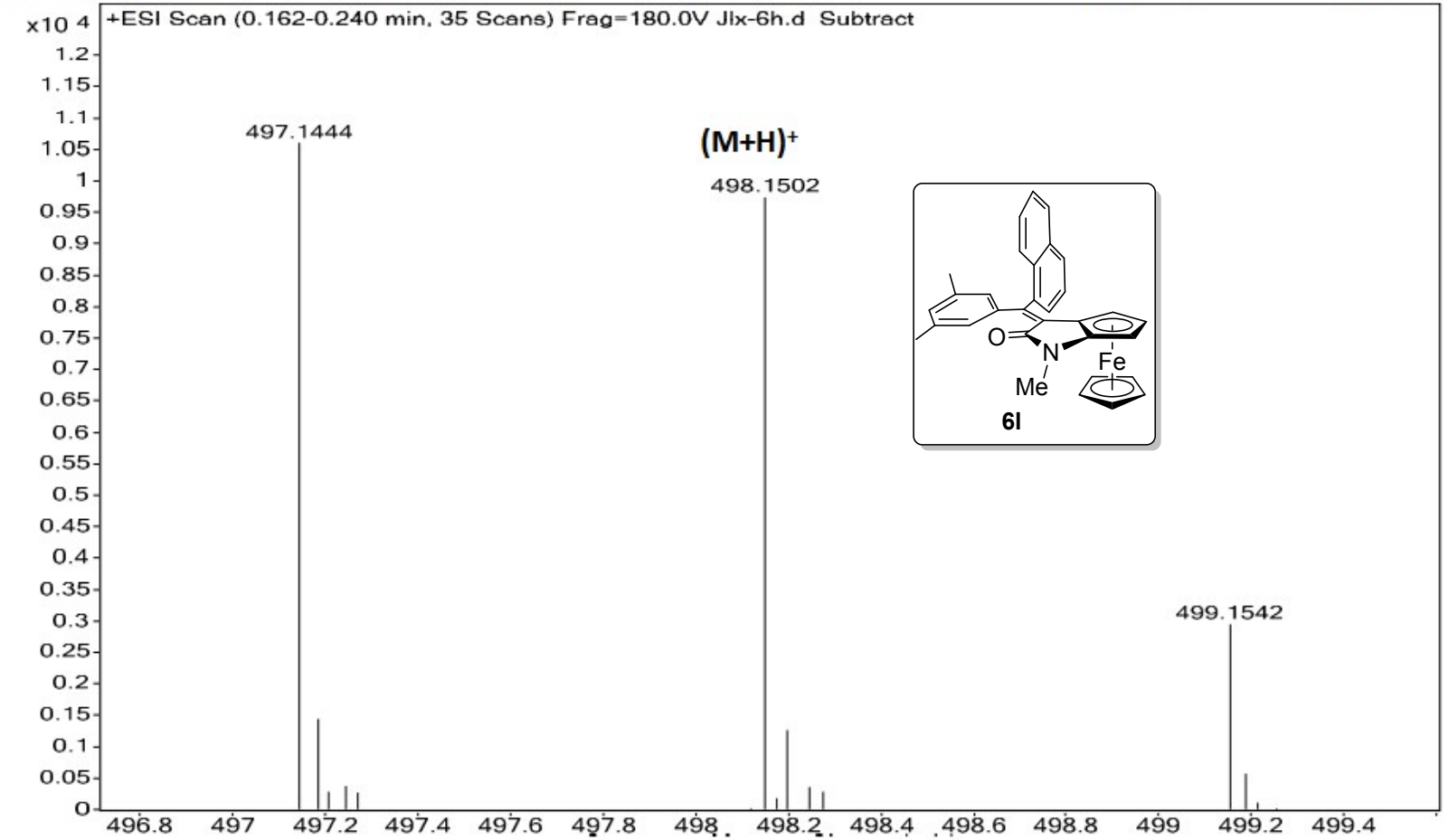
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	8.834	BB	0.3638	7113.98242	305.38953	94.5484
2	13.659	BB	0.2728	410.18692	23.36188	5.4516

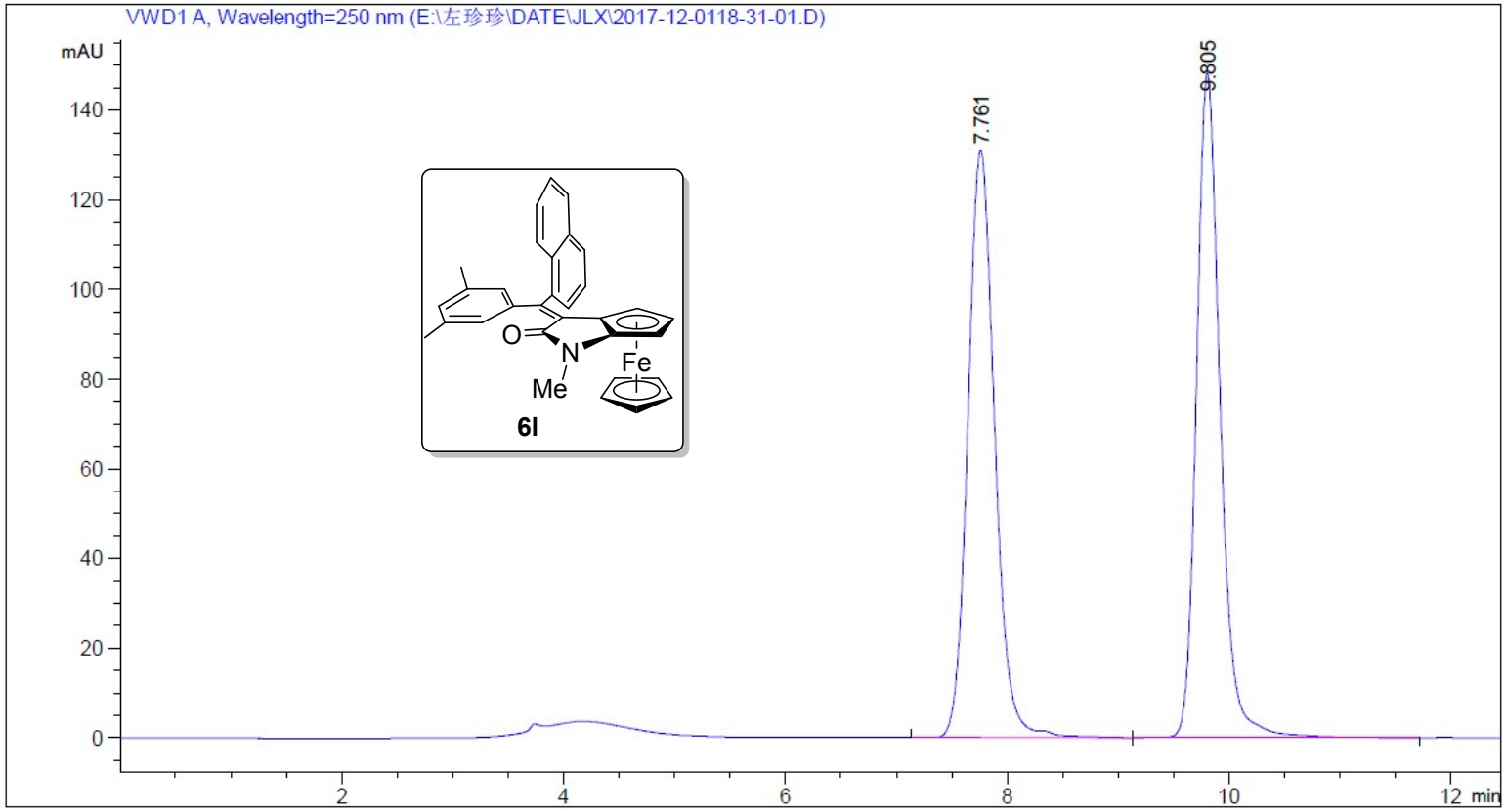
NMR、HMRS Spectra and HPLC Chromatographs of **6l :**



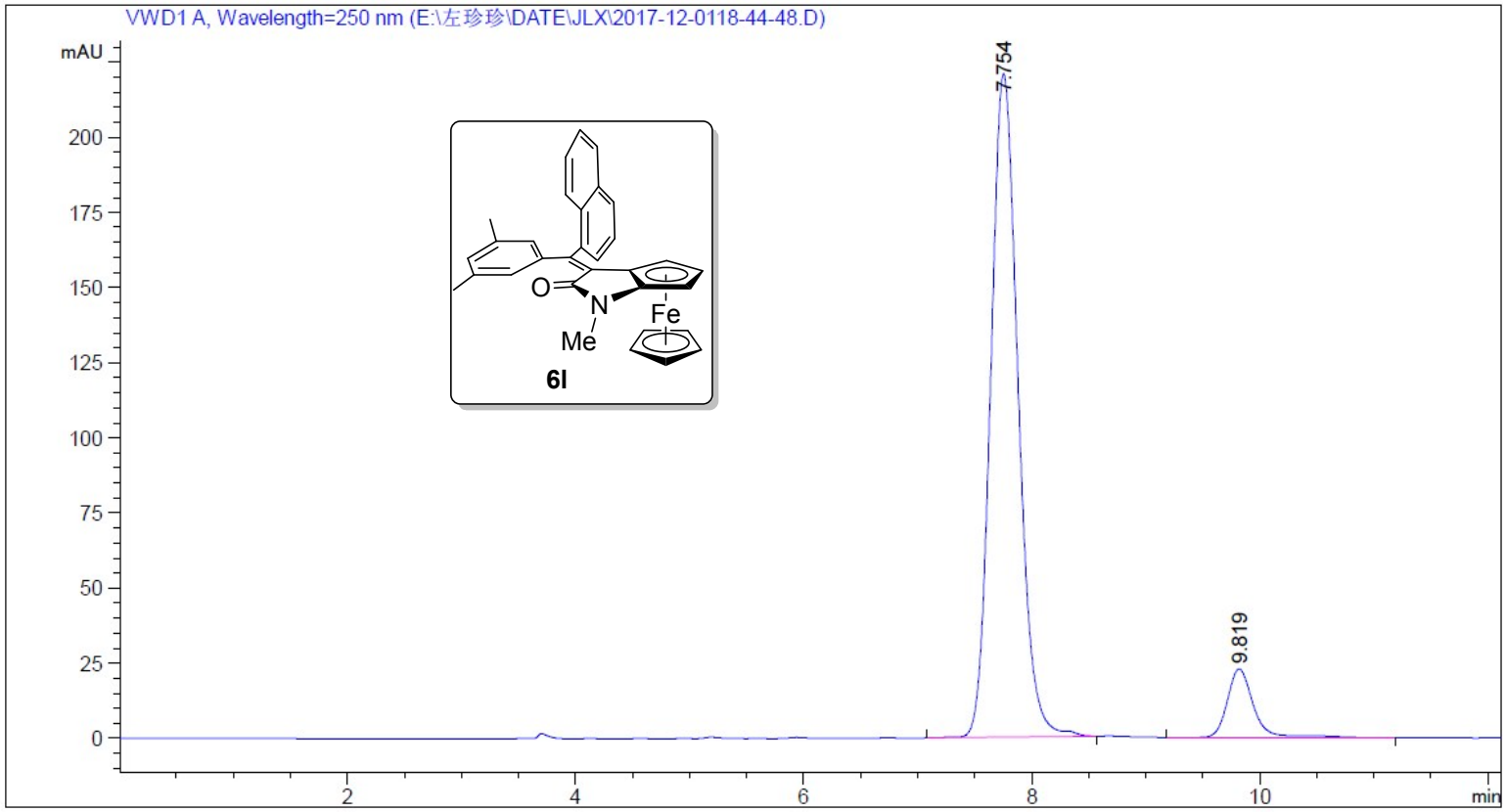

168.76
168.58
136.99
136.94
130.31
128.31
128.30
126.87
126.82
126.57
126.23
126.14
126.10
126.09
125.94
125.51
125.36
106.20
77.42
77.10
76.79
72.83
72.31
70.19
70.01
64.55
64.24
60.53
60.52
50.53
50.50
27.97
27.85
21.46
145.87
145.47
140.33
140.02
138.36
138.10
136.99
136.94
134.07
133.94
130.51
130.48
130.39
130.31
129.87
128.51
128.31
128.30
128.04
126.87
126.82
126.57
126.23
126.14
126.10
126.09
125.94
125.60
125.51
125.36
146 144 142 140 138 136 134 132 130 128 126 124
f1 (ppm)
O
N
Me
Fe
6l
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

Sample Name	Jlx-6h	**Position**	P1-A8	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	Jlx-6h.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	3/20/18 Tue 15:06:54



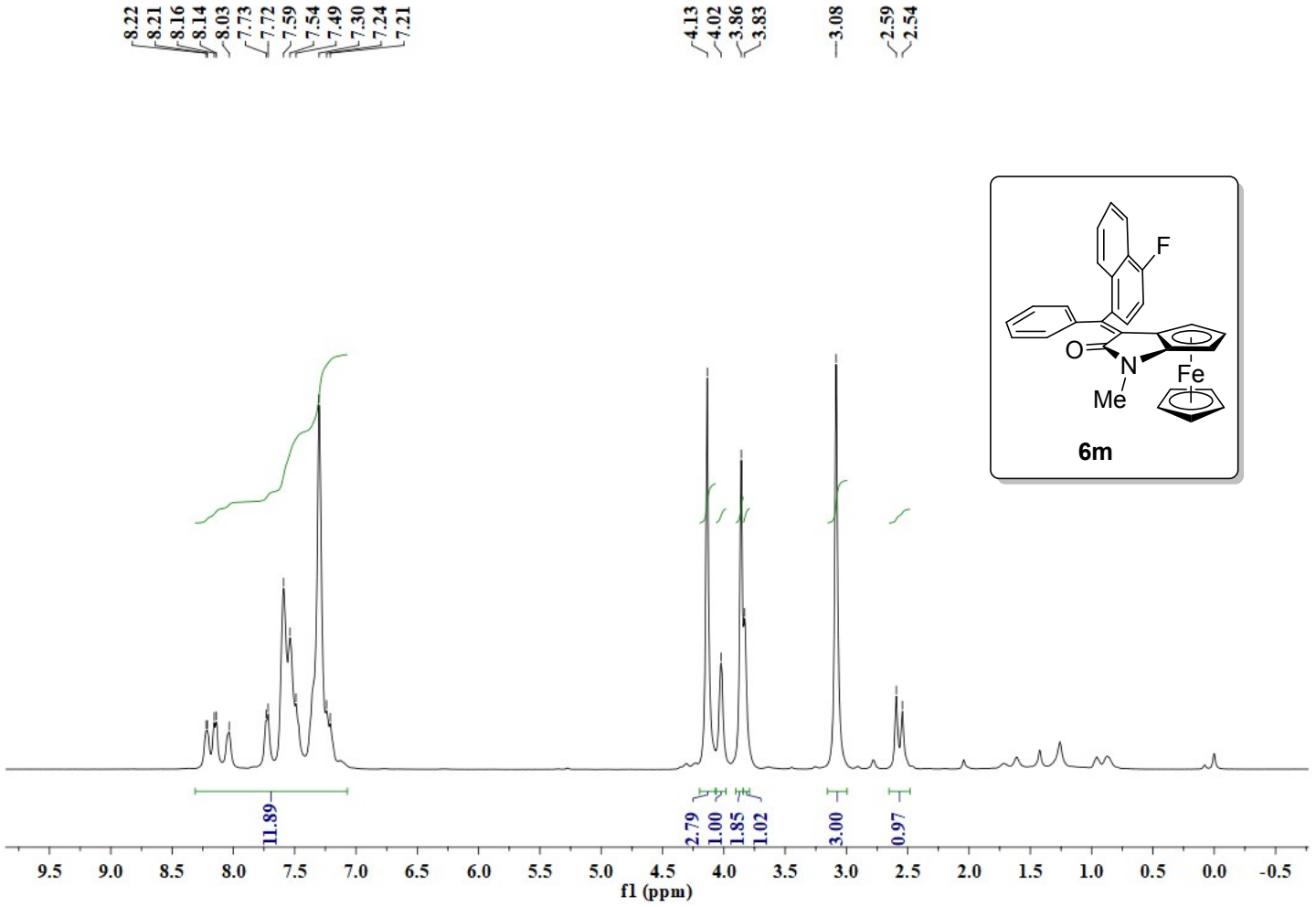


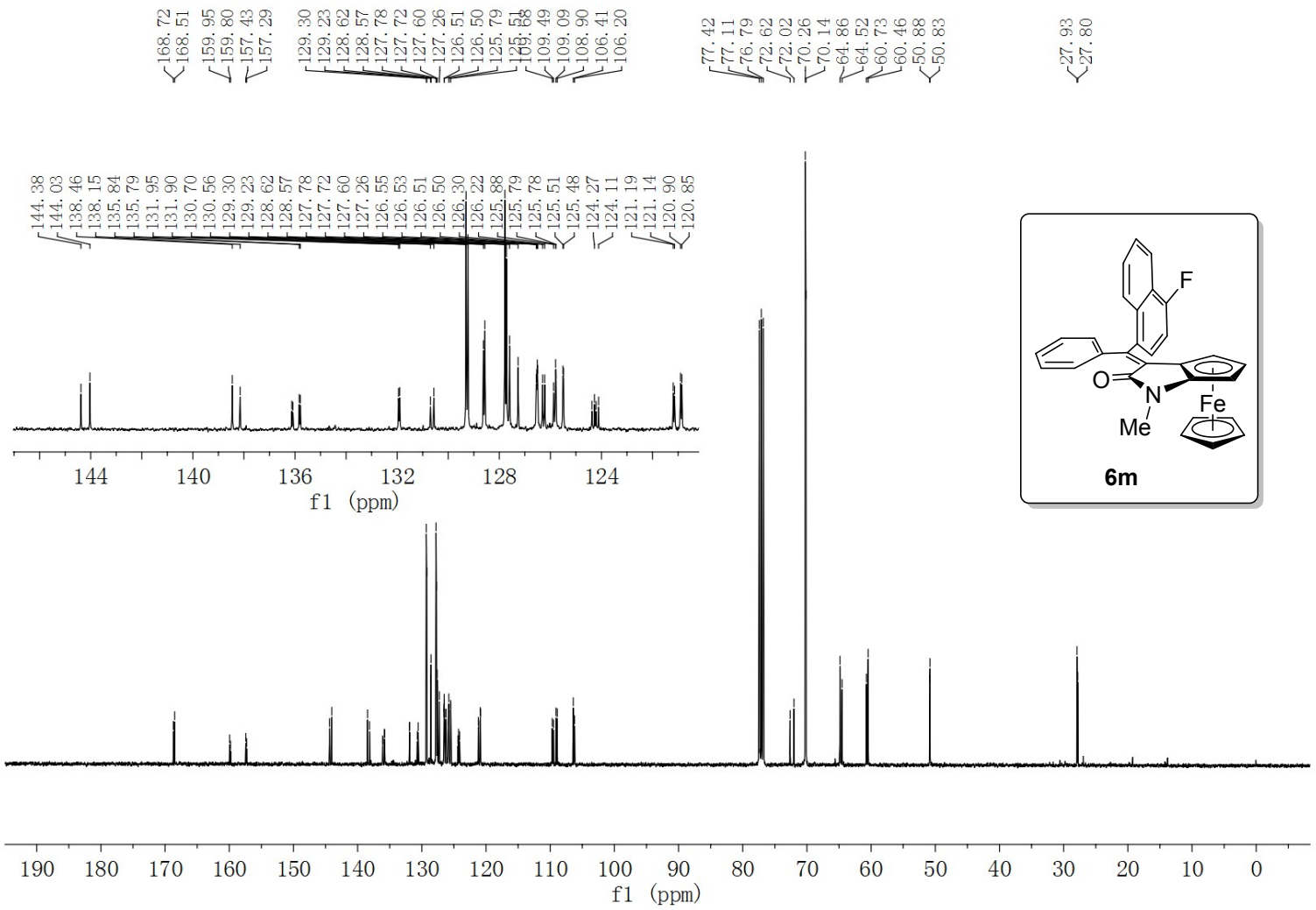
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.761	BB	0.2607	2206.07007	130.87776	49.9712
2	9.805	BB	0.2279	2208.61255	148.19824	50.0288

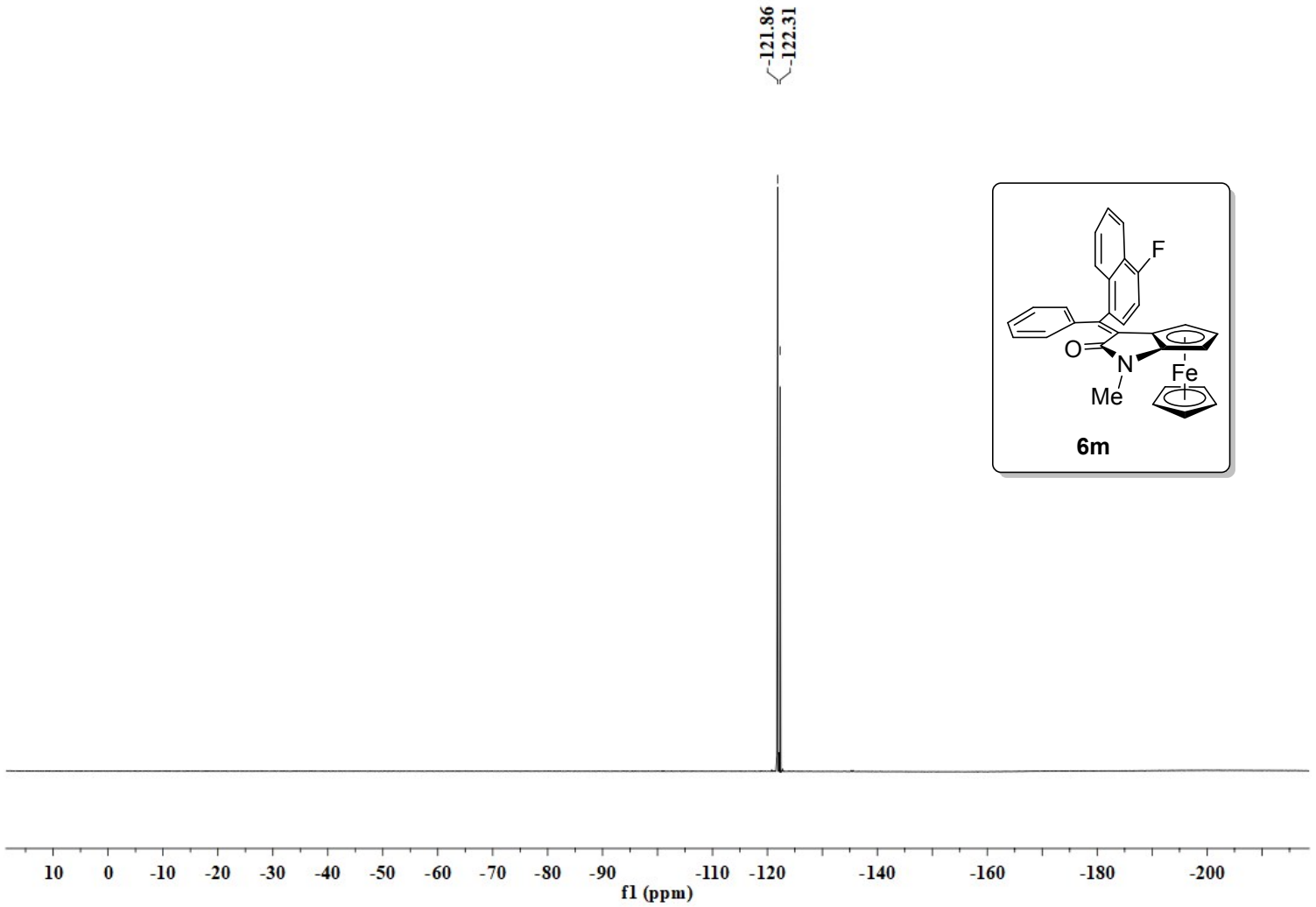


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.754	BB	0.2580	3670.32568	220.67119	90.7583
2	9.819	BB	0.2461	373.73914	22.93939	9.2417

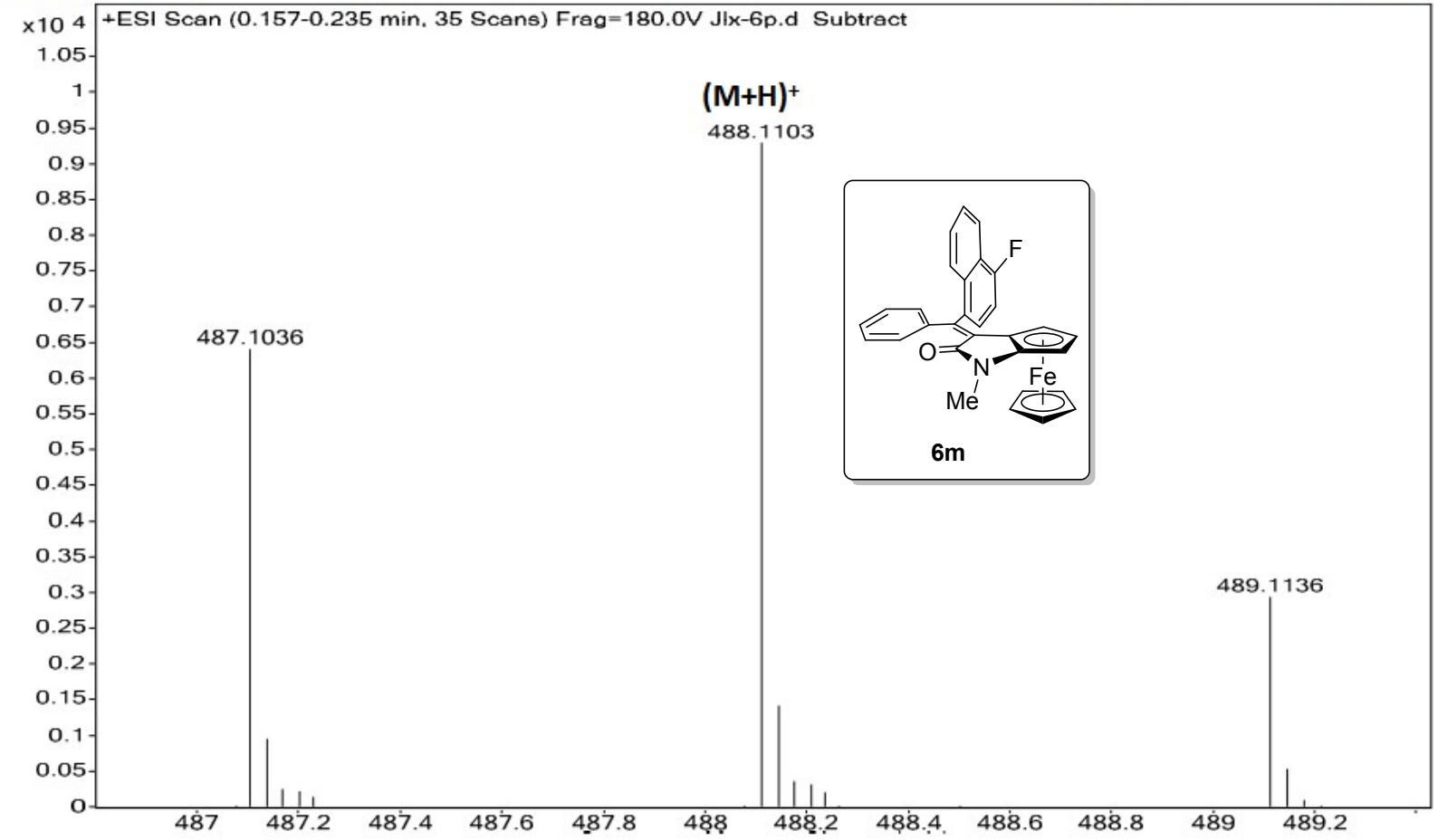
NMR、HMRS Spectra and HPLC Chromatographsof **6m :**

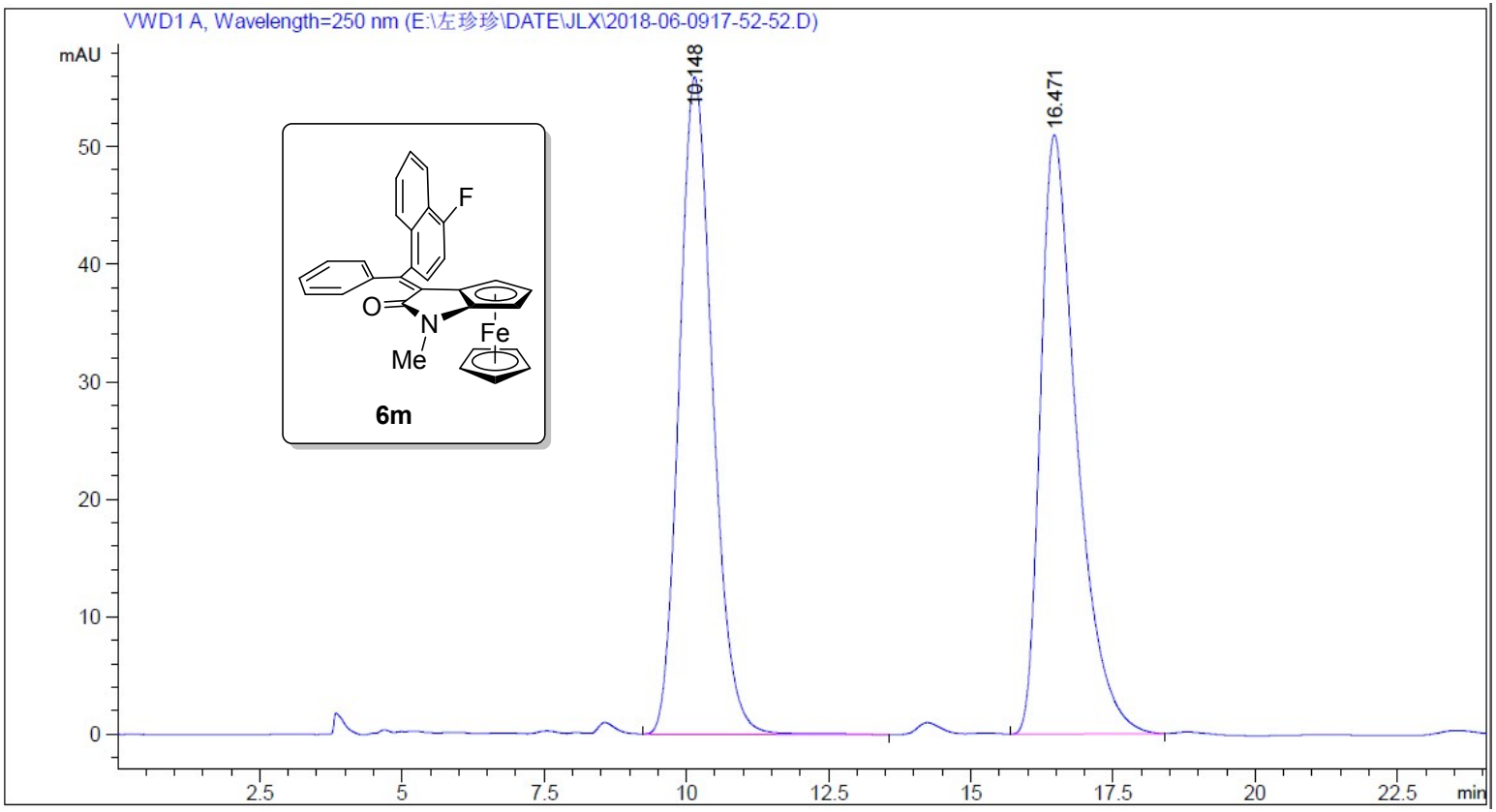



168.72
168.51
159.95
159.80
157.43
157.29
129.30
129.23
128.62
128.57
127.78
127.72
127.60
127.26
126.51
126.50
125.79
125.51
109.49
109.09
108.90
106.41
106.20
77.42
77.11
76.79
72.62
72.02
70.26
70.14
64.86
64.52
60.73
60.46
50.88
50.83
27.93
27.80
144.38
144.03
138.46
138.15
135.84
135.79
131.95
131.90
130.70
130.56
129.30
129.23
128.62
128.57
127.78
127.72
127.60
127.26
126.55
126.53
126.51
126.50
126.30
126.22
125.88
125.79
125.78
125.51
125.48
124.27
124.11
121.19
121.14
120.90
120.85
144
140
136
132
128
124
f1 (ppm)
F
O
N
Me
Fe
6m
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

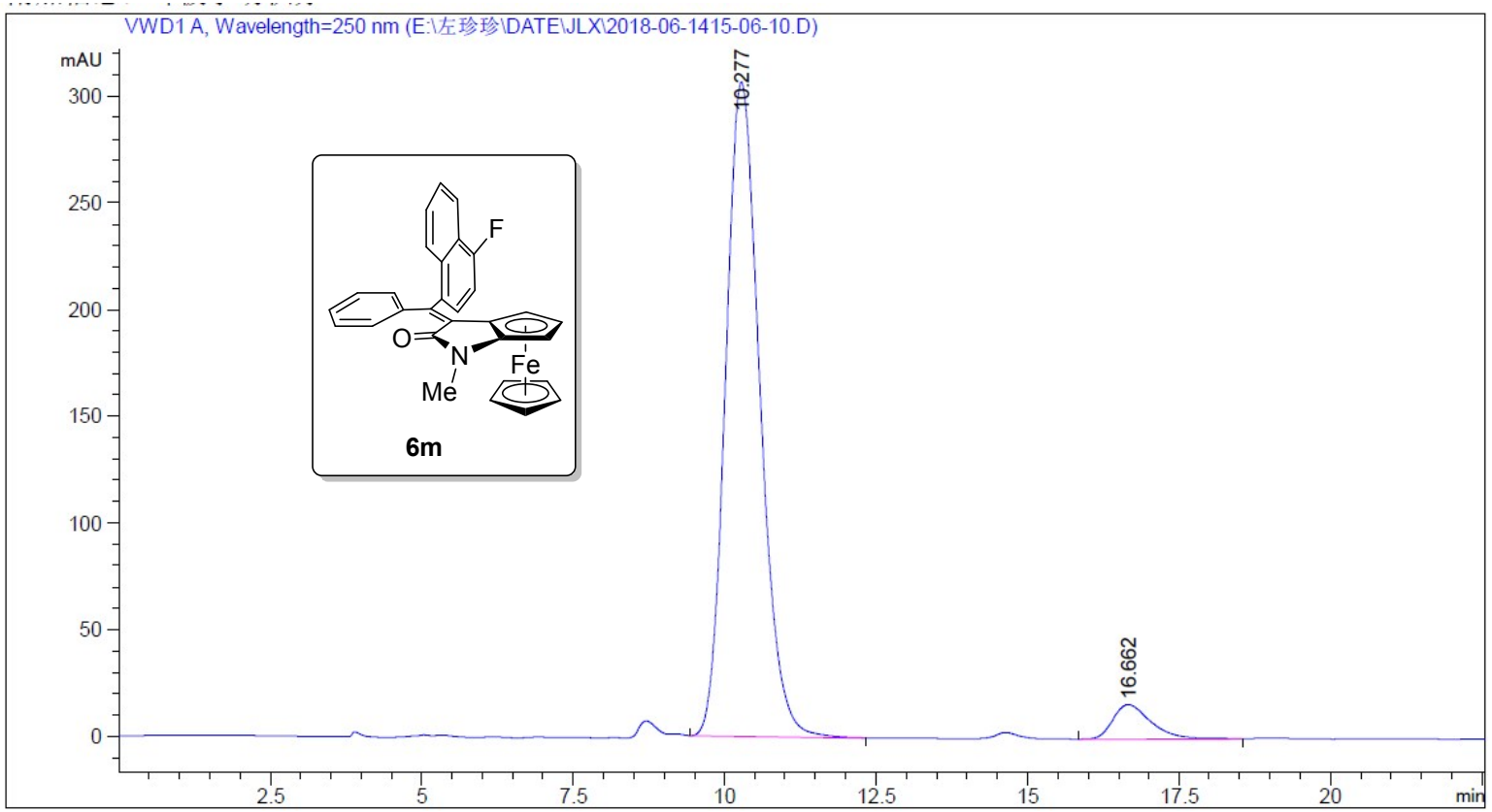

-121.86
-122.31
F
O
N
Me
Fe
6m
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-110
-120
-140
-160
-180
-200
f1 (ppm)

Sample Name	Jlx-6p	**Position**	P1-B7	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	Jlx-6p.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	3/20/18 Tue 15:23:29



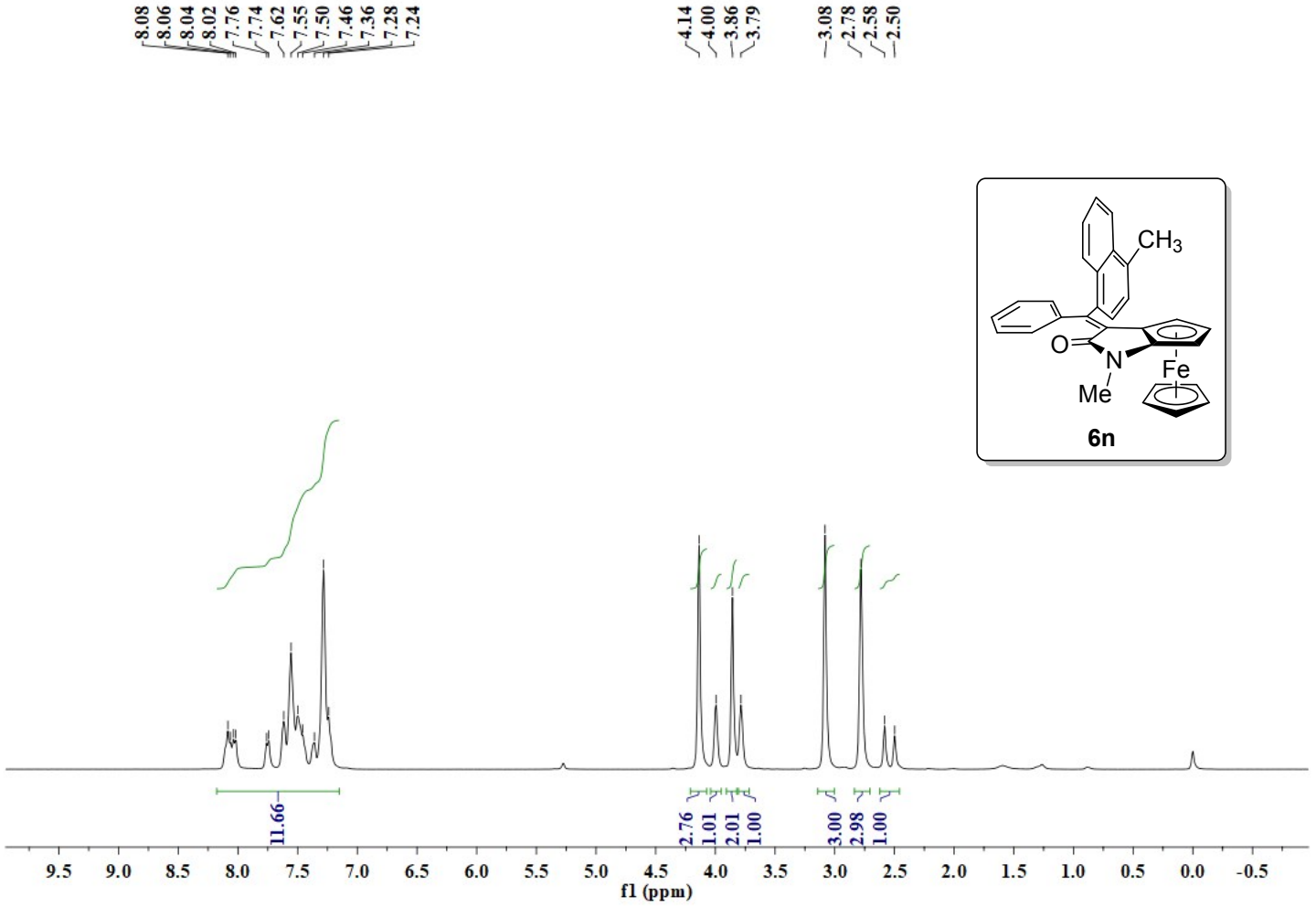


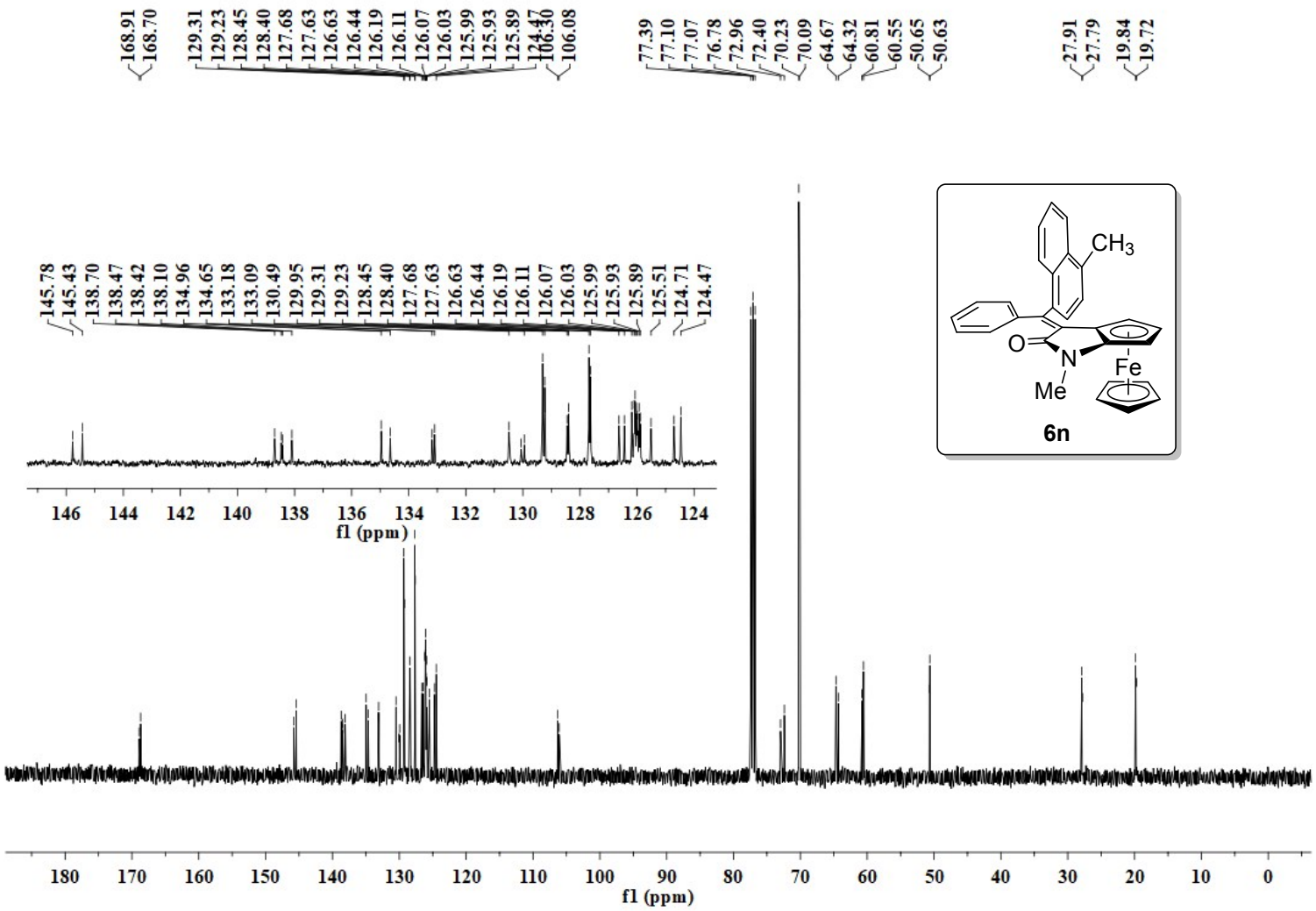
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	10.148	BB	0.6299	2290.15918	55.90253	50.2931
2	16.471	BB	0.6622	2263.46460	50.96308	49.7069



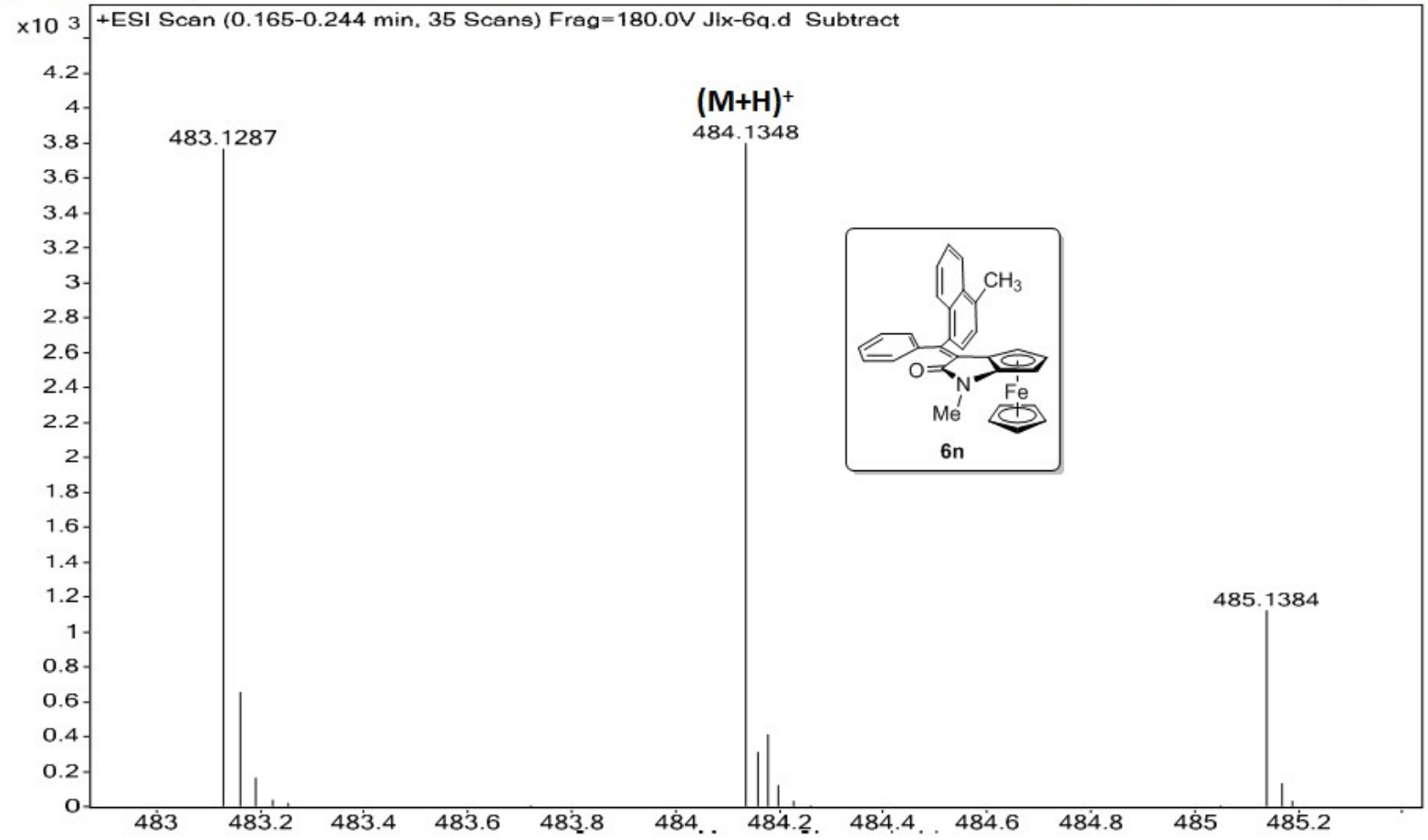
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	10.277	BB	0.6112	1.20673e4	306.60995	94.4762
2	16.662	BB	0.6597	705.54083	16.21382	5.5238

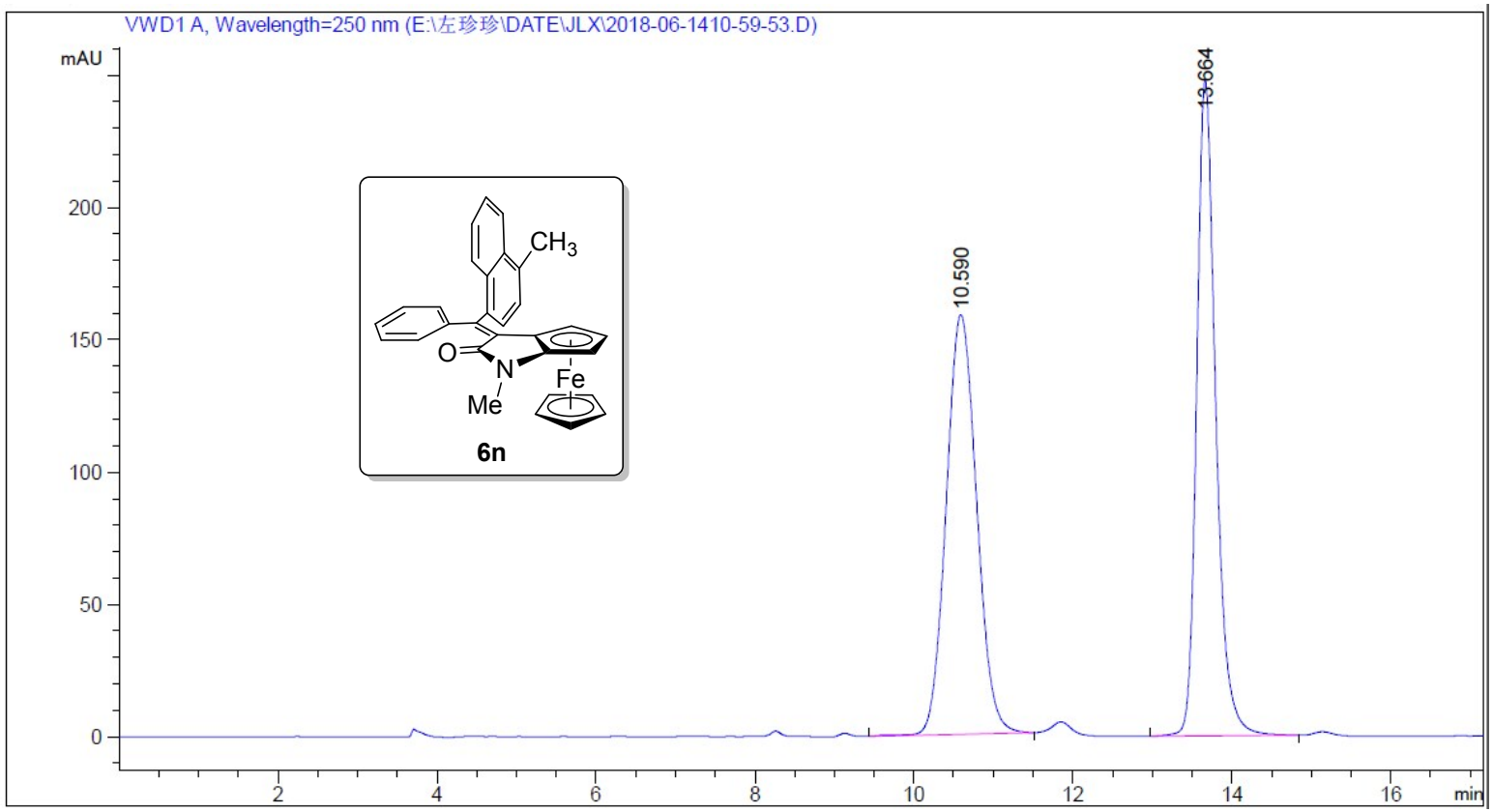
NMR、HMRS Spectra and HPLC Chromatographsof **6n**



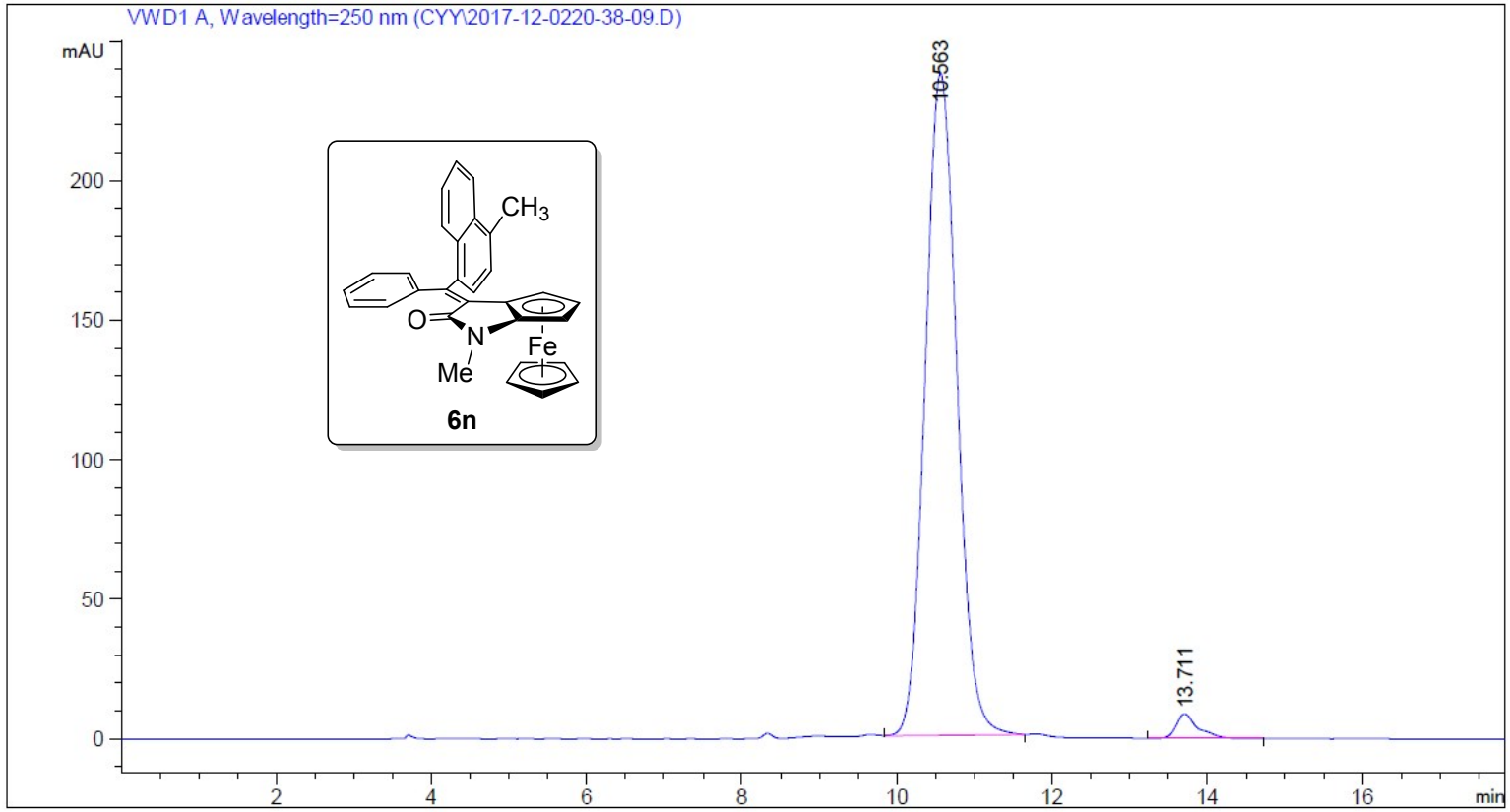

168.91
168.70
129.31
129.23
128.45
128.40
127.68
127.63
126.63
126.44
126.19
126.11
126.07
126.03
125.99
125.93
125.89
124.47
106.30
106.08
77.39
77.10
77.07
76.78
72.96
72.40
70.23
70.09
64.67
64.32
60.81
60.55
50.65
50.63
27.91
27.79
19.84
19.72
145.78
145.43
138.70
138.47
138.42
138.10
134.96
134.65
133.18
133.09
130.49
129.95
129.31
129.23
128.45
128.40
127.68
127.63
126.63
126.44
126.19
126.11
126.07
126.03
125.99
125.93
125.89
125.51
124.71
124.47
146 144 142 140 138 136 134 132 130 128 126 124
f1 (ppm)
CH3
O
N
Me
Fe
6n
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

Sample Name	Jlx-6q	**Position**	P1-B8	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	Jlx-6q.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	3/20/18 Tue 15:24:45



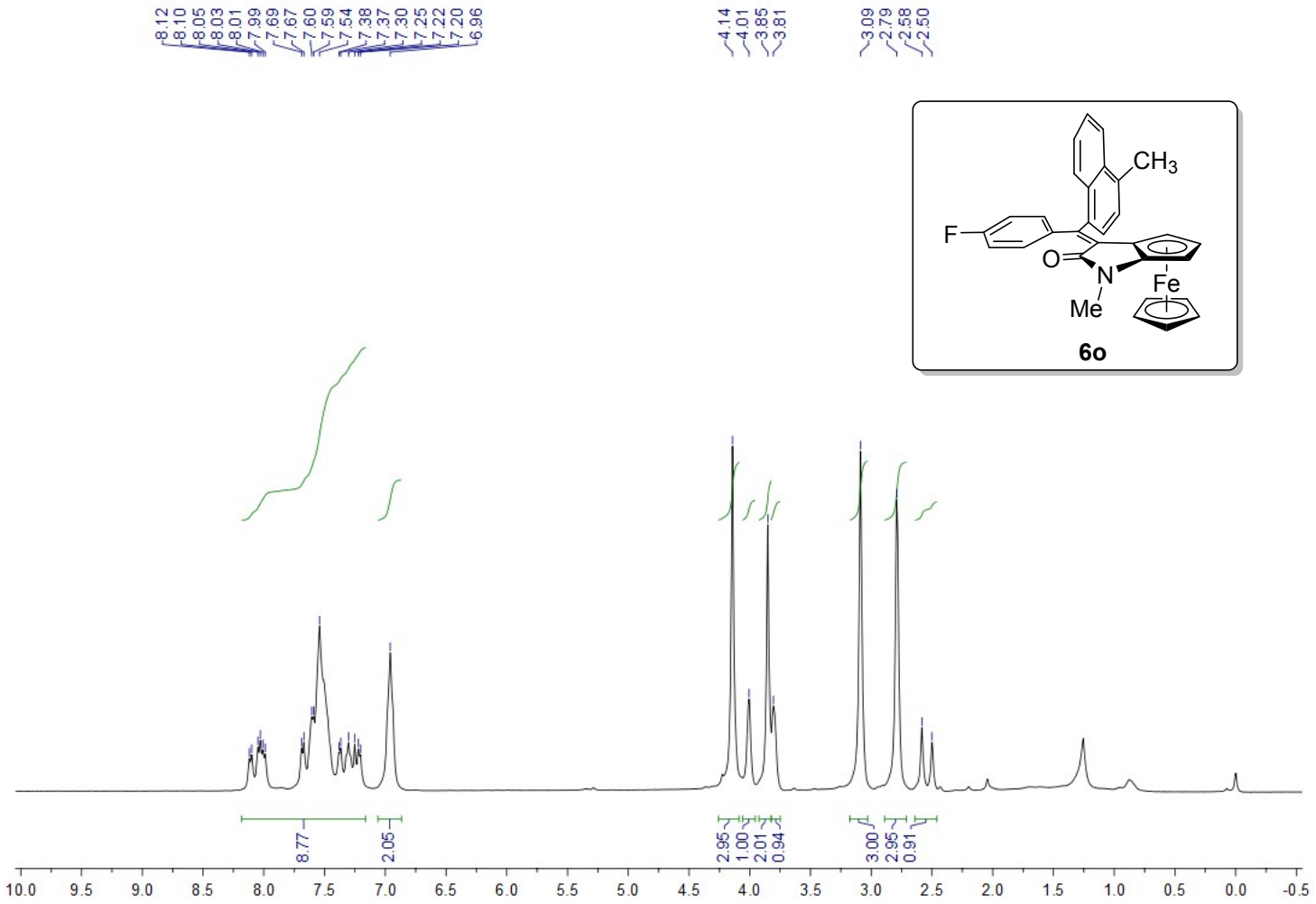


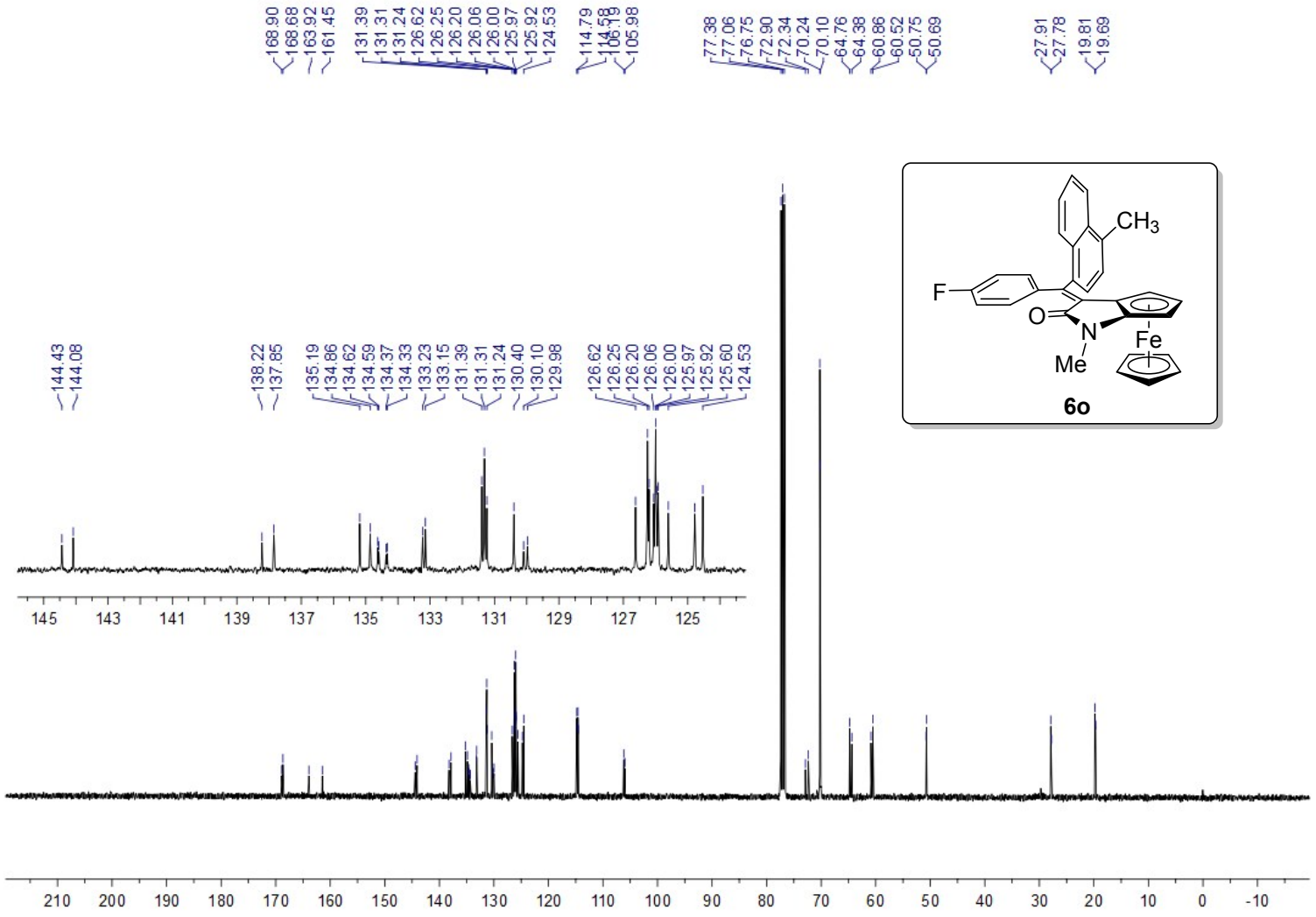
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	10.590	BB	0.4149	4222.96387	158.48151	50.5404
2	13.664	BB	0.2587	4132.66162	247.63560	49.4596

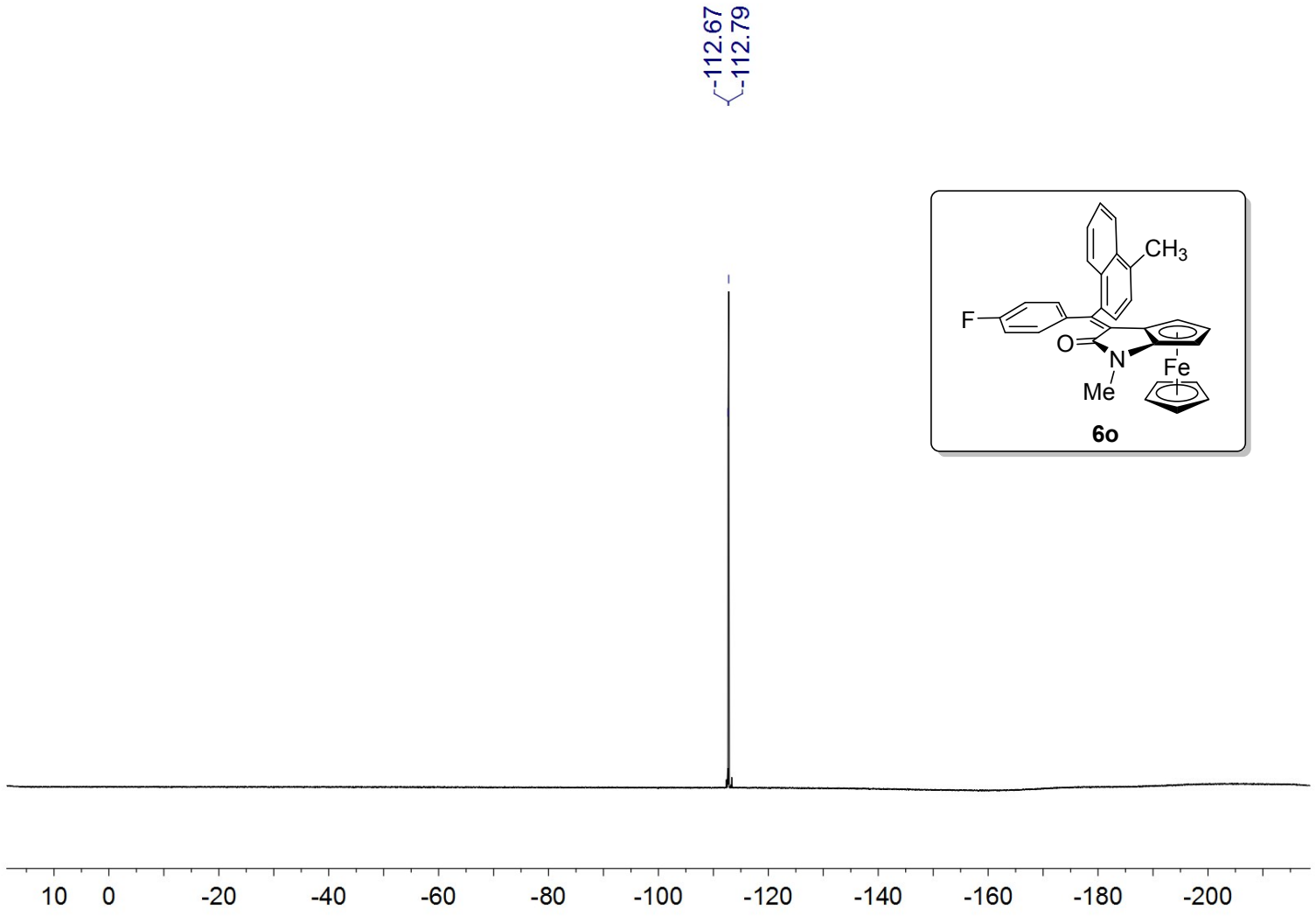


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	10.563	BB	0.4449	6727.74023	237.23781	97.5351
2	13.711	BB	0.2801	170.02568	8.84991	2.4649

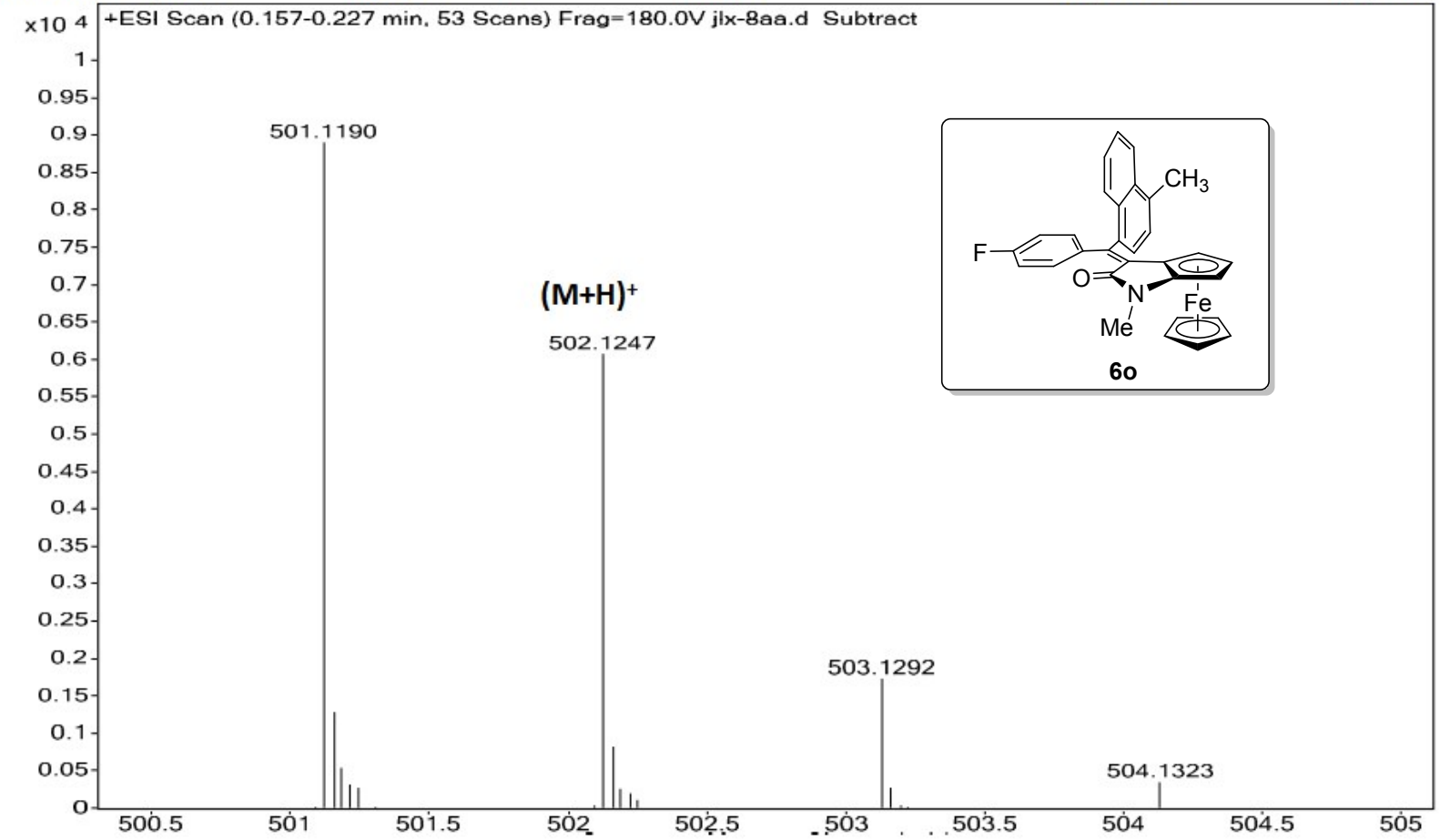
NMR、HMRS Spectra and HPLC Chromatographsof **6o :**

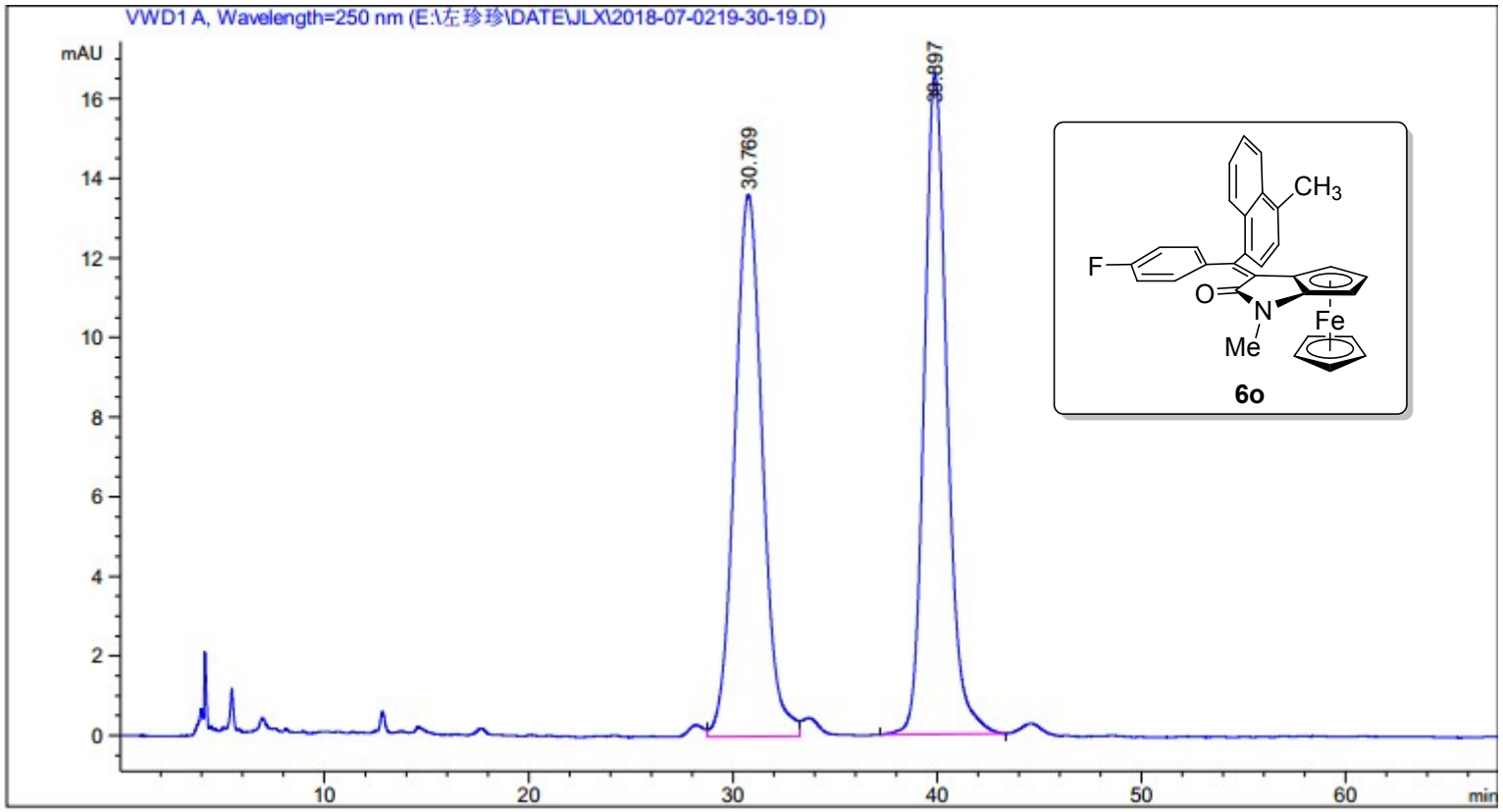



168.90
168.68
163.92
161.45
131.39
131.31
131.24
126.62
126.25
126.20
126.06
126.00
125.97
125.92
124.53
114.79
114.58
105.98
77.38
77.06
76.75
72.90
72.34
70.24
70.10
64.76
64.38
60.86
60.52
50.75
50.69
27.91
27.78
19.81
19.69
144.43
144.08
138.22
137.85
135.19
134.86
134.62
134.59
134.37
134.33
133.23
133.15
131.39
131.31
131.24
130.40
130.10
129.98
126.62
126.25
126.20
126.06
126.00
125.97
125.92
125.60
124.53
CH3
F
O
N
Me
Fe
6o
145
143
141
139
137
135
133
131
129
127
125
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

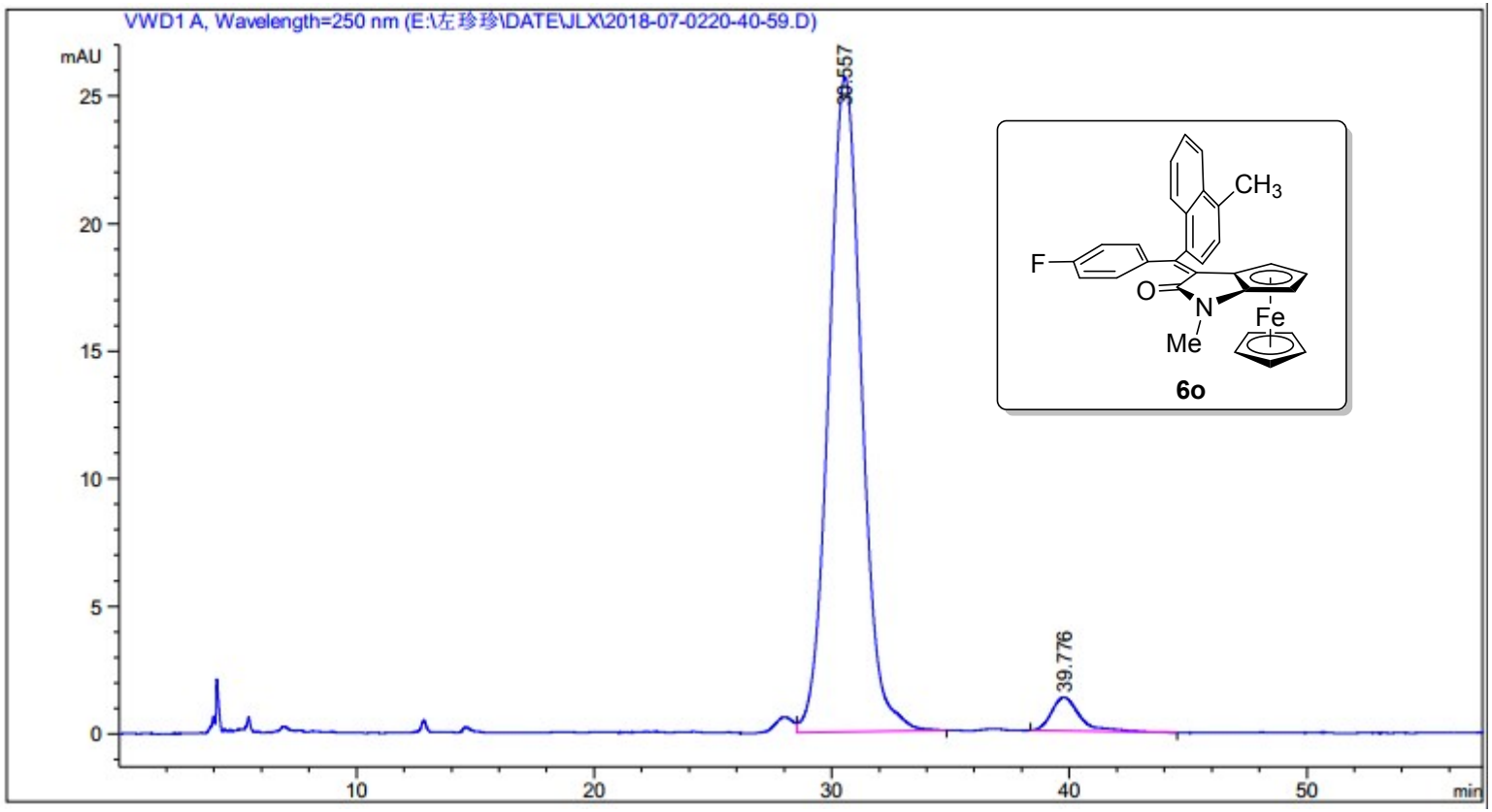

-112.67
-112.79
CH3
F
O
N
Me
Fe
6o
10
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200

Sample Name	jlx-8aa	**Position**	P1-A4	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
Data Filename	jlx-8aa.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	5/24/18 Thu 10:36:31



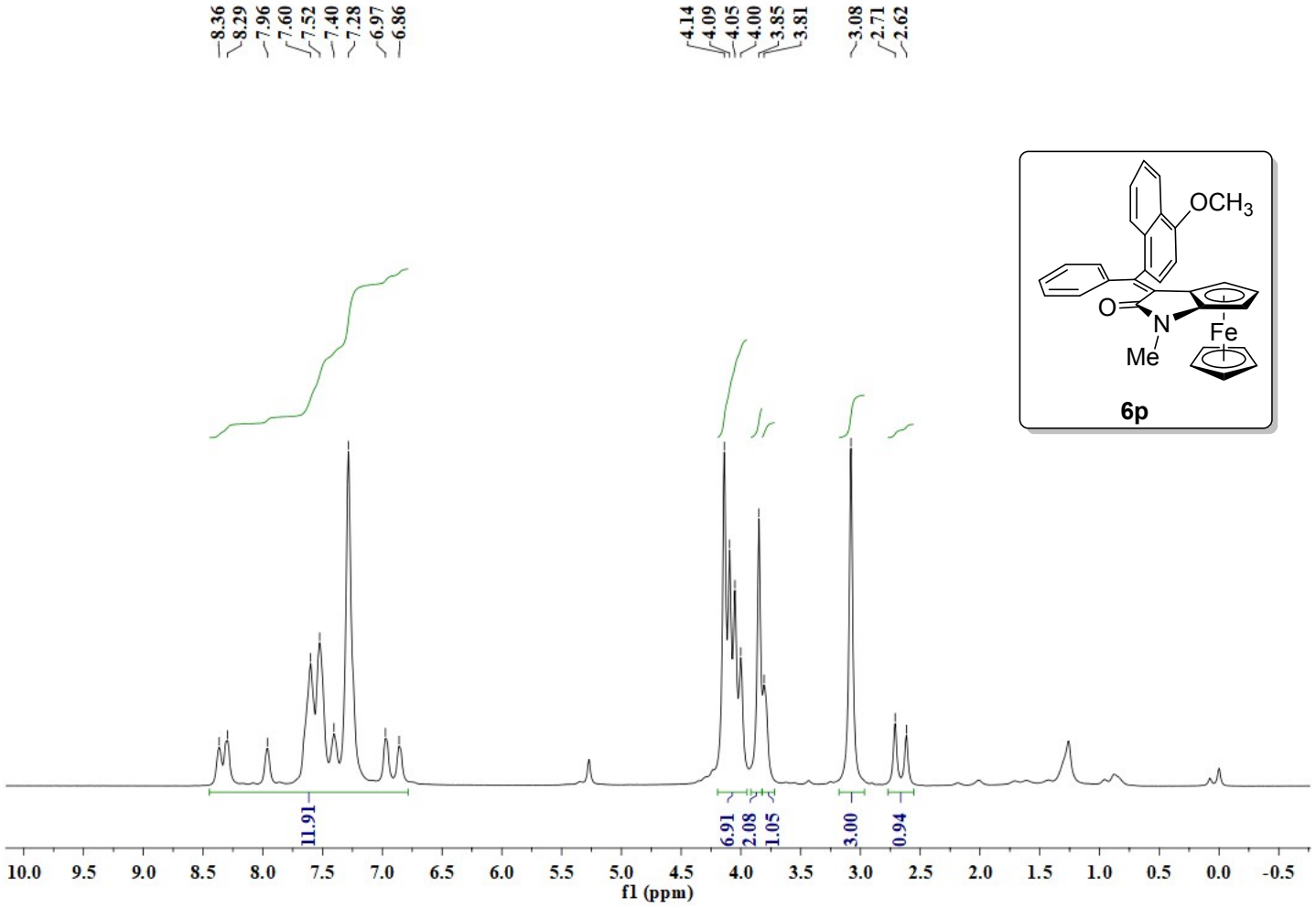


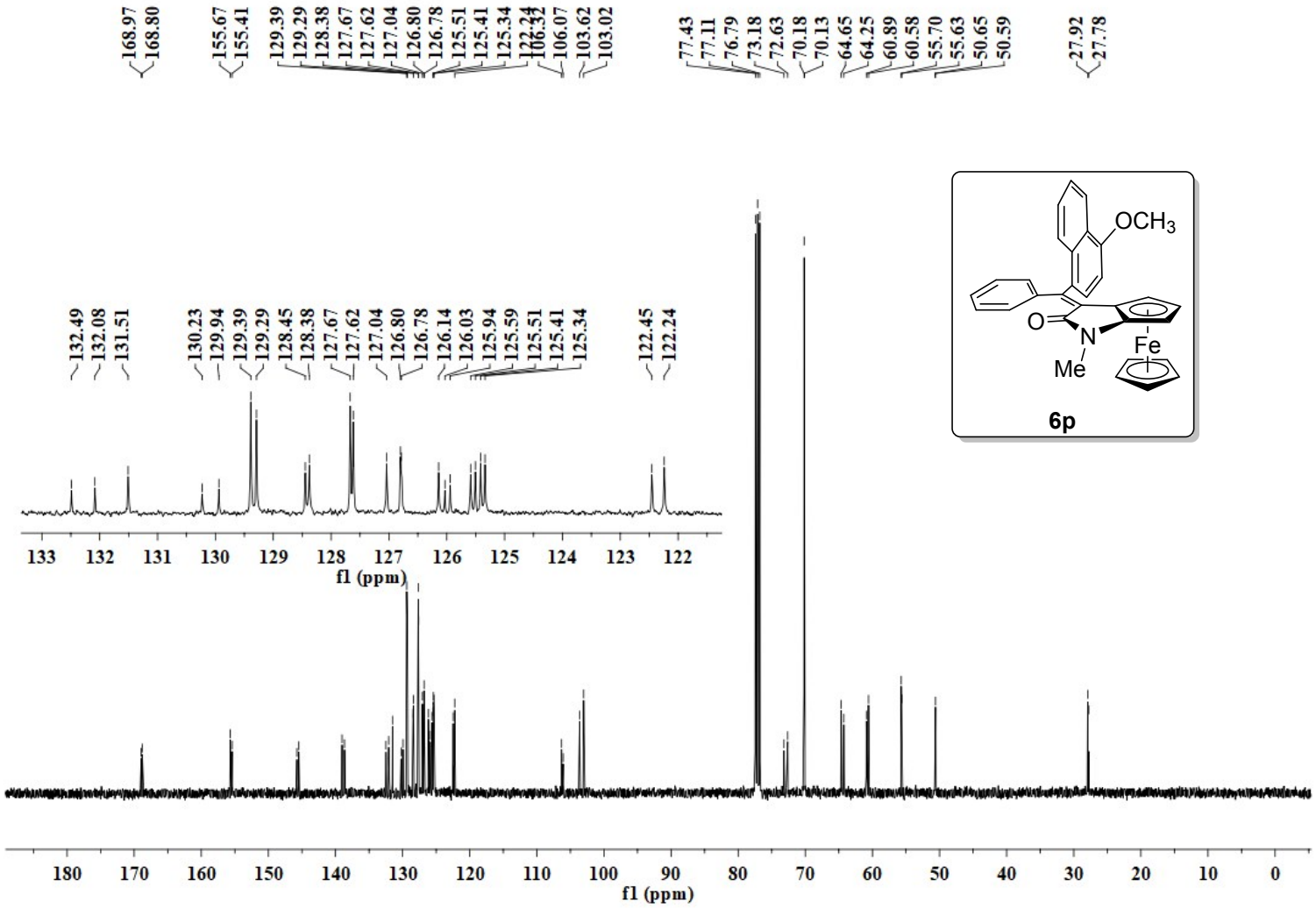
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	30.769	VV	1.4575	1290.27136	13.61601	49.9295
2	39.897	BB	1.1946	1293.91357	16.57693	50.0705



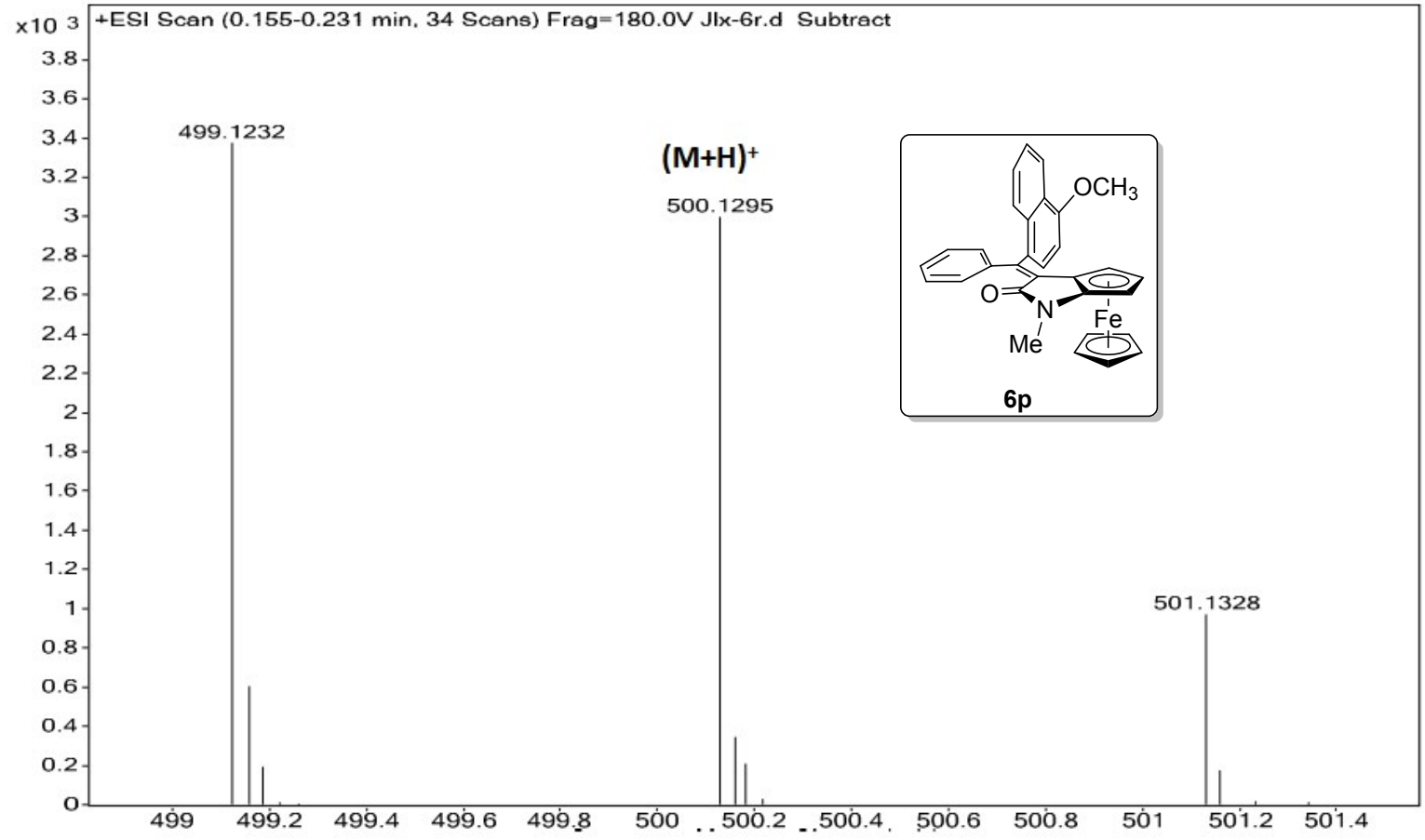
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	30.557	VB	1.4948	2468.47827	25.64843	95.6707
2	39.776	BB	1.1389	111.70461	1.32587	4.3293

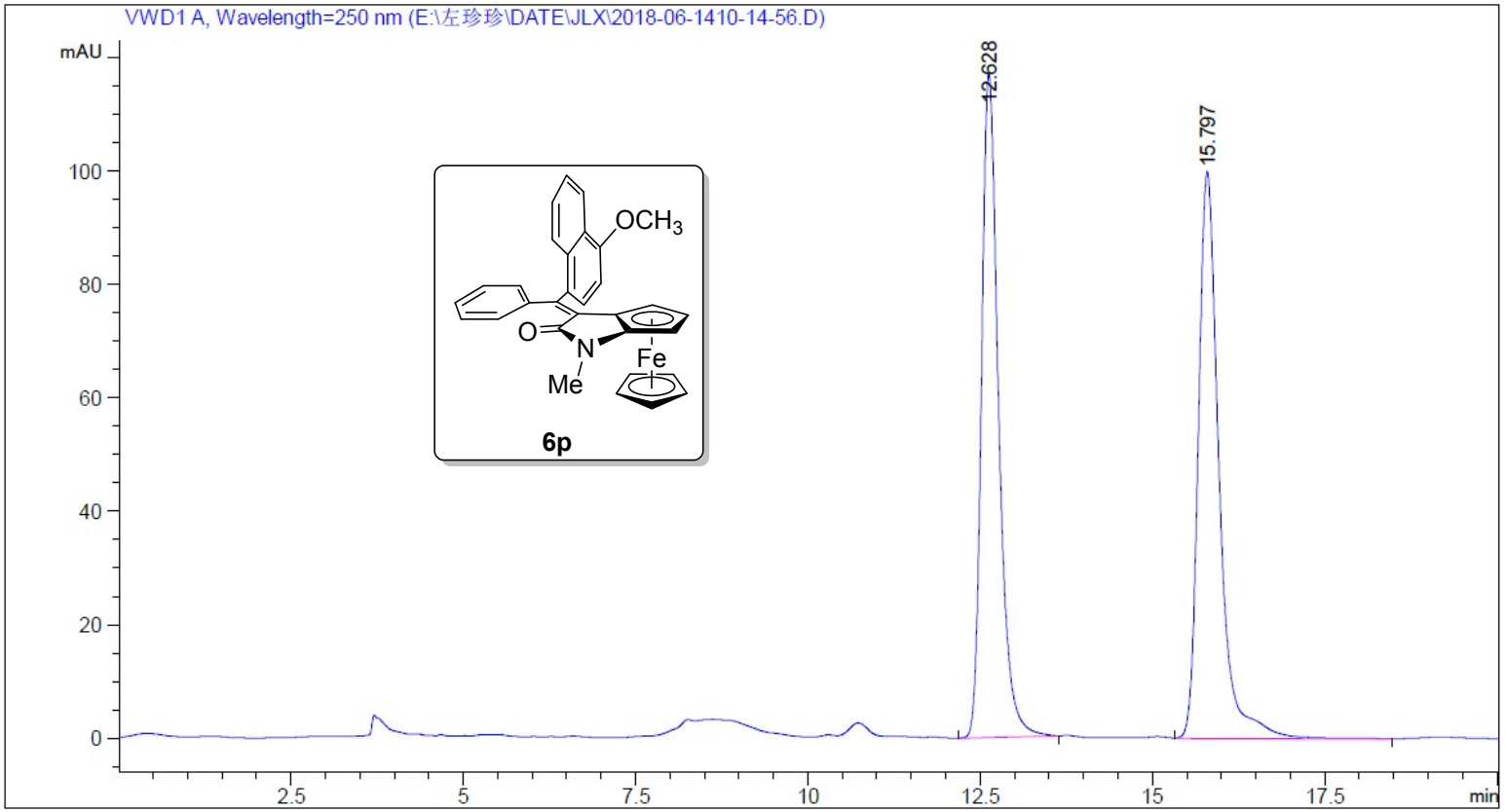
NMR、HMRS Spectra and HPLC Chromatographsof **6p :**



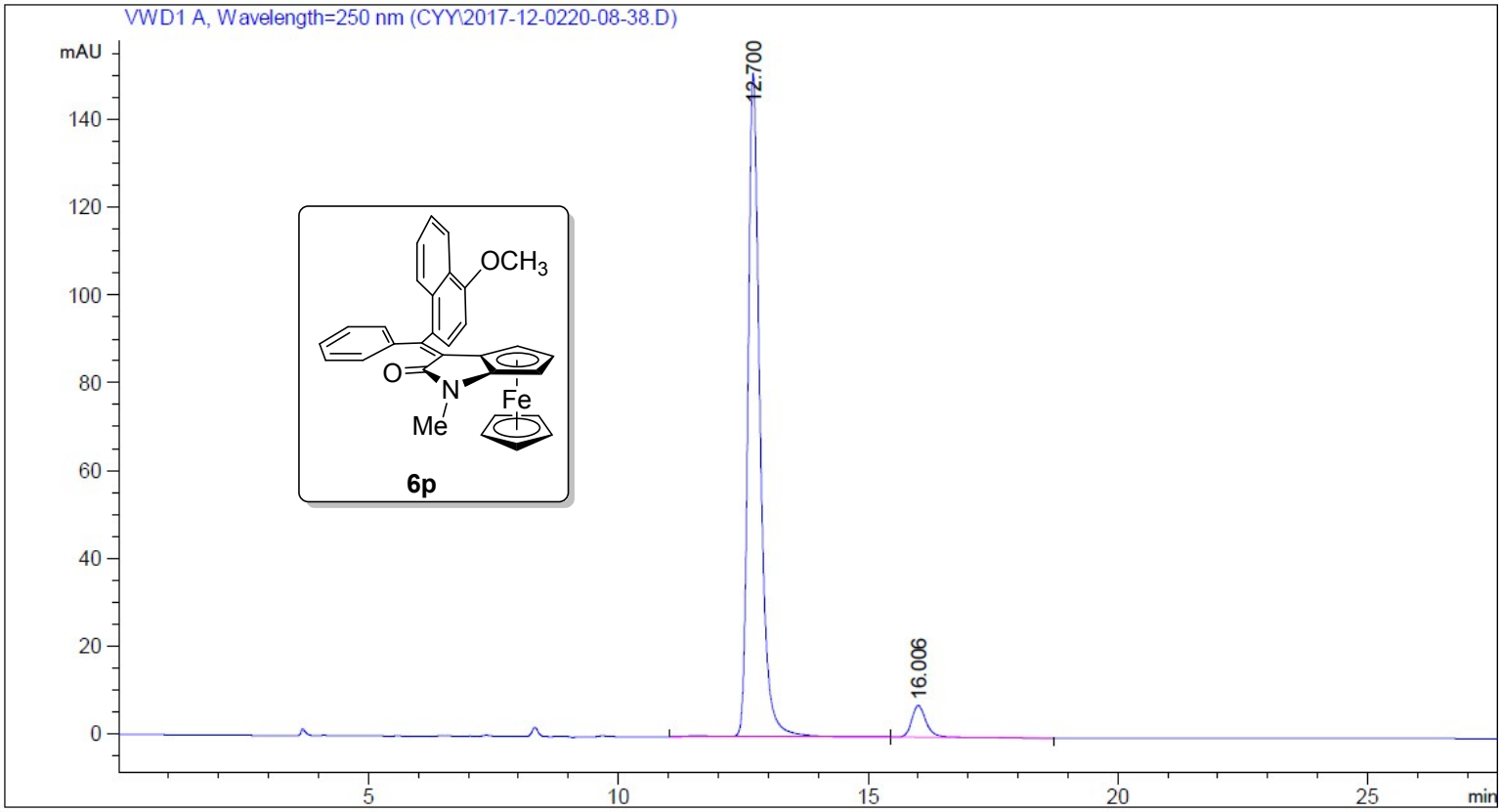

168.97
168.80
155.67
155.41
129.39
129.29
128.38
127.67
127.62
127.04
126.80
126.78
125.51
125.41
125.34
106.07
103.62
103.02
77.43
77.11
76.79
73.18
72.63
70.18
70.13
64.65
64.25
60.89
60.58
55.70
55.63
50.65
50.59
27.92
27.78
132.49
132.08
131.51
130.23
129.94
129.39
129.29
128.45
128.38
127.67
127.62
127.04
126.80
126.78
126.14
126.03
125.94
125.59
125.51
125.41
125.34
122.45
122.24
133 132 131 130 129 128 127 126 125 124 123 122
f1 (ppm)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
OCH3
O
N
Me
Fe
6p

Sample Name	Jlx-6r	**Position**	P1-B9	**Instrument Name**	Instrument 1	**User Name**	Agilent FSE
Inj Vol	0.2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	Jlx-6r.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	3/20/18 Tue 15:26:02



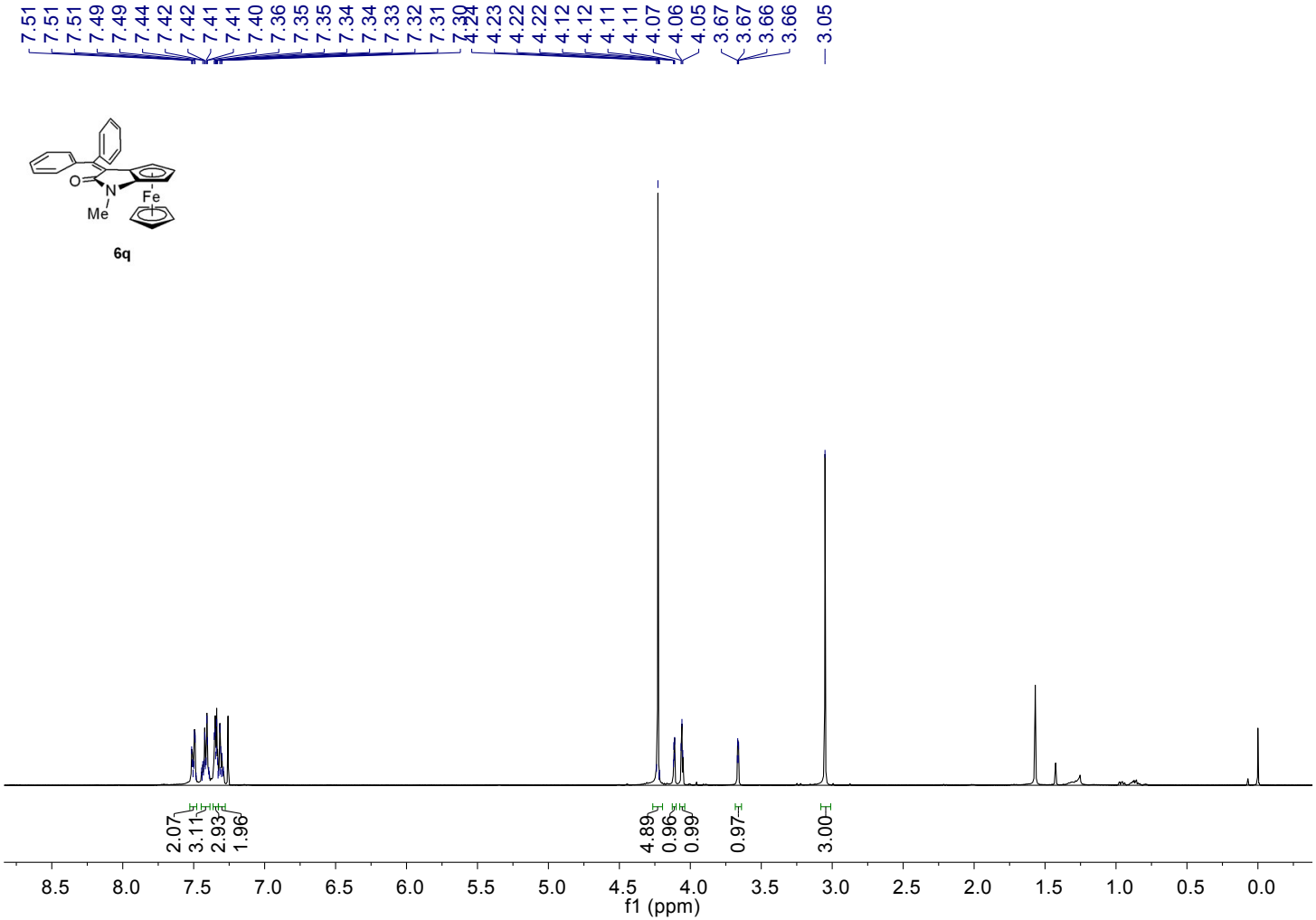


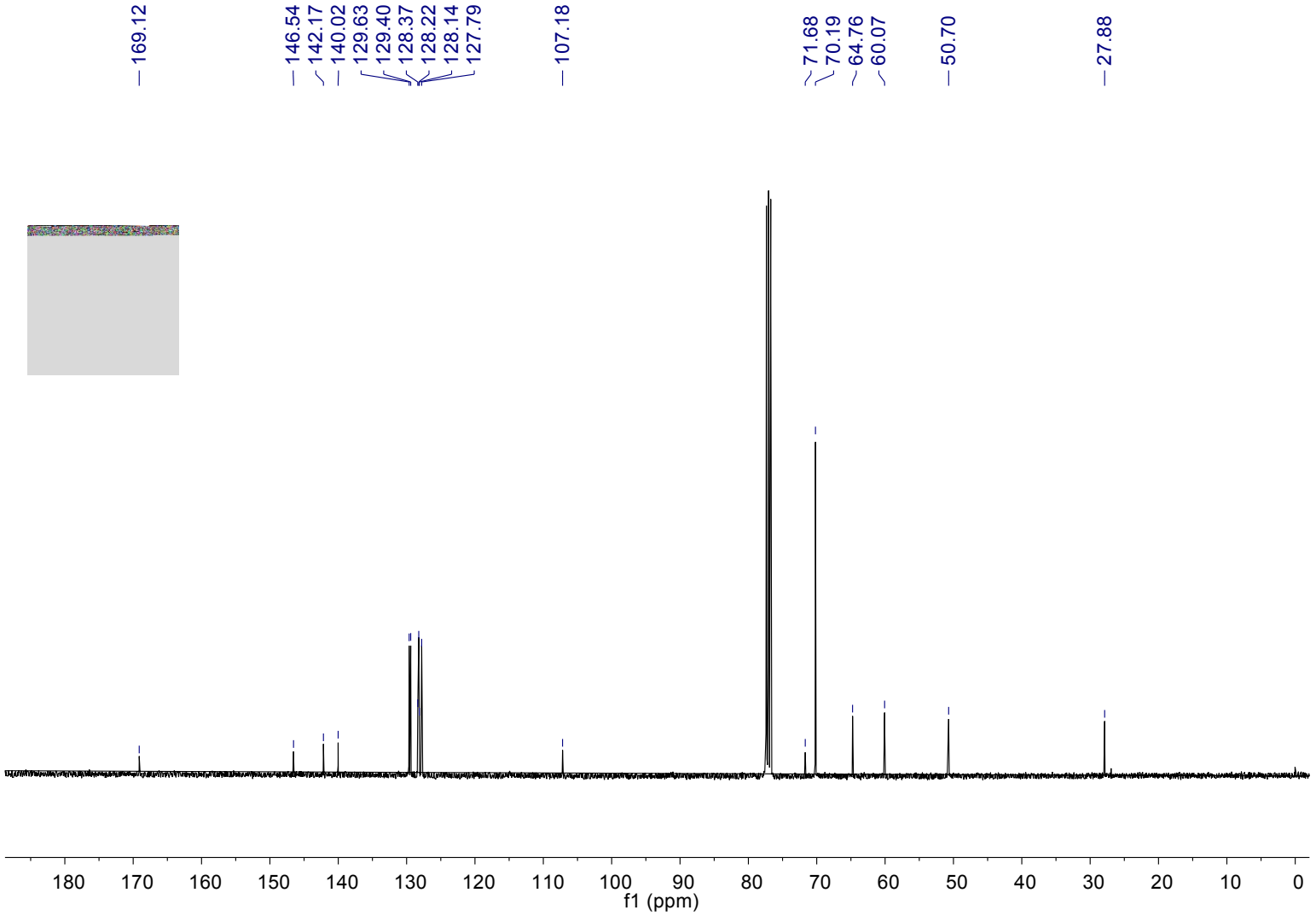
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.628	BB	0.2571	2010.97864	116.67024	49.1306
2	15.797	BB	0.3157	2082.14941	99.69502	50.8694

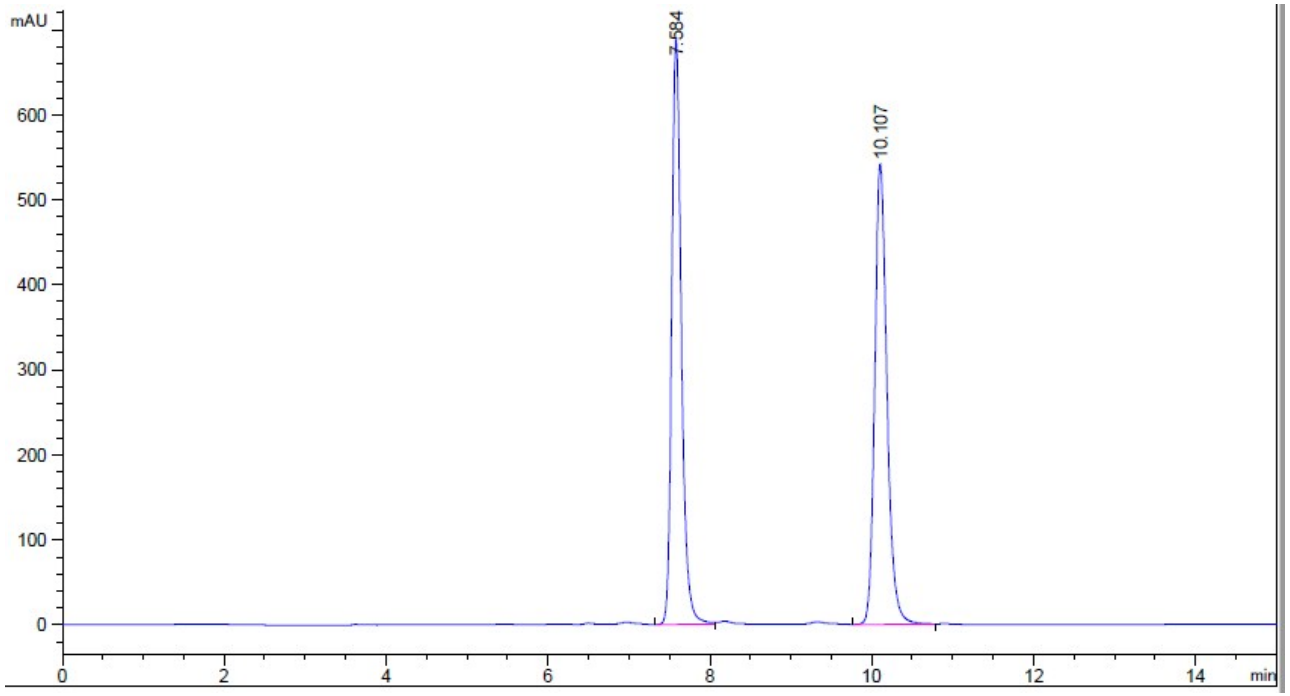


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.700	BB	0.2540	2537.66504	151.05618	94.4717
2	16.006	BB	0.3097	148.49881	7.22754	5.5283

NMR and HPLC Chromatographs of **6q :**

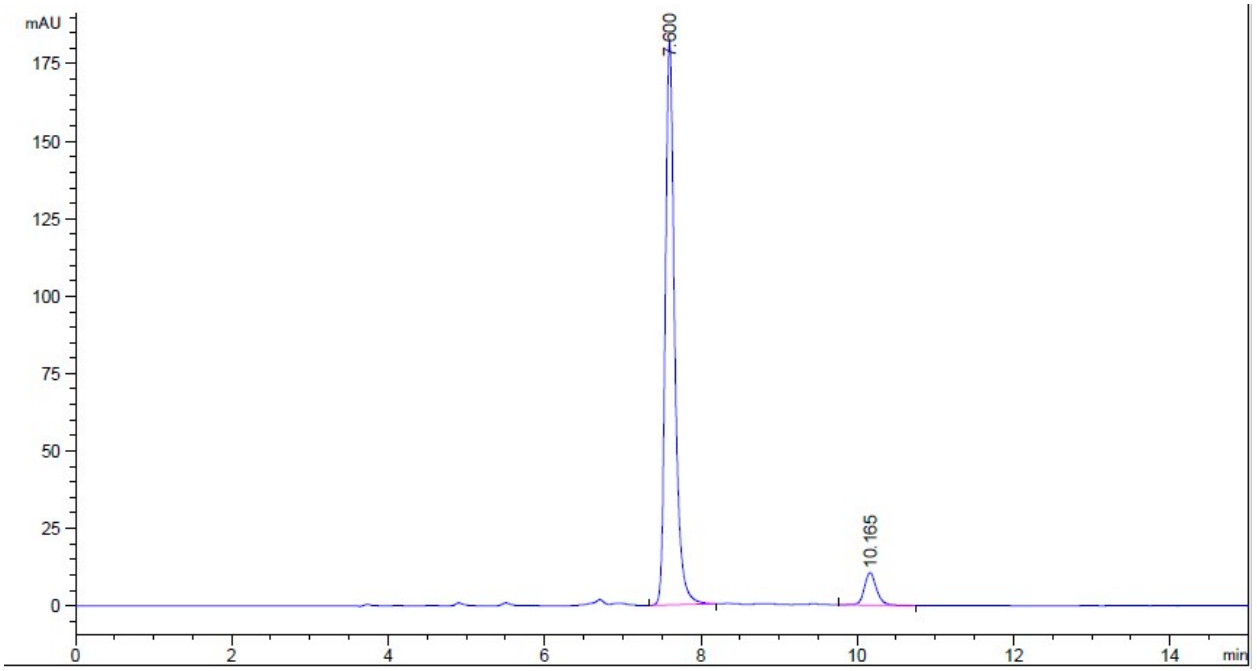



169.12
146.54
142.17
140.02
129.63
129.40
128.37
128.22
128.14
127.79
107.18
71.68
70.19
64.76
60.07
50.70
27.88
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



信号 1: VWD1 A, Wavelength=250 nm

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.584	BV	0.1254	5684.93750	688.05481	50.0479
2	10.107	BB	0.1603	5674.05957	541.37012	49.9521



信号 1: VWD1 A, Wavelength=250 nm

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.600	BB	0.1261	1512.76465	181.84796	92.9775
2	10.165	BB	0.1644	114.25712	10.54263	7.0225