# Supplementary Materials

# $\alpha$-Hydroxylactams as efficient entries to diversely functionalized ferrociphenols: Synthesis and anticancer activity studies

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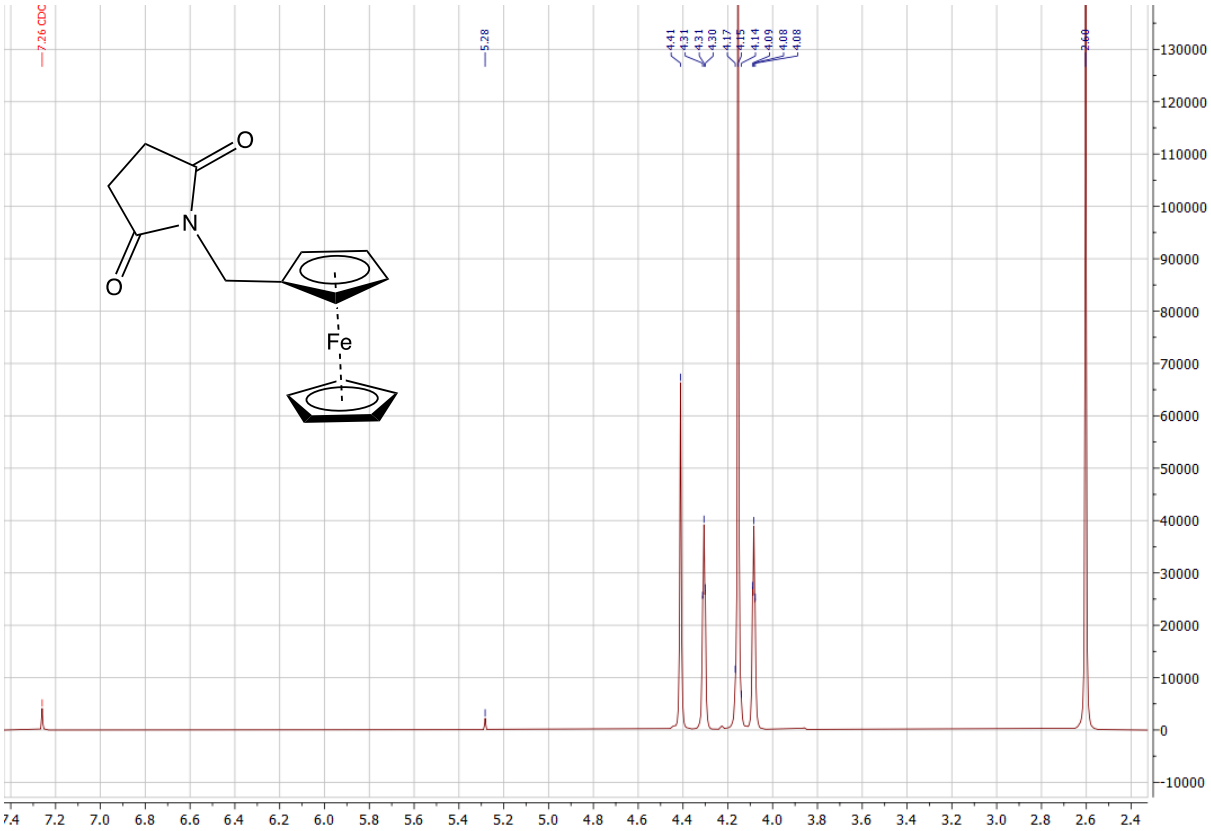
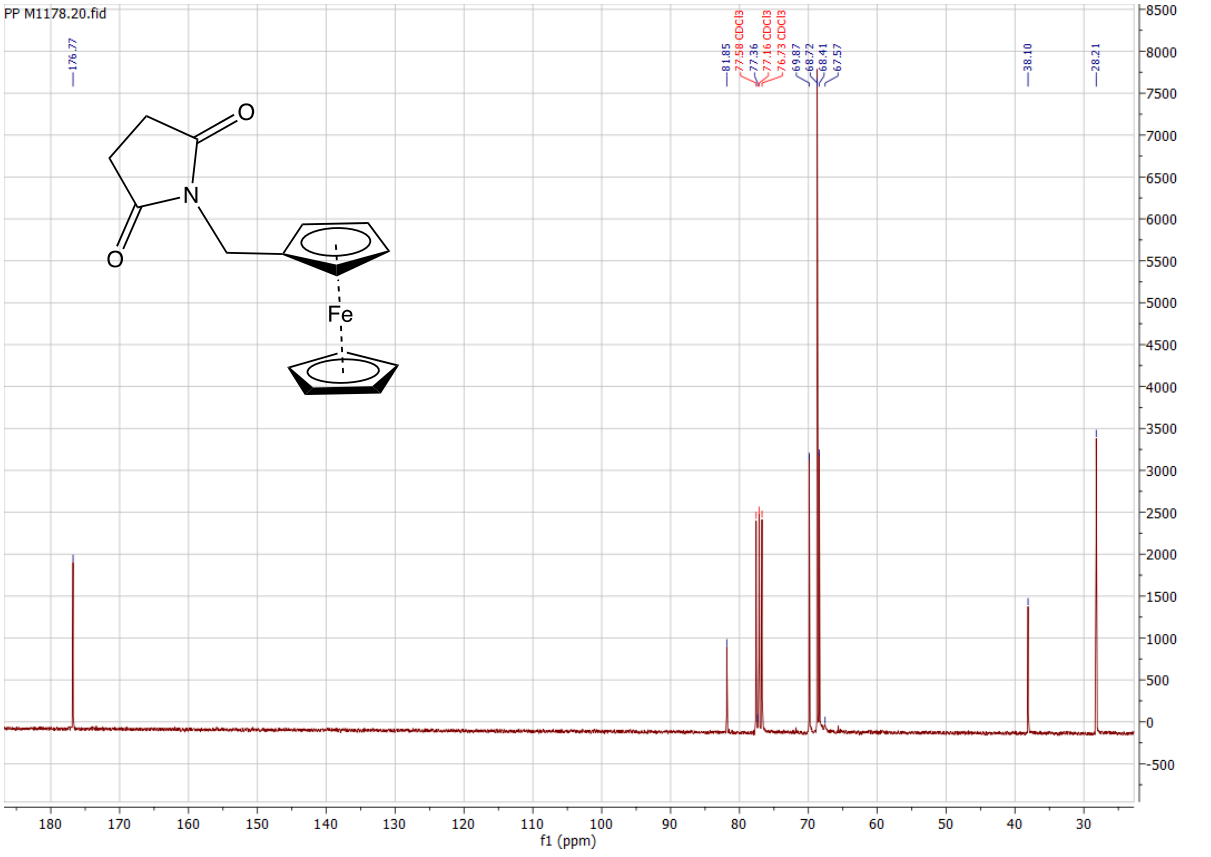
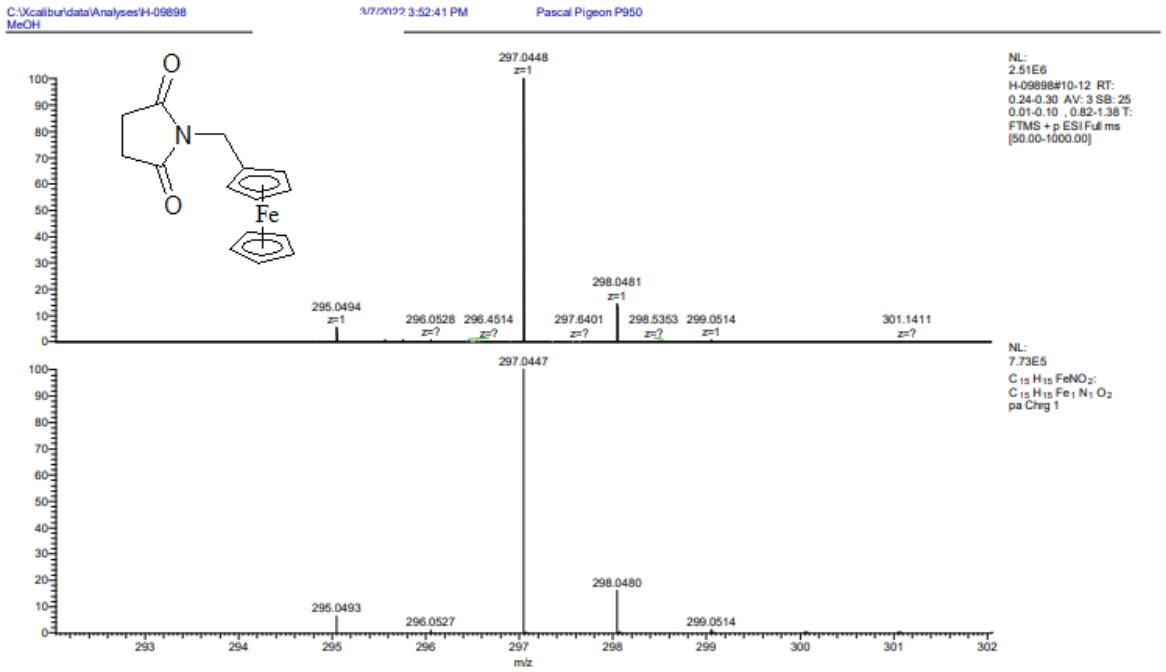
**Figure S1**: $^{1}H$ (in $CDCl_3$), $^{13}C$ (in $CDCl_3$) NMR, HR-MS and IR data for compound **3a**






# Experimental/theoretical isotopic pattern MS spectrum

**Error = 0.4 ppm; Relative Intensity (%) 100**

**HRMS (ESI) m/z: [M]+ Calcd for C15H15FeNO2 297.0447 . Found 297.0448; (Error: 0.4 ppm).**

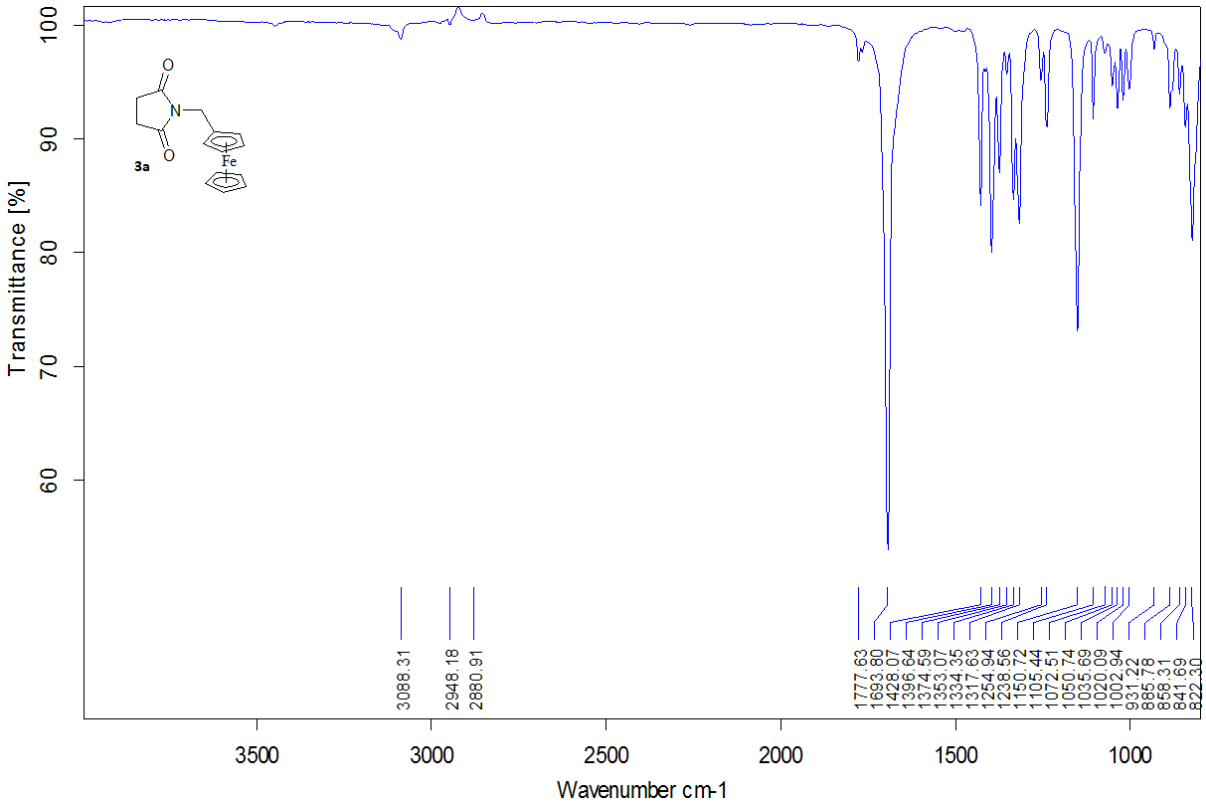
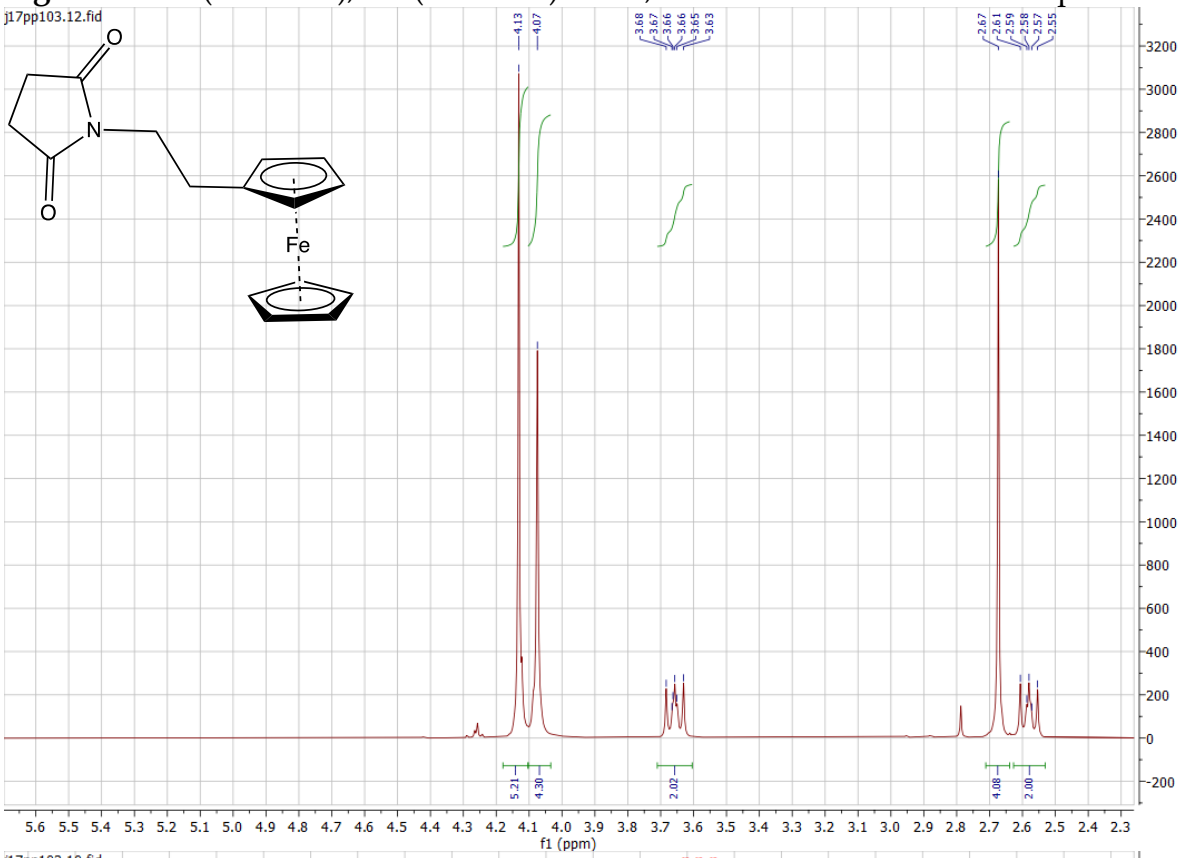
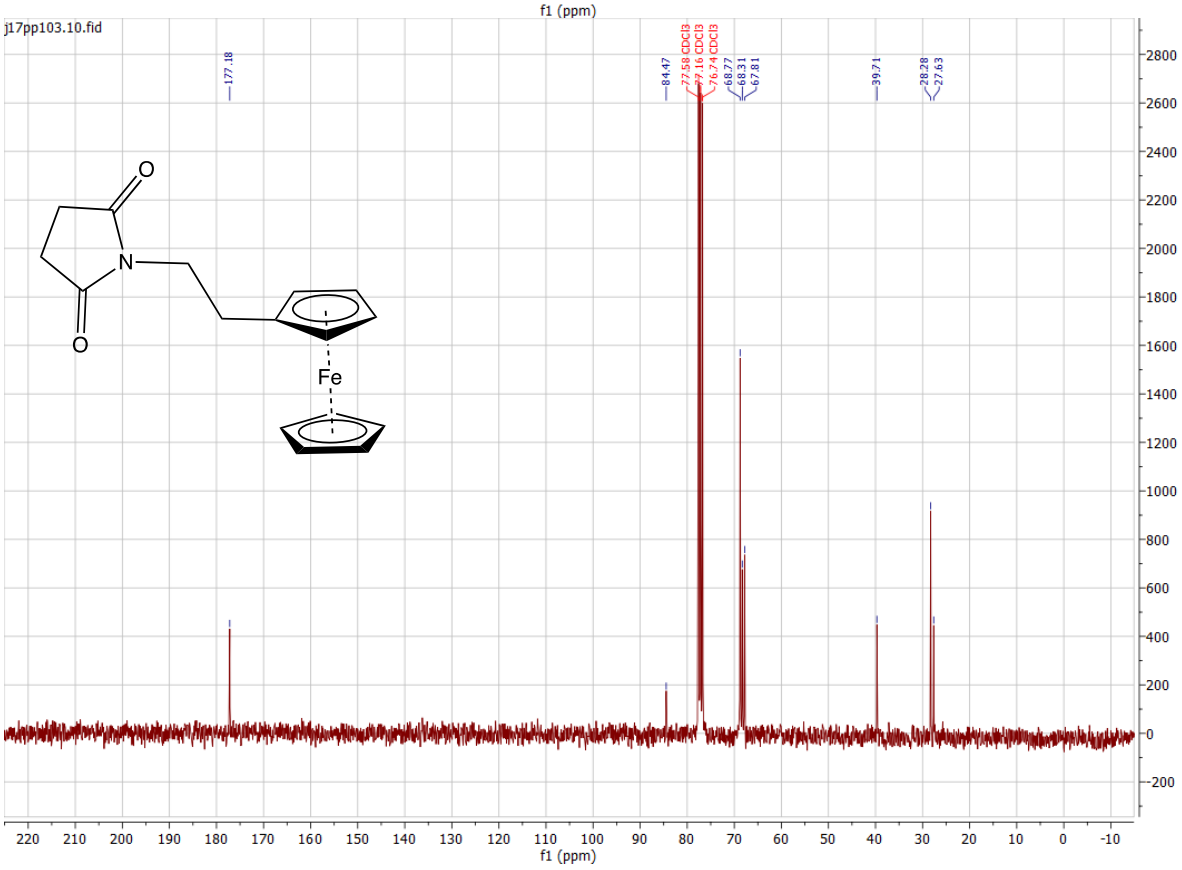


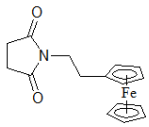
**Figure S2**: $^{1}H$ (in $CDCl_3$), $^{13}C$ (in $CDCl_3$) NMR, HR-MS and IR data for compound **3b**



**Single Mass Analysis**
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

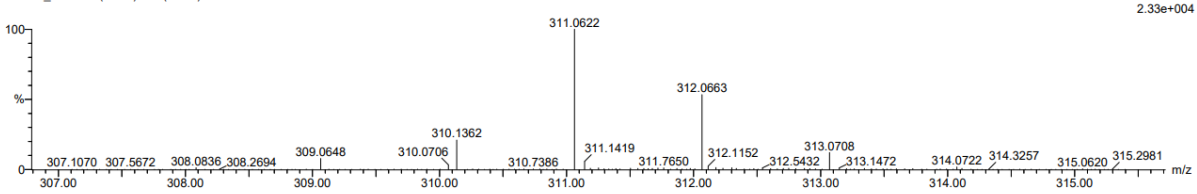
Monoisotopic Mass, Odd Electron Ions
291 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 1-120 N: 0-10 O: 0-10 Fe: 1-1



06-Sep-2013 5::7::2
ENSCP_P729 21 (0.572) Cm (18:24)

MeOH

LCT Premier XE KE483
1: TOF MS ES+
2.33e+004




| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 5.0 | 5.0 | 100.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 311.0622 | 311.0609 | 1.3 | 4.2 | 9.0 | 724.2 | 0.0 | C16 H17 N O2 Fe |

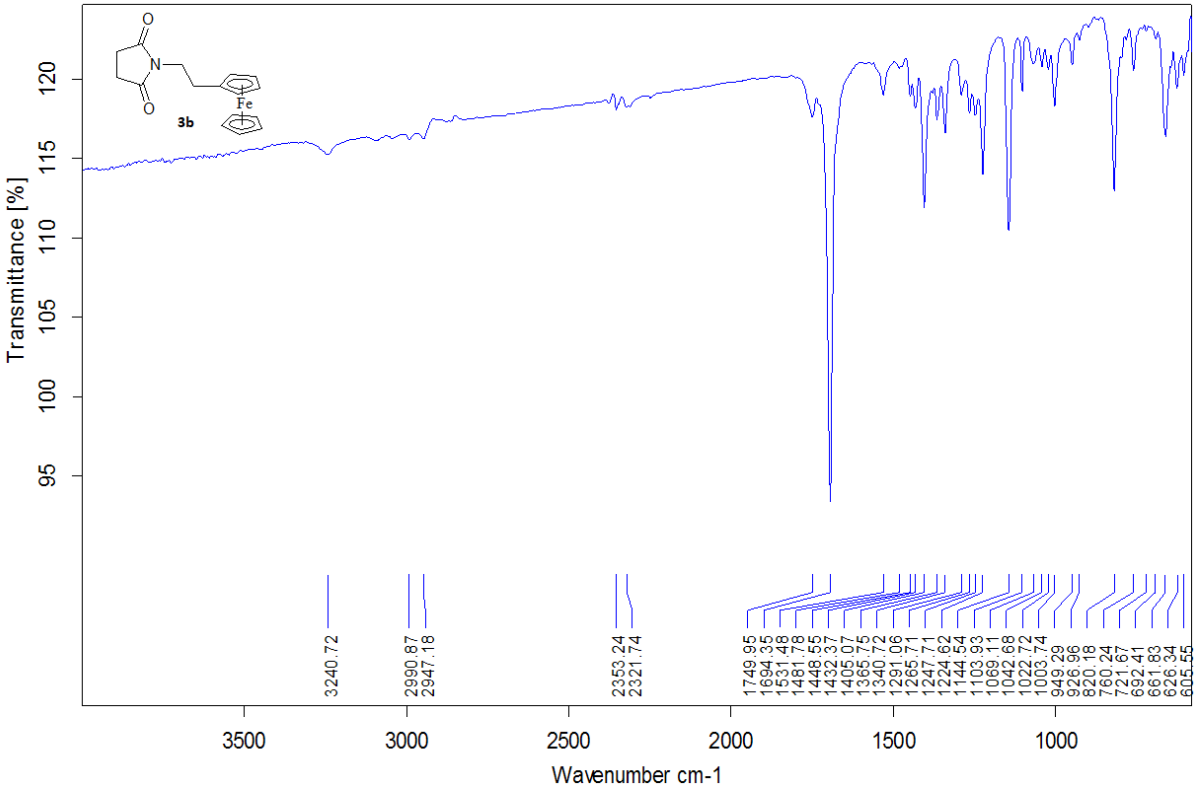
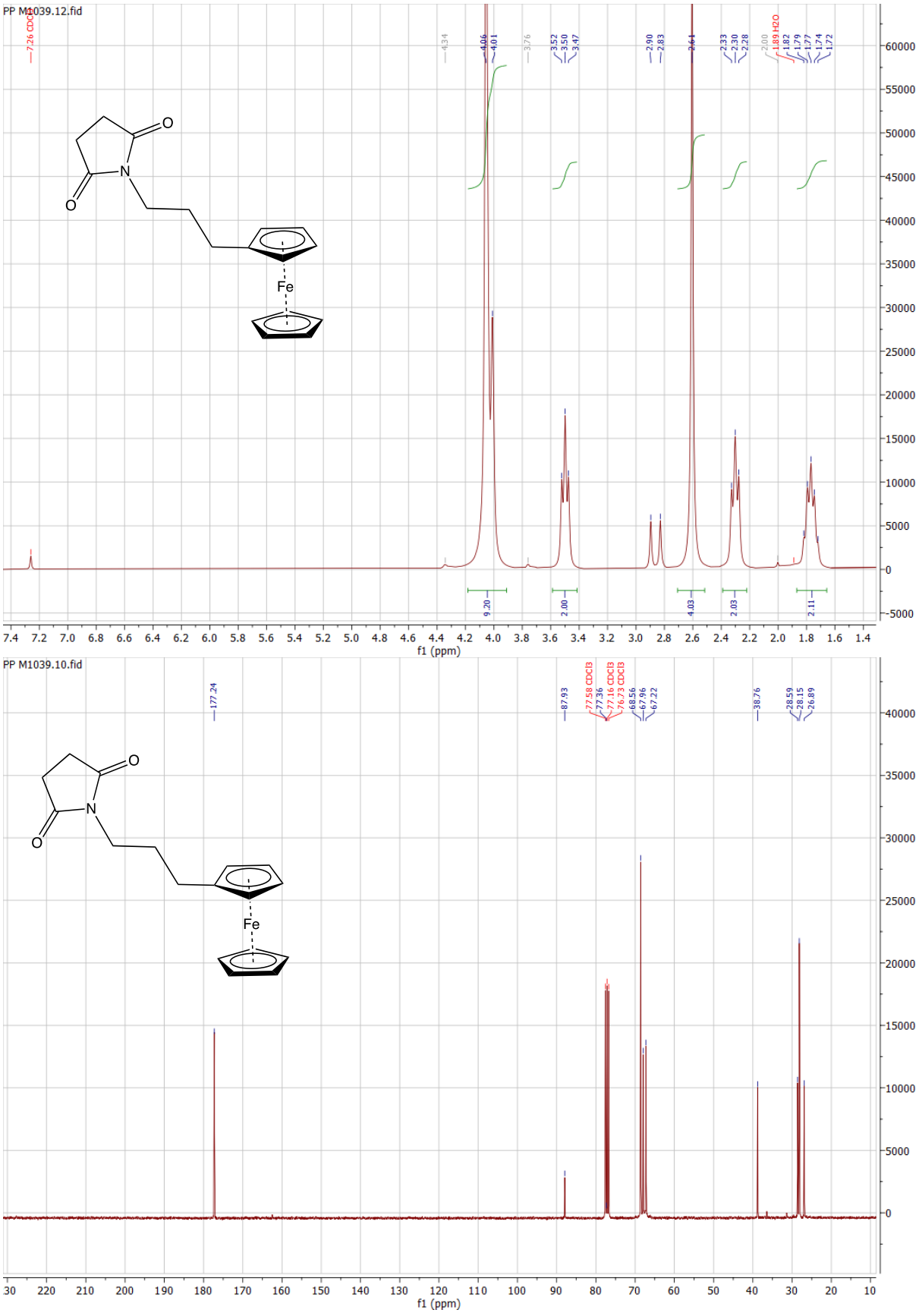
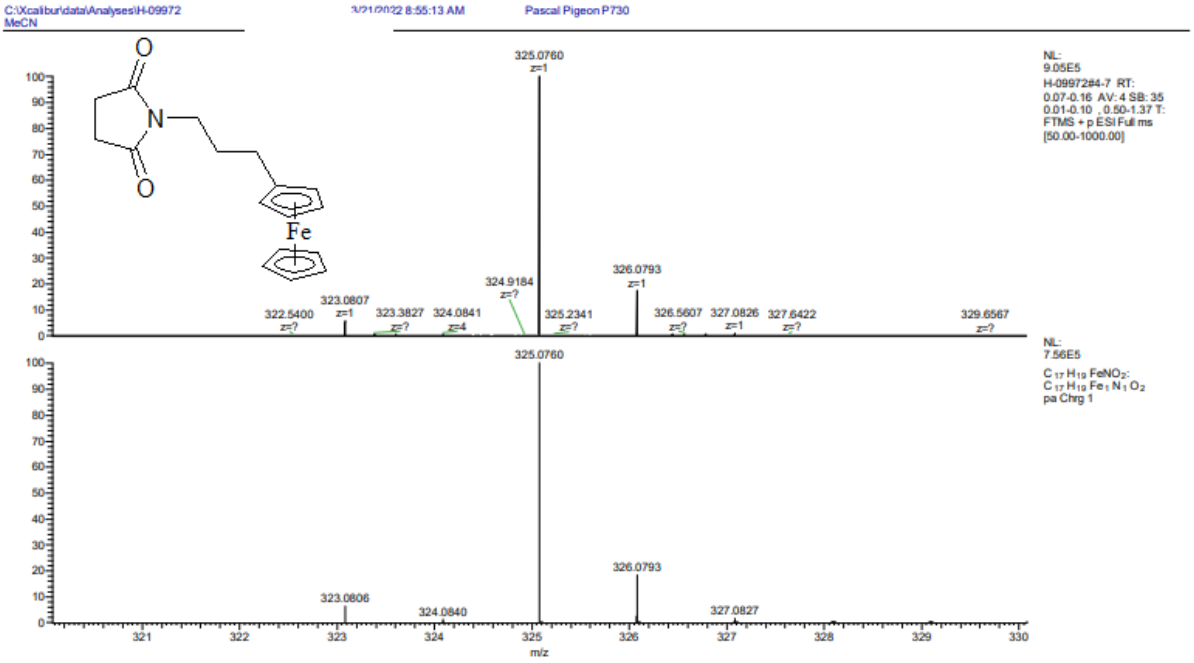


**Figure S3**: $^{1}H$ (in $CDCl_3$), $^{13}C$ (in $CDCl_3$) NMR, HR-MS and IR data for compound **3c**






# Experimental/theoretical isotopic pattern MS spectrum

**Error = 0.1 ppm; Relative Intensity (%) 100**

**HRMS (ESI) m/z: [M]+ Calcd for C17H19FeNO2 325.0760 . Found 325.076; (Error: 0.1 ppm).**

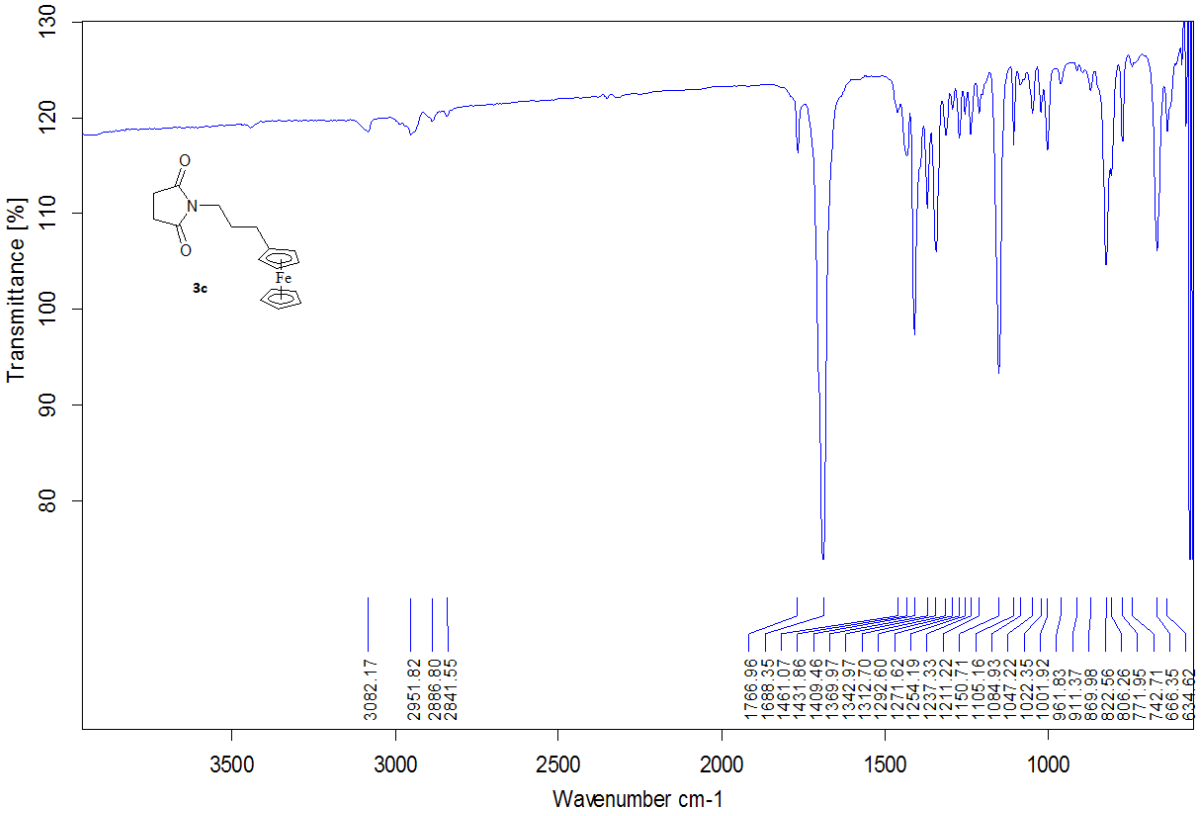
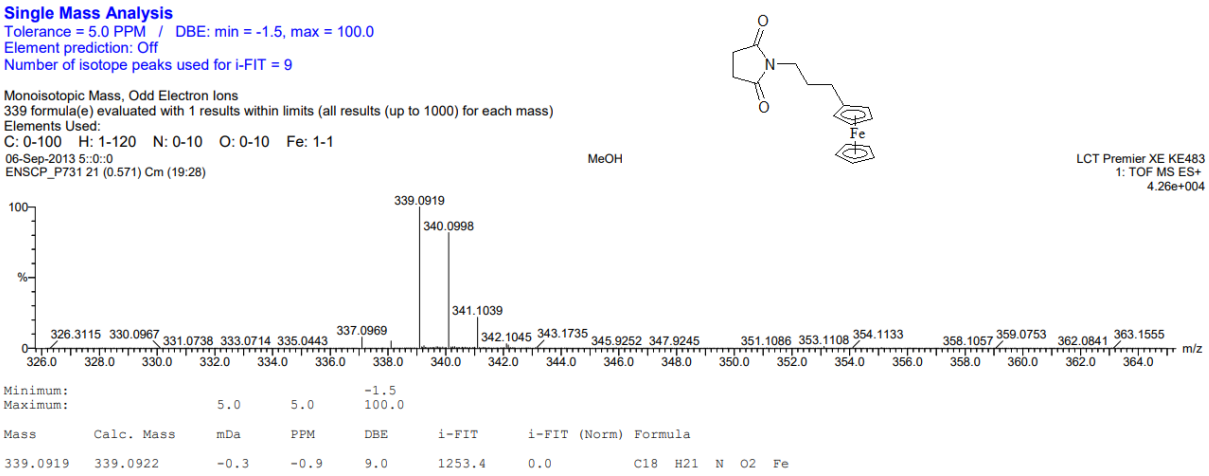


**Figure S4**: HR-MS and IR data for compound **3d**



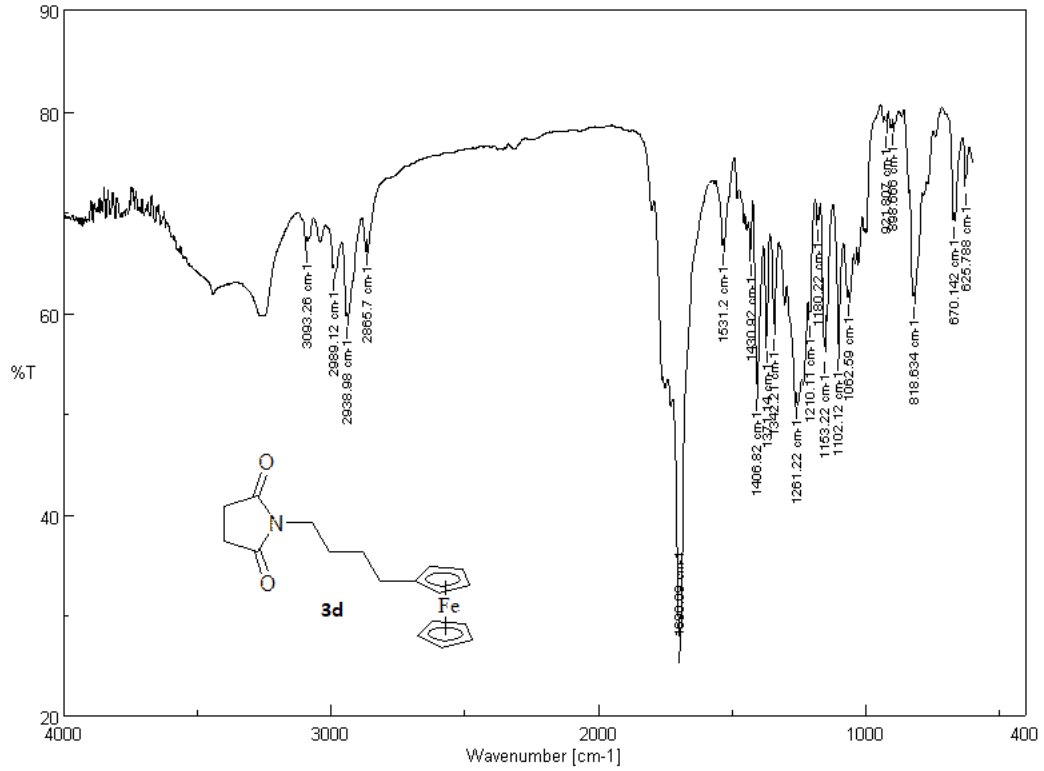
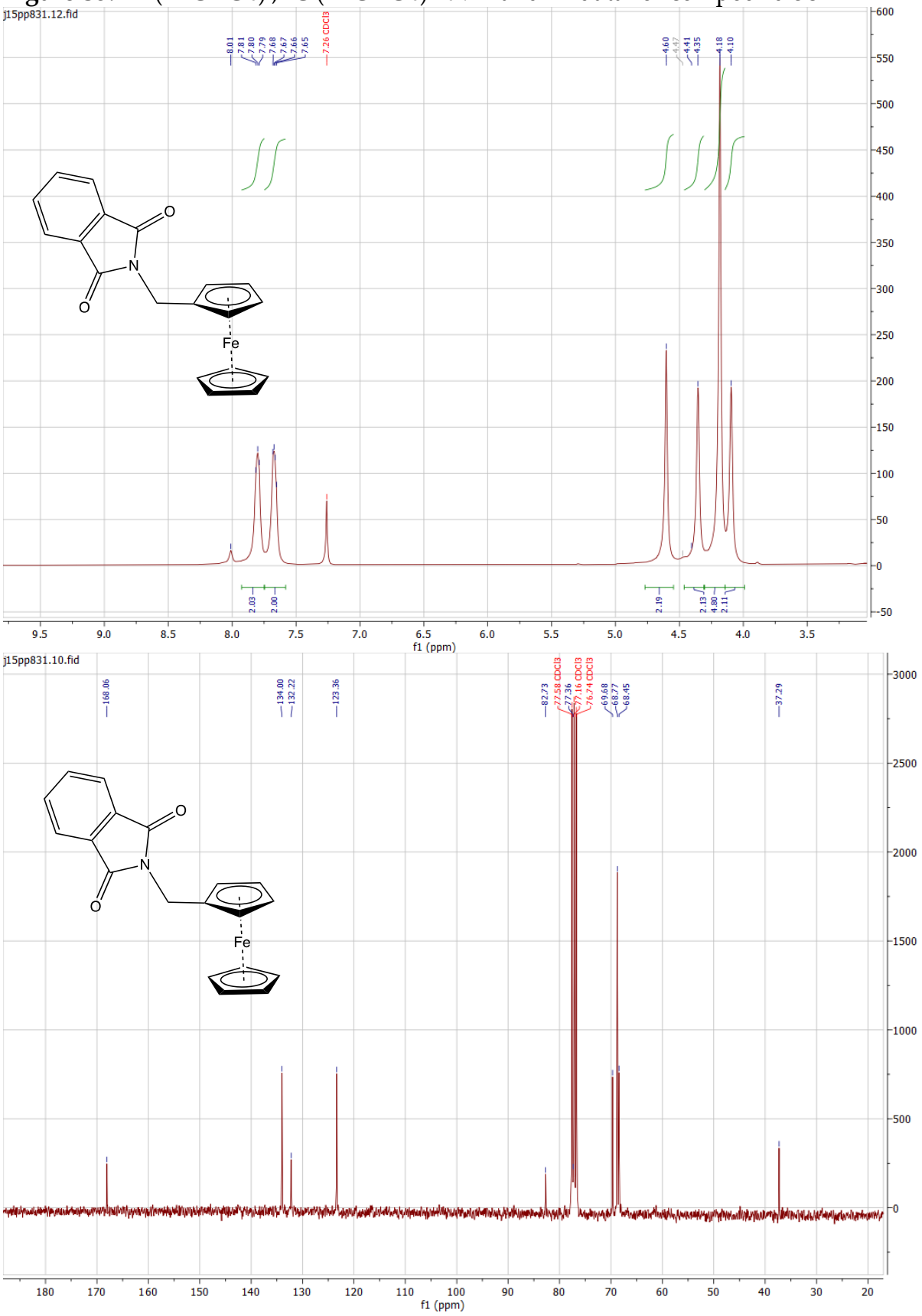



**Figure S5**: $^{1}H$ (in $CDCl_3$) ,$^{13}C$ (in $CDCl_3$) NMR and IR data for compound **3e**



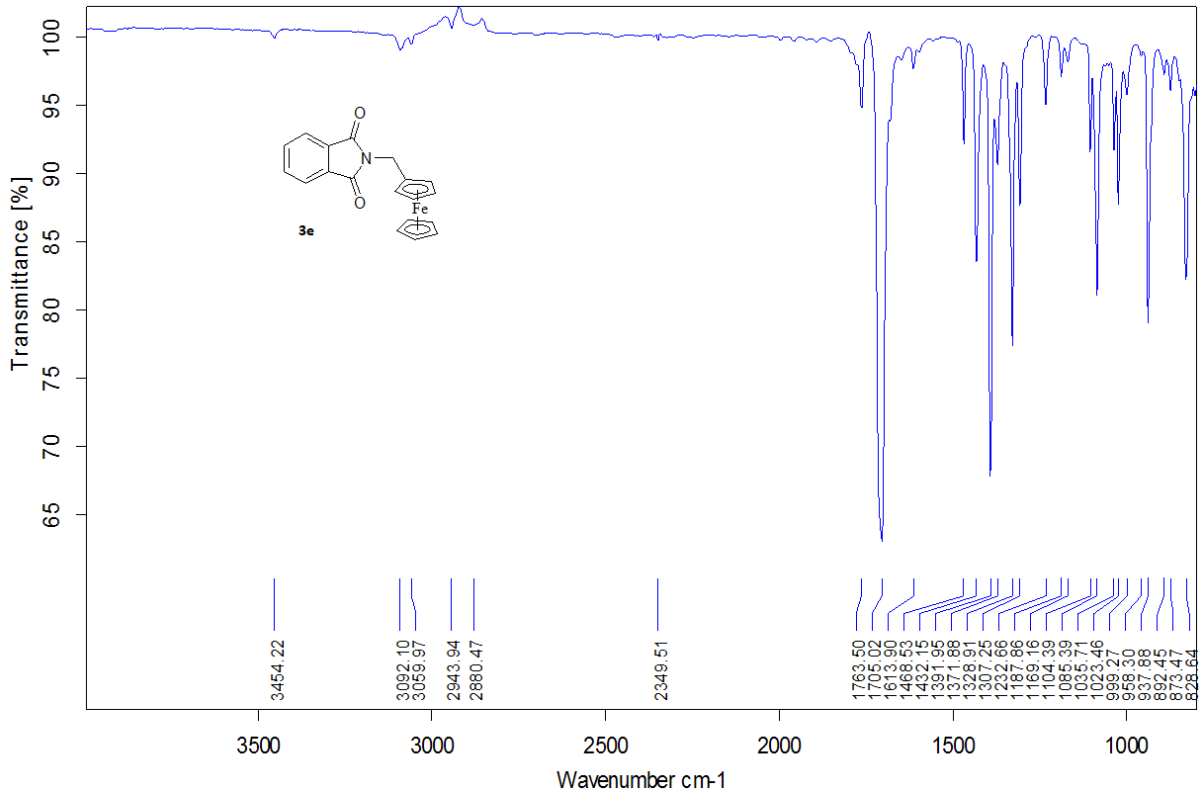
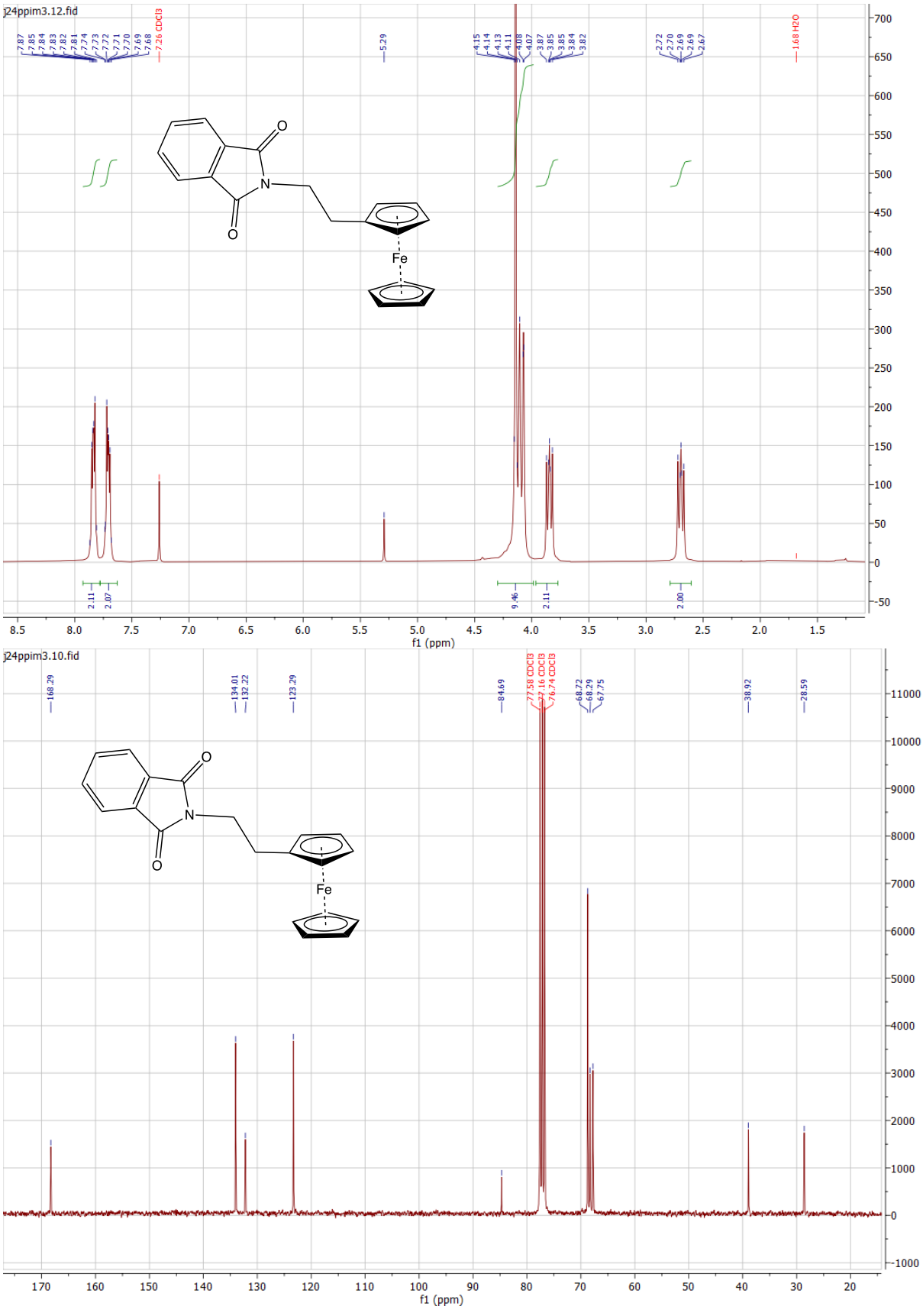
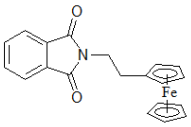

Transmittance [%]
100
95
90
85
80
75
70
65
3e
3454.22
3092.10
3059.97
2943.94
2880.47
2349.51
1763.50
1705.02
1613.90
1468.53
1432.15
1391.95
1371.88
1328.91
1307.25
1232.66
1187.86
1169.16
1104.39
1085.39
1035.71
1023.46
999.27
958.30
937.88
892.45
873.47
828.64
3500
3000
2500
2000
1500
1000
Wavenumber cm-1

**Figure S6**: $^{1}H$ (in $CDCl_3$), $^{13}C$ (in $CDCl_3$) NMR HR-MS and IR for compound **3f**



**Single Mass Analysis**
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

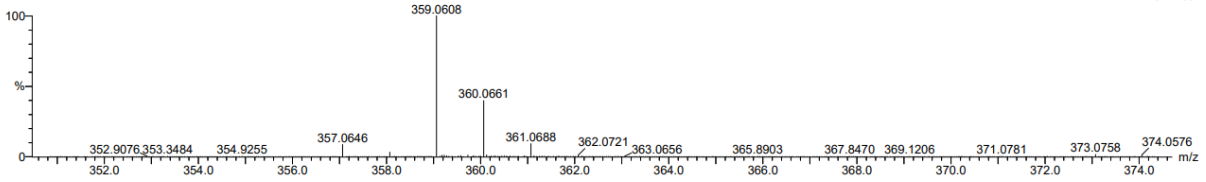
Monoisotopic Mass, Odd Electron Ions
365 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 1-120 N: 0-10 O: 0-10 Fe: 1-1




06-Sep-2013 5::9::2
ENSCP_P654 28 (0.714) Cm (28:39)

MeOH

LCT Premier XE KE483
1: TOF MS ES+
2.02e+004




| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 5.0 | 5.0 | 100.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 359.0608 | 359.0609 | -0.1 | -0.3 | 13.0 | 920.5 | 0.0 | C20 H17 N O2 Fe |
| | 359.0600 | 0.8 | 2.2 | 1.0 | 930.3 | 9.7 | C4 H17 N9 O7 Fe |

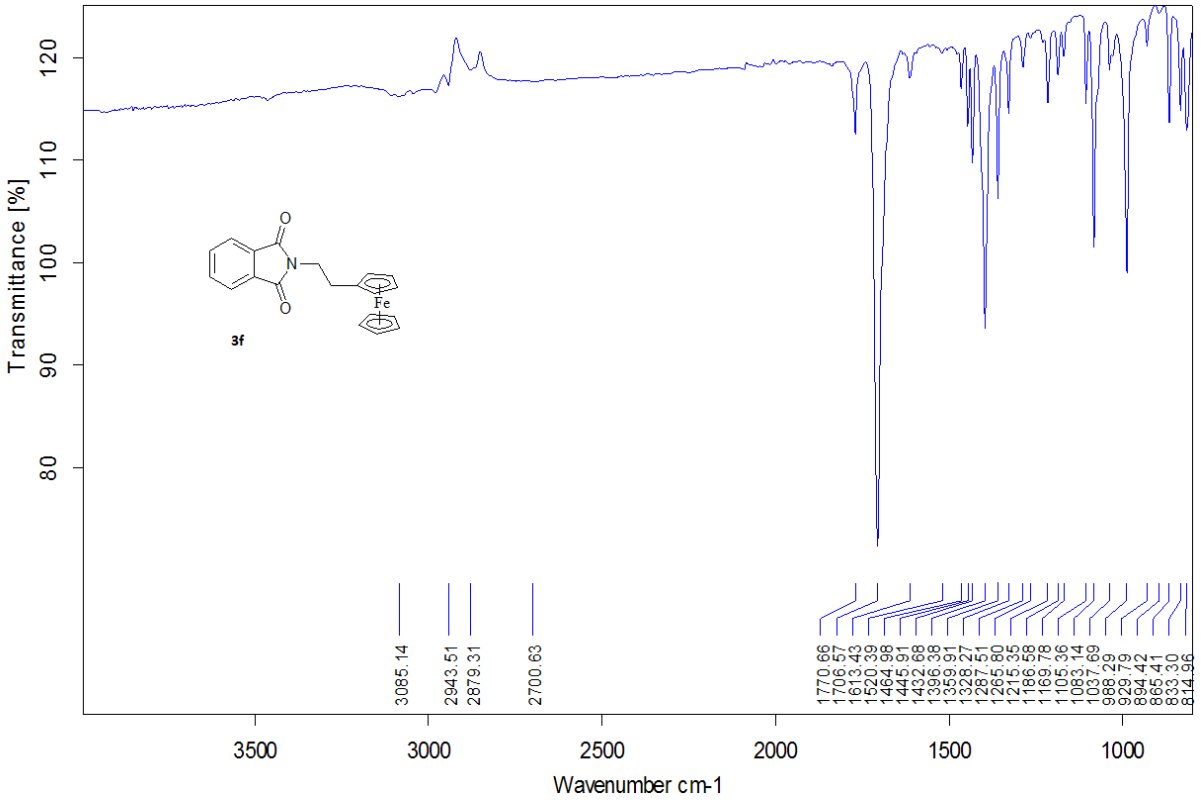
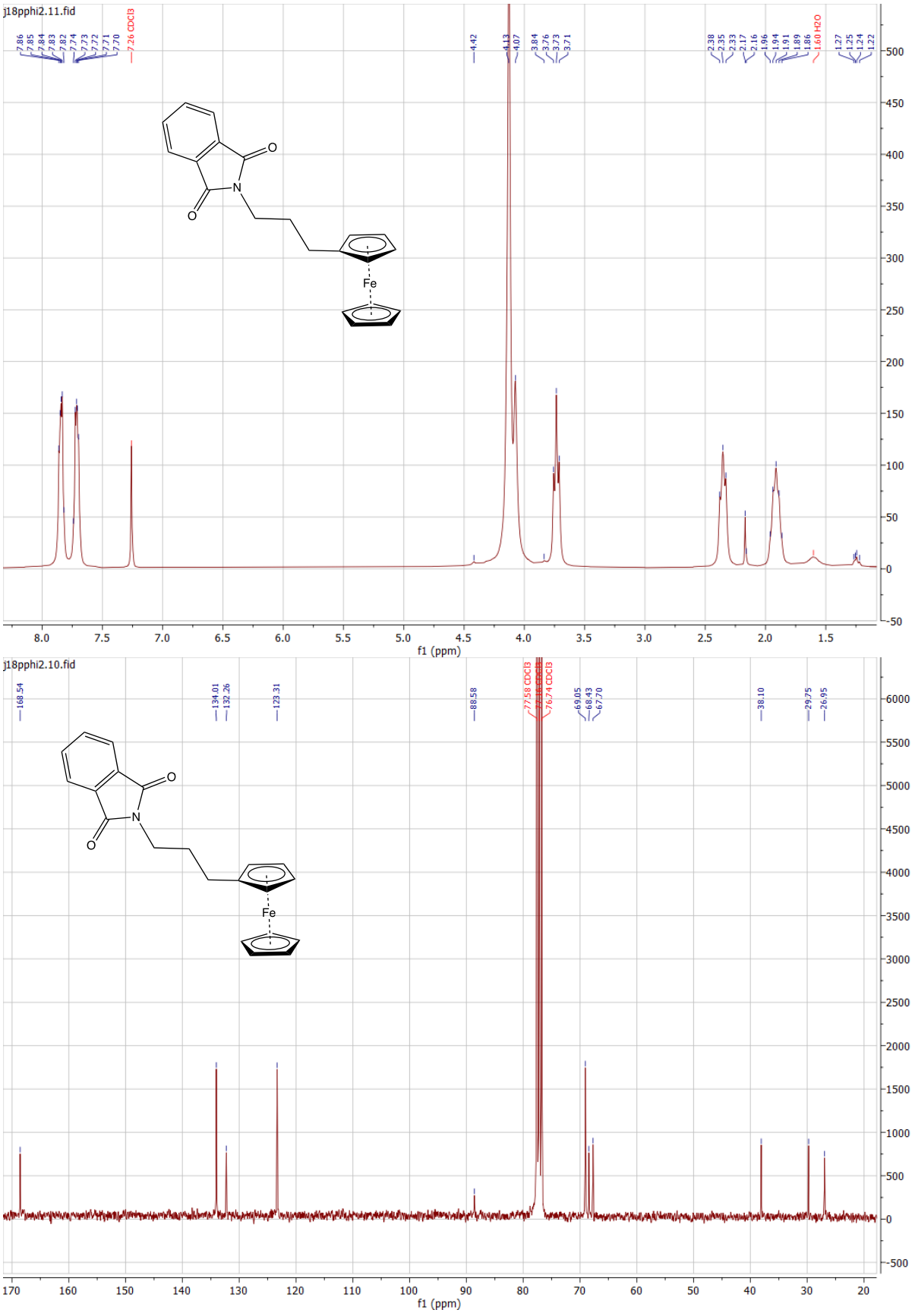
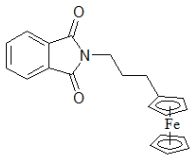


**Figure S7**: $^{1}H$ (in $CDCl_3$), $^{13}C$ (in $CDCl_3$) NMR, HR-MS and IR data for compound **3g**



**Single Mass Analysis**
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

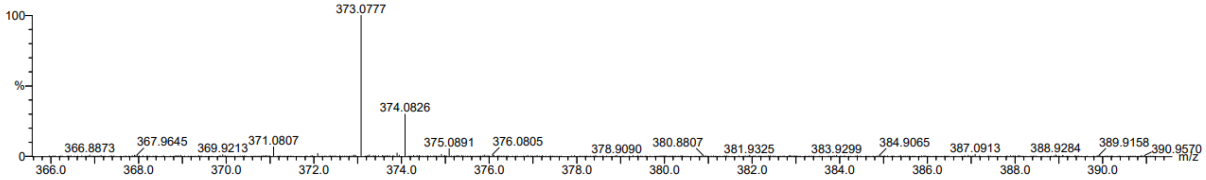
Monoisotopic Mass, Odd Electron Ions
156 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 1-150 H: 1-150 N: 0-3 O: 0-10 Fe: 1-1




19-Jun-2013 3::2::0
ENSCP_P659 57 (1.384) Cm (55:60)

ACN

LCT Premier XE KE483
1: TOF MS ES+
1.96e+003




| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 5.0 | 5.0 | 100.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 373.0777 | 373.0765 | 1.2 | 3.2 | 13.0 | 457.1 | 0.0 | C21 H19 N O2 Fe |
| | 373.0784 | -0.7 | -1.9 | 0.0 | 463.7 | 6.6 | C9 H23 N3 O9 Fe |

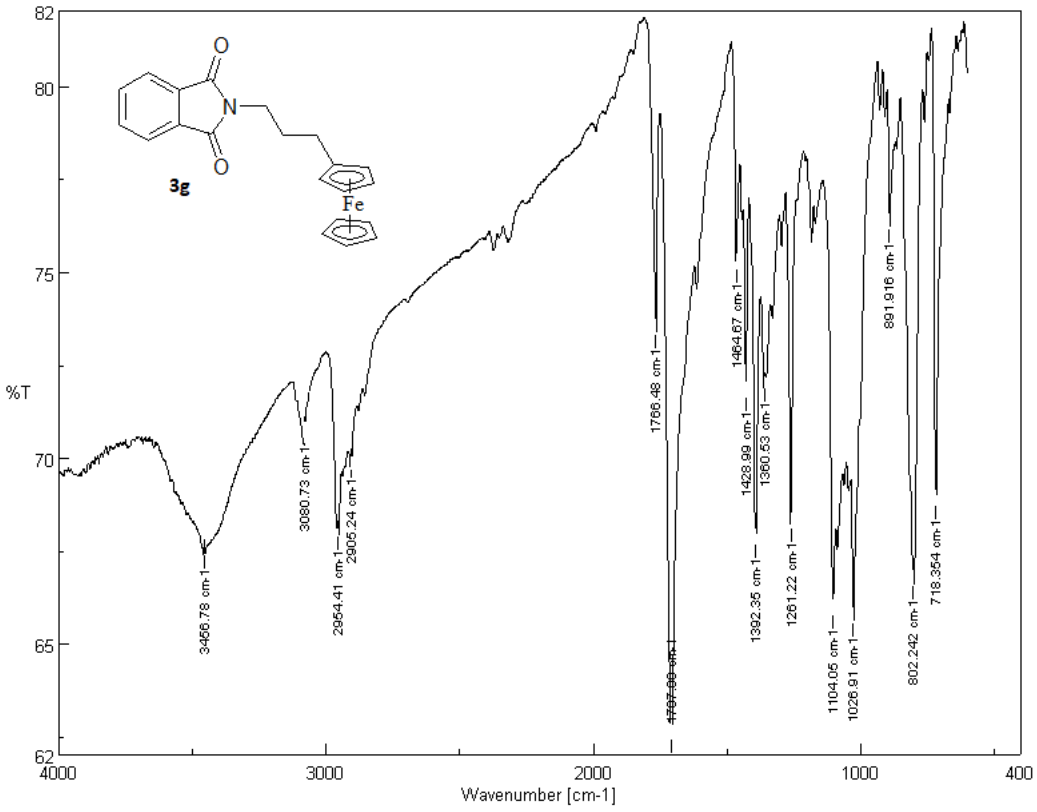
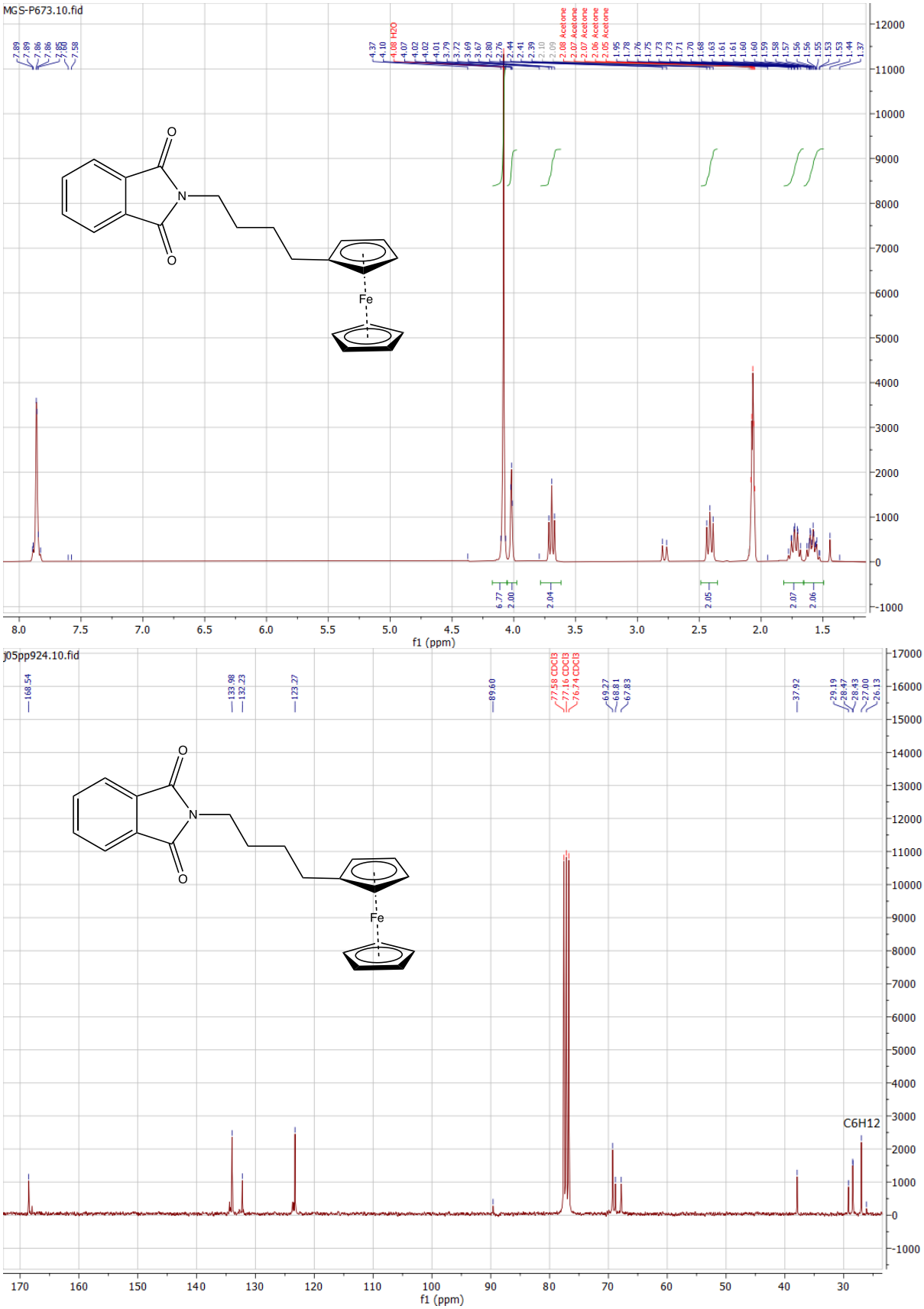
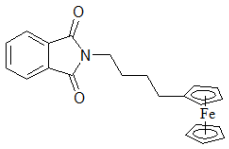


**Figure S8**: $^{1}H$ (in acetone-$d_6$), $^{13}C$ (in $CDCl_3$) NMR, HR-MS and IR data for compound **3h**



**Single Mass Analysis**
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

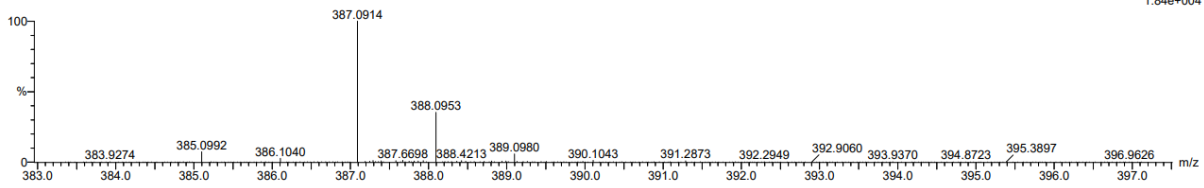
Monoisotopic Mass, Odd Electron Ions
164 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 1-150 H: 1-150 N: 0-3 O: 0-10 Fe: 1-1




19-Jun-2013 2::4::4
ENSCP_P673 49 (1.204) Cm (47:54)

ACN

LCT Premier XE KE483
1: TOF MS ES+
1.84e+004




| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 5.0 | 5.0 | 100.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 387.0914 | 387.0922 | -0.8 | -2.1 | 13.0 | 800.1 | 0.0 | C22 H21 N O2 Fe |

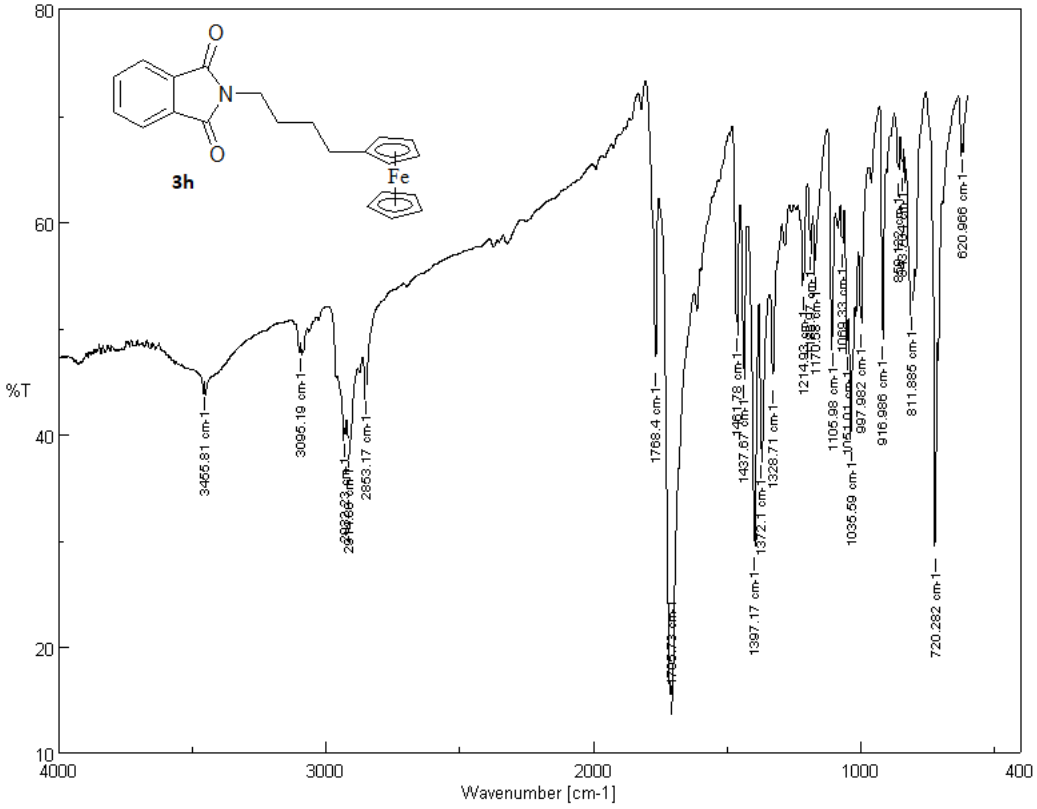
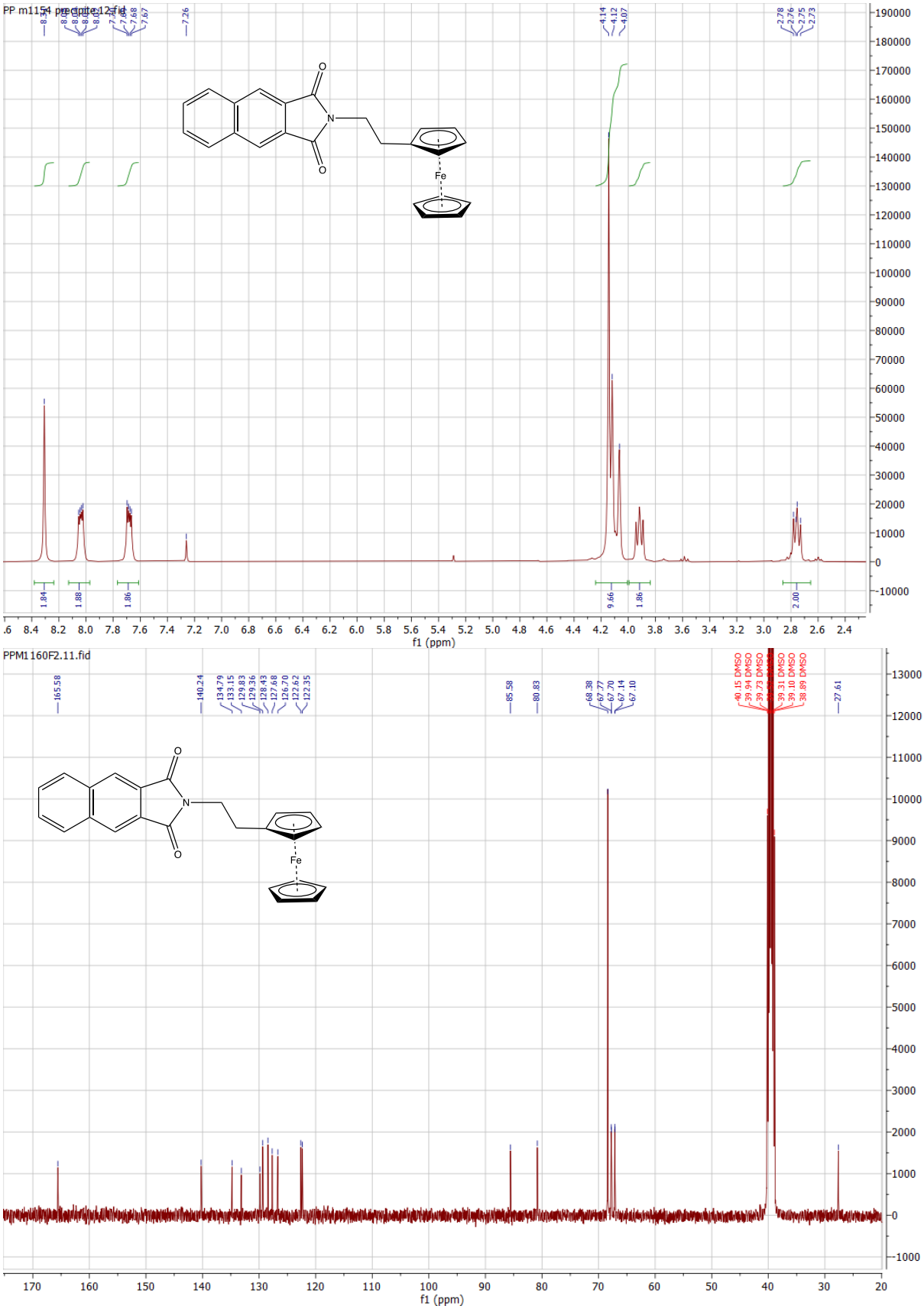
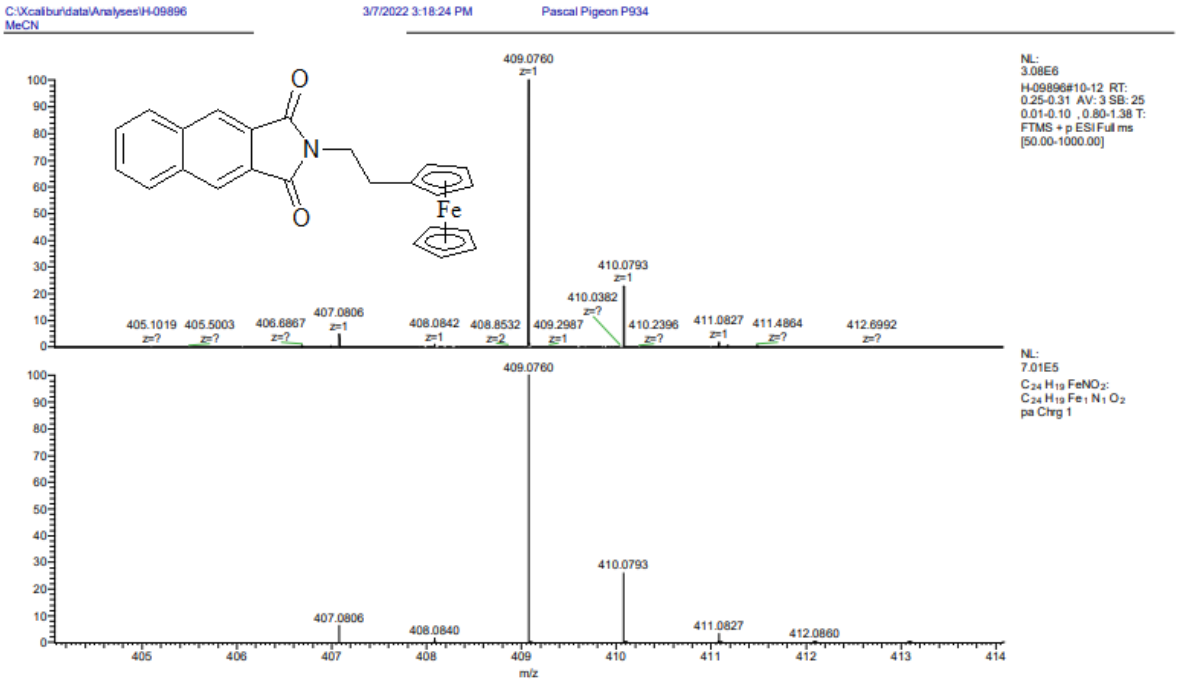


**Figure S9**: $^{1}H$ (in $CDCl_3$), $^{13}C$ (in DMSO-$d_6$) NMR, HR-MS and IR data for compound **3i**






# Experimental/theoretical isotopic pattern MS spectrum

**Error = 0.1 ppm; Relative Intensity (%) 100**

**HRMS (ESI) m/z: [M]+ Calcd for C24H19FeNO2 409.0760 . Found 409.076; (Error: 0.1 ppm).**

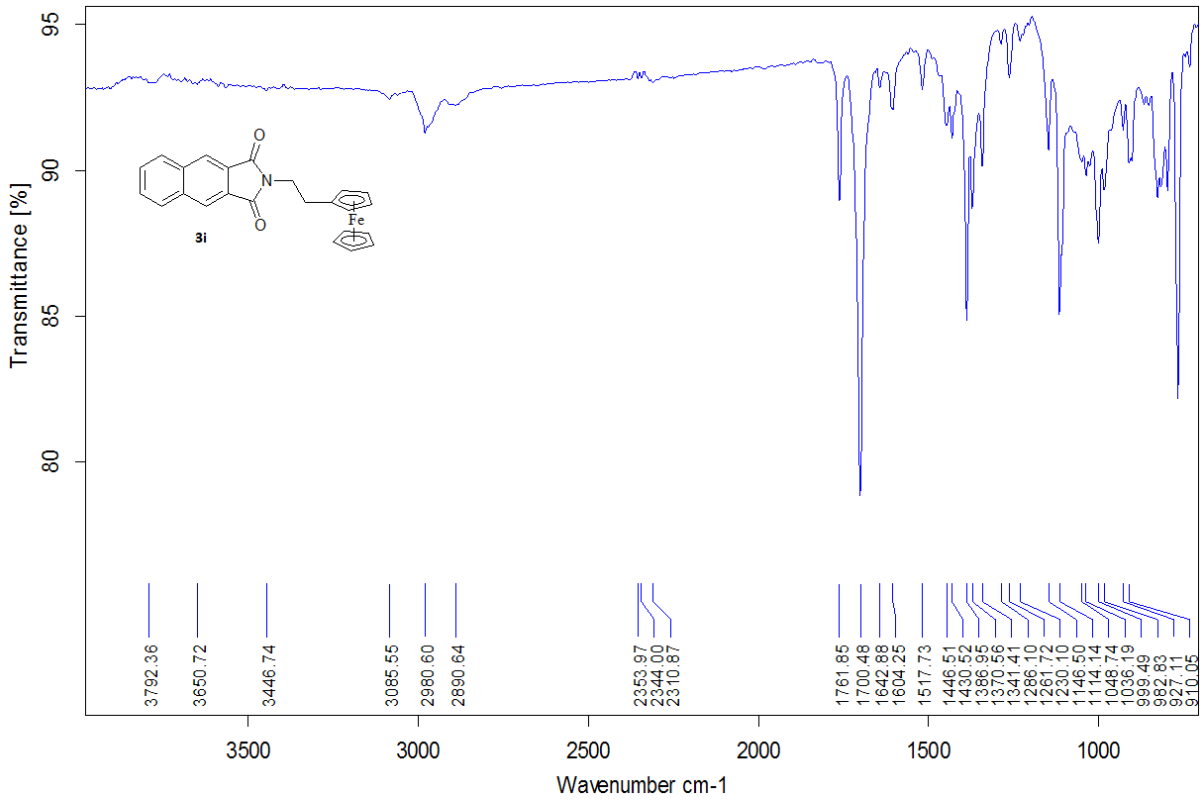
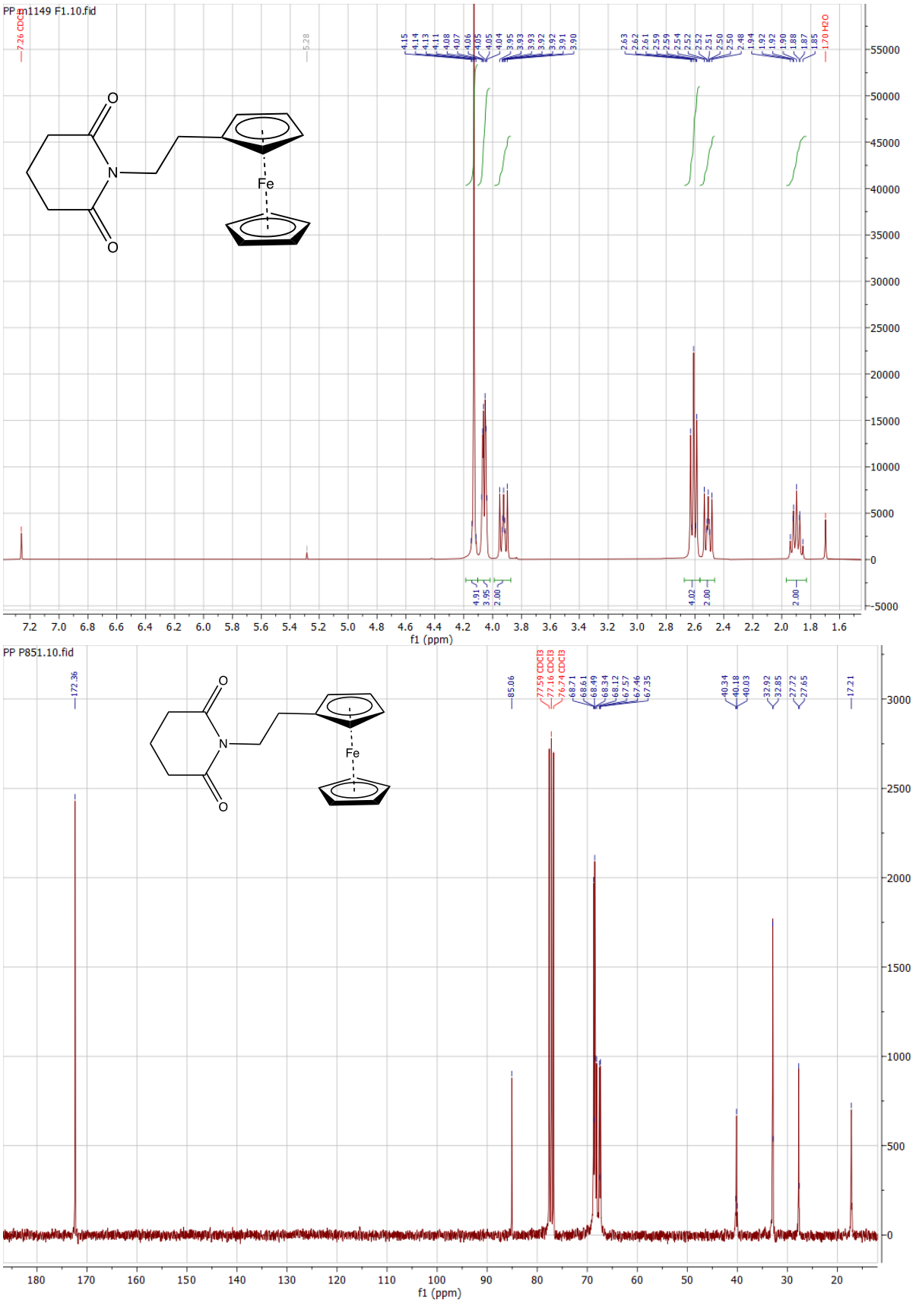
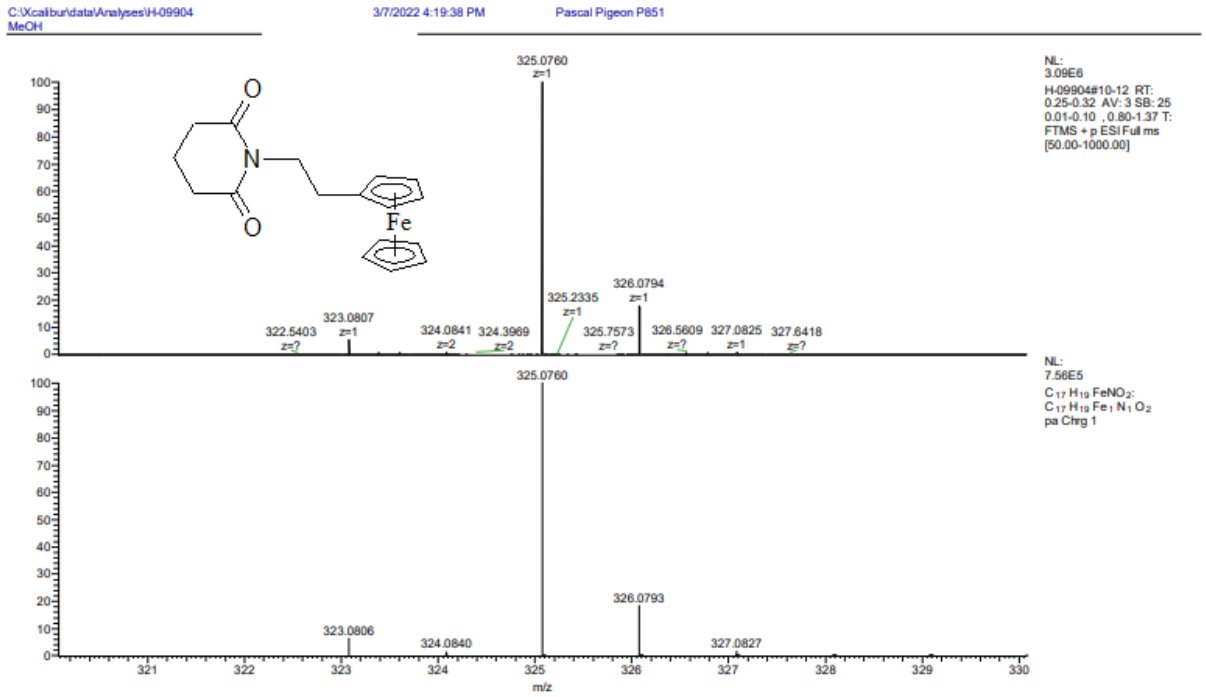


**Figure S10**: $^{1}H$ (in $CDCl_3$), $^{13}C$ (in $CDCl_3$) NMR, HR-MS and IR data for compound **3j**






# Experimental/theoretical isotopic pattern MS spectrum

**Error = 0.1 ppm; Relative Intensity (%) 100**

**HRMS (ESI) m/z: [M]+ Calcd for C17H19FeNO2 325.0760 . Found 325.076; (Error: 0.1 ppm).**

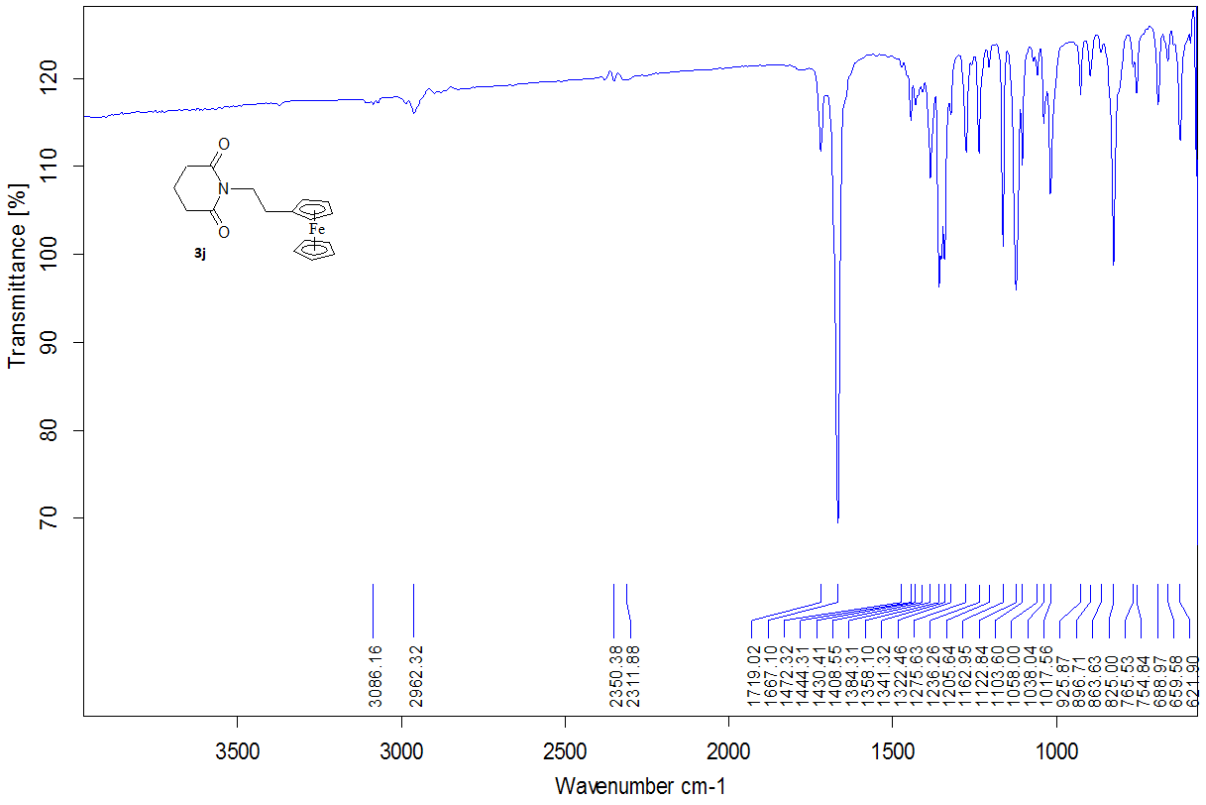
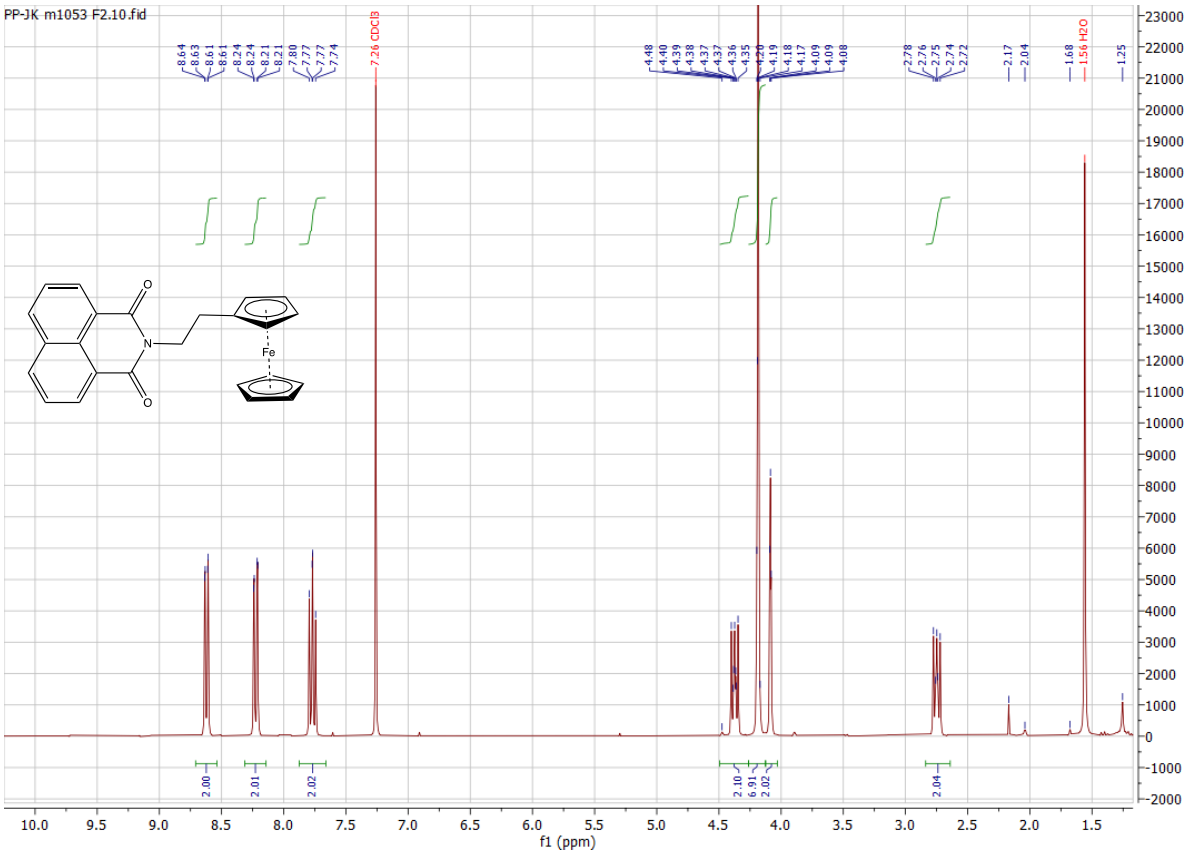
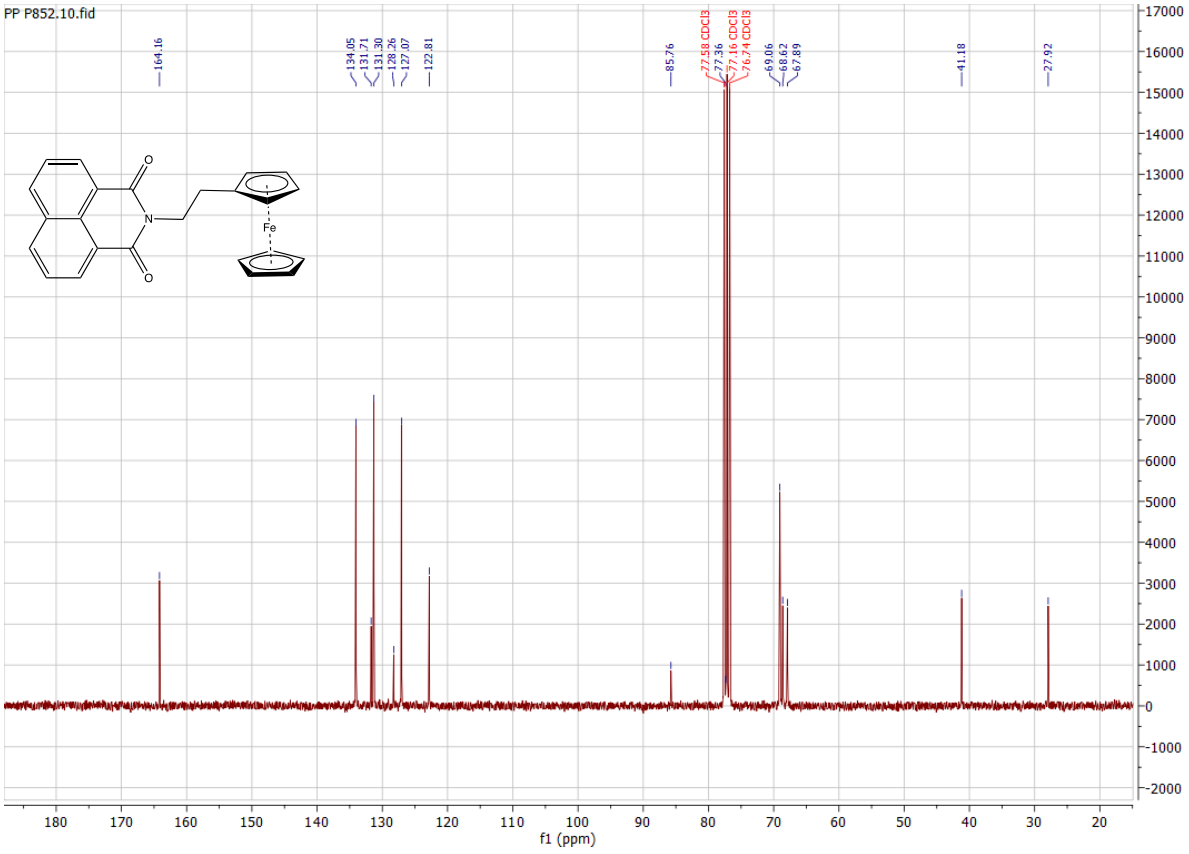
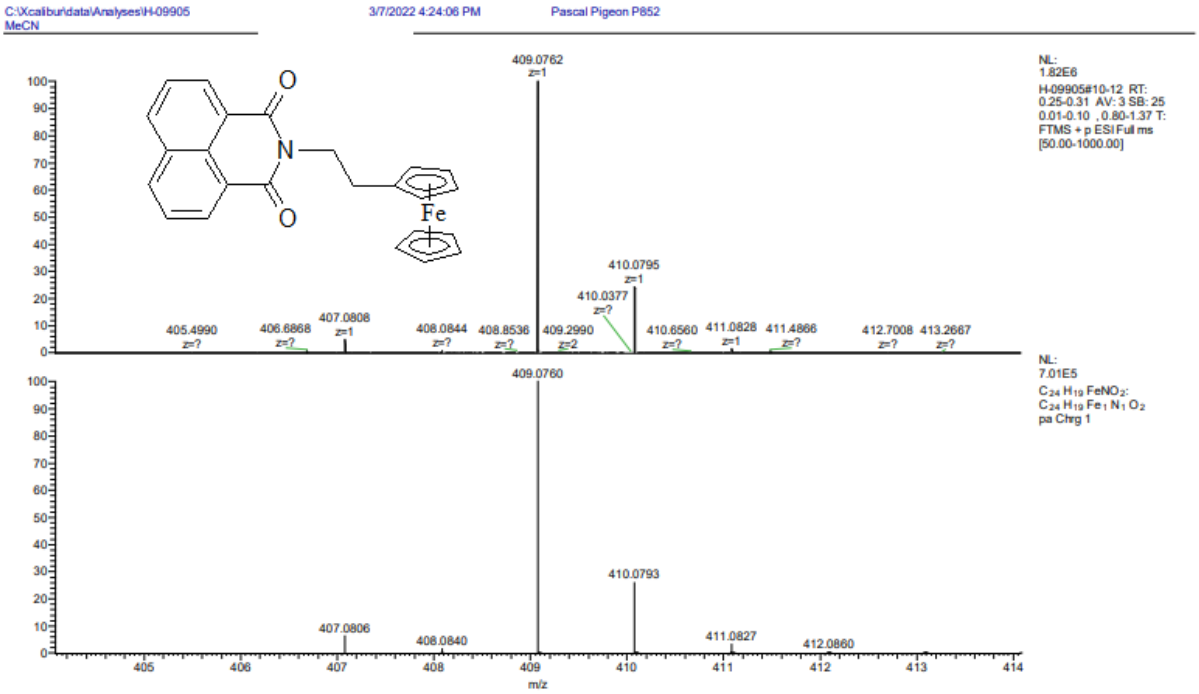


**Figure S11**: $^{1}H$ (in $CDCl_3$), $^{13}C$ (in $CDCl_3$) NMR, HR-MS and IR data for compound **3k**






# Experimental/theoretical isotopic pattern MS spectrum

**Error = 0.6 ppm; Relative Intensity (%) 100**

**HRMS (ESI) m/z: [M]+ Calcd for C24H19FeNO2 409.0760 . Found 409.0762; (Error: 0.6 ppm).**

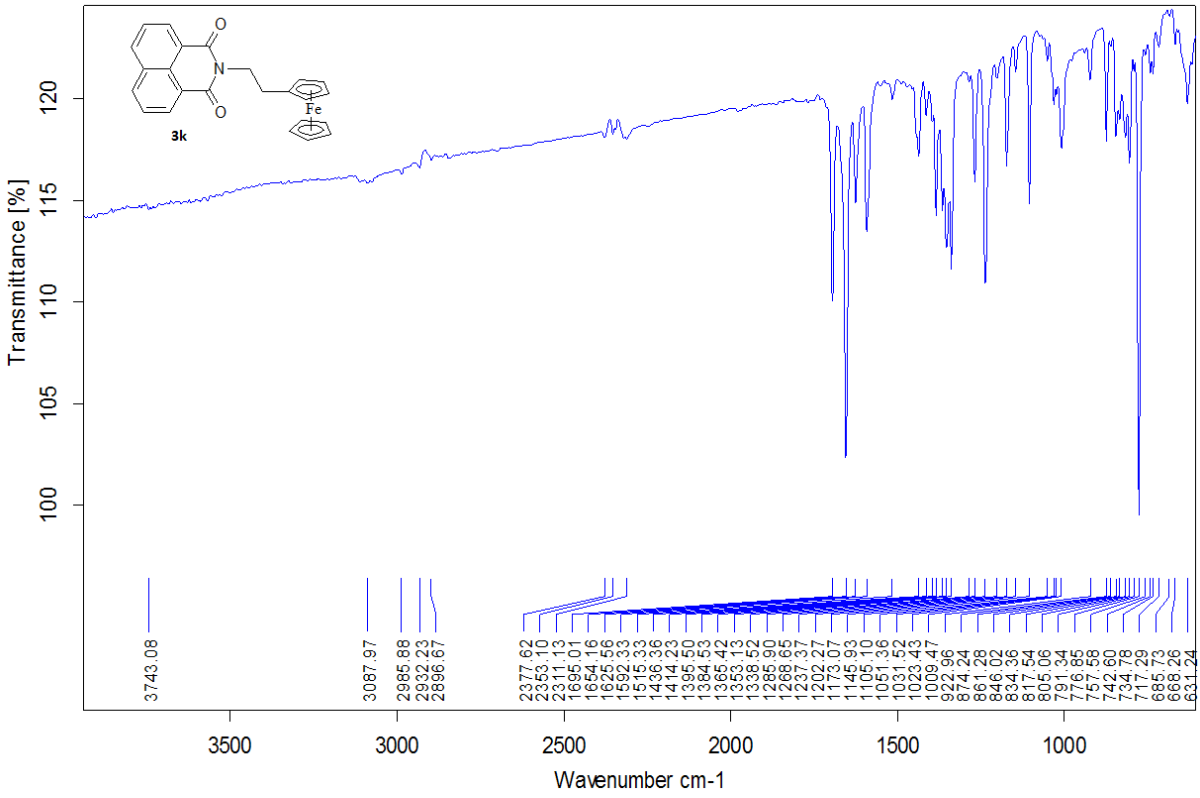
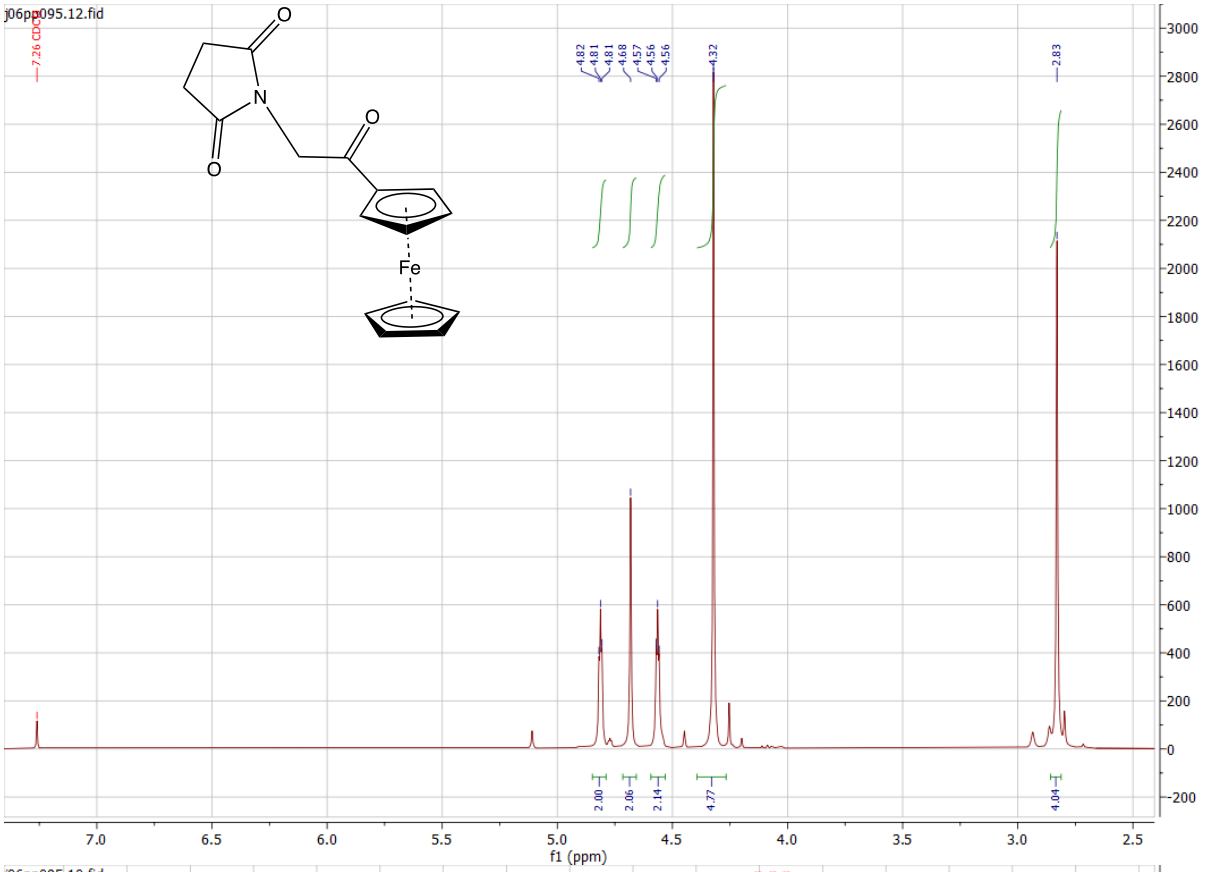
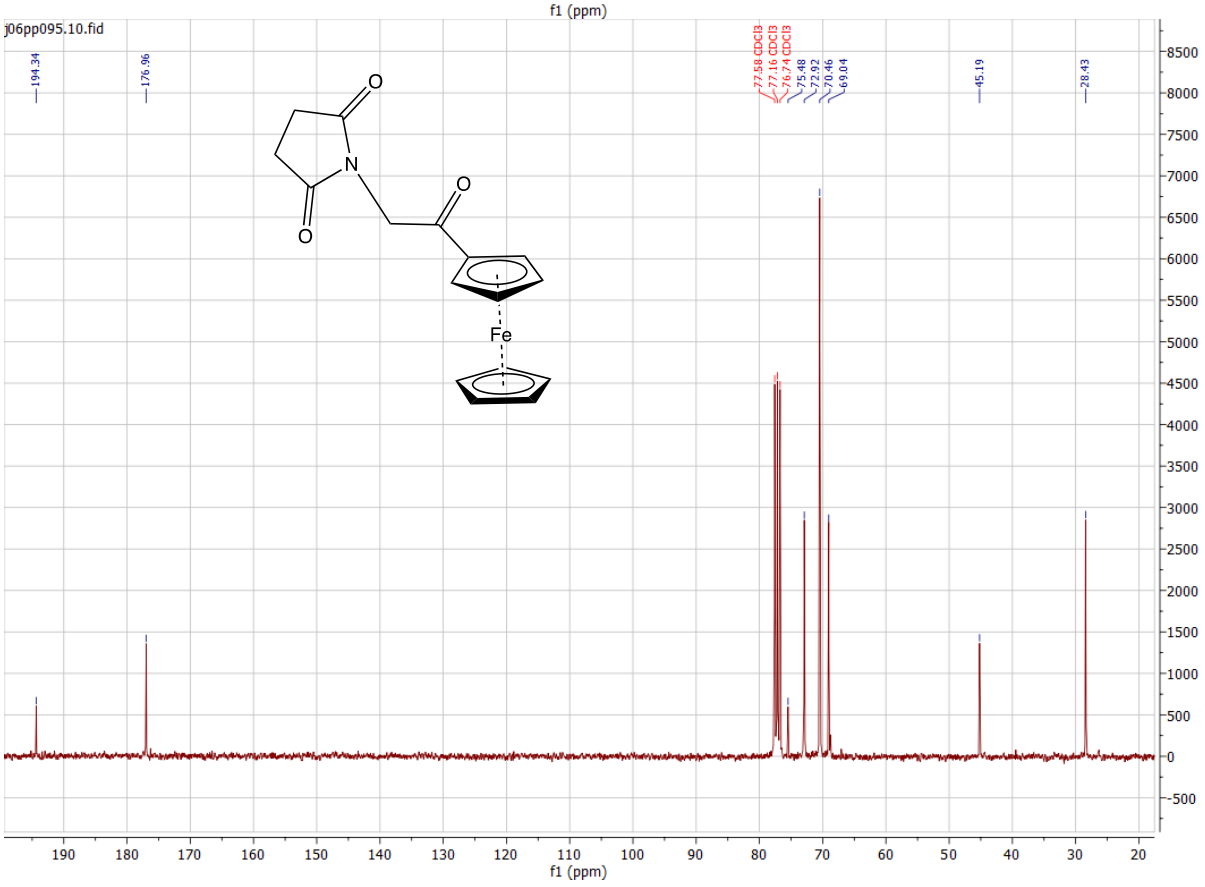
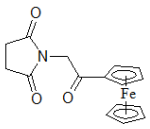


**Figure S12**: $^{1}H$ (in in $CDCl_3$), $^{13}C$ (in in $CDCl_3$) NMR, HR-MS and IR data for compound **4b**



**Single Mass Analysis**
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

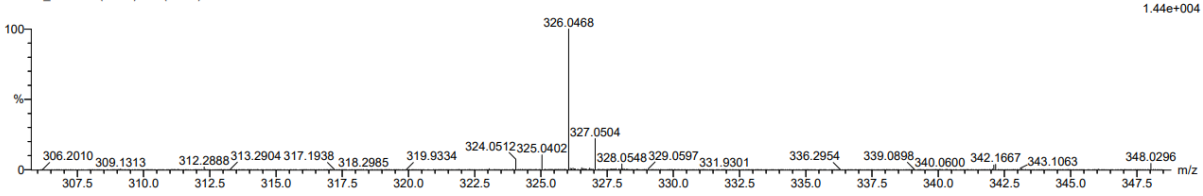


Monoisotopic Mass, Even Electron Ions
310 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 1-120 N: 0-10 O: 0-10 Fe: 1-1

06-Sep-2013 5::1::7
ENSCP_P737 26 (0.681) Cm (26:32)

MeOH

LCT Premier XE KE483
1: TOF MS ES+
1.44e+004




| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 5.0 | 5.0 | 100.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 326.0468 | 326.0480 | -1.2 | -3.7 | 9.5 | 763.4 | 0.0 | C16 H16 N O3 Fe |
| | 326.0453 | 1.5 | 4.6 | 10.5 | 770.9 | 7.5 | C12 H12 N7 O Fe |

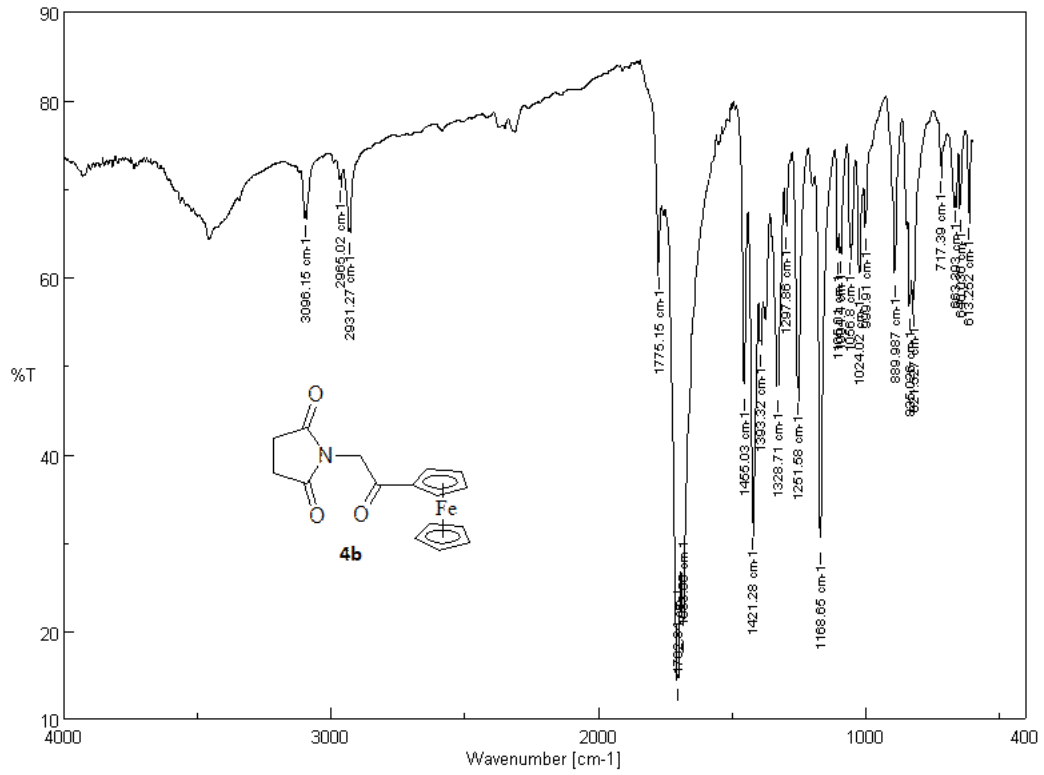
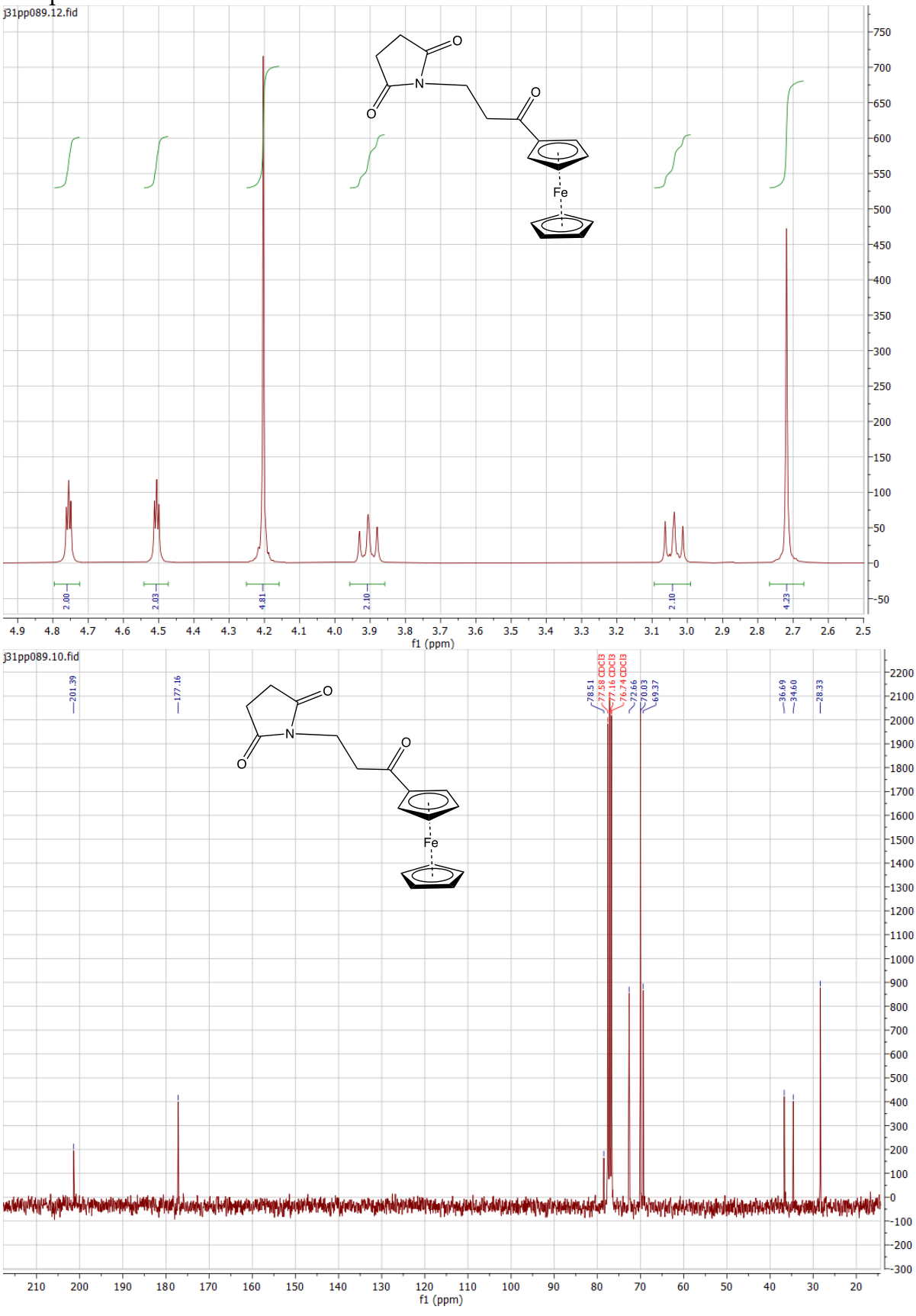
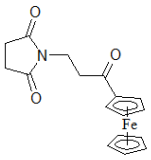


**Figure S13**: $^{1}H$ (in in $CDCl_3$), $^{13}C$ (in in $CDCl_3$) NMR, HR-MS and IR data for compound **4c**



**Single Mass Analysis**
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

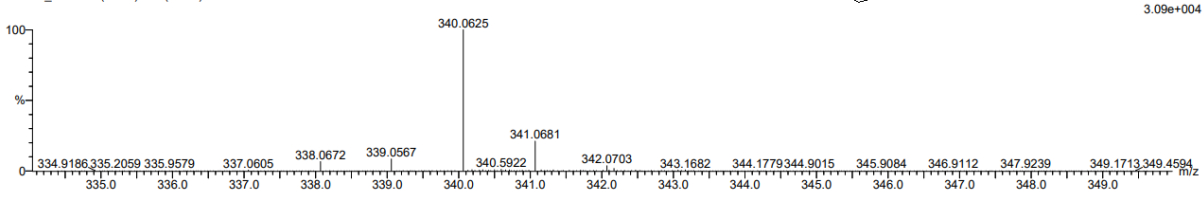
Monoisotopic Mass, Even Electron Ions
332 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 1-120 N: 0-10 O: 0-10 Fe: 1-1



06-Sep-2013 5::8::9
ENSCP_P724 24 (0.625) Cm (24:31)

MeOH

LCT Premier XE KE483
1: TOF MS ES+
3.09e+004




| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 5.0 | 5.0 | 100.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 340.0625 | 340.0636 | -1.1 | -3.2 | 9.5 | 975.5 | 0.0 | C17 H18 N O3 Fe |
| | 340.0609 | 1.6 | 4.7 | 10.5 | 982.2 | 6.7 | C13 H14 N7 O Fe |

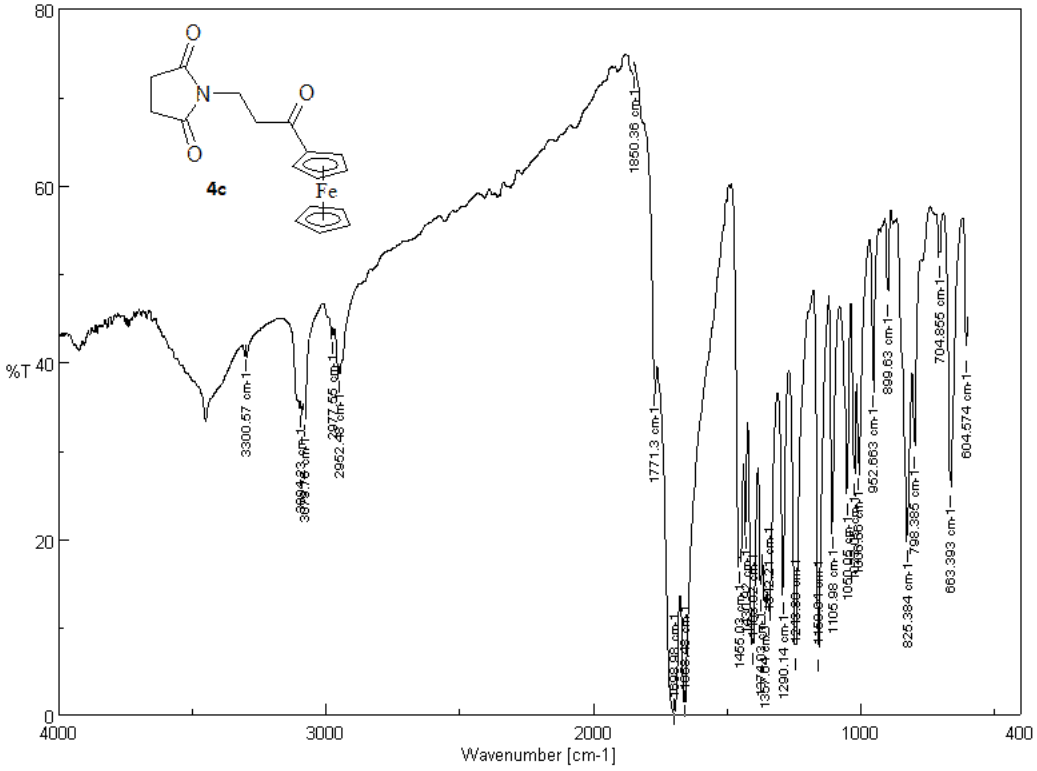
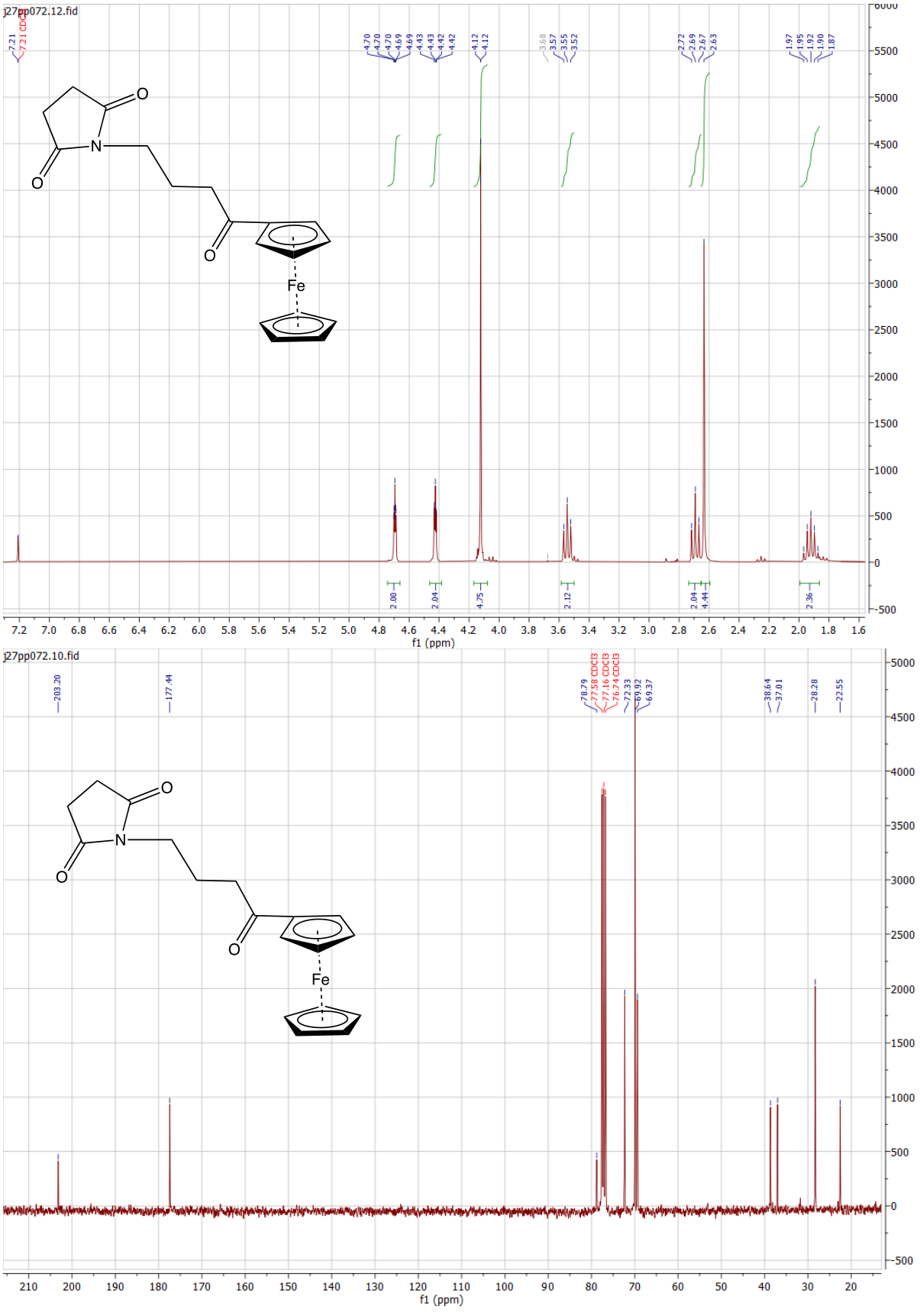
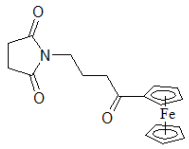


**Figure S14**: $^{1}H$ (in $CDCl_3$), $^{13}C$ (in $CDCl_3$) NMR, HR-MS and IR data for compound **4d**



**Single Mass Analysis**
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

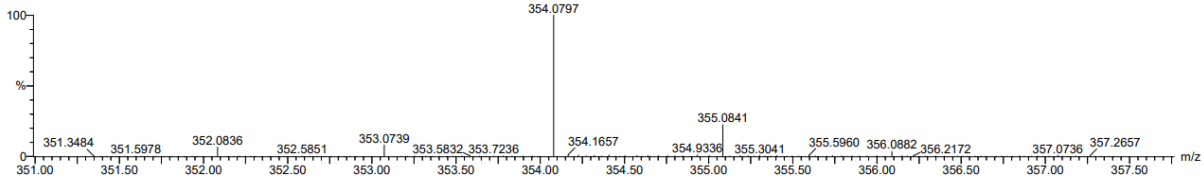
Monoisotopic Mass, Even Electron Ions
356 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 1-120 N: 0-10 O: 0-10 Fe: 1-1



06-Sep-2013 5::3::2
ENSCP_P726 21 (0.573) Cm (20:28)

MeOH

LCT Premier XE KE483
1: TOF MS ES+
4.84e+004




| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 5.0 | 5.0 | 100.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 354.0797 | 354.0793 | 0.4 | 1.1 | 9.5 | 604.1 | 0.0 | C18 H20 N O3 Fe |

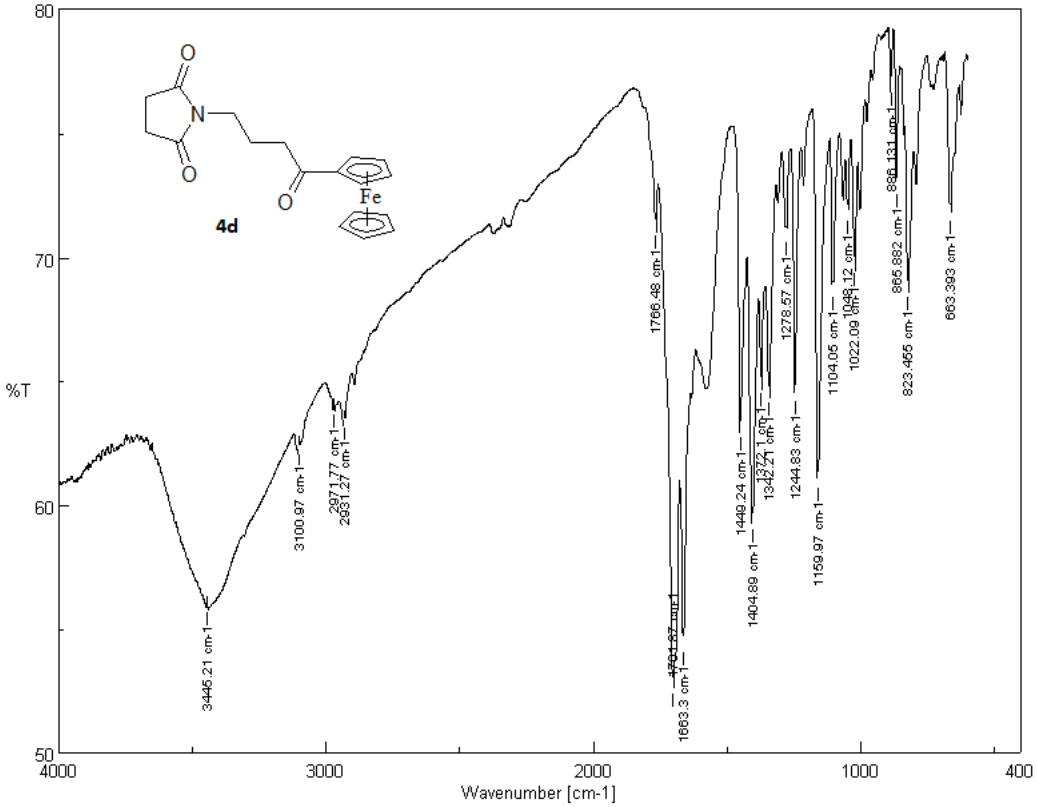
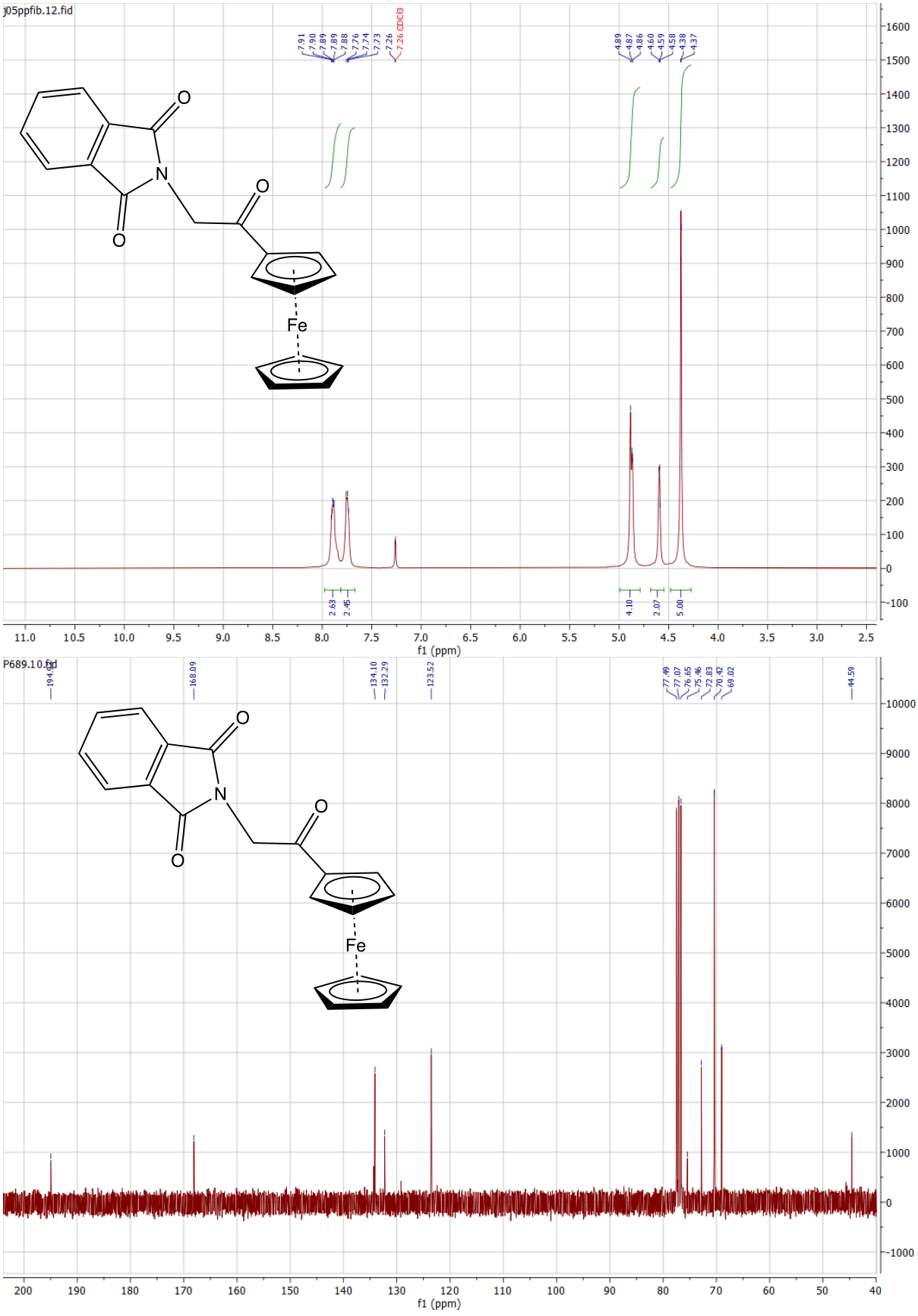


**Figure S15**: $^{1}H$ (in $CDCl_3$), $^{13}C$ (in $CDCl_3$) NMR, HR-MS and IR data for compound **4f**

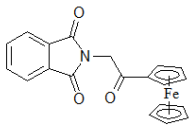


**Single Mass Analysis**
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

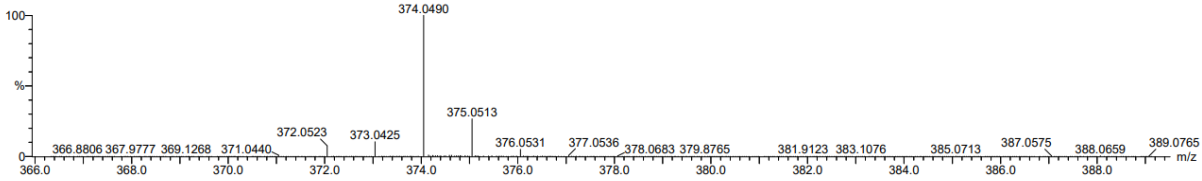
Monoisotopic Mass, Even Electron Ions
382 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 1-120 N: 0-10 O: 0-10 Fe: 1-1

06-Sep-2013 5::8::1
ENSCP_P689 25 (0.661) Cm (25:32)

MeOH



LCT Premier XE KE483
1: TOF MS ES+
2.57e+004




| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | 5.0 | 5.0 | -1.5 | | | |
| Maximum: | | | | 100.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 374.0490 | 374.0480 | 1.0 | 2.7 | 13.5 | 836.7 | 0.0 | C20 H16 N O3 Fe |
| | 374.0498 | -0.8 | -2.1 | 0.5 | 849.4 | 12.7 | C8 H20 N3 O10 Fe |

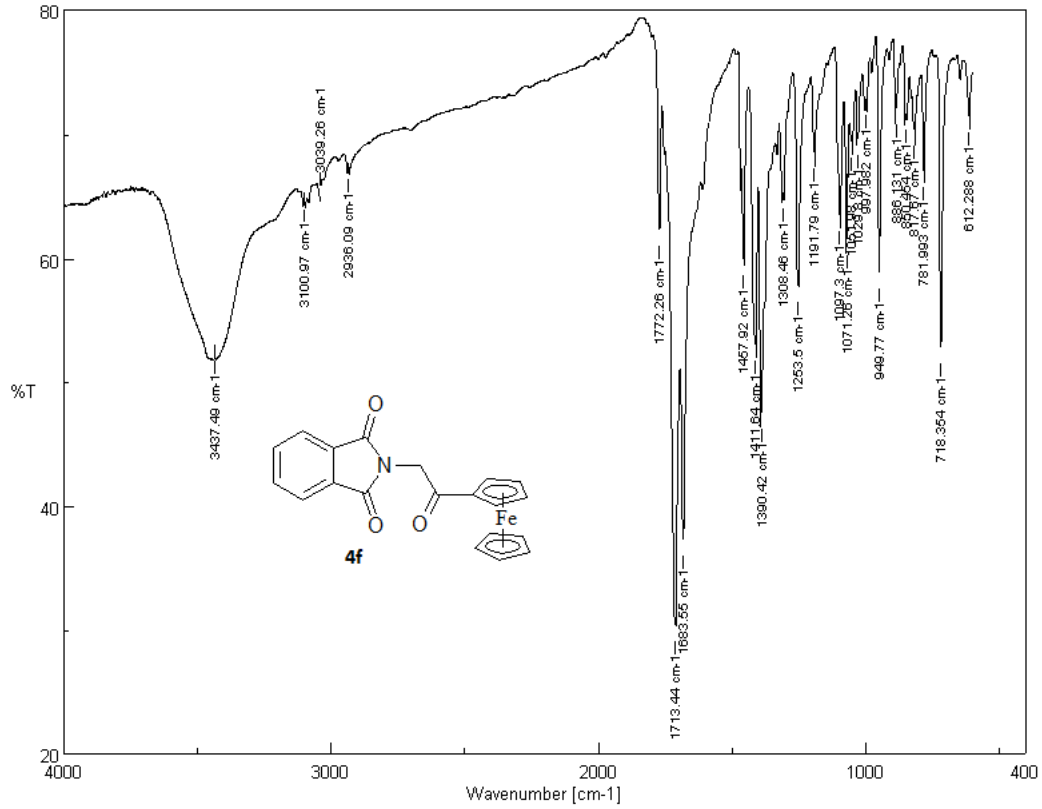
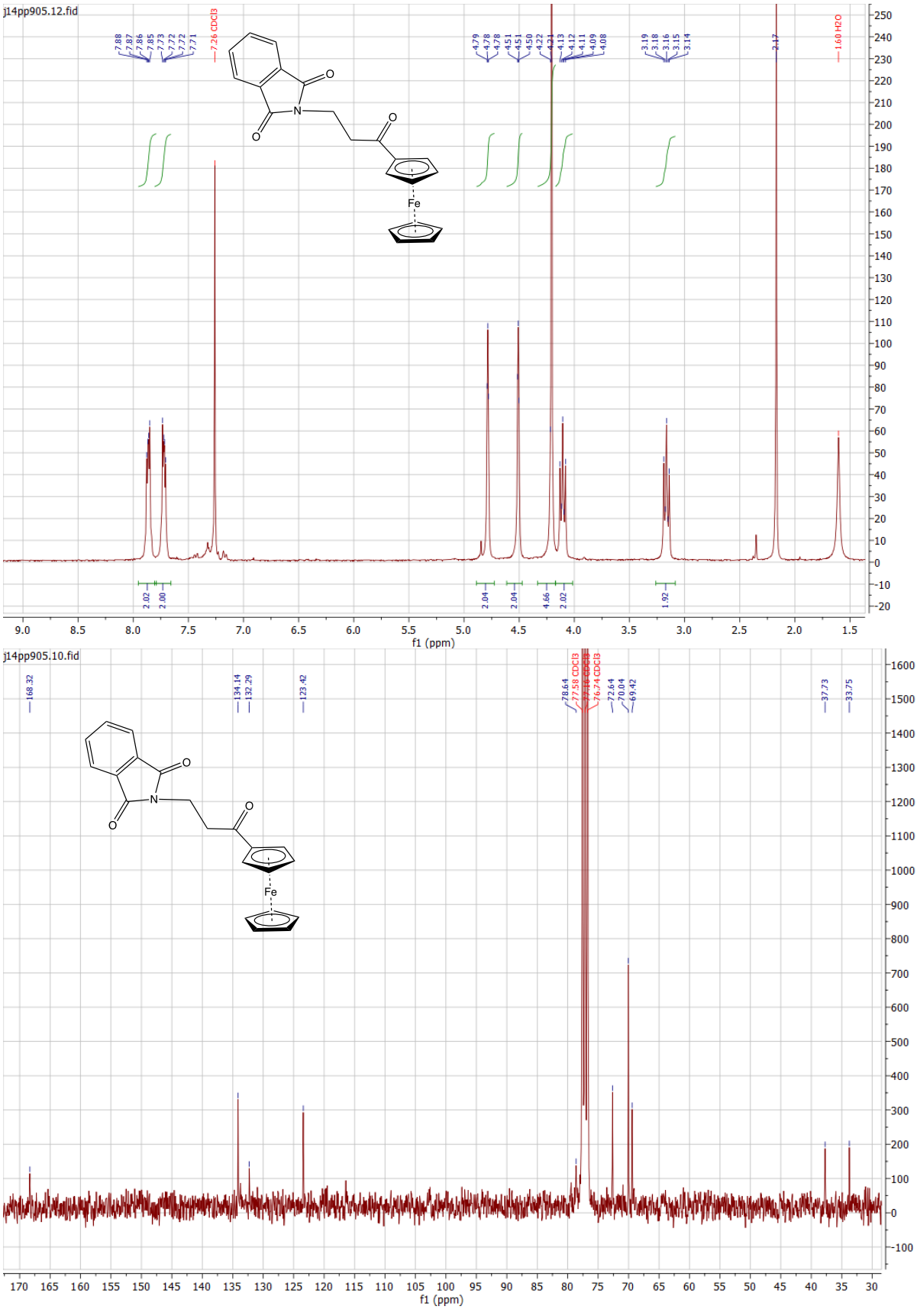
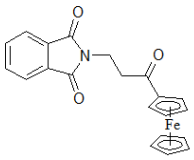


**Figure S16**: $^{1}H$ (in $CDCl_3$), $^{13}C$ (in $CDCl_3$) NMR, HR-MS and IR data for compound **4g**



**Single Mass Analysis**
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

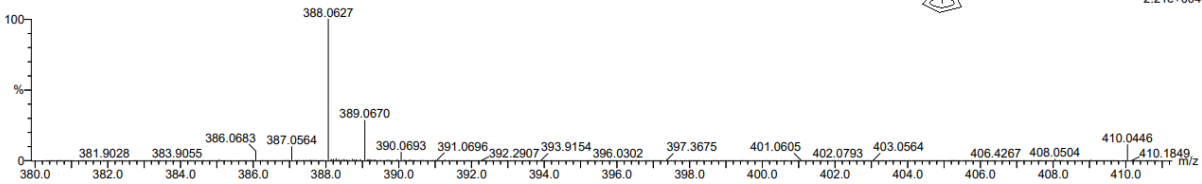
Monoisotopic Mass, Even Electron Ions
401 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 1-120 N: 0-10 O: 0-10 Fe: 1-1




06-Sep-2013 5::2::1
ENSCP_P662 26 (0.680) Cm (26:32)

MeOH

LCT Premier XE KE483
1: TOF MS ES+
2.21e+004




| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 5.0 | 5.0 | 100.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 388.0627 | 388.0636 | -0.9 | -2.3 | 13.5 | 795.1 | 0.0 | C21 H18 N O3 Fe |
| | 388.0609 | 1.8 | 4.6 | 14.5 | 803.3 | 8.2 | C17 H14 N7 O Fe |
| | 388.0628 | -0.1 | -0.3 | 1.5 | 811.9 | 16.8 | C5 H18 N9 O8 Fe |

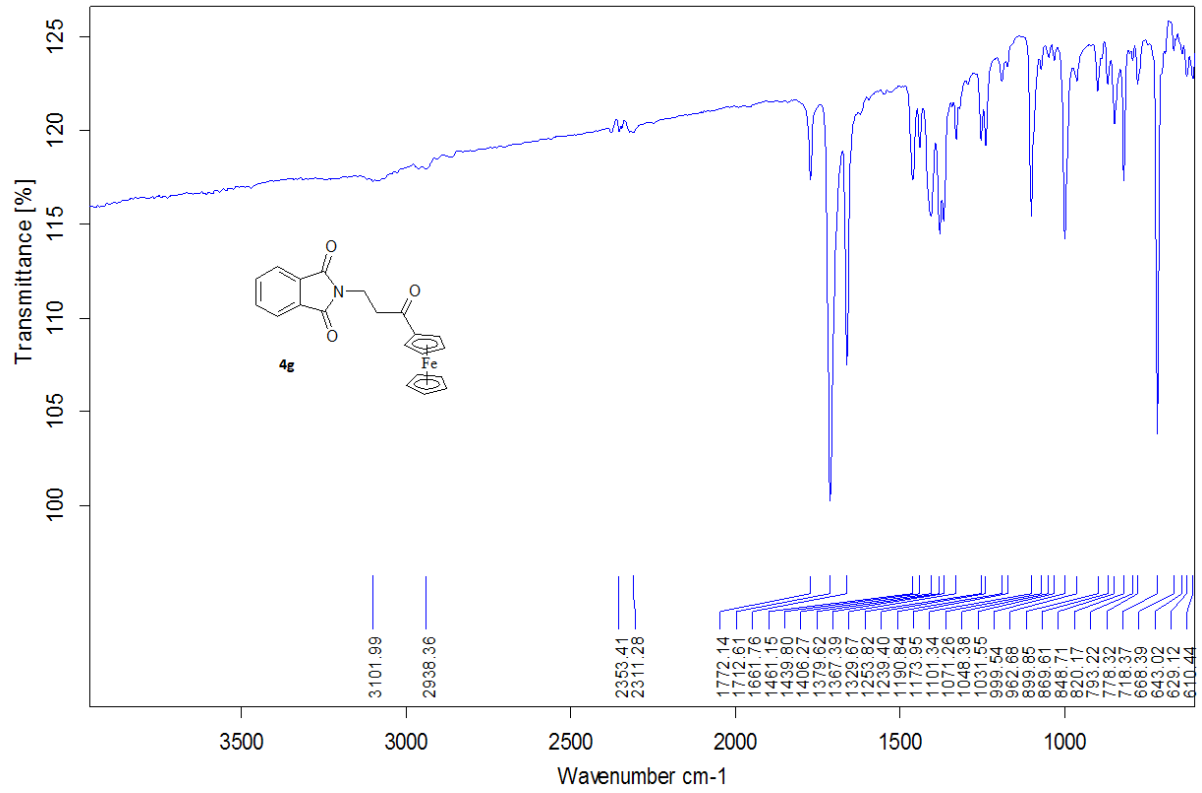
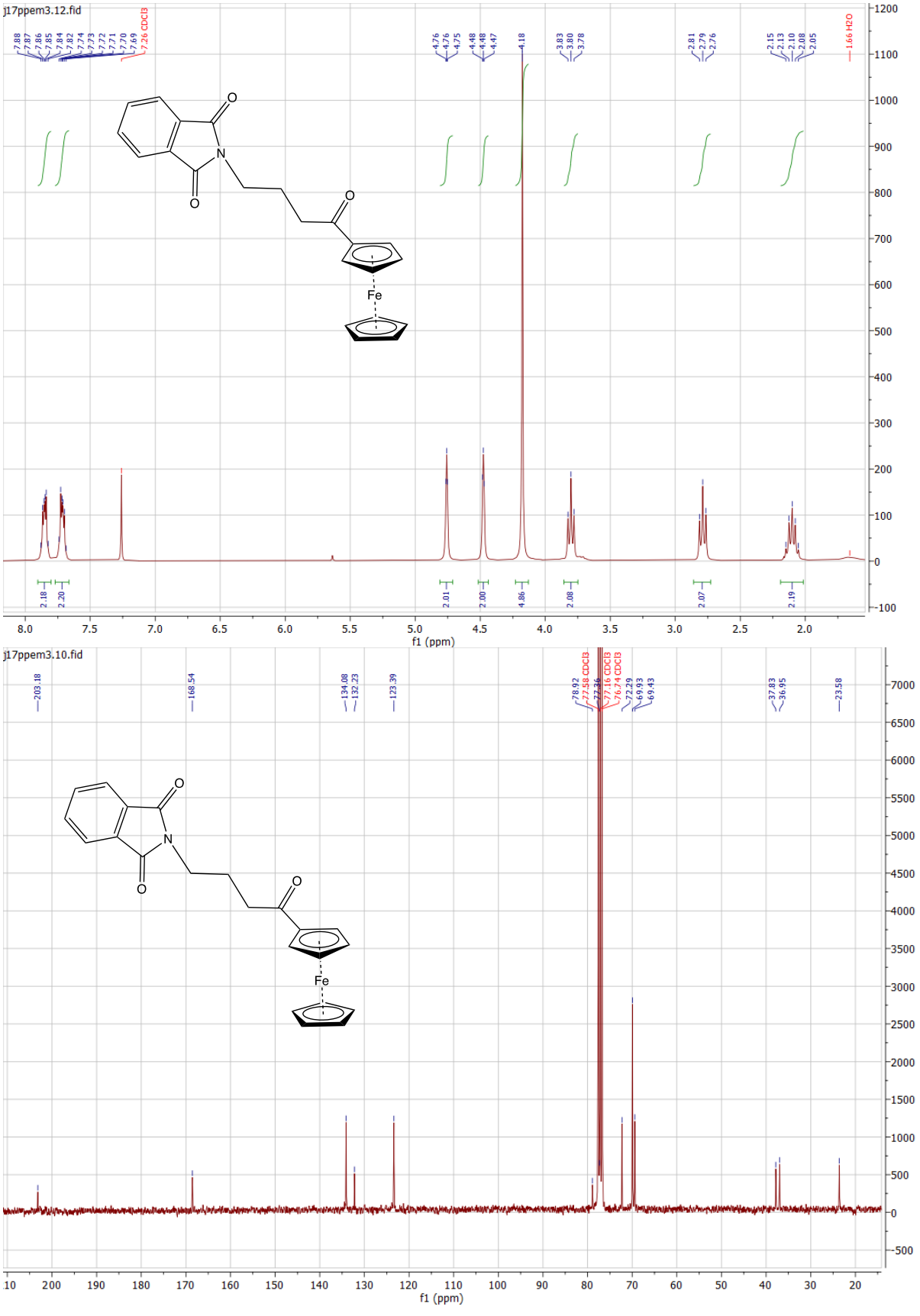
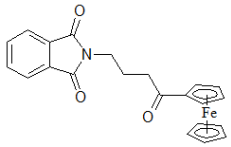


**Figure S17**: $^{1}H$ (in $CDCl_3$), $^{13}C$ (in $CDCl_3$) NMR, HR-MS and IR data for compound **4h**



**Single Mass Analysis**
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

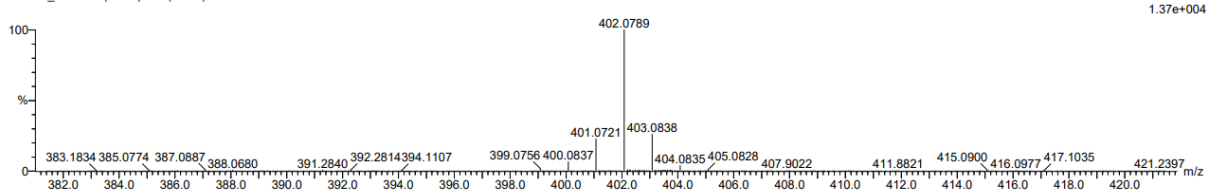
Monoisotopic Mass, Even Electron Ions
423 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 1-120 N: 0-10 O: 0-10 Fe: 1-1




06-Sep-2013 5::5::9
ENSCP_P671 28 (0.715) Cm (28:38)

MeOH

LCT Premier XE KE483
1: TOF MS ES+
1.37e+004




| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 5.0 | 5.0 | 100.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 402.0789 | 402.0793 | -0.4 | -1.0 | 13.5 | 810.4 | 0.0 | C22 H20 N O3 Fe |
| | 402.0784 | 0.5 | 1.2 | 1.5 | 824.7 | 14.3 | C6 H20 N9 O8 Fe |

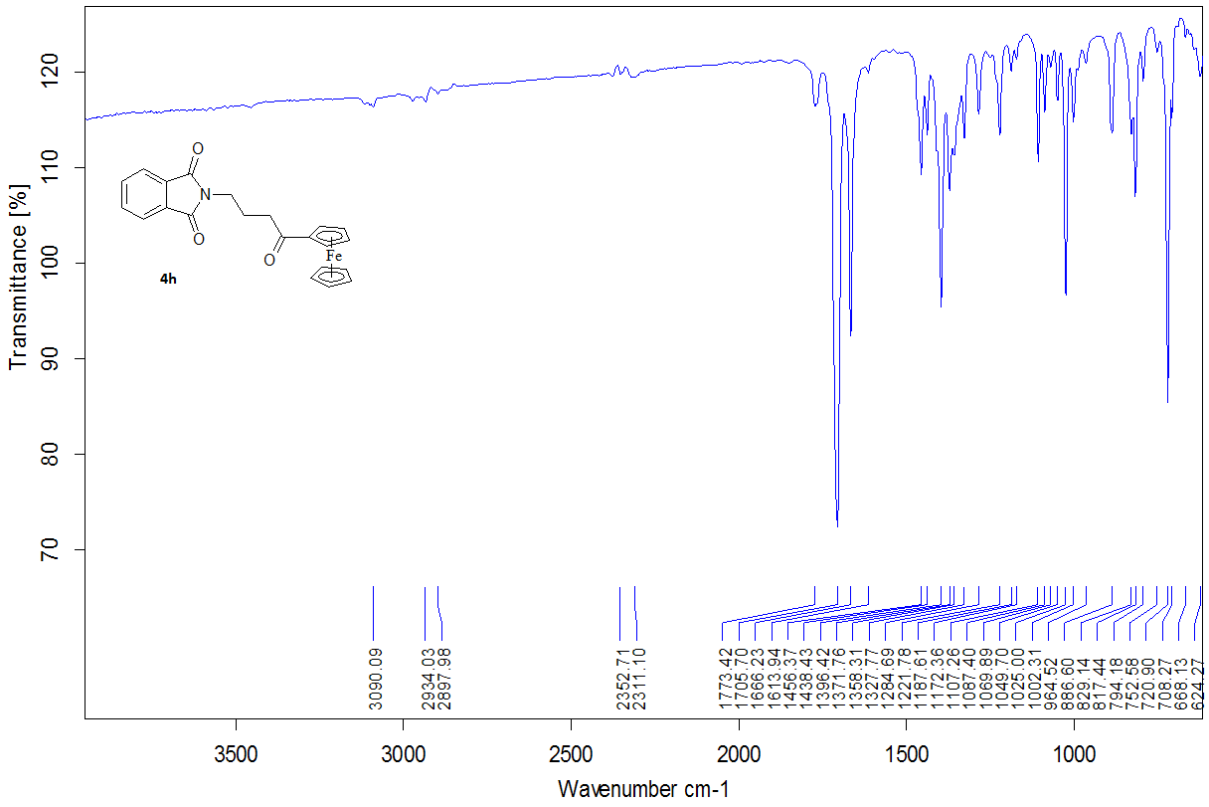
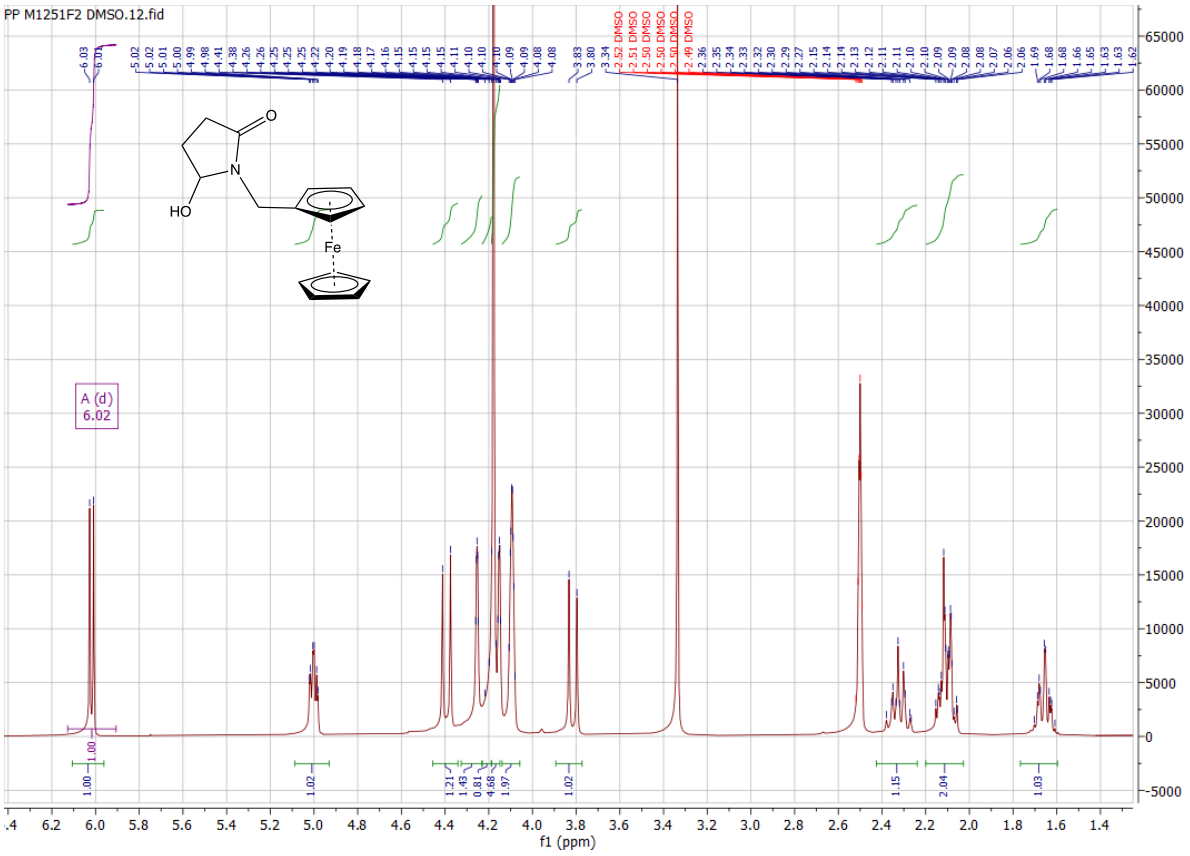
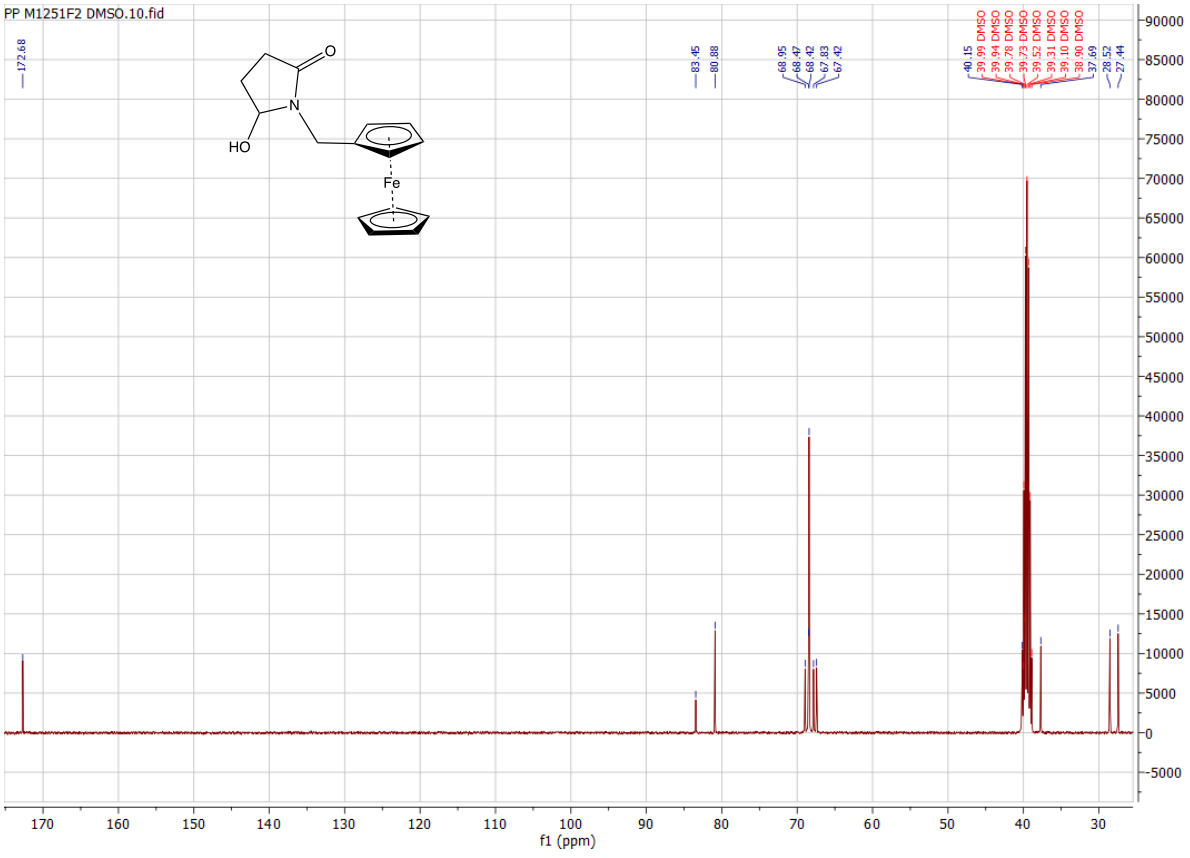
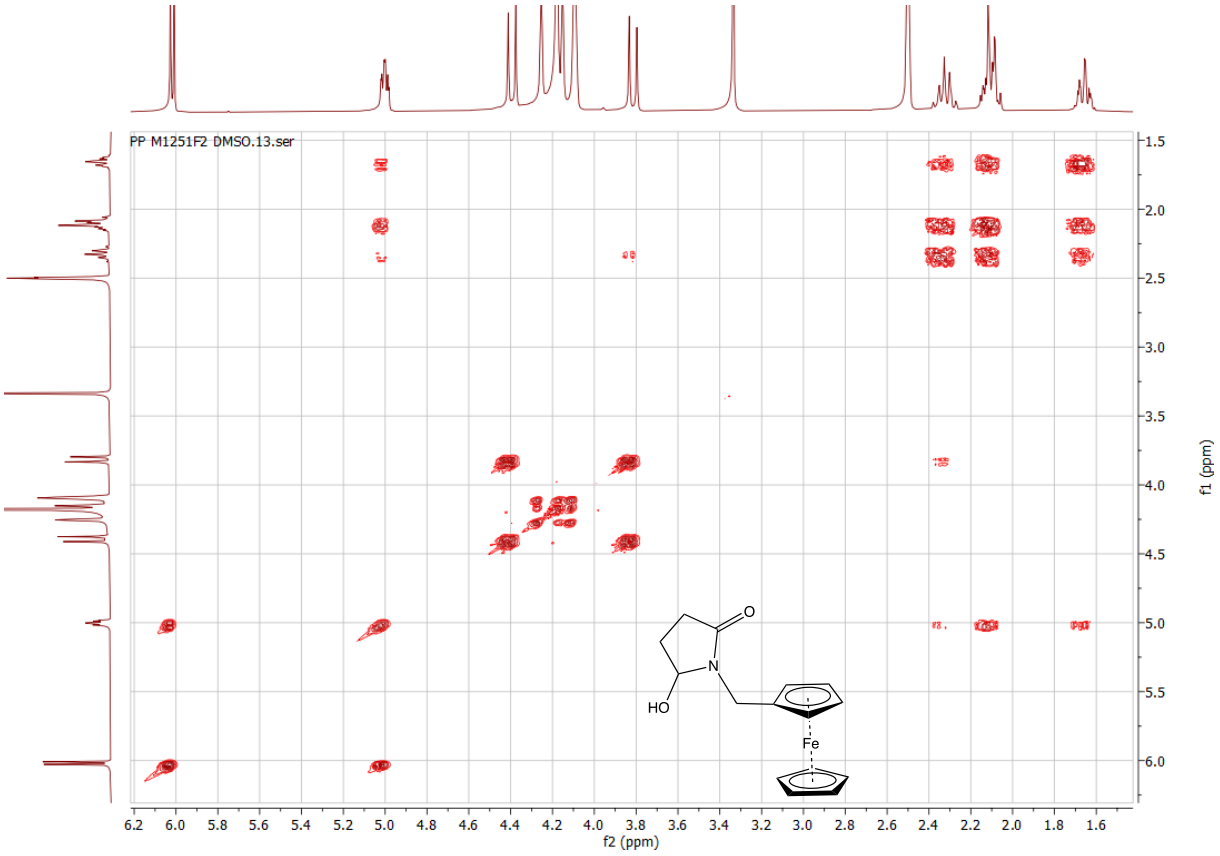
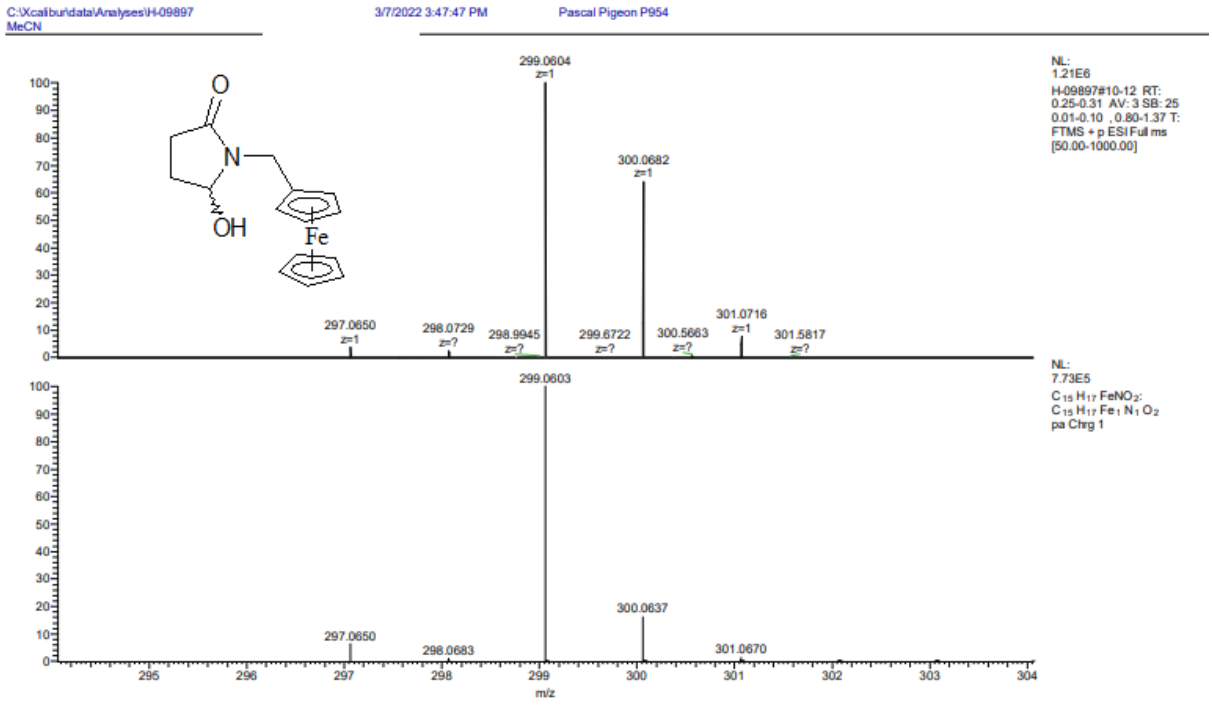


**Figure S18**: $^{1}H$ (in DMSO-$d_6$), $^{13}C$ (in DMSO-$d_6$), COSY (in DMSO-$d_6$) NMR, NMR, HR-MS and IR data for compound **6a**






# Experimental/theoretical isotopic pattern MS spectrum

**Error = 0.3 ppm; Relative Intensity (%) 100**

**HRMS (ESI) m/z: [M]+ Calcd for C15H17FeNO2 299.0603 . Found 299.0604; (Error: 0.3 ppm).**

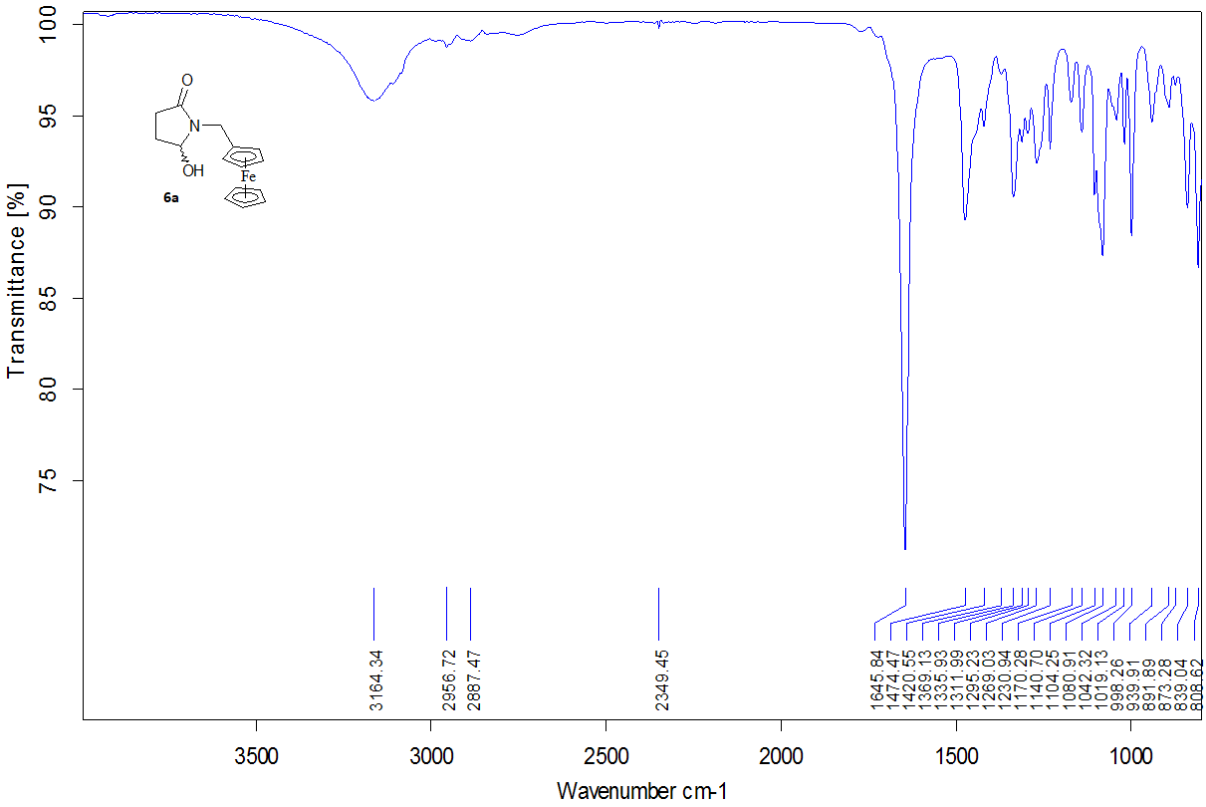
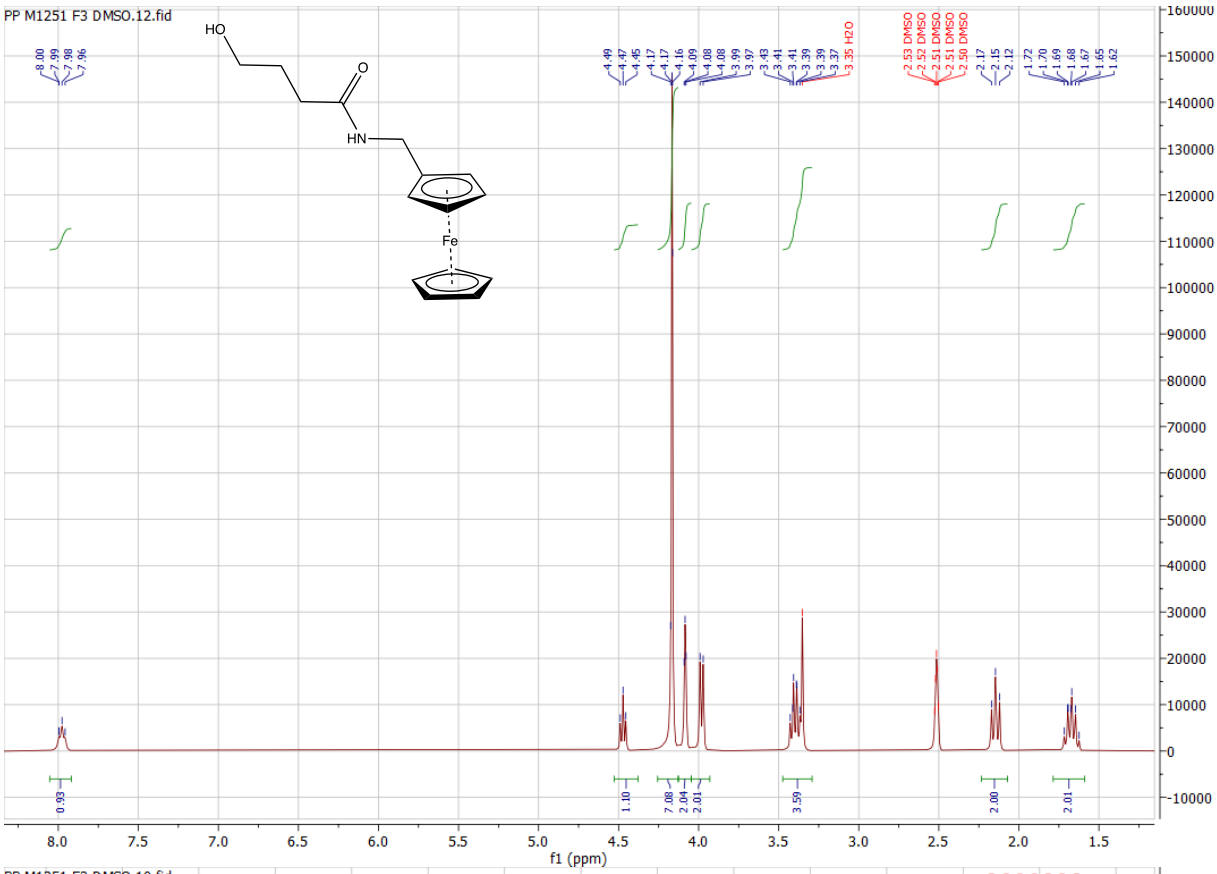
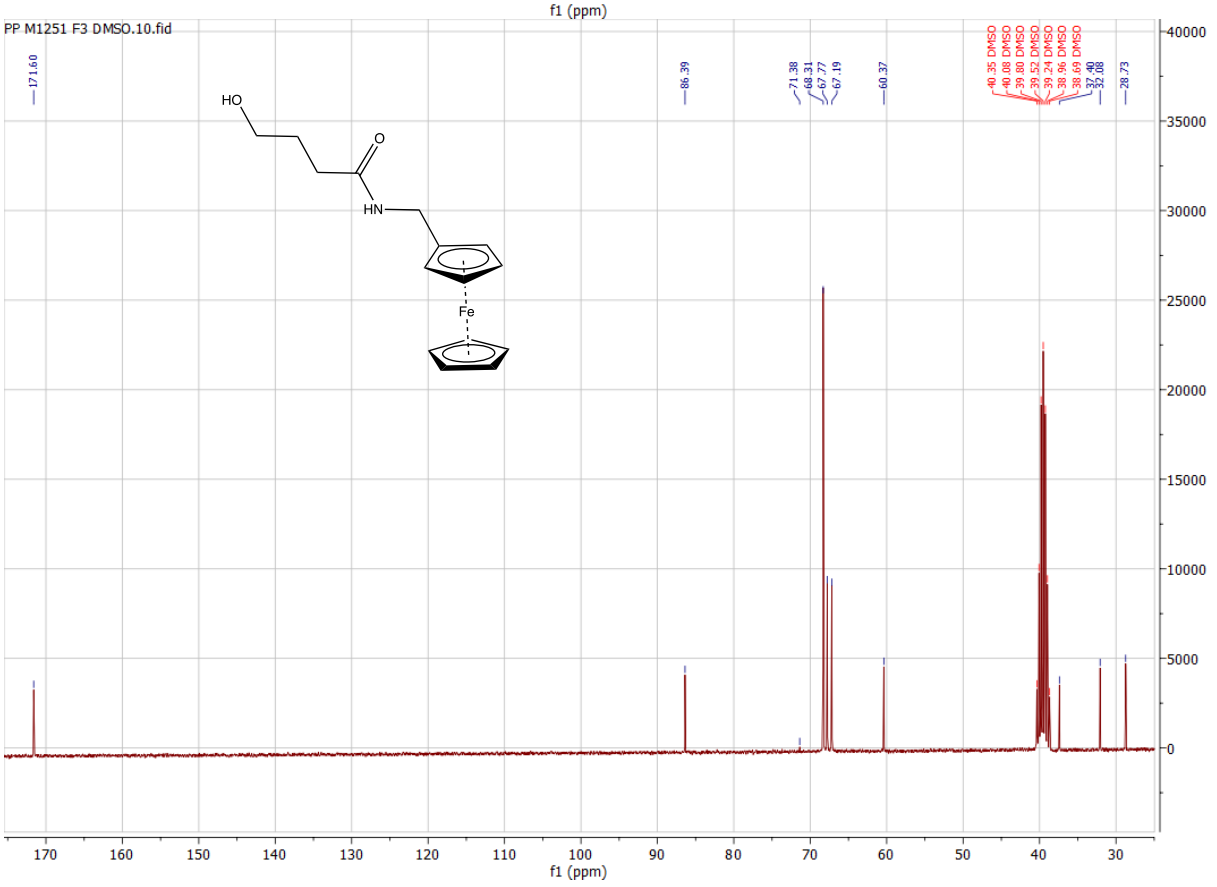
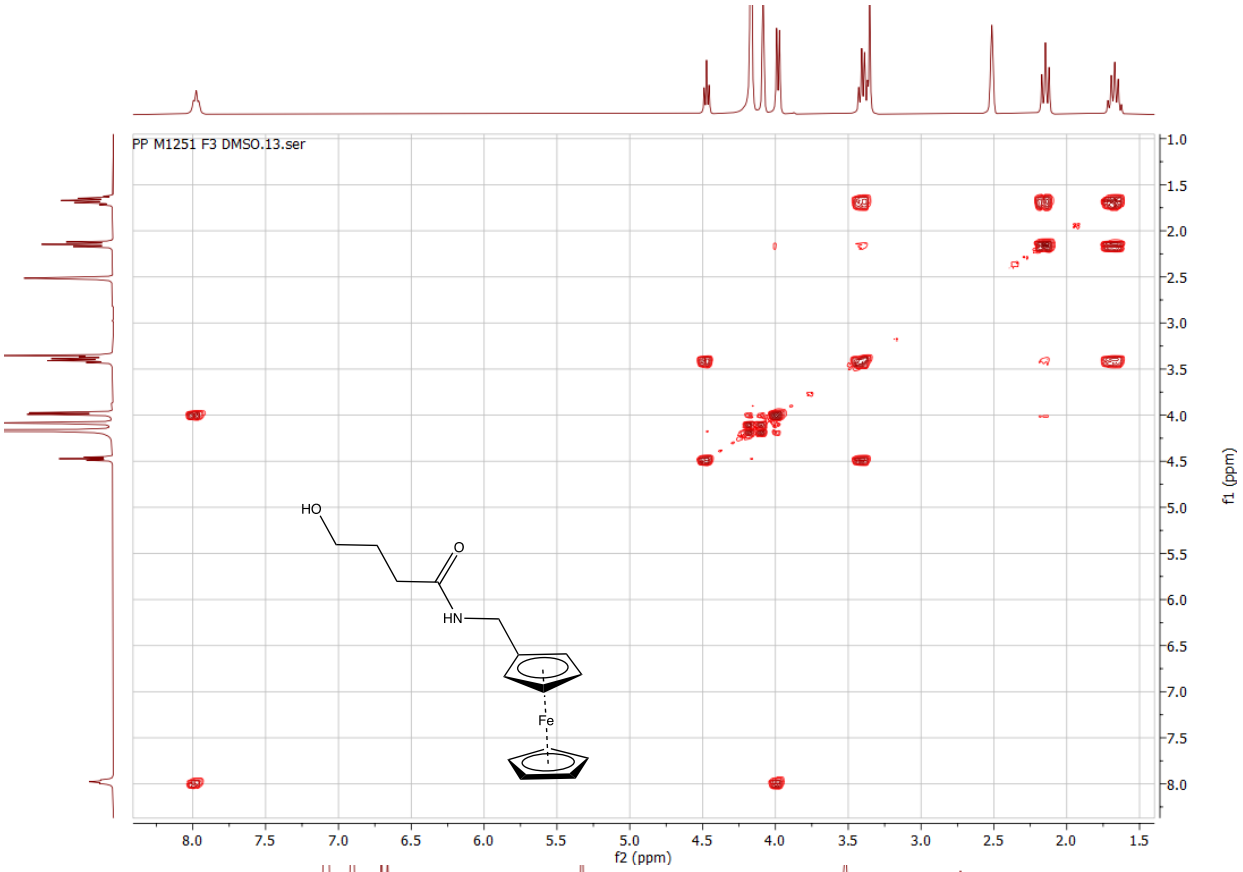
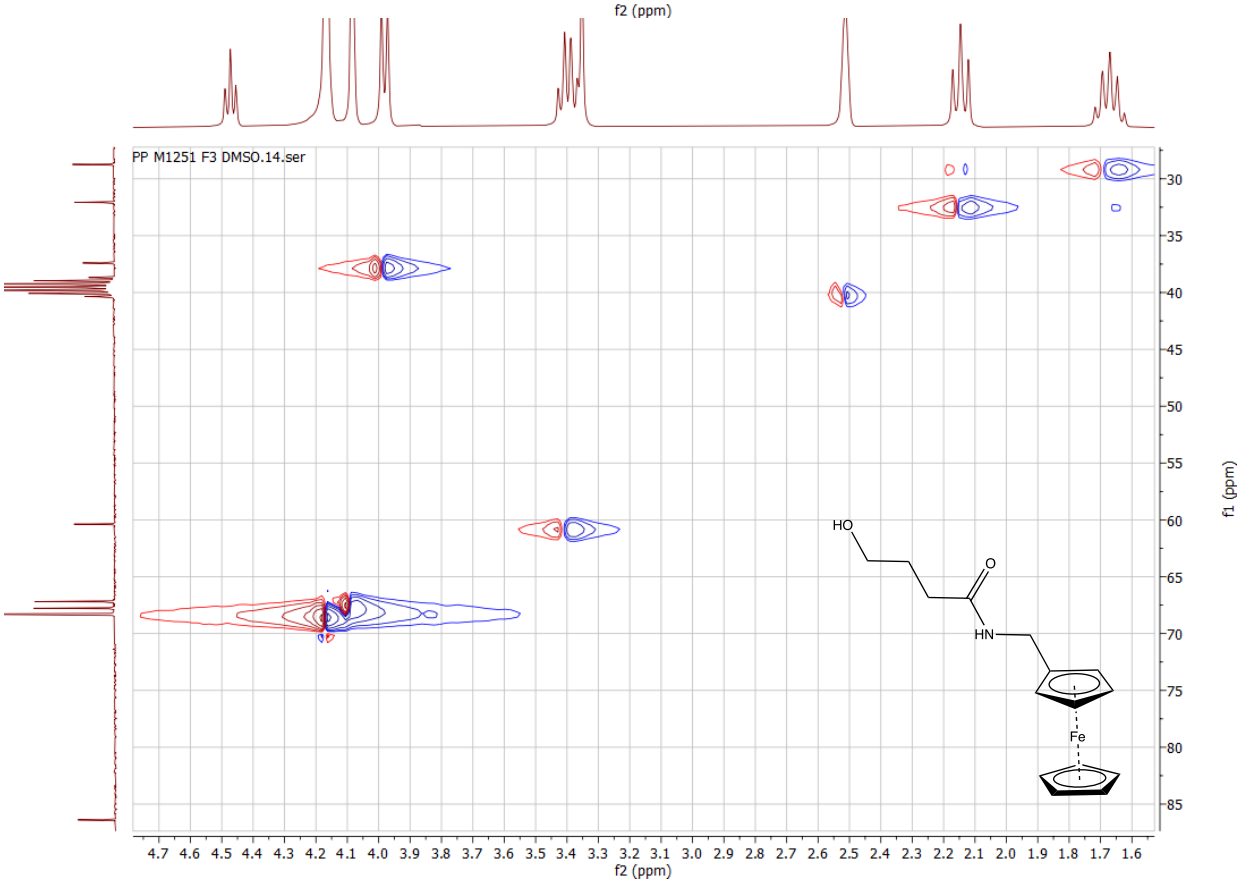

Transmittance [%]
100
95
90
85
80
75
3500
3000
2500
2000
1500
1000
Wavenumber cm-1
3164.34
2956.72
2887.47
2349.45
1645.84
1474.47
1420.55
1369.13
1335.93
1311.99
1295.23
1269.03
1230.94
1170.28
1140.70
1104.25
1080.91
1042.32
1019.13
998.26
939.91
891.89
873.28
839.04
808.62
O
N
OH
Fe
6a

**Figure S19**: $^{1}H$ (in DMSO-$d_6$), $^{13}C$ (in DMSO-$d_6$), COSY (in DMSO-$d_6$), HMQC (in DMSO-$d_6$) NMR and IR data for compound **7a**




PP M1251 F3 DMSO.13.ser
HO
O
HN
Fe
f2 (ppm)
f1 (ppm)


PP M1251 F3 DMSO.14.ser
HO
O
HN
Fe
f2 (ppm)
f1 (ppm)

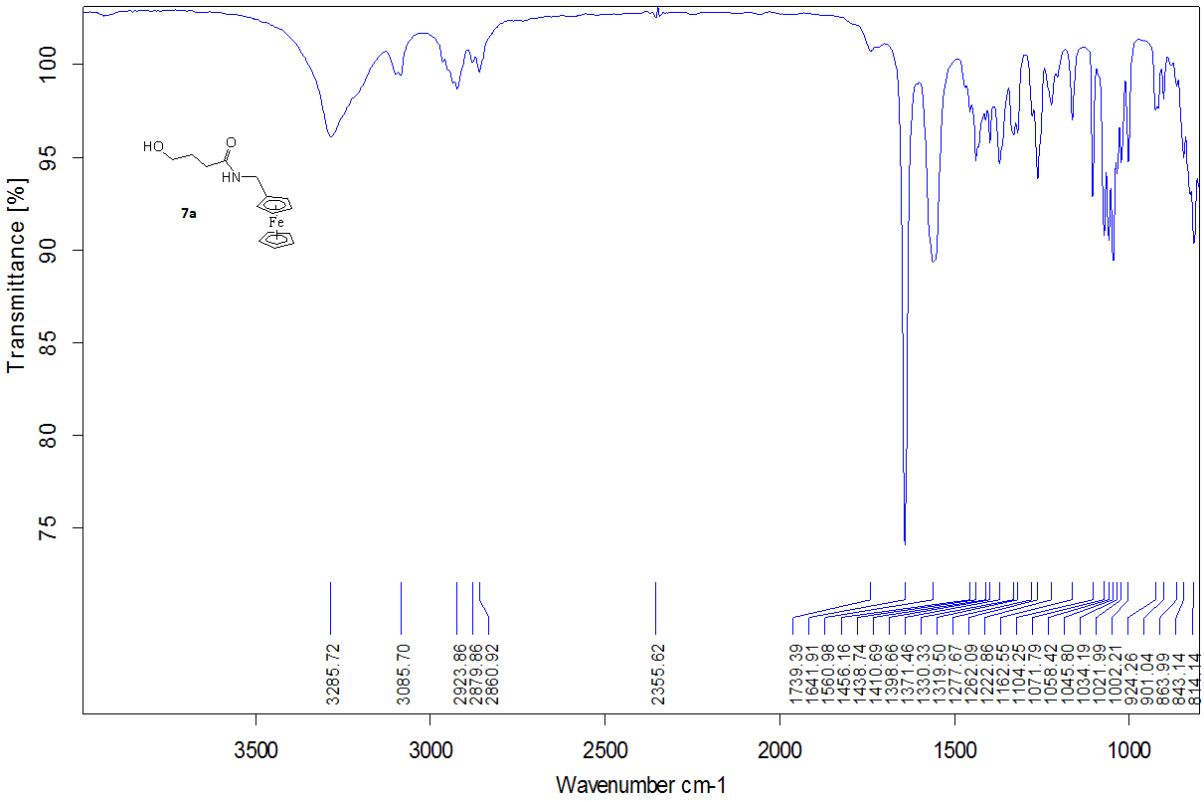

Transmittance [%]
100
95
90
85
80
75
HO
O
HN
Fe
7a
3285.72
3085.70
2923.86
2879.86
2860.92
2355.62
1739.39
1641.91
1560.98
1456.16
1438.74
1410.69
1398.66
1371.46
1330.33
1319.50
1277.67
1262.09
1222.86
1162.55
1104.25
1071.79
1058.42
1045.60
1034.19
1021.99
1002.21
924.26
901.04
863.99
843.14
814.14
3500
3000
2500
2000
1500
1000
Wavenumber cm-1

**Figure S20**: $^{1}H$ (in DMSO-$d_6$) NMR for compound **6b**

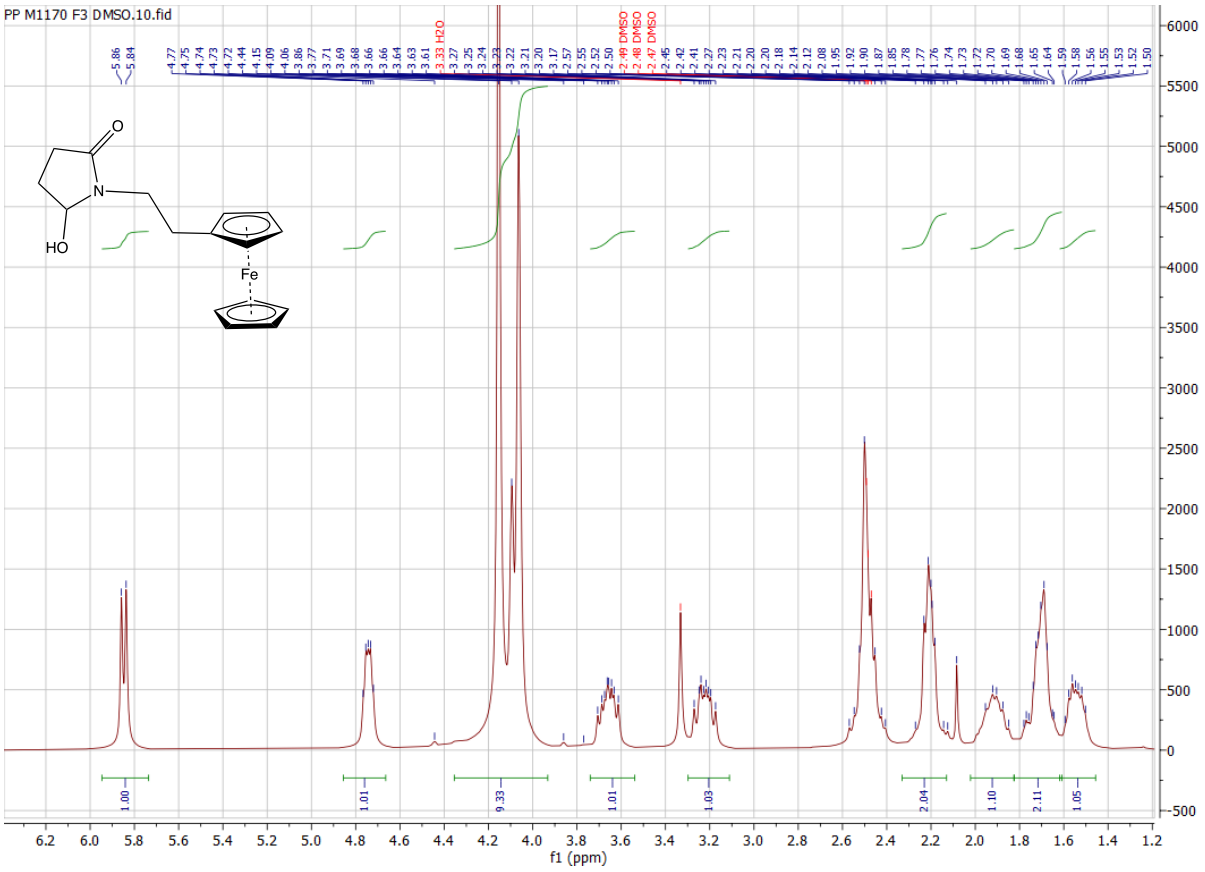
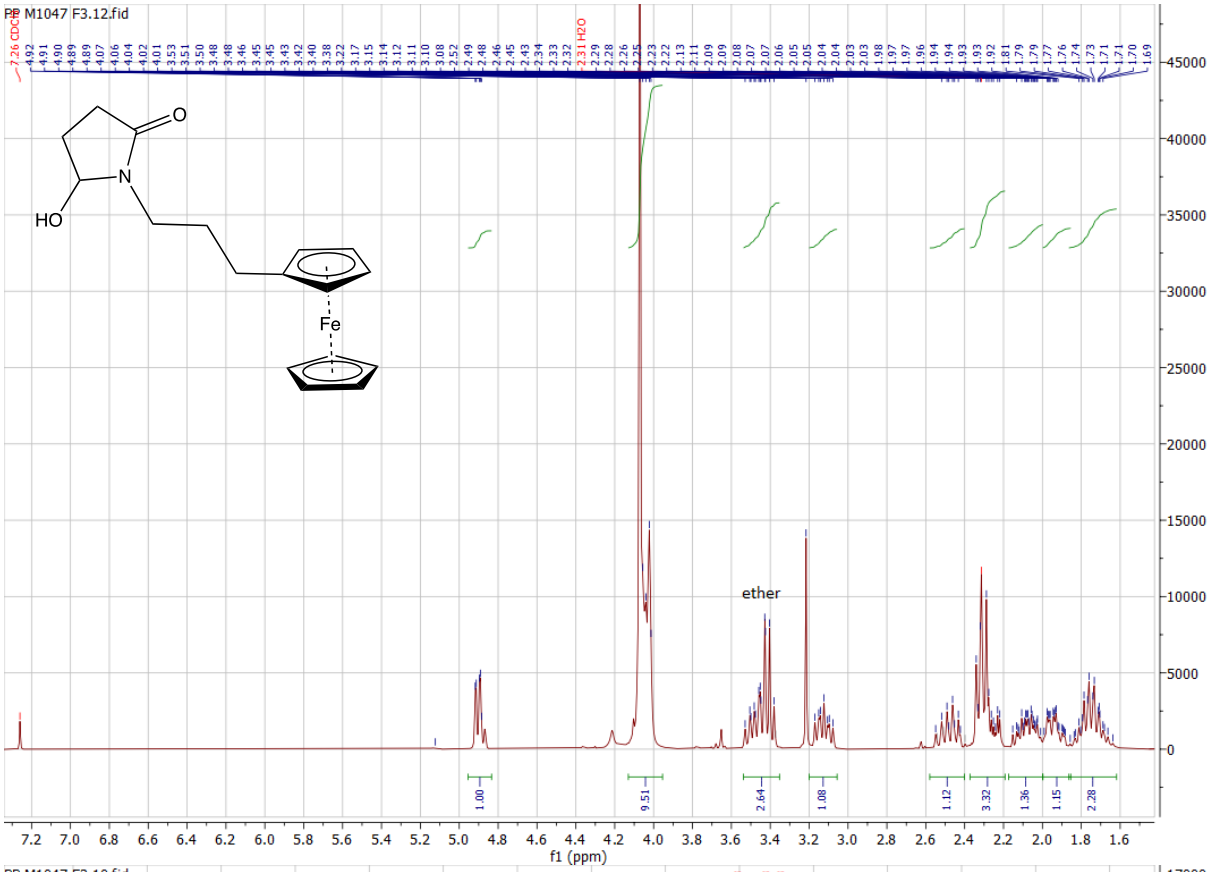
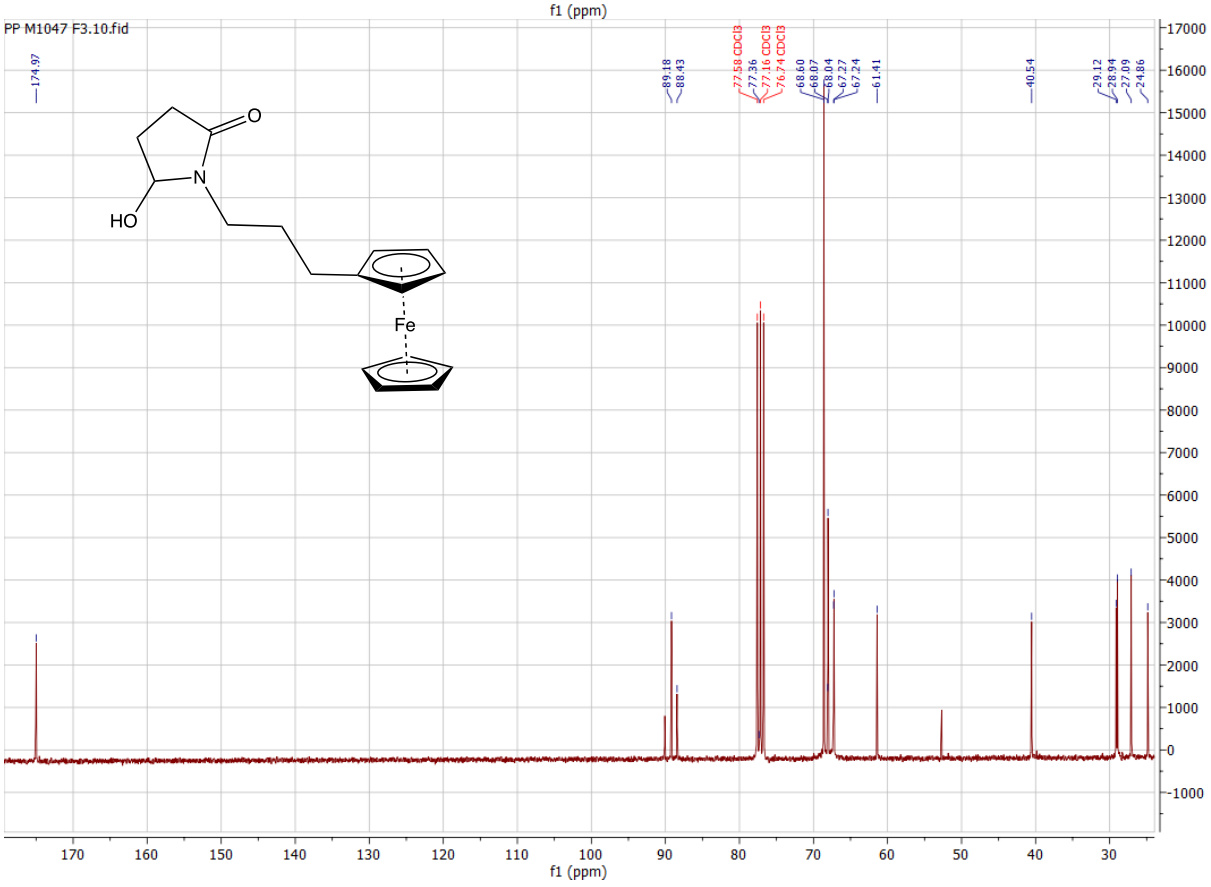
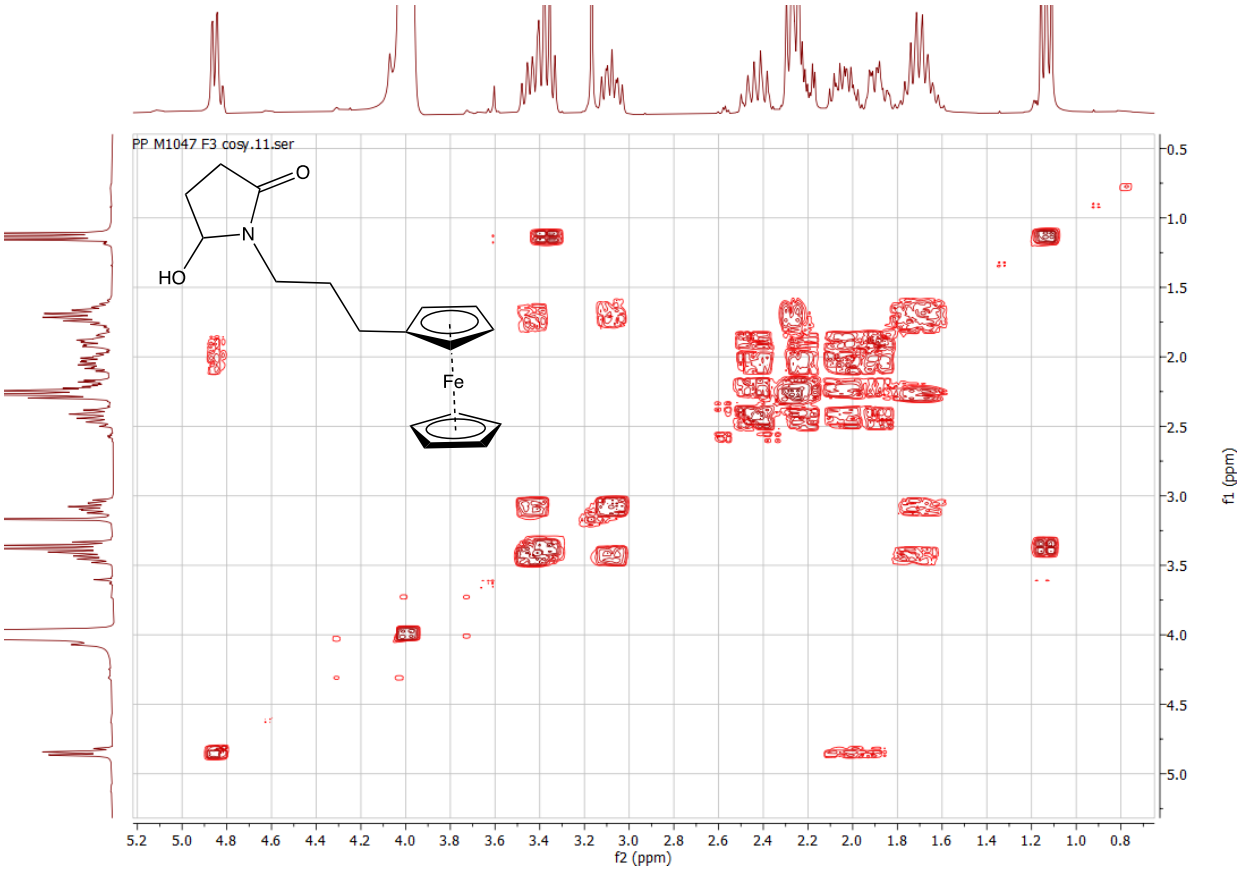
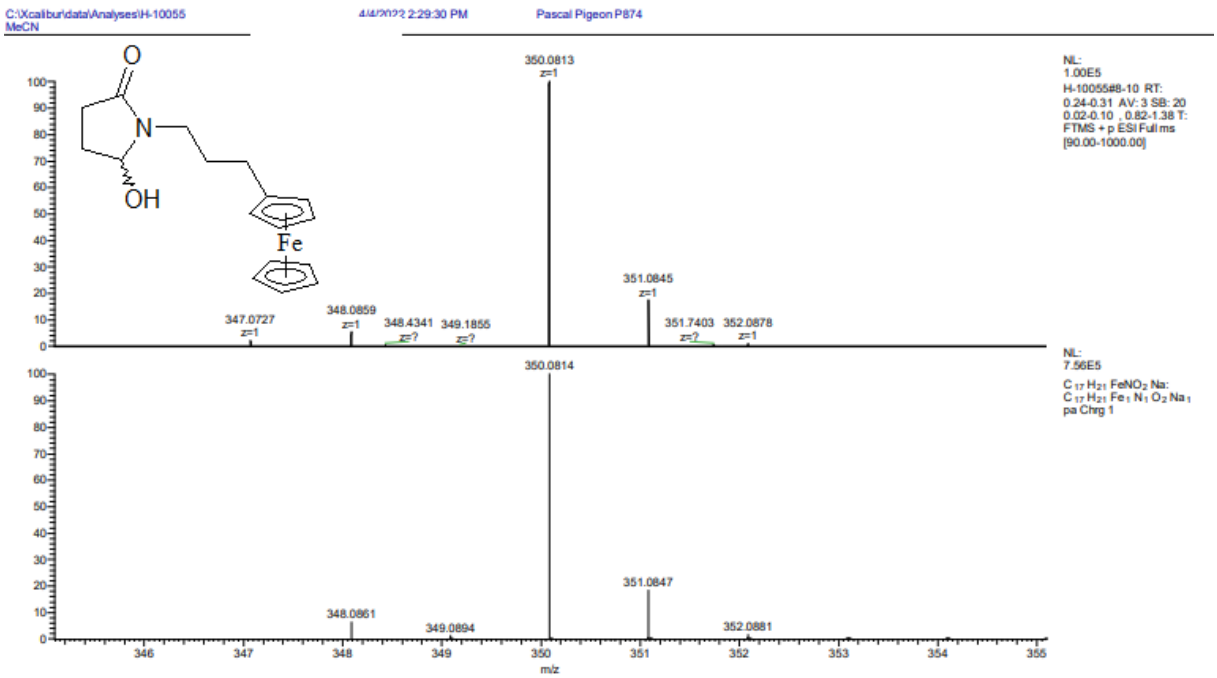


**Figure S21**: $^{1}H$ (in $CDCl_3$), $^{13}C$ (in $CDCl_3$), COSY (in $CDCl_3$) NMR, HR-MS and IR data for compound **6c**






# Experimental/theoretical isotopic pattern MS spectrum

**Error = -0.2 ppm; Relative Intensity (%) 100**

**HRMS (ESI) m/z: [M+Na]+ Calcd for C17H21FeNO2Na 350.0814. Found 350.0813; (Error: -0.2 ppm).**

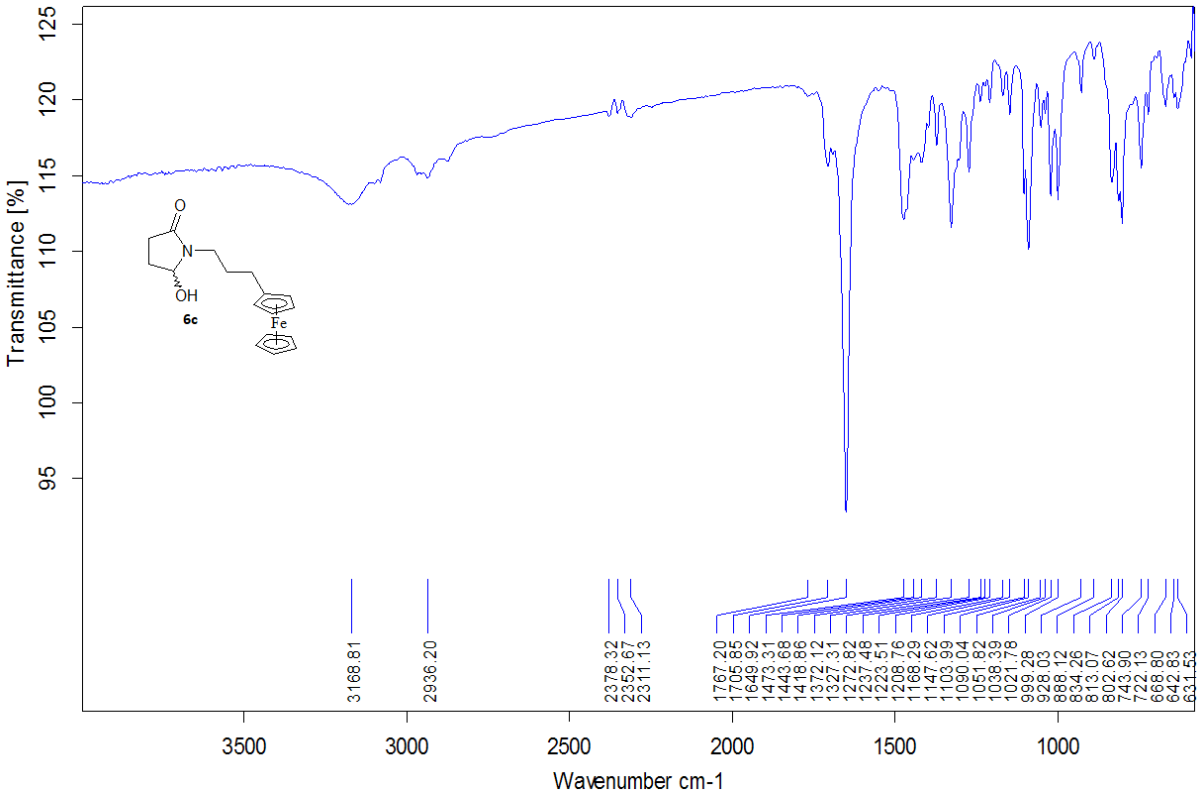
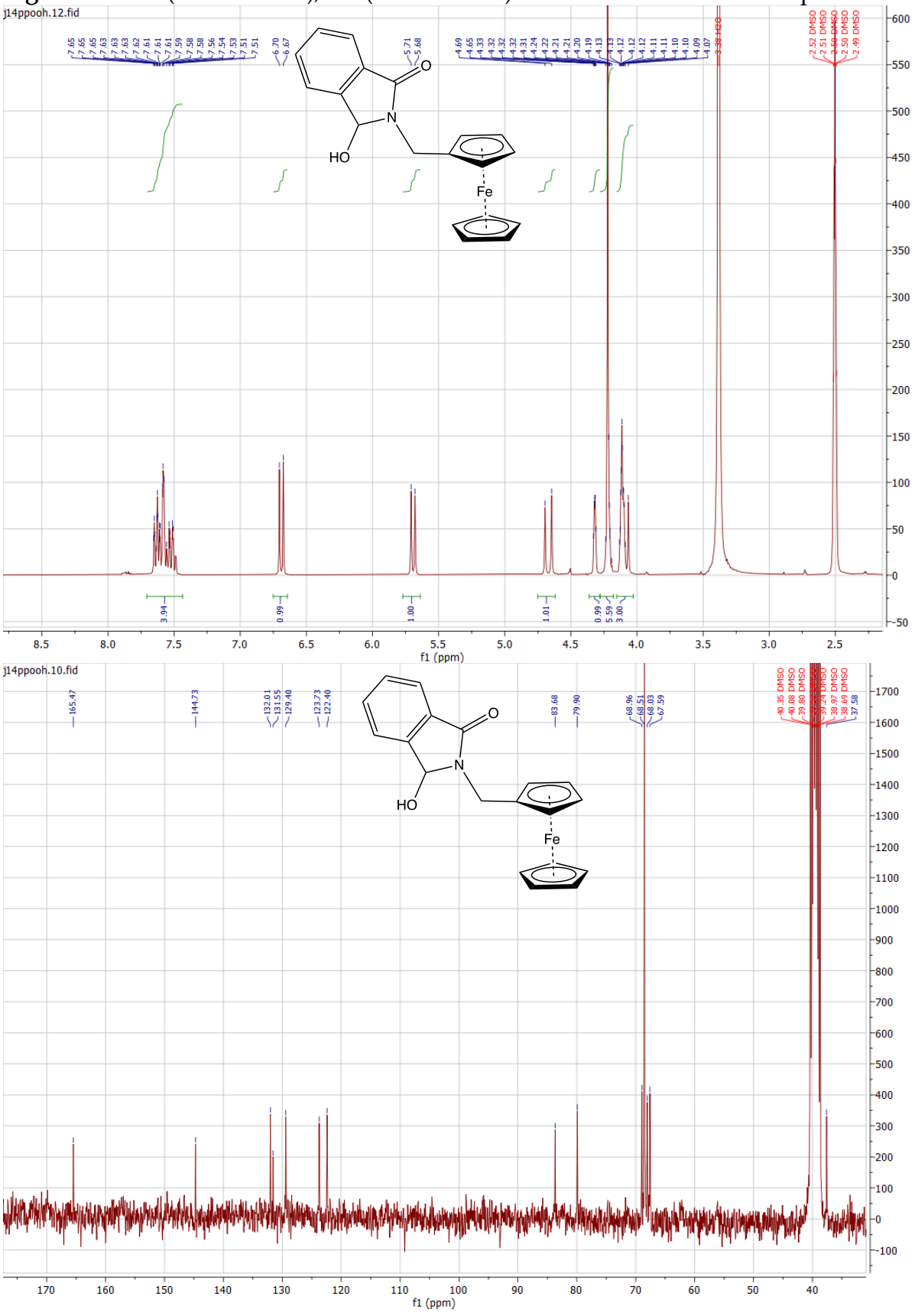

Transmittance [%]
125
120
115
110
105
100
95
O
N
OH
6c
Fe
3168.81
2936.20
2378.32
2352.67
2311.13
1767.20
1705.85
1649.92
1473.31
1443.68
1418.86
1372.12
1327.31
1272.82
1237.48
1223.51
1208.76
1168.29
1147.62
1103.99
1090.04
1051.82
1038.39
1021.78
999.28
928.03
888.12
834.26
813.07
802.62
743.90
722.13
668.80
642.83
631.53
3500
3000
2500
2000
1500
1000
Wavenumber cm-1

**Figure S22**: $^{1}H$ (in DMSO-$d_6$), $^{13}C$ (in DMSO-$d_6$) NMR and IR data for compound **6e**



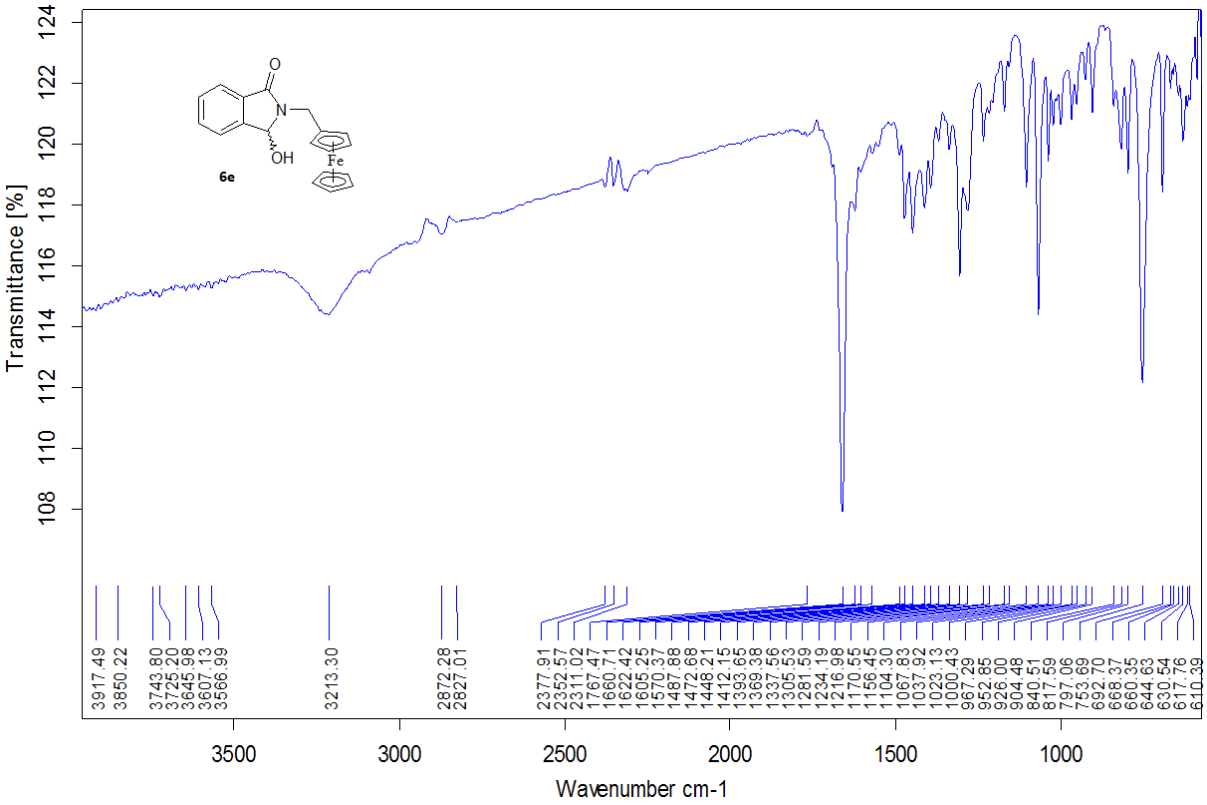
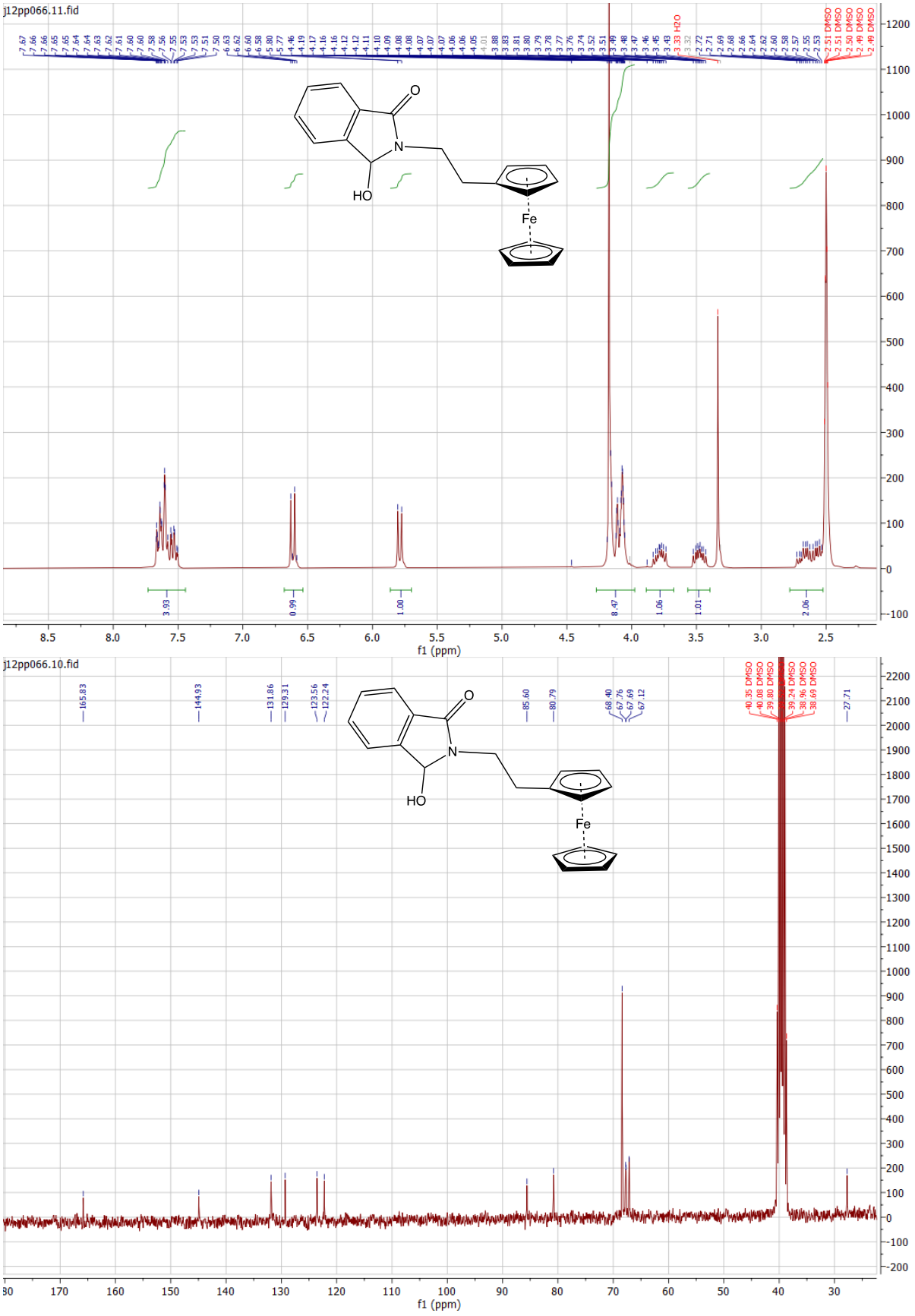

Transmittance [%]
108
110
112
114
116
118
120
122
124
O
N
OH
Fe
6e
3917.49
3850.22
3743.80
3725.20
3645.98
3607.13
3566.99
3213.30
2872.28
2827.01
2377.91
2352.57
2311.02
1767.47
1660.71
1622.42
1605.25
1570.37
1487.88
1472.69
1448.21
1412.15
1393.65
1369.38
1337.56
1305.53
1281.59
1234.19
1216.98
1170.55
1156.45
1104.30
1067.83
1037.92
1023.13
1000.43
967.29
952.85
926.00
904.48
840.51
817.59
797.06
753.69
692.70
668.37
660.35
644.63
630.54
617.76
610.39
3500
3000
2500
2000
1500
1000
Wavenumber cm-1

**Figure S23**: $^{1}H$ (in DMSO-$d_6$), $^{13}C$ (in DMSO-$d_6$) NMR, HR-MS and IR data for compound **6f**

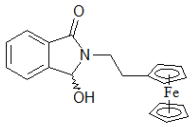


**Single Mass Analysis**
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

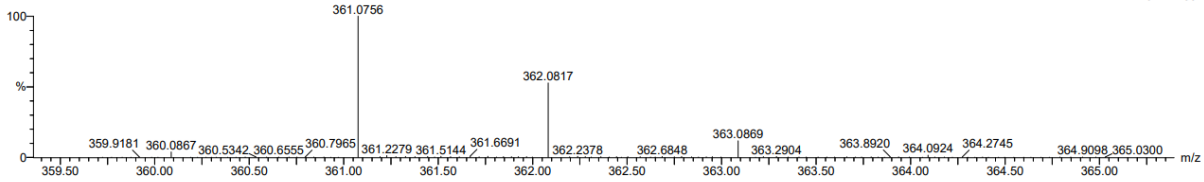
Monoisotopic Mass, Odd Electron Ions
152 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 1-150 H: 1-150 N: 0-3 O: 0-10 Fe: 1-1

19-Jun-2013 2::5::3
ENSCP_P677 37 (0.932) Cm (31:44)

ACN



LCT Premier XE KE483
1: TOF MS ES+
6.17e+004




| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 5.0 | 5.0 | 100.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 361.0756 | 361.0765 | -0.9 | -2.5 | 12.0 | 751.7 | 0.0 | C20 H19 N O2 Fe |

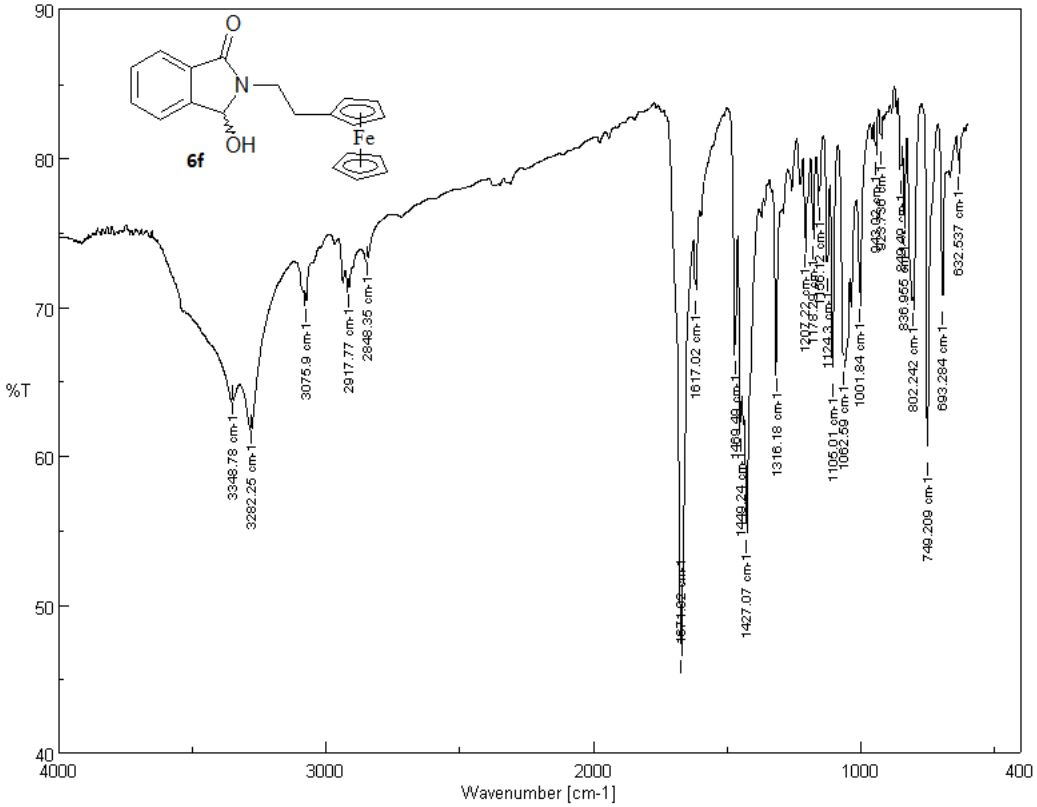
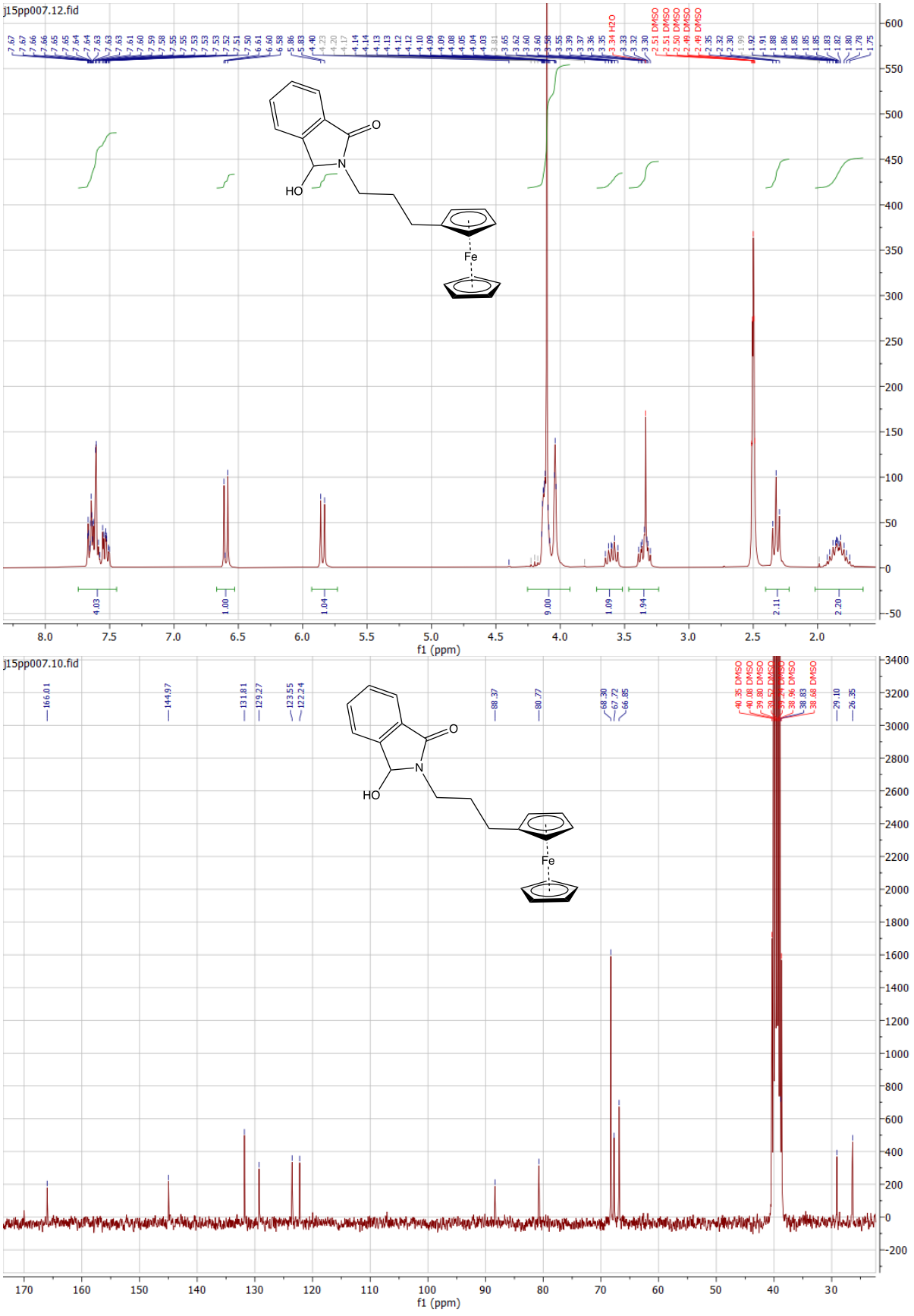


**Figure S24**: $^{1}H$ (in DMSO-$d_6$), $^{13}C$ (in DMSO-$d_6$) NMR, HR-MS and IR data for compound **6g**

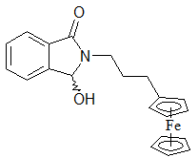


**Single Mass Analysis**
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

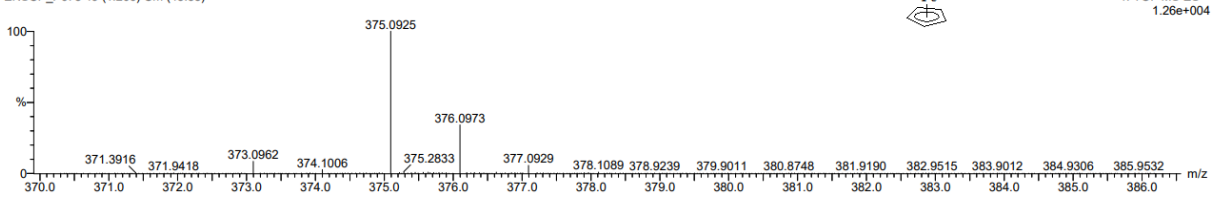
Monoisotopic Mass, Odd Electron Ions
160 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 1-150 H: 1-150 N: 0-3 O: 0-10 Fe: 1-1

19-Jun-2013 3::0::1
ENSCP_P678 49 (1.206) Cm (48:58)

ACN




LCT Premier XE KE483
1: TOF MS ES+
1.26e+004




| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 5.0 | 5.0 | 100.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 375.0925 | 375.0922 | 0.3 | 0.8 | 12.0 | 788.0 | 0.0 | C21 H21 N O2 Fe |
| | 375.0940 | -1.5 | -4.0 | -1.0 | 795.2 | 7.2 | C9 H25 N3 O9 Fe |

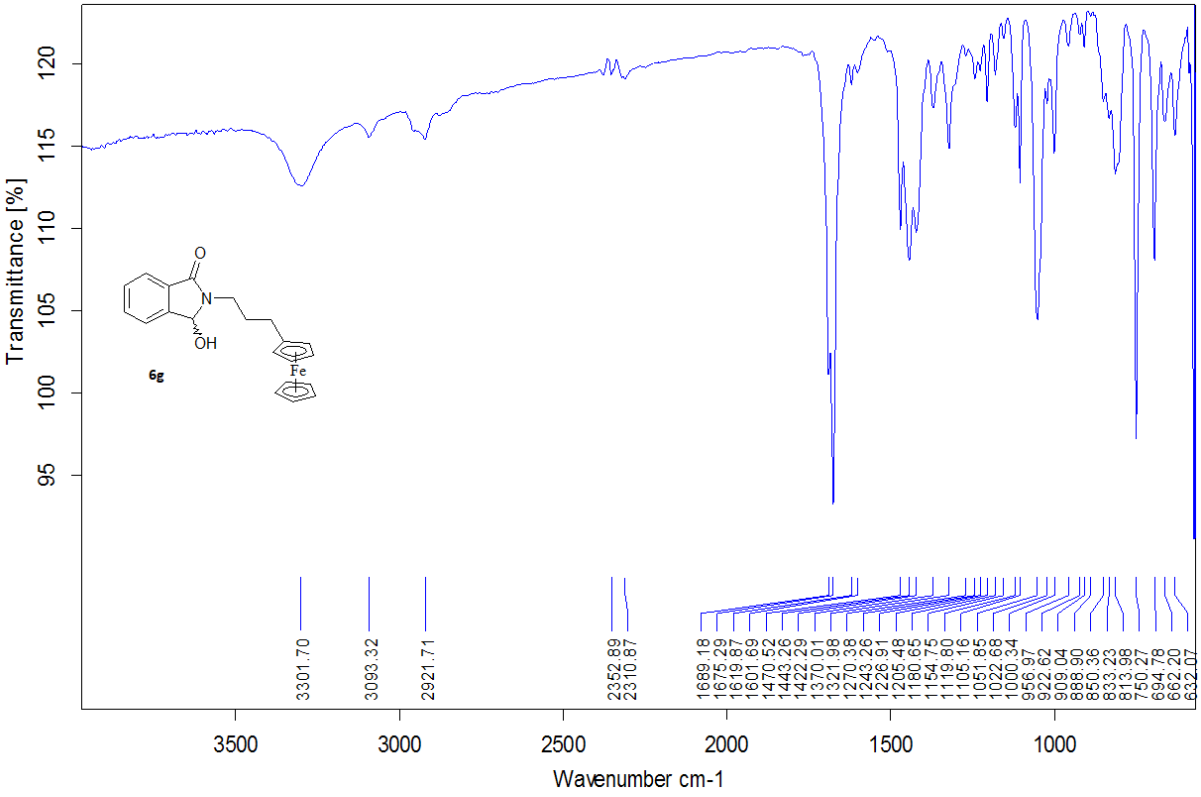
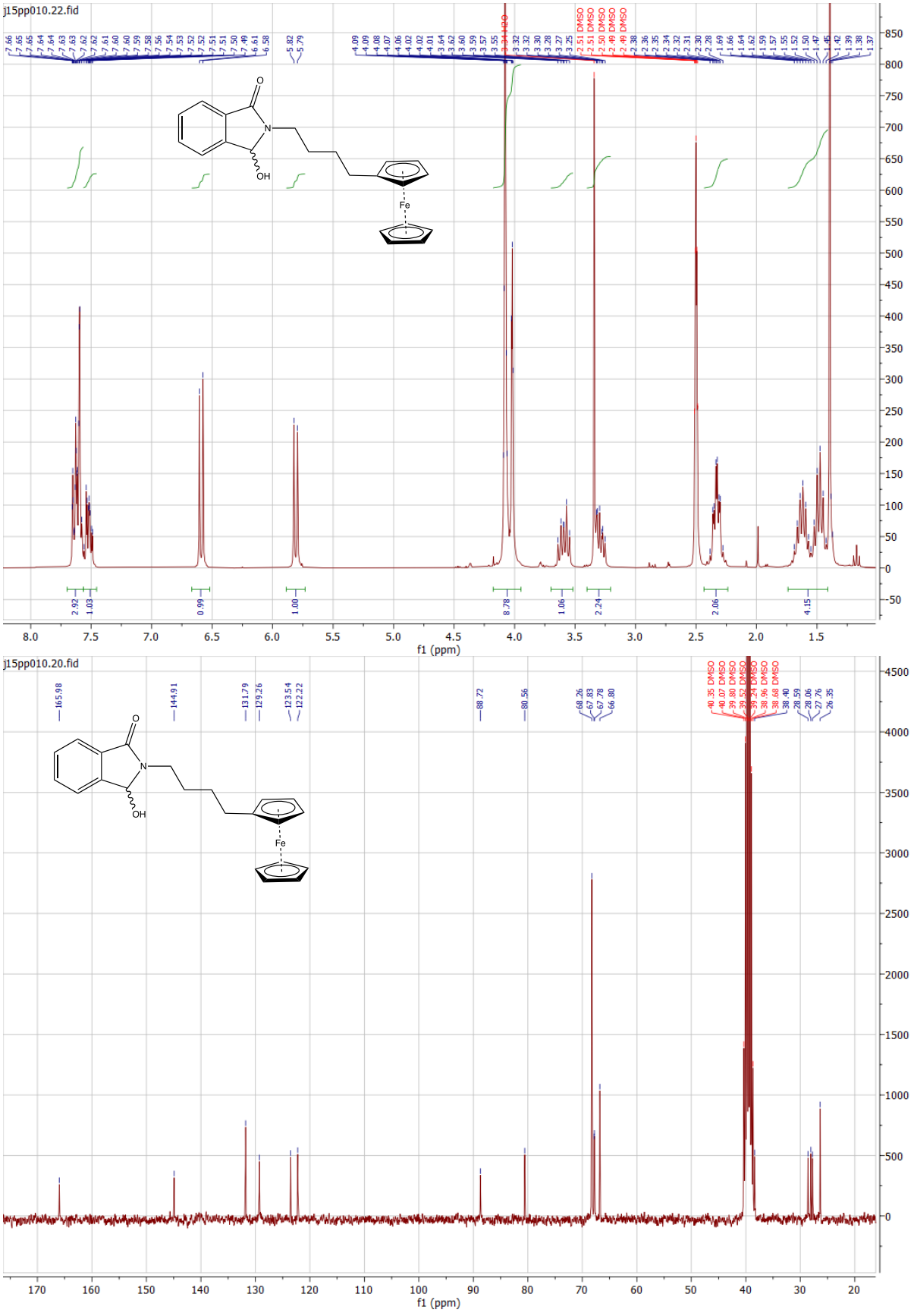
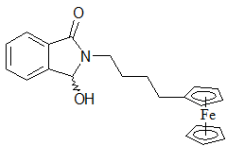


**Figure S25**: $^{1}H$ (in DMSO-$d_6$) and $^{13}C$ (in DMSO-$d_6$) NMR and HR-MS data for compound **6h**



**Single Mass Analysis**
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

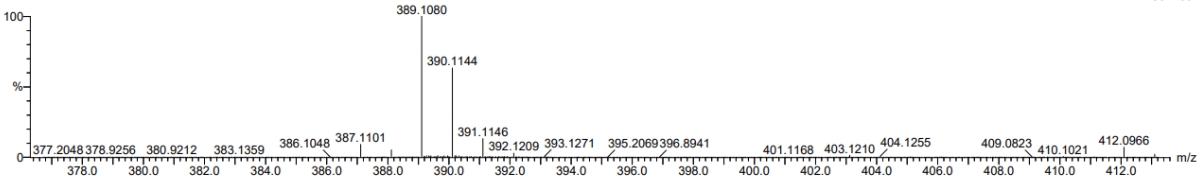
Monoisotopic Mass, Odd Electron Ions
412 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 1-120 N: 0-10 O: 0-10 Fe: 1-1




06-Sep-2013 5::7::4
ENSCP_P679 29 (0.753) Cm (29:39)

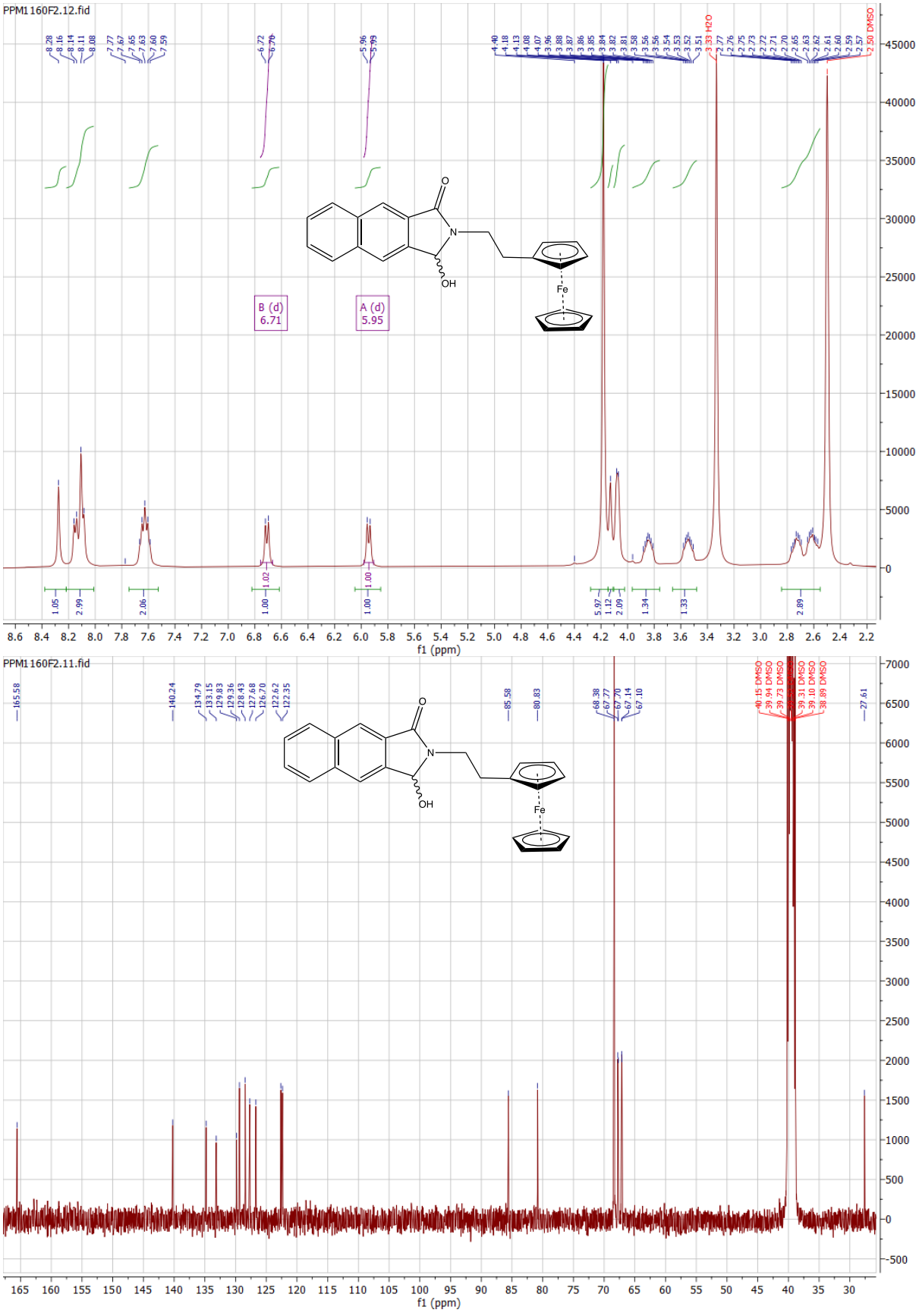
MeOH

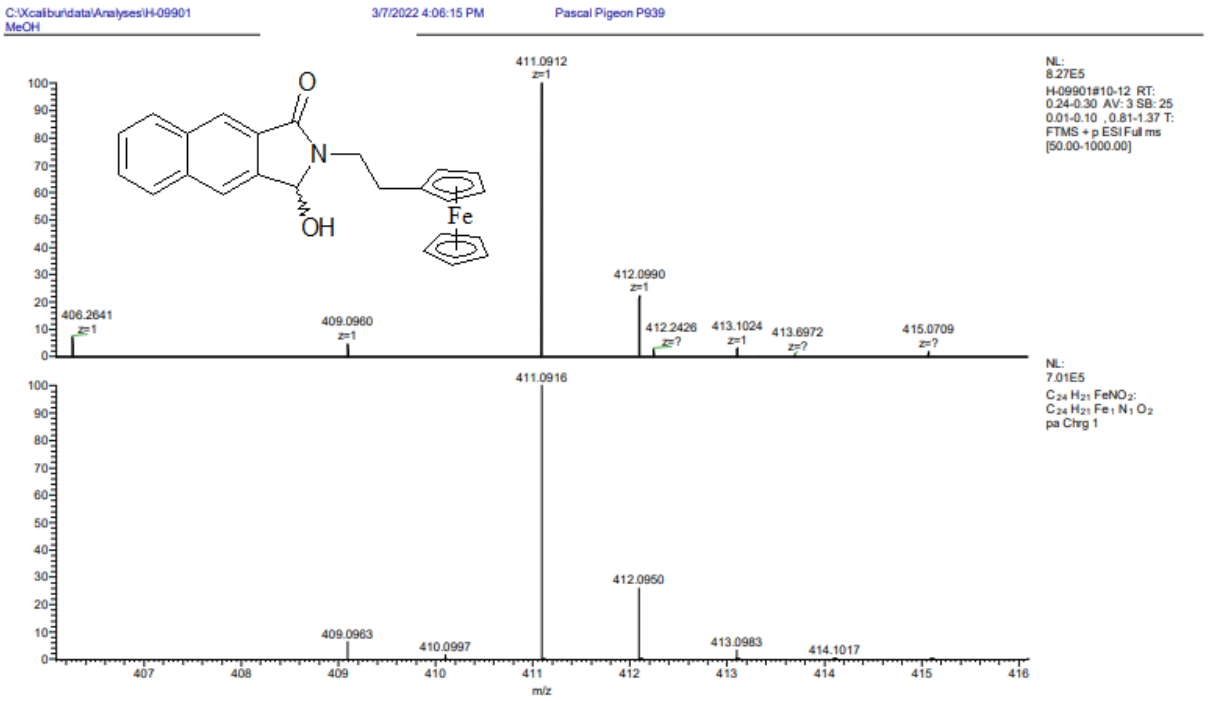
LCT Premier XE KE483
1: TOF MS ES+
2.55e+004




| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 5.0 | 5.0 | 100.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 389.1080 | 389.1078 | 0.2 | 0.5 | 12.0 | 1020.1 | 0.0 | C22 H23 N O2 Fe |
| | 389.1097 | -1.7 | -4.4 | -1.0 | 1023.3 | 3.2 | C10 H27 N3 O9 Fe |
| | 389.1070 | 1.0 | 2.6 | 0.0 | 1026.1 | 6.1 | C6 H23 N9 O7 Fe |

**Figure S26**: $^{1}H$ (in DMSO-$d_6$), $^{13}C$ (in DMSO-$d_6$) NMR, HR-MS and IR data for compound **6i**






# Experimental/theoretical isotopic pattern MS spectrum

**Error = -1.0 ppm; Relative Intensity (%) 100**

**HRMS (ESI) m/z: [M]+ Calcd for C24H21FeNO2 411.0916 . Found 411.0912; (Error: -1.0 ppm).**

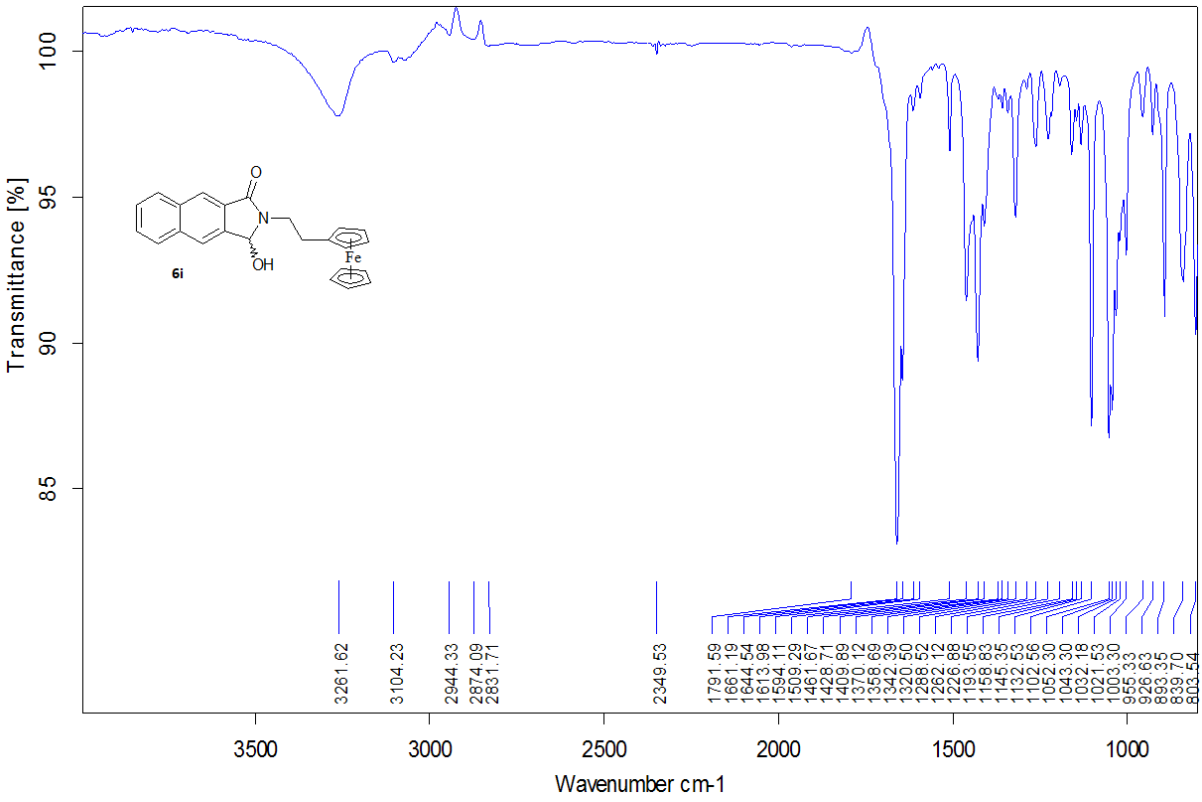


**Figure S27**: $^{1}H$ (in $CDCl_3$), COSY (in $CDCl_3$) NMR data for compound **6j**

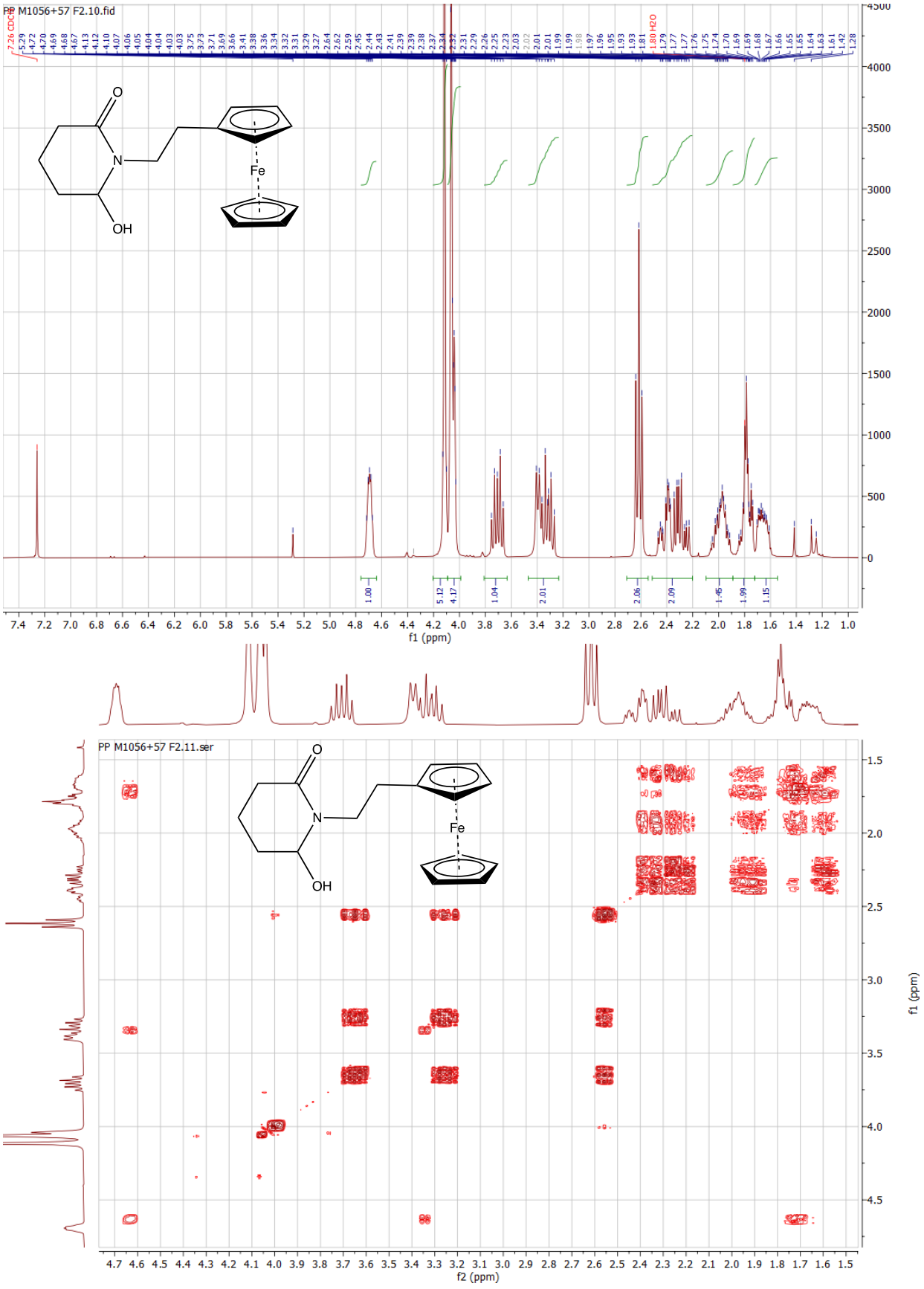
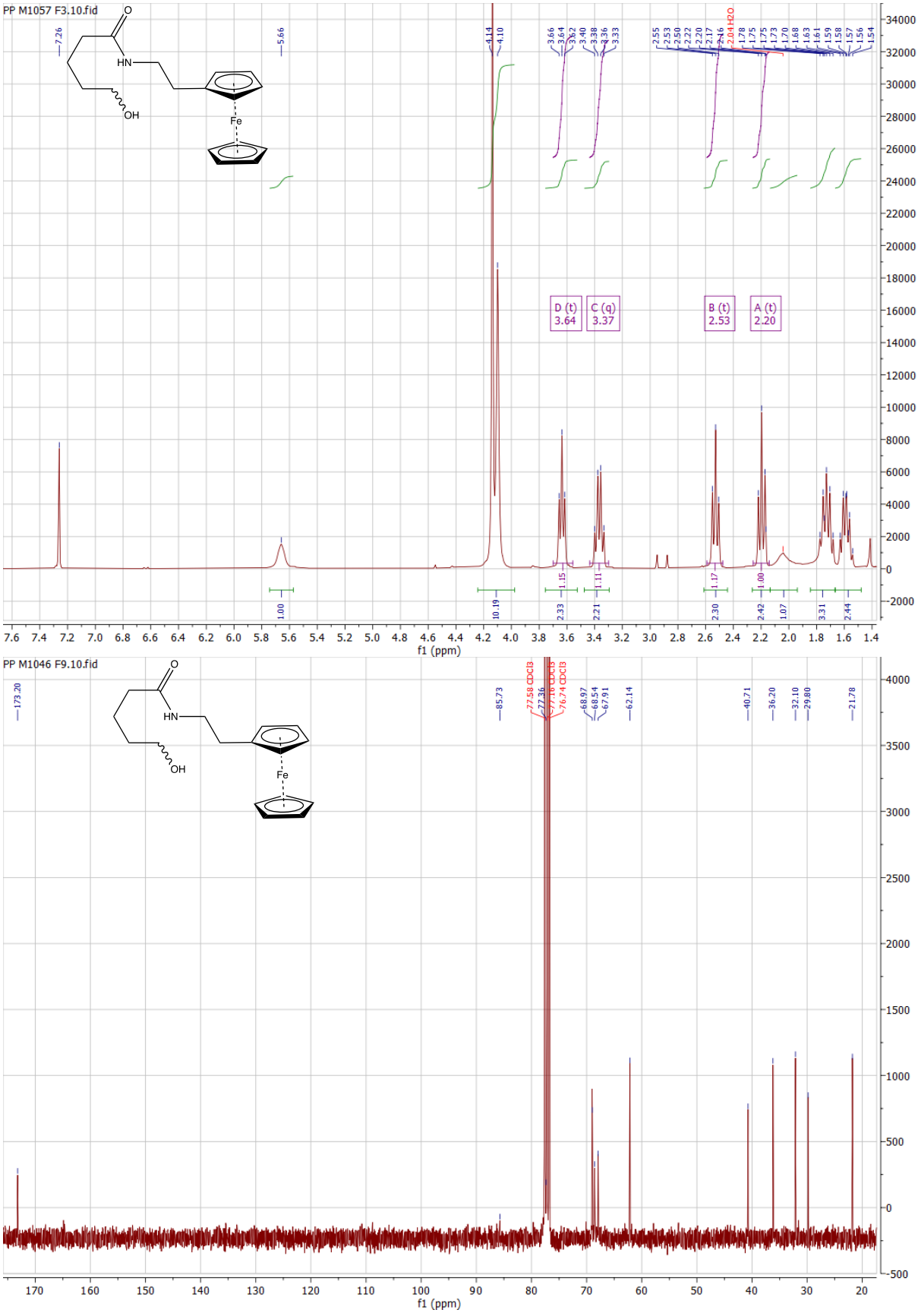


**Figure S28**: $^{1}H$ (in $CDCl_3$), $^{13}C$ (in $CDCl_3$) NMR and IR data for compound **7j**



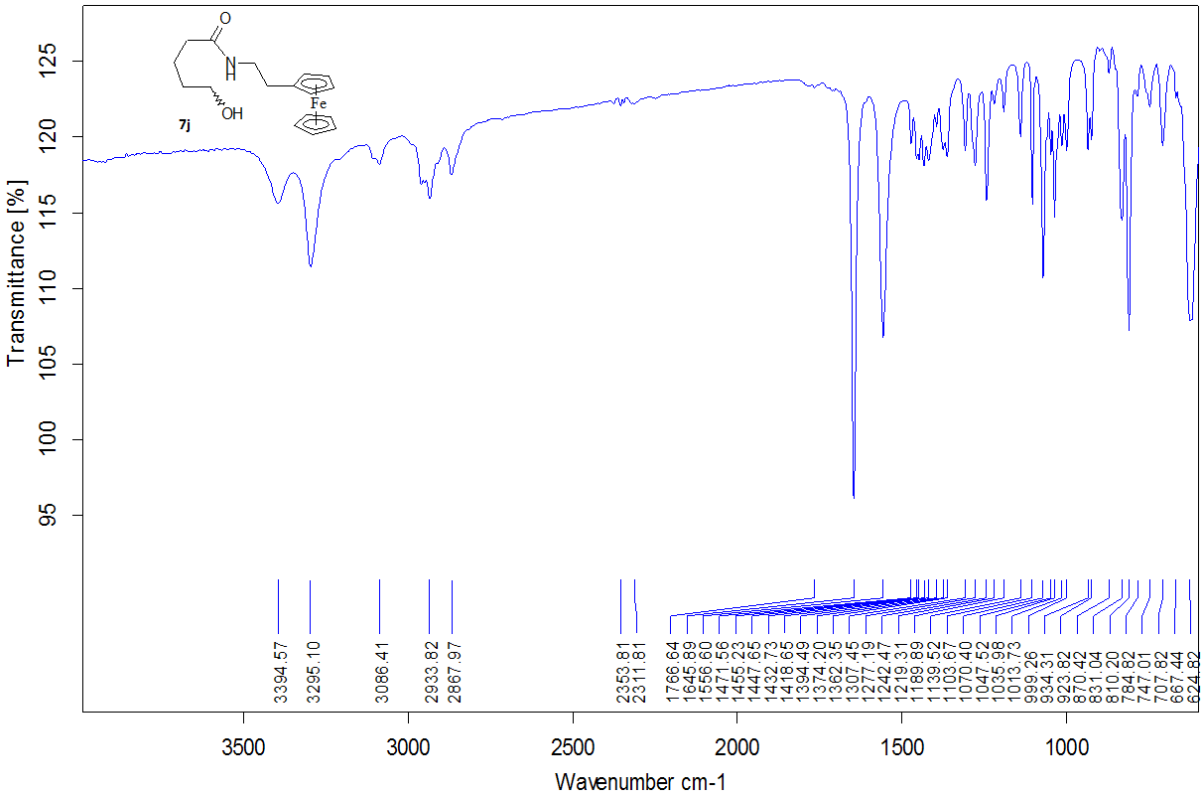
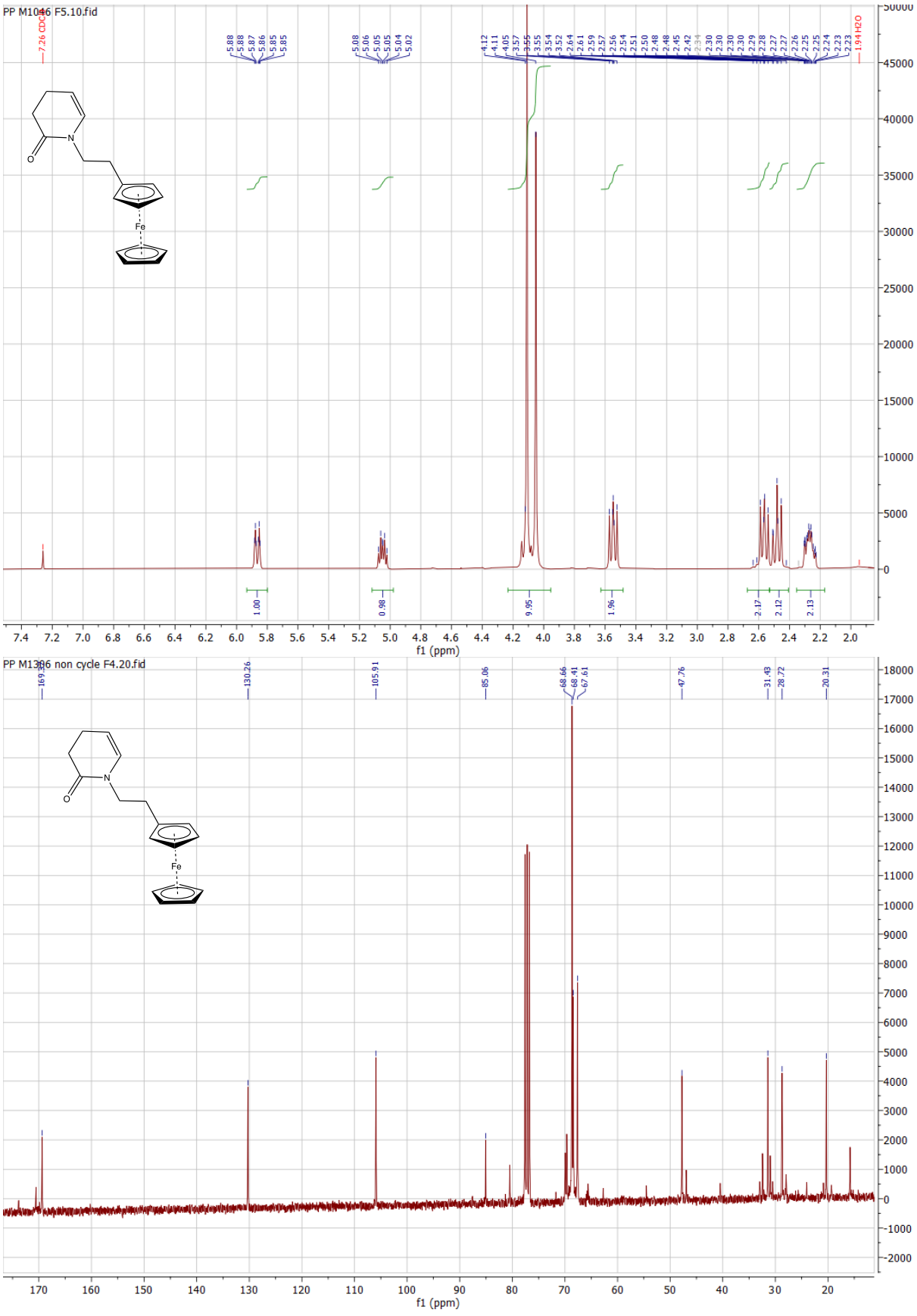
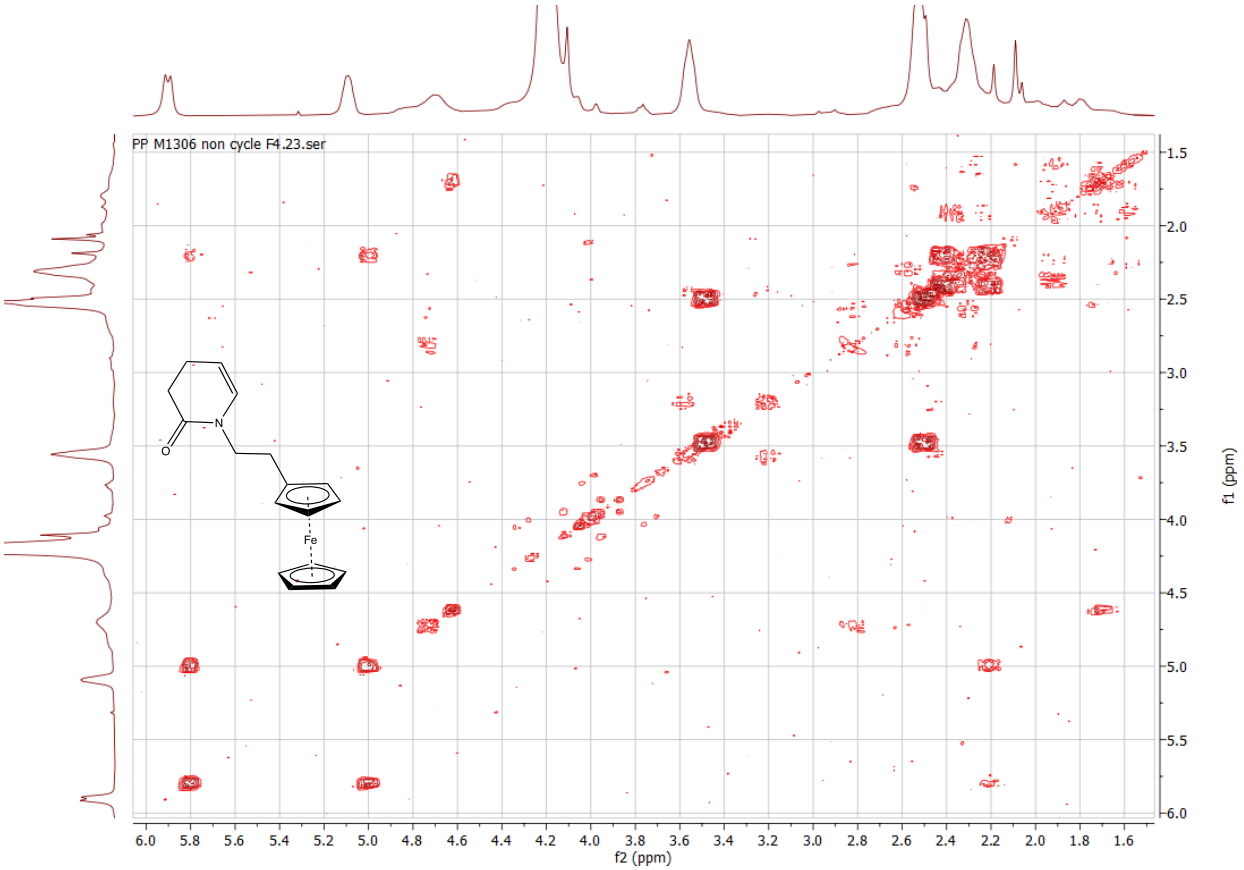
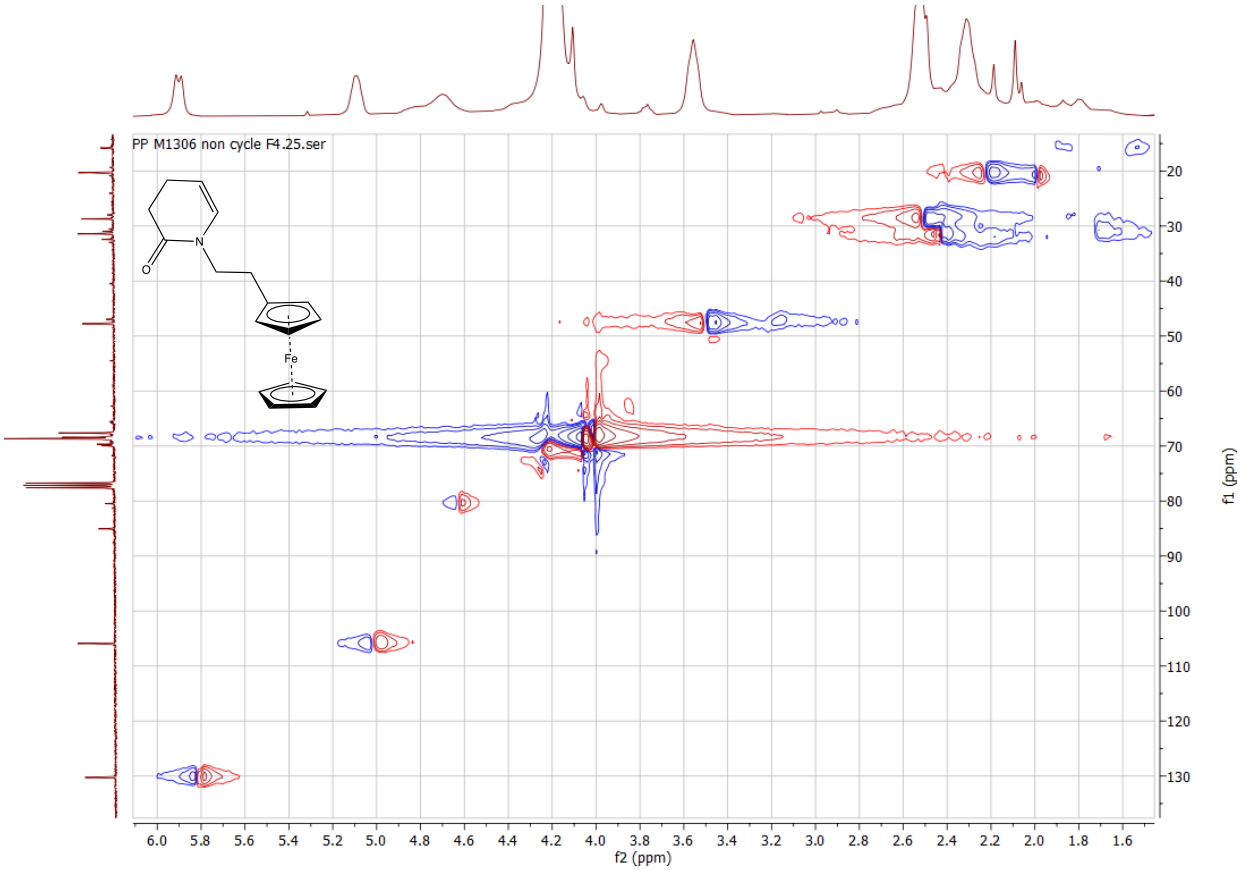

7j
Transmittance [%]
95
100
105
110
115
120
125
3500
3000
2500
2000
1500
1000
Wavenumber cm-1
3394.57
3295.10
3086.41
2933.82
2867.97
2353.81
2311.81
1766.64
1645.89
1556.60
1471.56
1455.23
1447.65
1432.73
1418.65
1394.49
1374.20
1362.35
1307.45
1277.19
1242.47
1219.31
1189.89
1139.52
1103.67
1070.40
1047.52
1035.98
1013.73
999.26
934.31
923.82
870.42
831.04
810.20
784.82
747.01
707.82
667.44
624.82

**Figure S29**: $^{1}H$ (in $CDCl_3$), $^{13}C$ (in $CDCl_3$), COSY (in $CDCl_3$), HMQC (in $CDCl_3$) NMR and IR data for compound **8j**




PP M1306 non cycle F4.23.ser
N
O
Fe
f2 (ppm)
f1 (ppm)


PP M1306 non cycle F4.25.ser
N
O
Fe
f2 (ppm)
f1 (ppm)

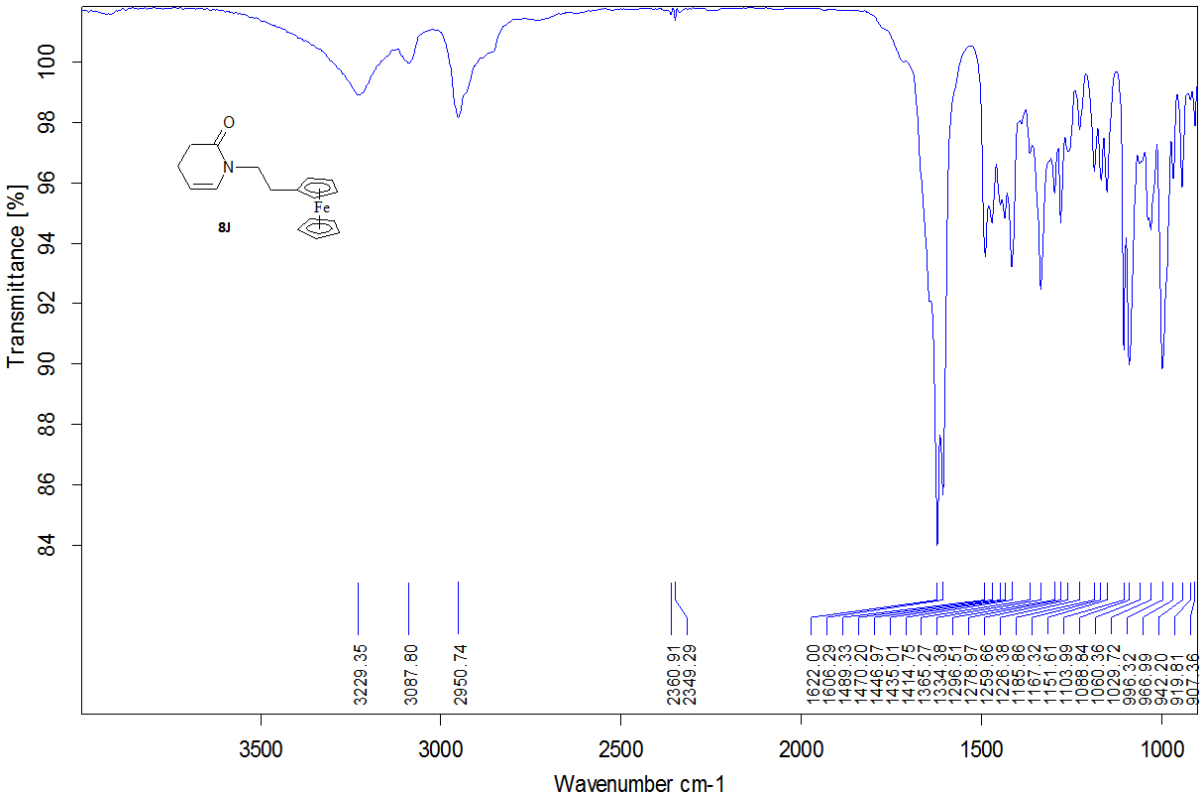
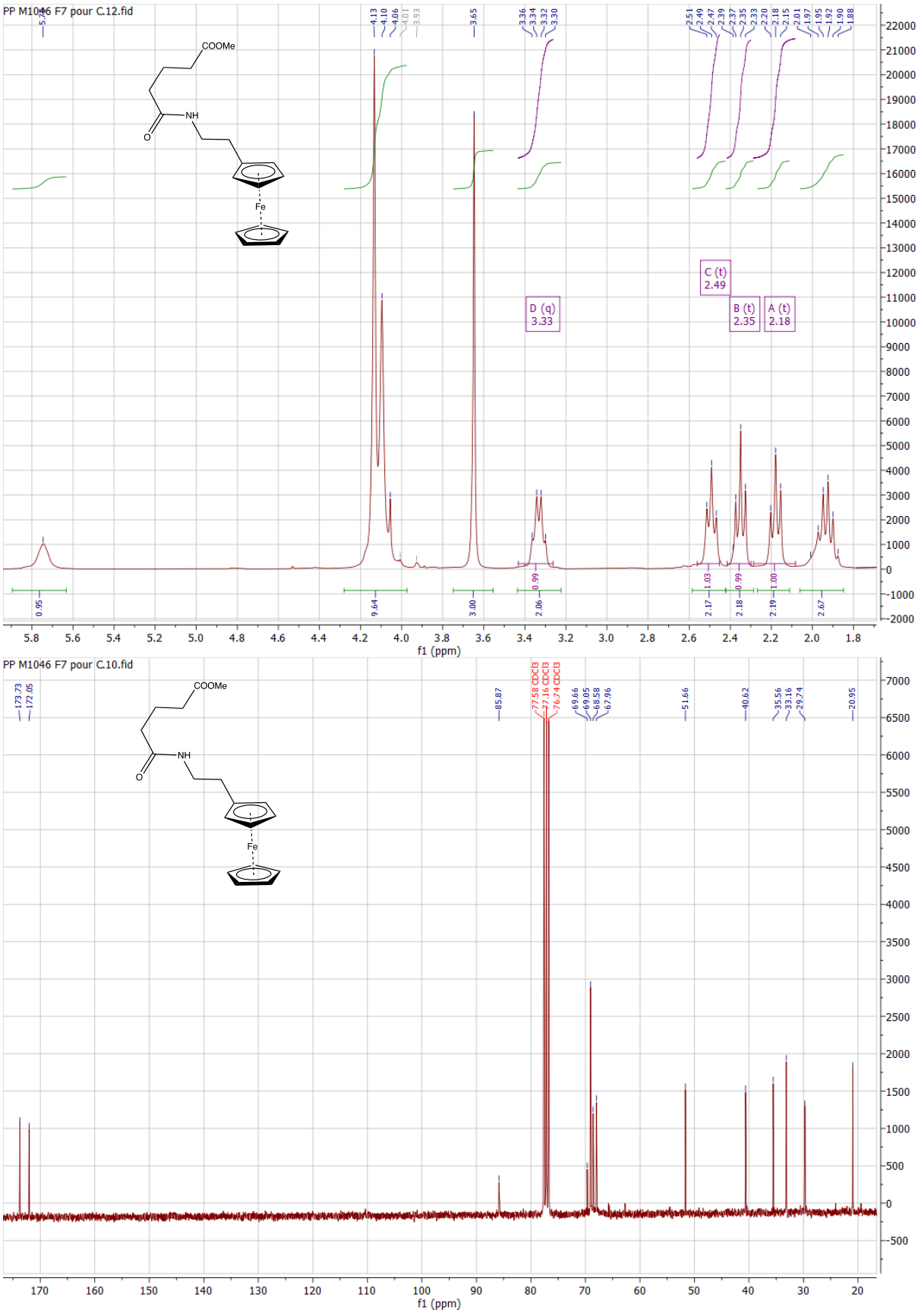

Transmittance [%]
100
98
96
94
92
90
88
86
84
O
N
Fe
8J
3229.35
3087.80
2950.74
2360.91
2349.29
1622.00
1606.29
1489.33
1470.20
1446.97
1435.01
1414.75
1365.27
1334.38
1296.51
1278.97
1259.66
1226.38
1185.86
1167.32
1151.61
1103.99
1088.84
1060.36
1029.72
996.32
966.99
942.20
919.81
907.36
3500
3000
2500
2000
1500
1000
Wavenumber cm-1

**Figure S30**: $^{1}H$ (in $CDCl_3$), $^{13}C$ (in $CDCl_3$) NMR and IR data for compound **9j**



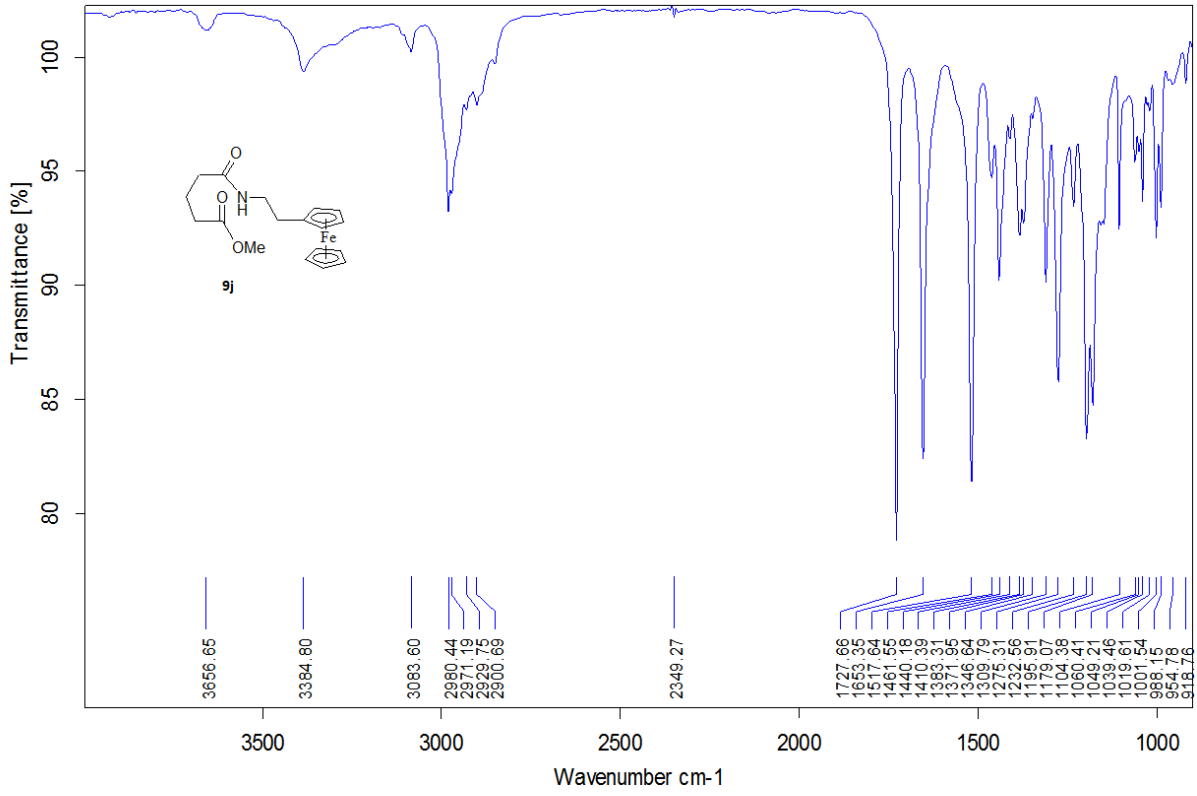
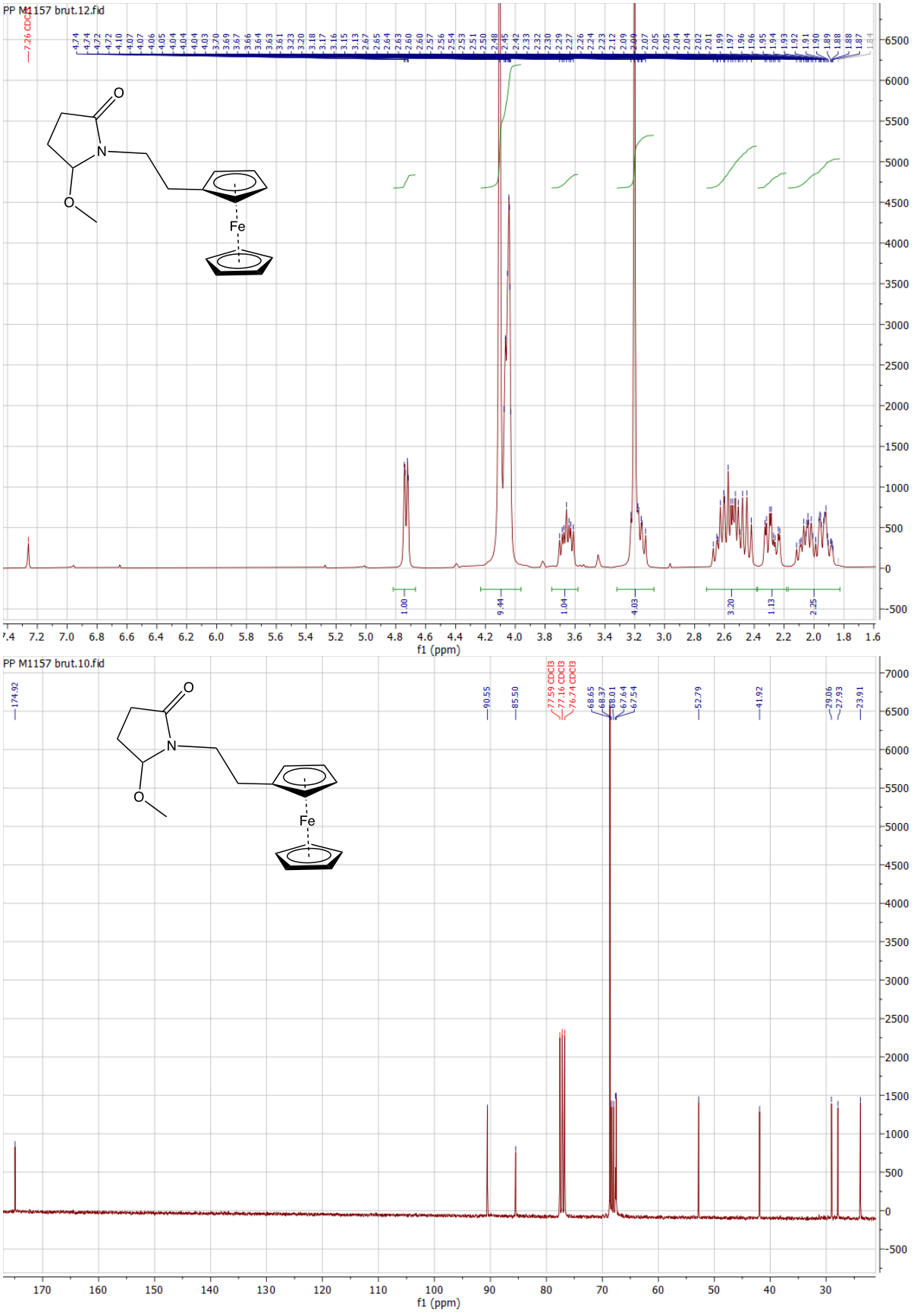
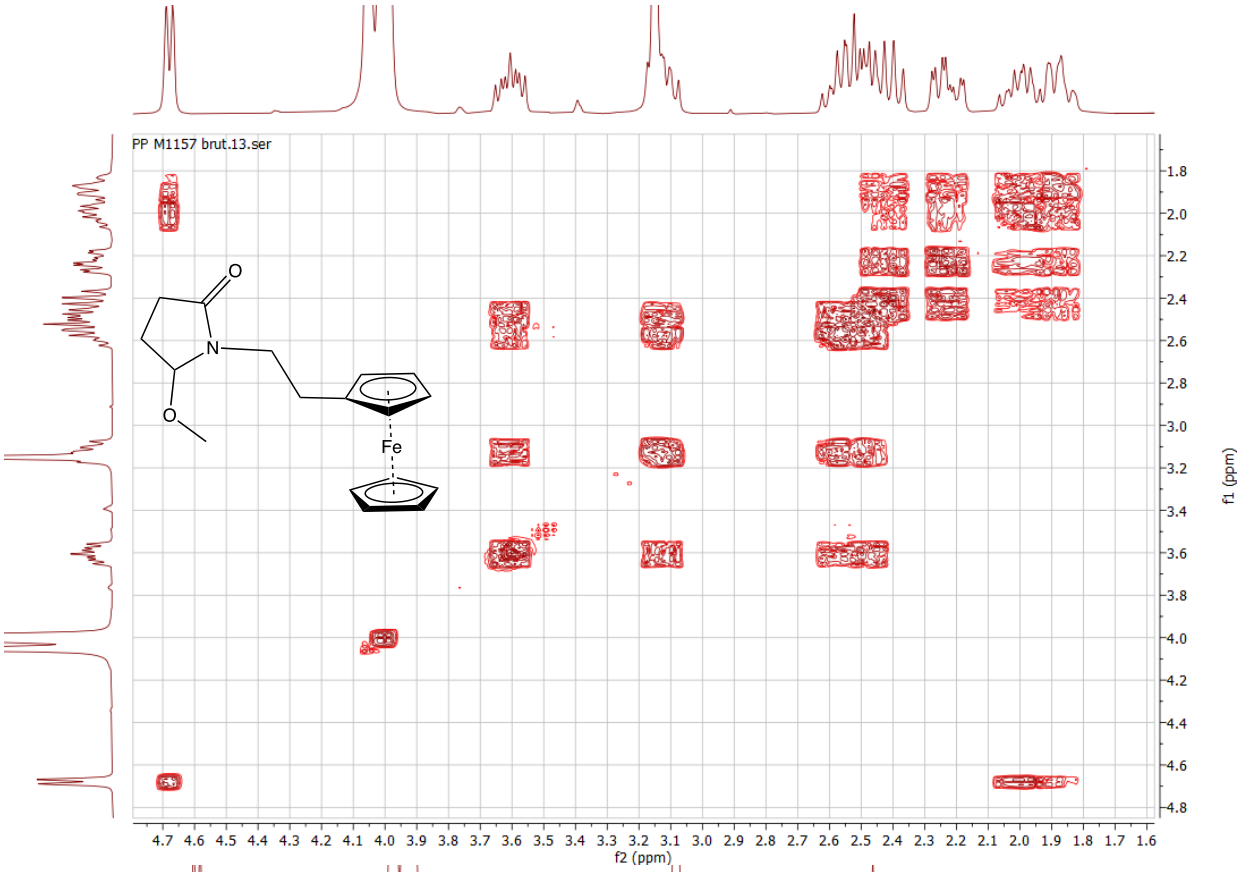
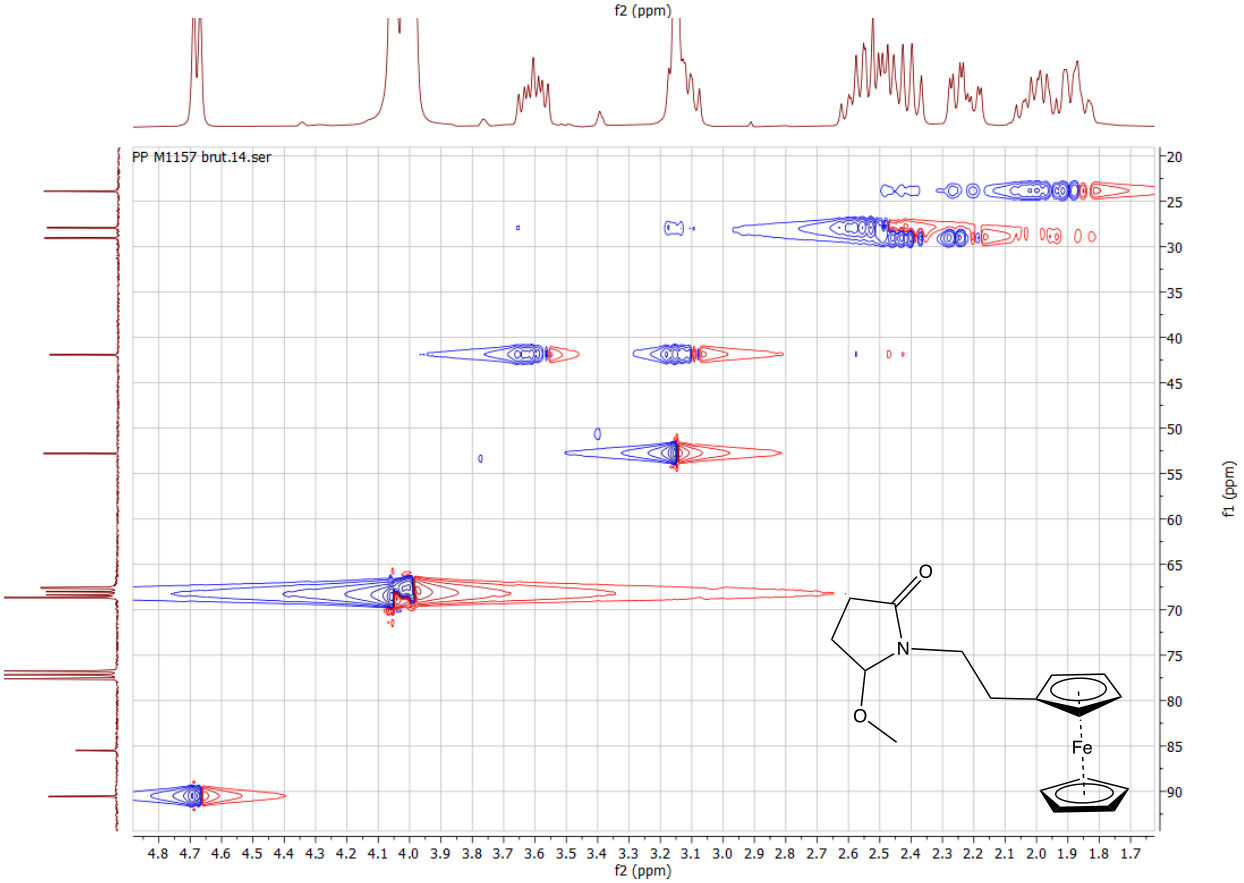
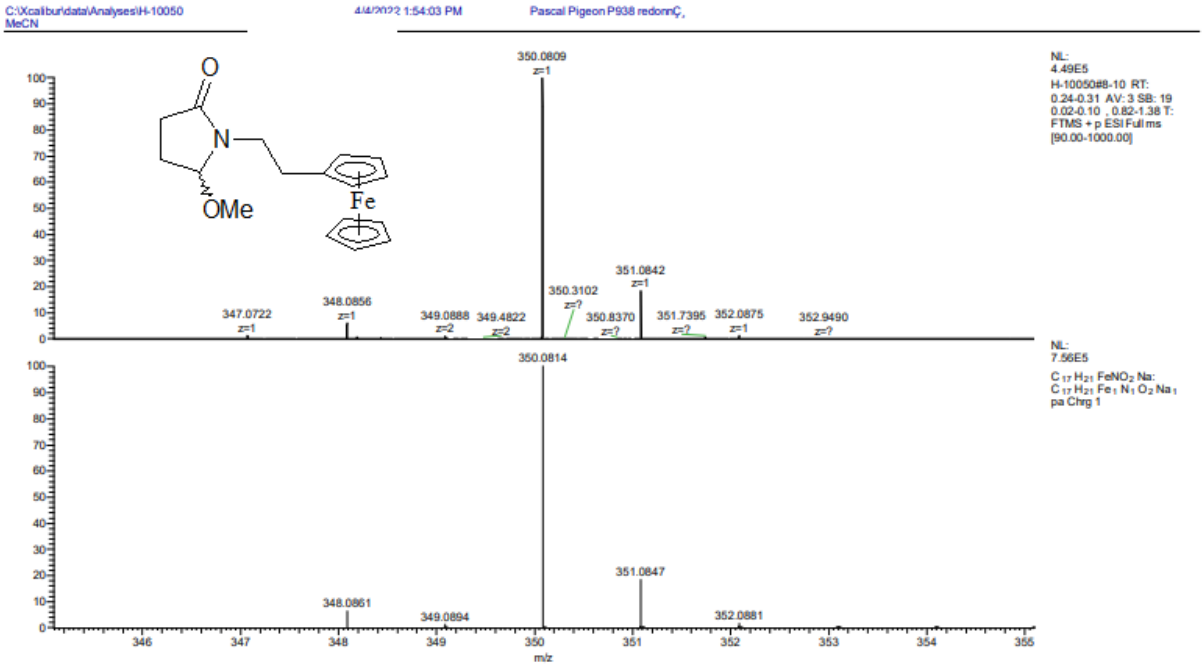

Transmittance [%]
100
95
90
85
80
O
O
N
H
OMe
Fe
9j
3656.65
3384.80
3083.60
2980.44
2971.19
2929.75
2900.69
2349.27
1727.66
1653.35
1517.64
1461.55
1440.18
1410.39
1383.31
1371.95
1346.64
1309.79
1275.31
1232.56
1195.91
1179.07
1104.38
1060.41
1049.21
1039.46
1019.61
1001.54
988.15
954.78
918.76
3500
3000
2500
2000
1500
1000
Wavenumber cm-1

**Figure S31**: $^{1}H$ (in $CDCl_3$), $^{13}C$ (in $CDCl_3$), COSY (in $CDCl_3$), HMQC (in $CDCl_3$) NMR, HR-MS and IR data for compound **10b**




PP M1157 brut.13.ser
O
N
O
Fe
f2 (ppm)
f1 (ppm)


PP M1157 brut.14.ser
O
N
O
Fe
f2 (ppm)
f1 (ppm)




# Experimental/theoretical isotopic pattern MS spectrum

**Error = -1.4 ppm; Relative Intensity (%) 100**

**HRMS (ESI) m/z: [M+Na]+ Calcd for C17H21FeNO2Na 350.0814. Found 350.0809; (Error: -1.4 ppm).**

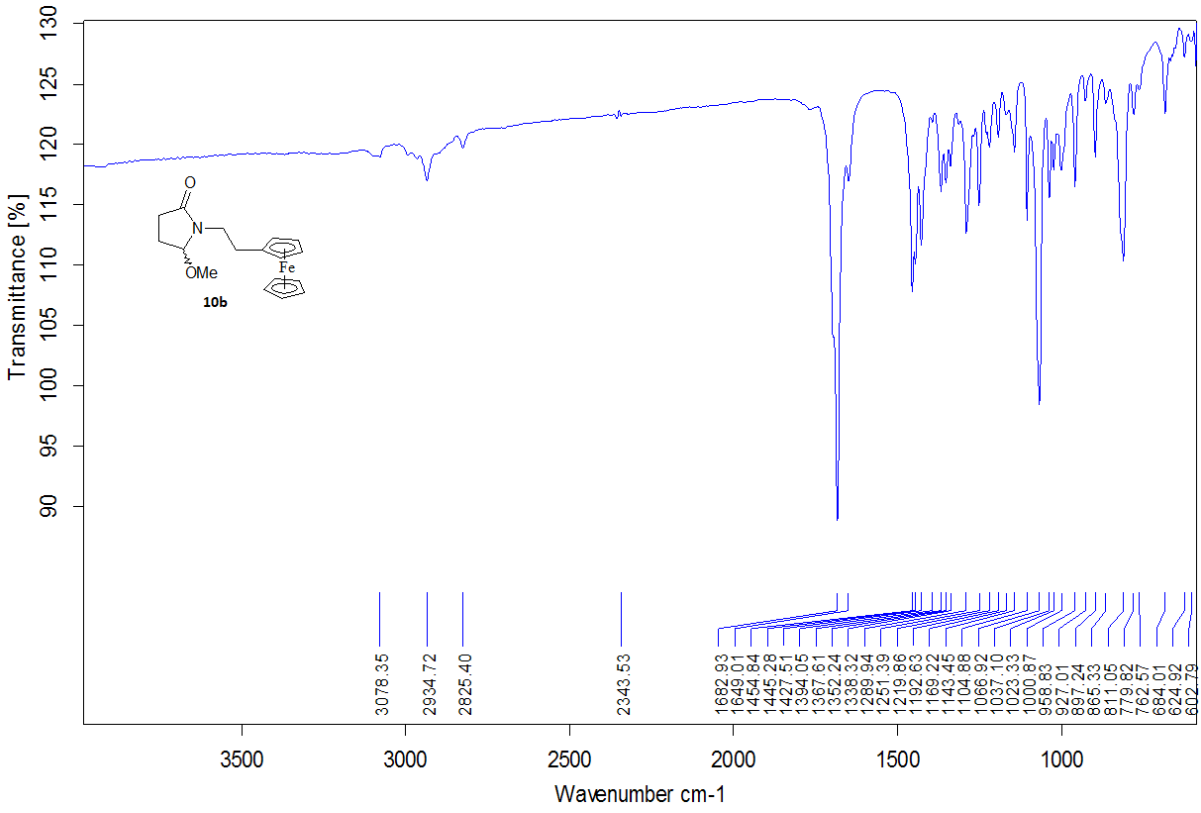
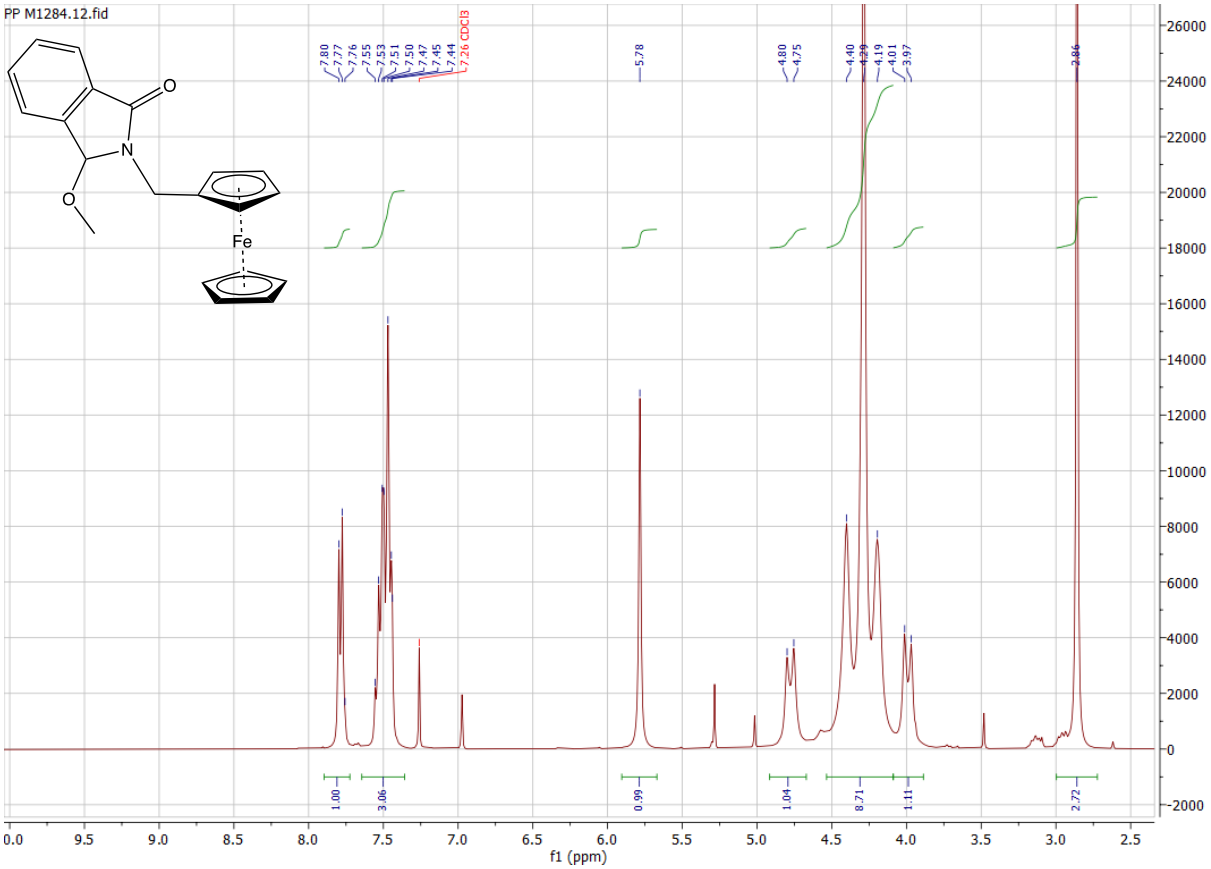
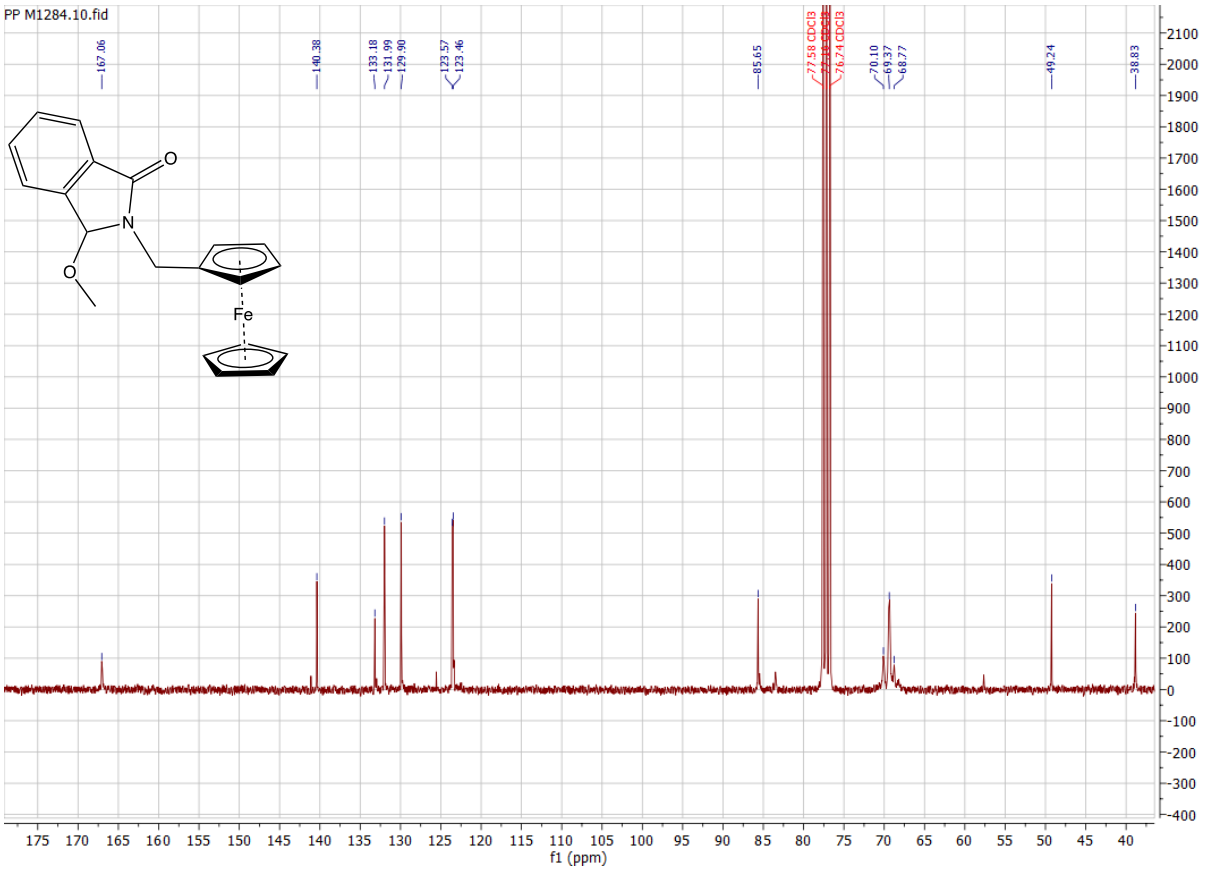
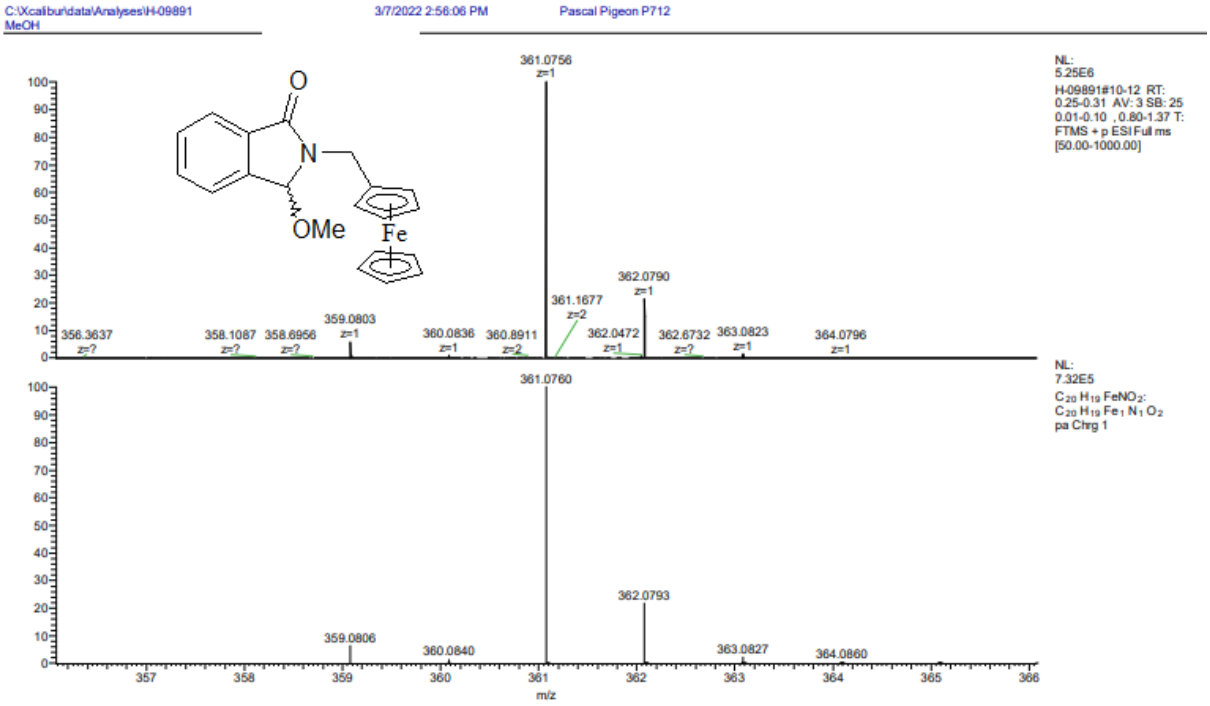


**Figure S32**: $^{1}H$ (in $CDCl_3$), $^{13}C$ (in $CDCl_3$) NMR, HR-MS and IR data for compound **10e**






# Experimental/theoretical isotopic pattern MS spectrum

**Error = -1.0 ppm; Relative Intensity (%) 100**

**HRMS (ESI) m/z: [M]+ Calcd for C20H19FeNO2 361.0760 . Found 361.0756; (Error: -1.0 ppm).**

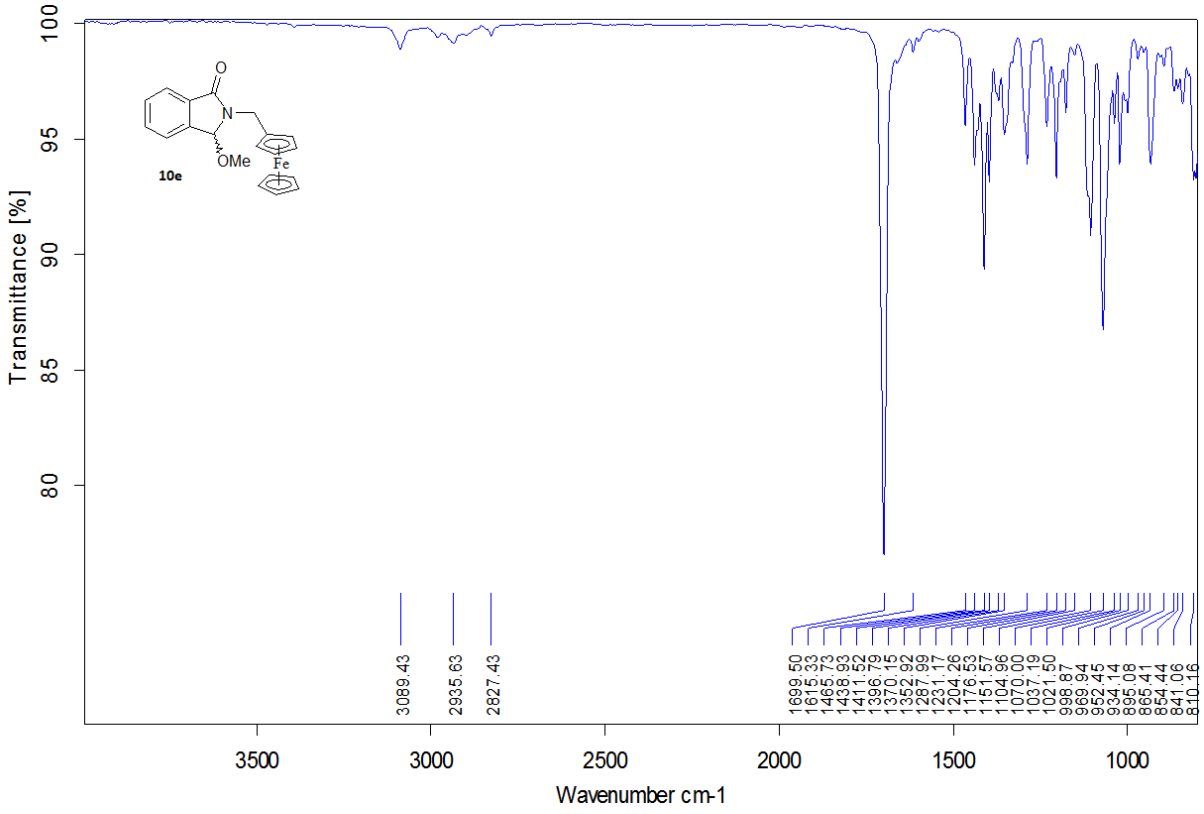
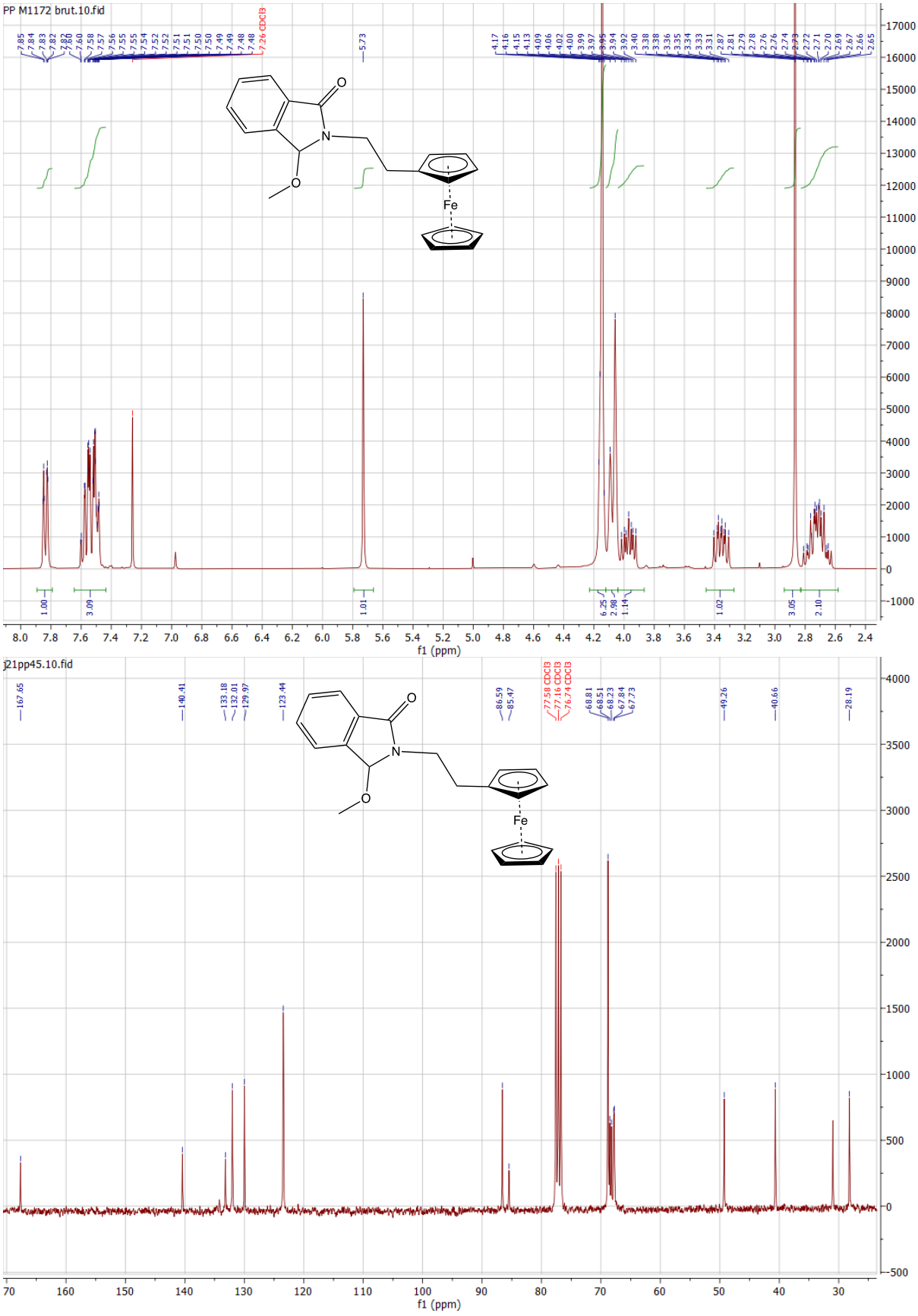
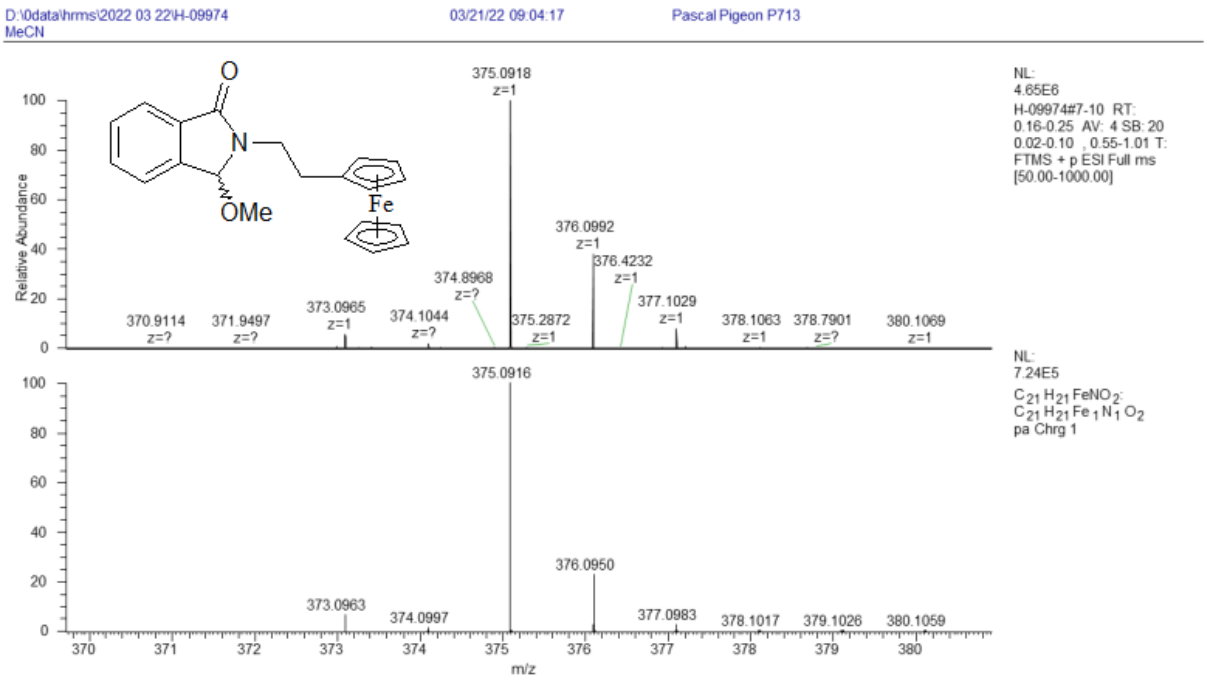


**Figure S33**: $^{1}H$ (in $CDCl_3$), $^{13}C$ (in $CDCl_3$) NMR, HR-MS and IR data for compound **10f**






# Experimental/theoretical isotopic pattern MS spectrum

**Error = 0.2 ppm; Relative Intensity (%) 100**

**HRMS (ESI) m/z: [M+H]+ Calcd for C21H21FeNO2H 376.0994. Found 376.0995; (Error: 0.2 ppm).**

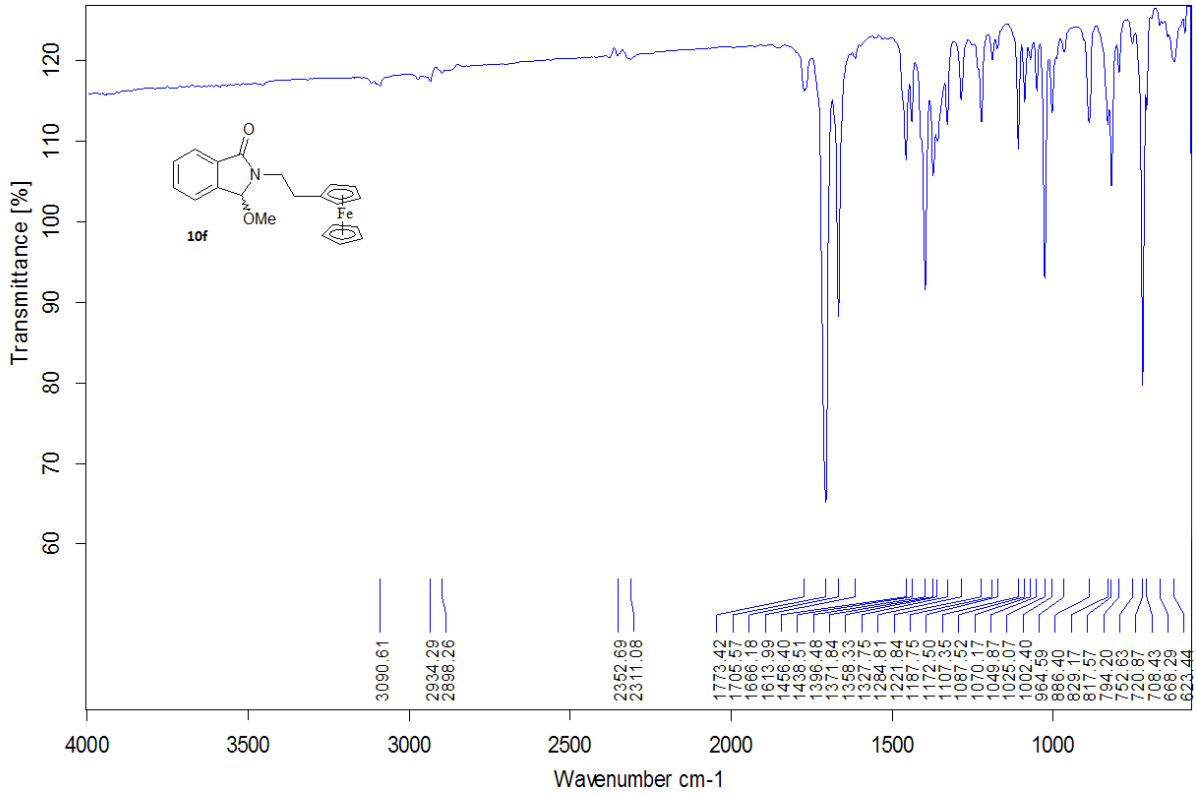
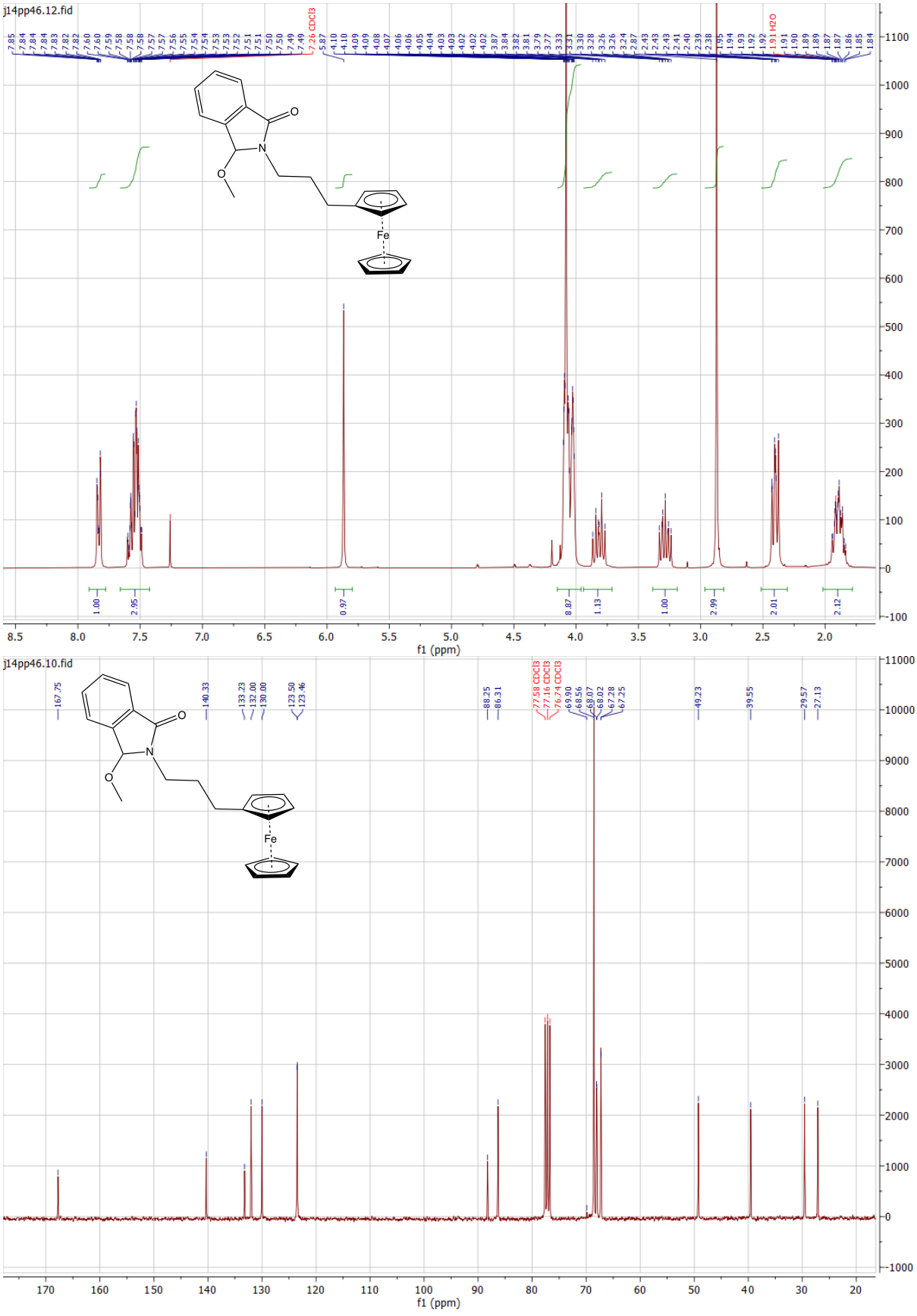
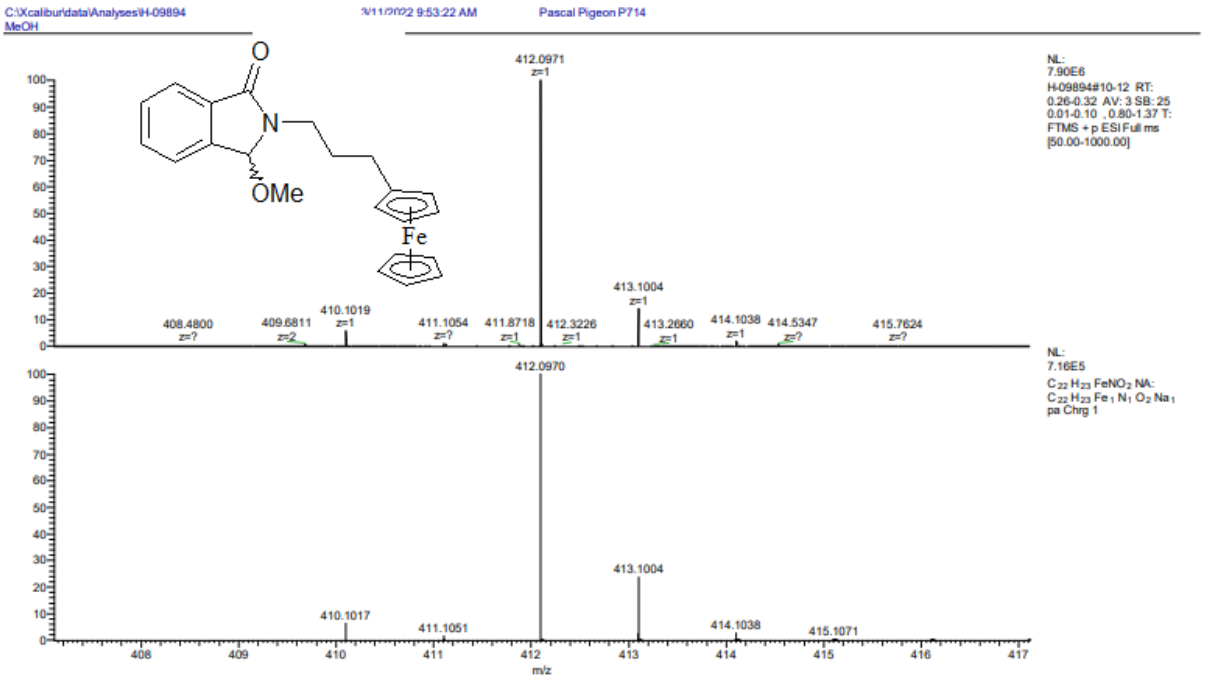


**Figure S34**: $^{1}H$ (in $CDCl_3$), $^{13}C$ (in $CDCl_3$) NMR, HR-MS and IR data for compound **10g**






# Experimental/theoretical isotopic pattern MS spectrum

**Error = 0.2 ppm; Relative Intensity (%) 100**

**HRMS (ESI) m/z: [M]+ Calcd for C22H23FeNO2Na 412.0970 . Found 412.0971; (Error: 0.2 ppm).**

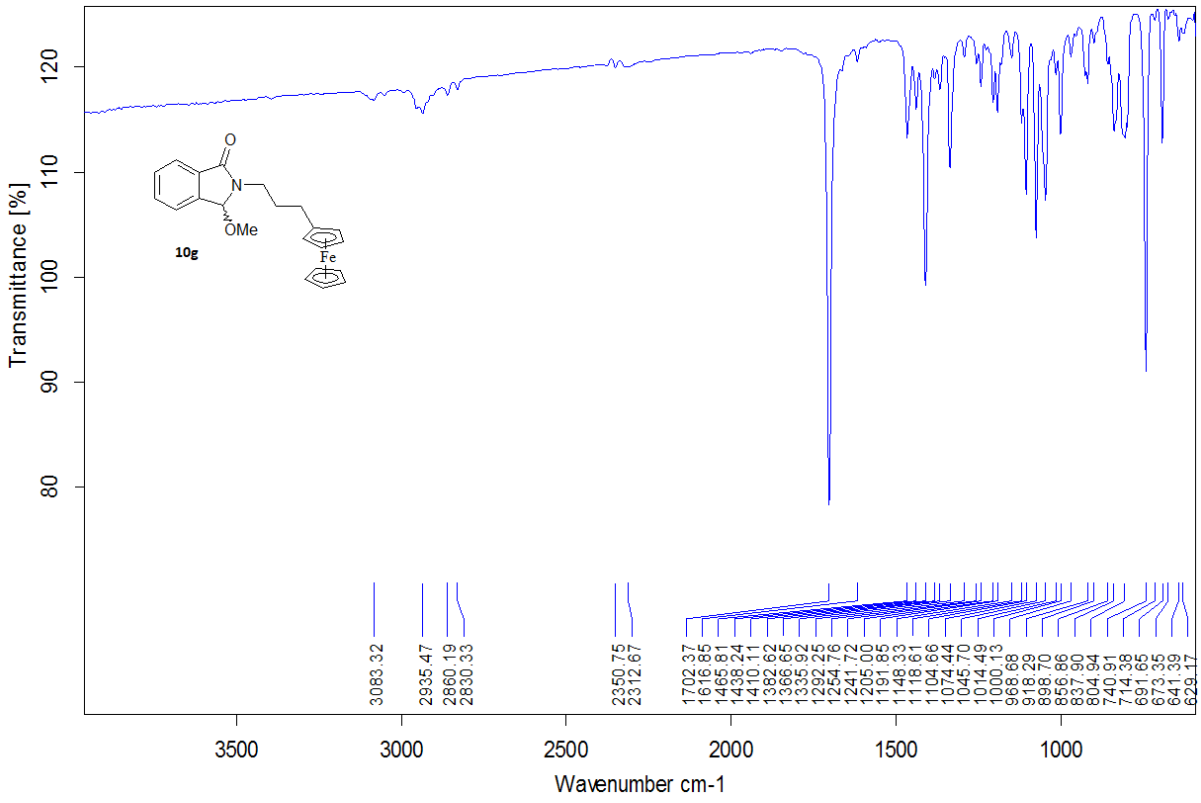
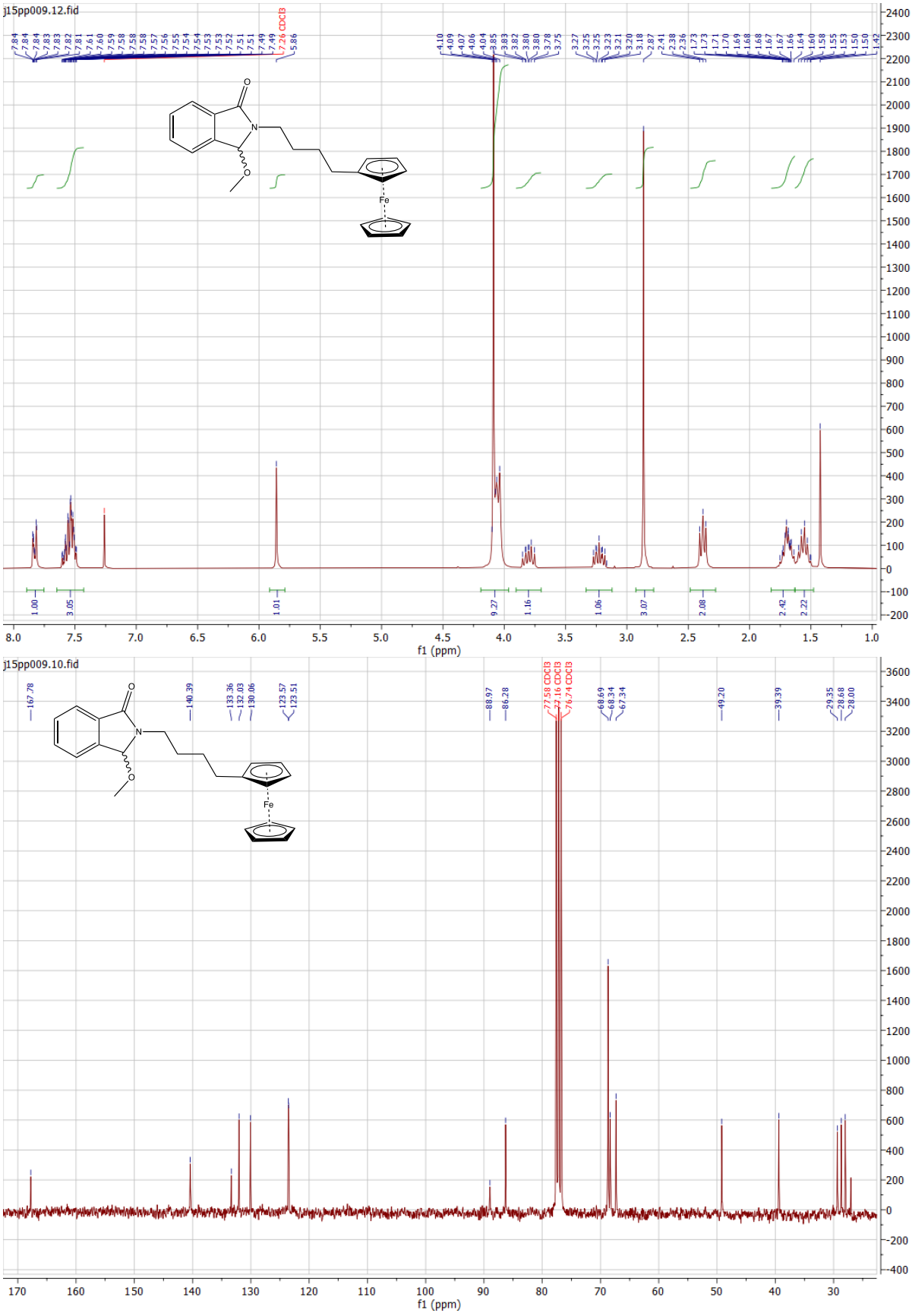
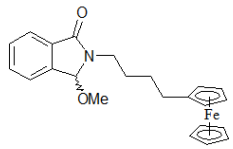


**Figure S35**: $^{1}H$ (in $CDCl_3$), $^{13}C$ (in $CDCl_3$) NMR, HR-MS and IR data for compound **10h**



**Single Mass Analysis**
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

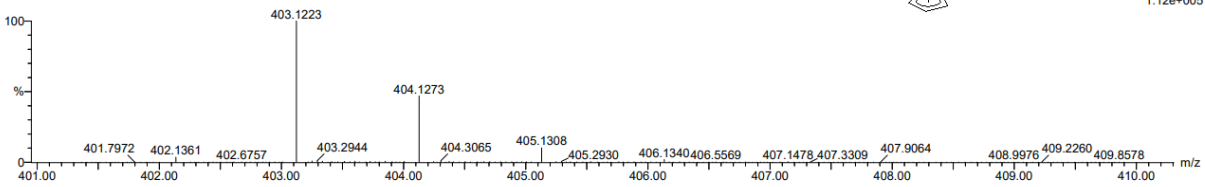
Monoisotopic Mass, Odd Electron Ions
174 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 1-150 H: 1-150 N: 0-3 O: 0-10 Fe: 1-1




19-Jun-2013 2::1::6
ENSCP_P715 37 (0.932) Cm (32:47)

ACN

LCT Premier XE KE483
1: TOF MS ES+
1.12e+005




| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 5.0 | 5.0 | 100.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 403.1223 | 403.1235 | -1.2 | -3.0 | 12.0 | 1238.0 | 0.0 | C23 H25 N O2 Fe |

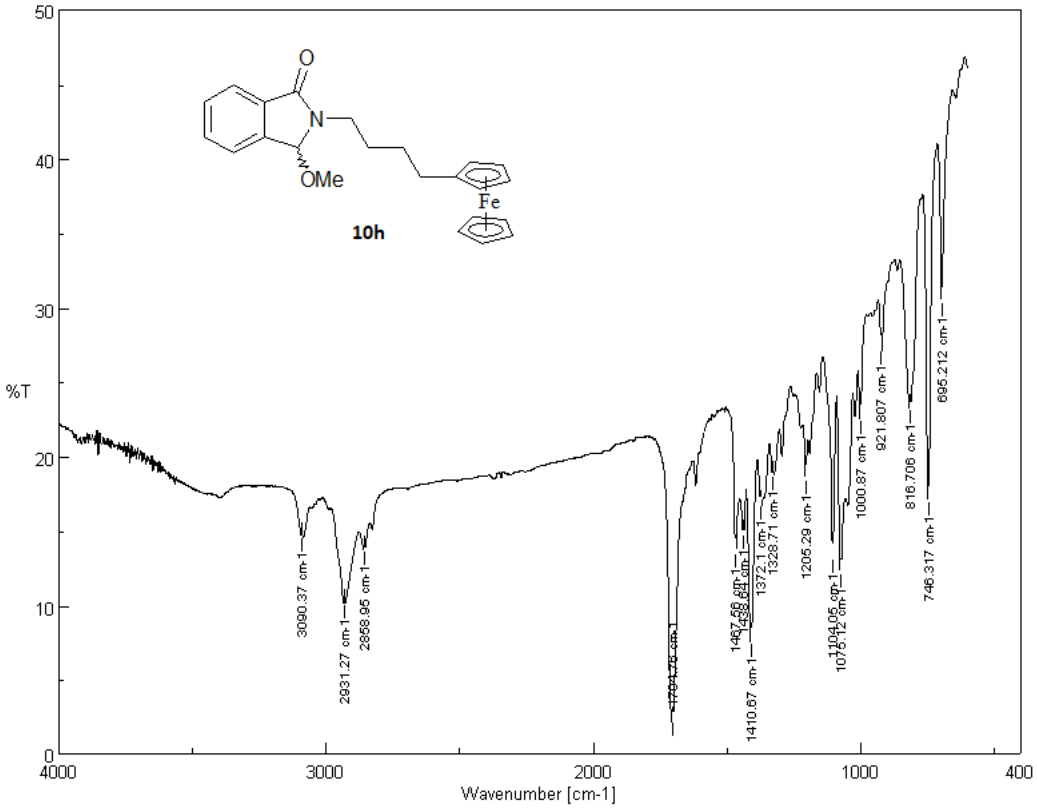
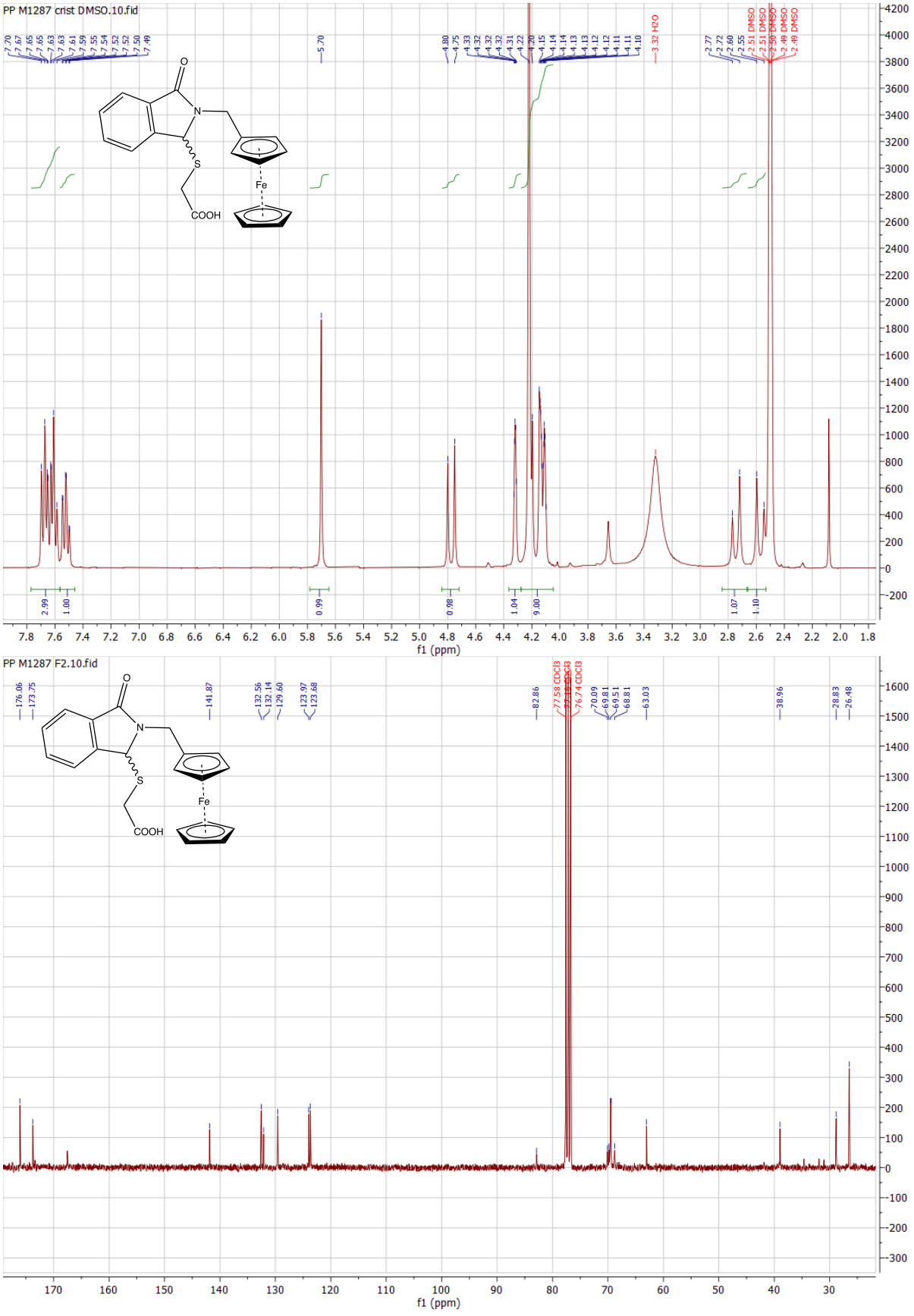
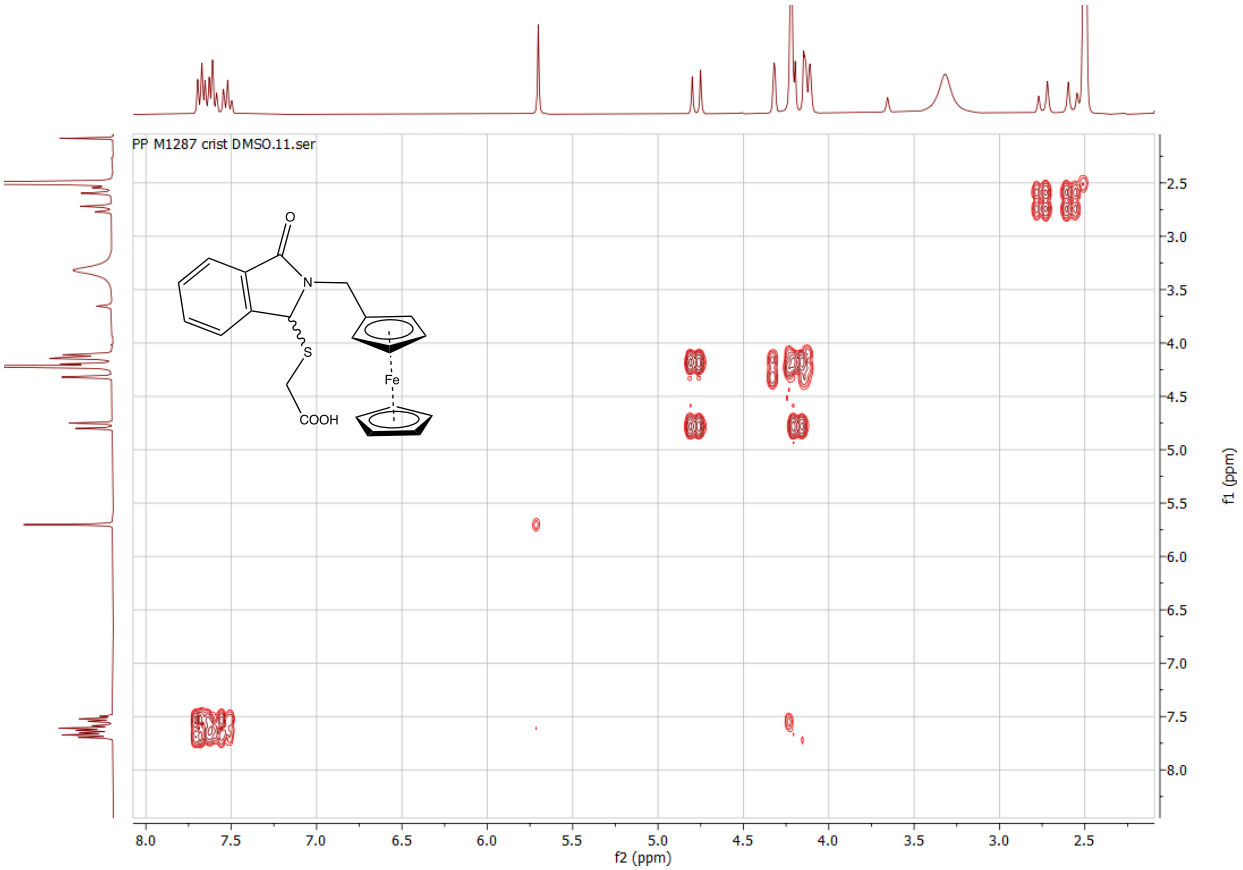
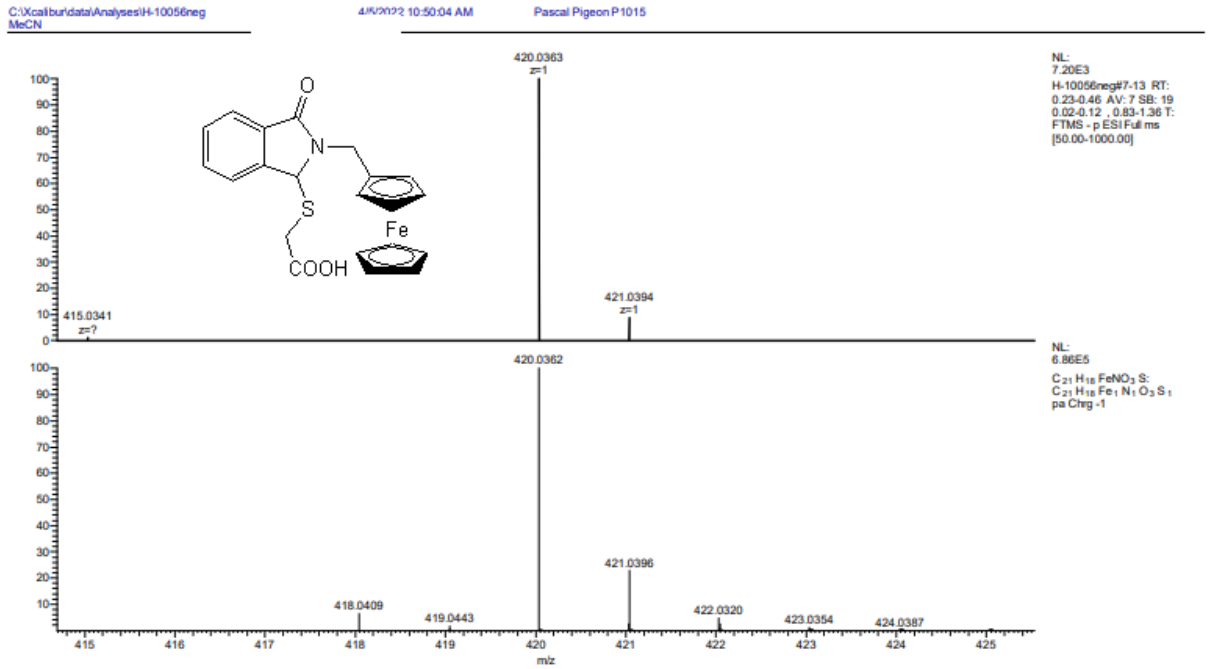


**Figure S36**: $^{1}H$ (in DMSO-$d_6$), $^{13}C$ (in $CDCl_3$), COSY (in DMSO-$d_6$) NMR, HR-MS and IR data for compound **11**






# Experimental/theoretical isotopic pattern MS spectrum

**Error = 0.9 ppm; Relative Intensity (%) 100**

**HRMS (ESI) m/z: [M] 1- Calcd for C21H18FeNO3S420.0362 . Found 420.0366; (Error: 0.9 ppm).**

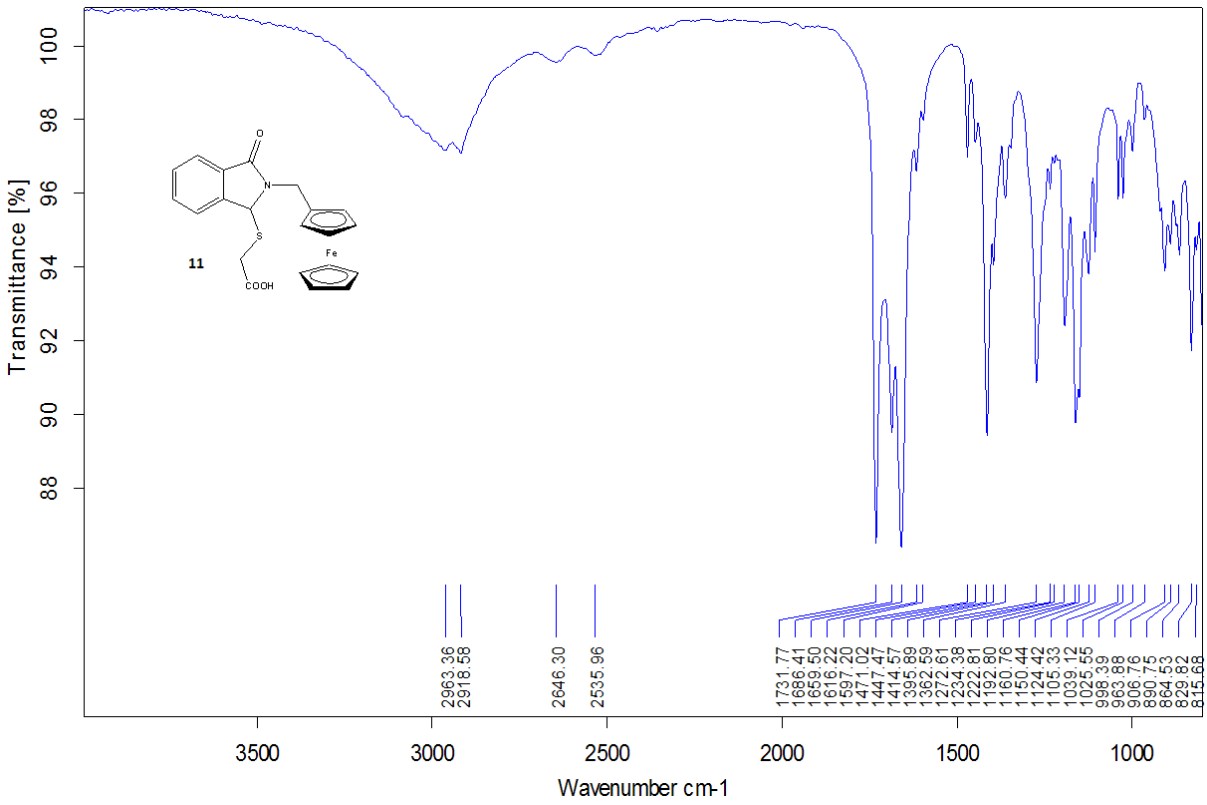
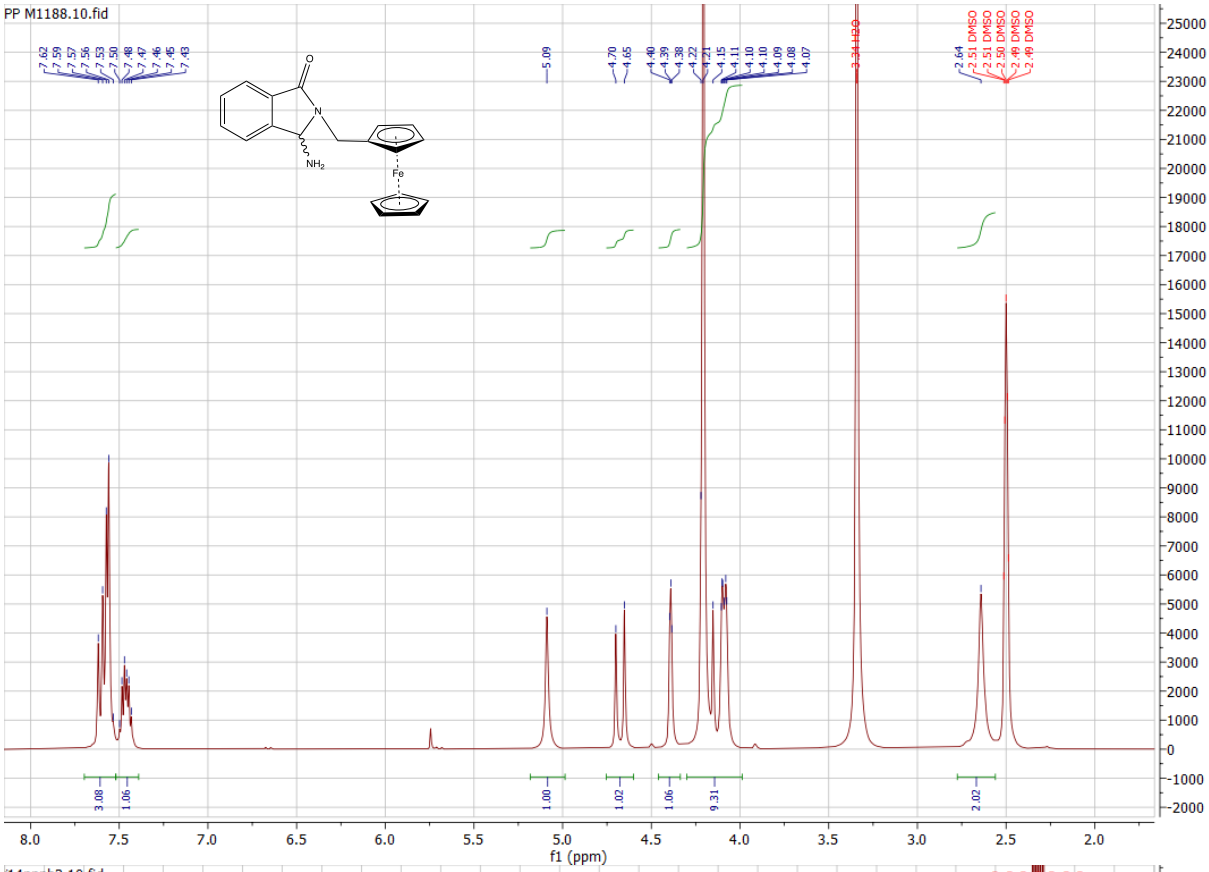
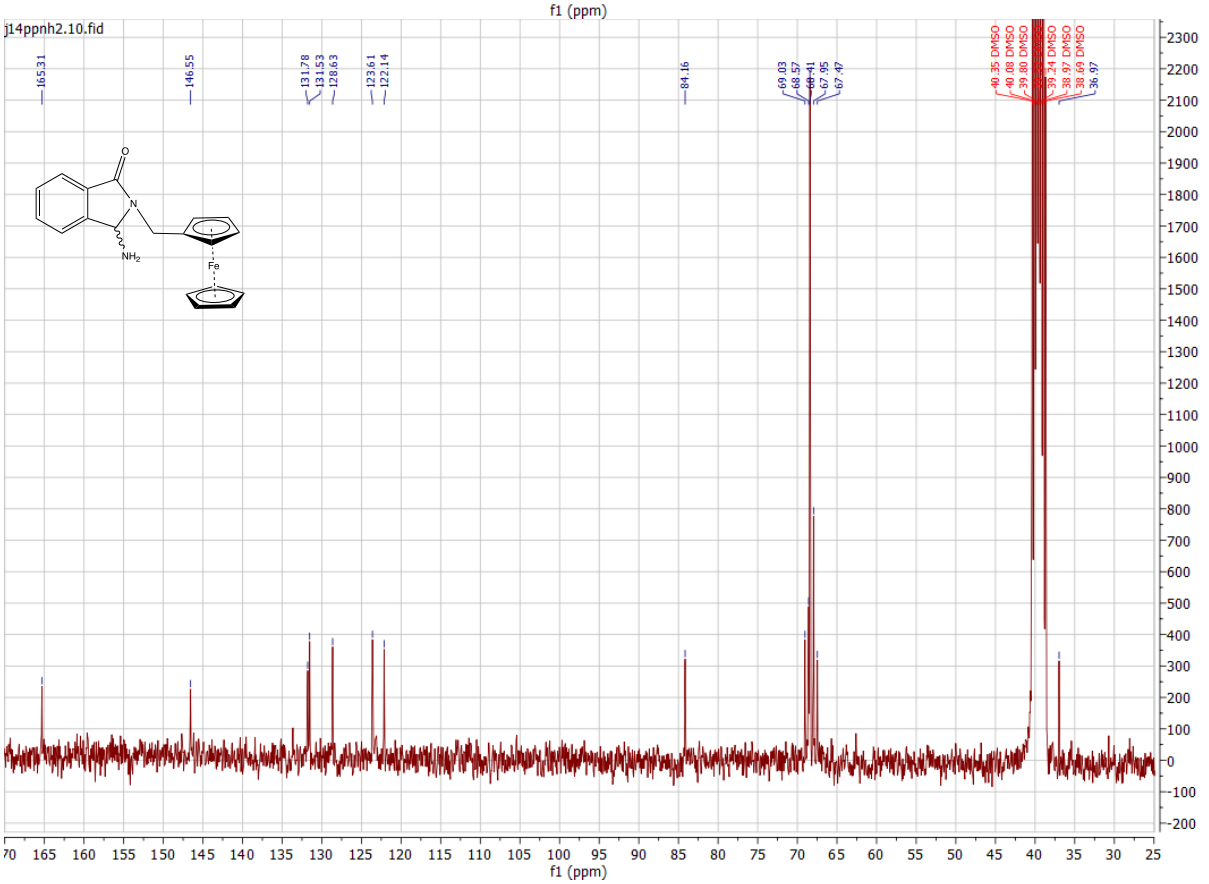
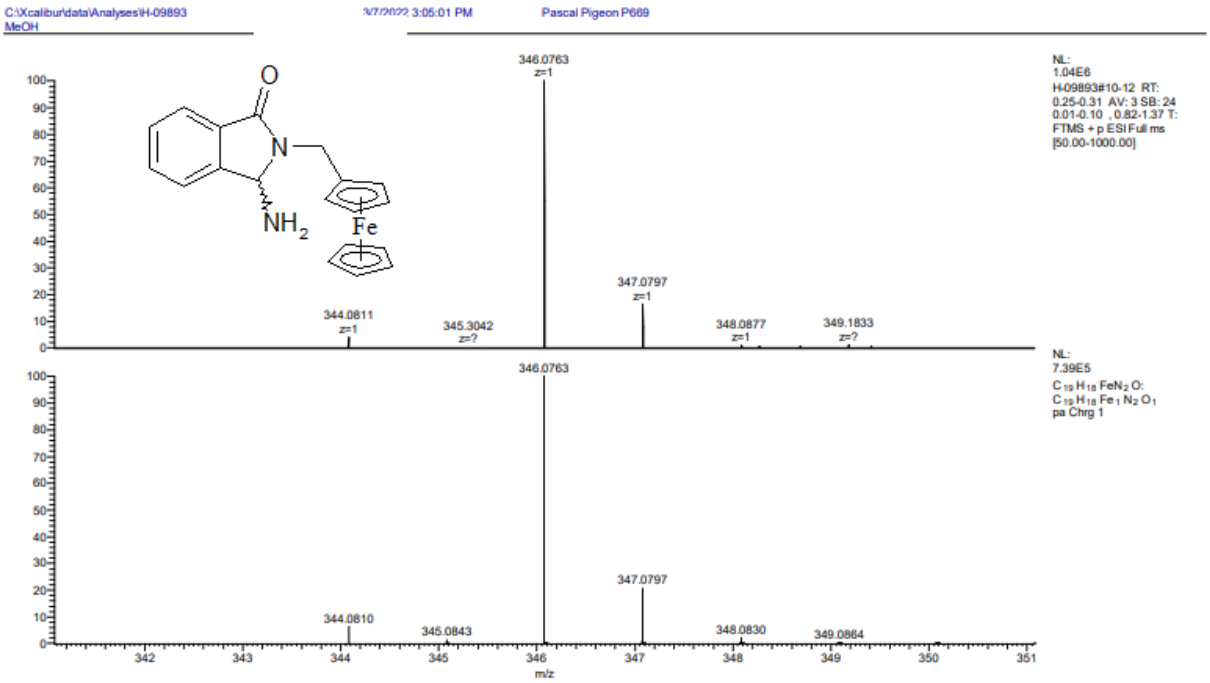

Transmittance [%]
100
98
96
94
92
90
88
O
N
S
Fe
COOH
11
2963.36
2918.58
2646.30
2535.96
1731.77
1686.41
1659.50
1616.22
1597.20
1471.02
1447.47
1414.57
1395.89
1362.59
1272.61
1234.38
1222.81
1192.80
1160.76
1150.44
1124.42
1105.33
1039.12
1025.55
998.39
963.88
906.76
890.75
864.53
829.82
815.68
3500
3000
2500
2000
1500
1000
Wavenumber cm-1

**Figure S37**: $^{1}H$ (in DMSO-$d_6$), $^{13}C$ (in DMSO-$d_6$) NMR, HR-MS and IR data for compound **13**






# Experimental/theoretical isotopic pattern MS spectrum

**Error = 0.0 ppm; Relative Intensity (%) 100**

**HRMS (ESI) m/z: [M]+ Calcd for C19H18FeN2O 346.0763 . Found 346.0763; (Error: 0.0 ppm).**

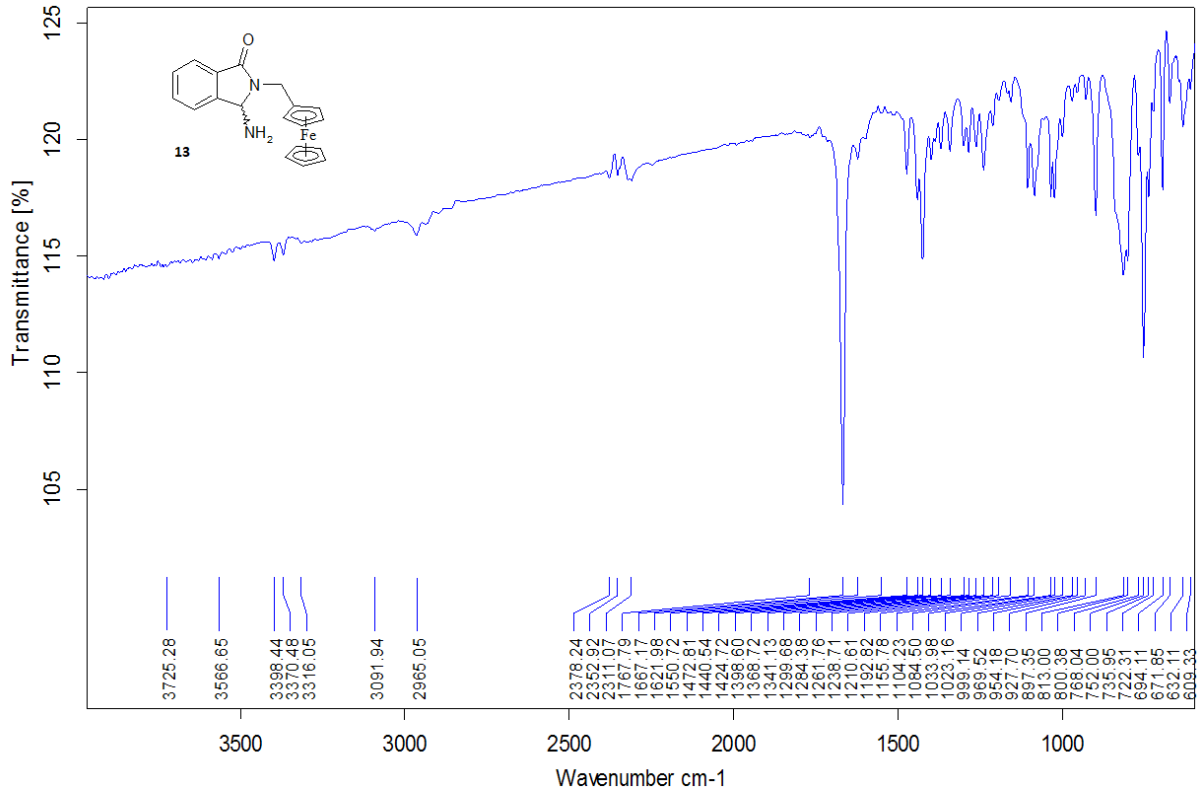
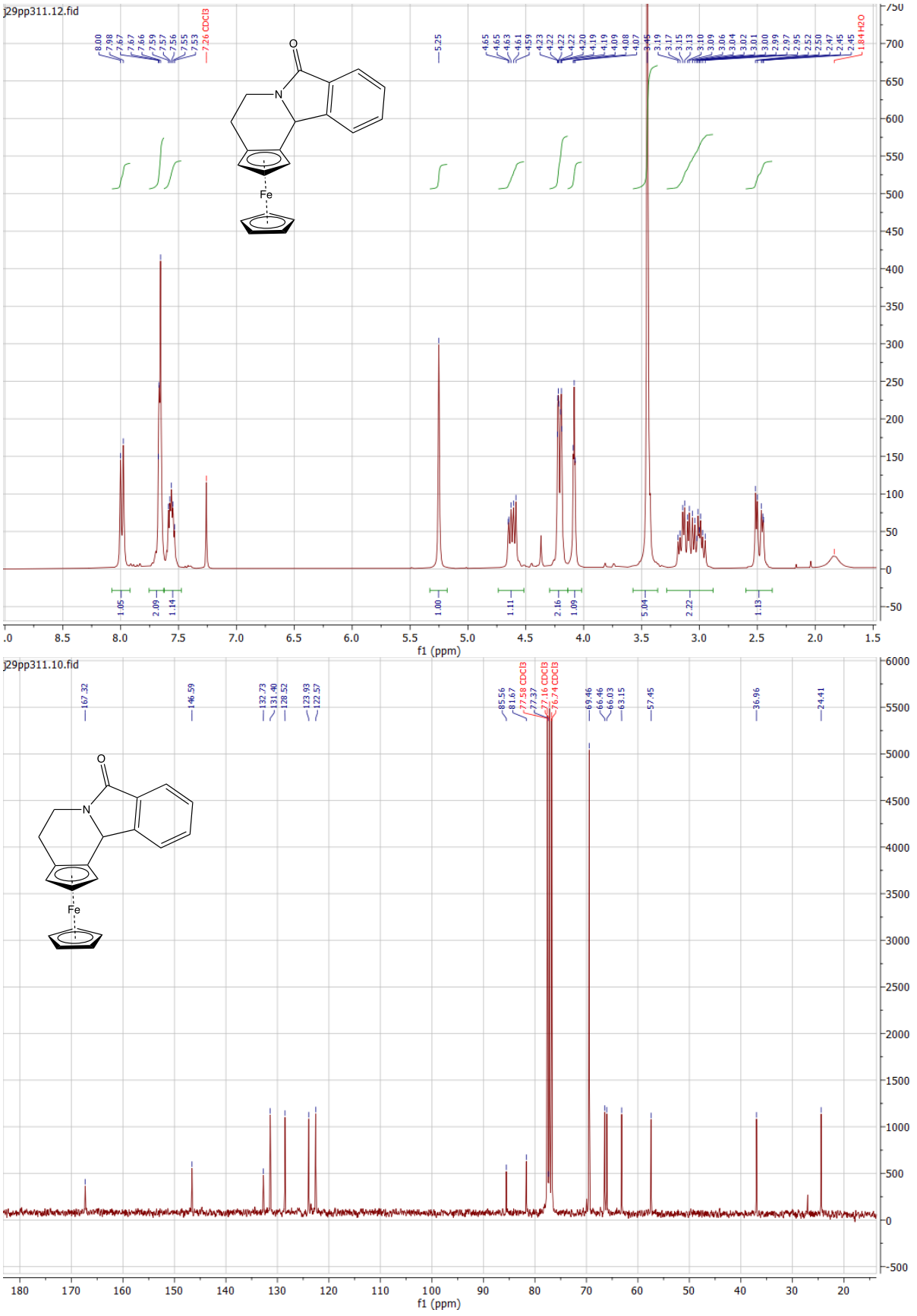
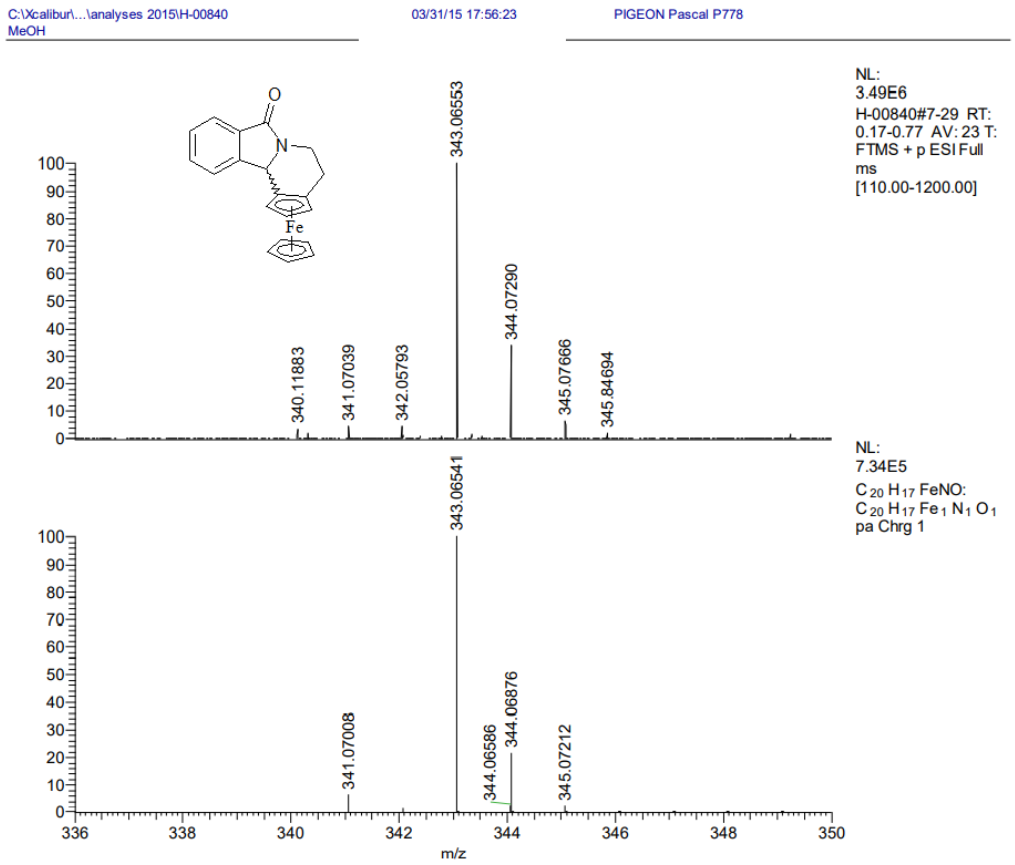


**Figure S38**: $^{1}H$ (in $CDCl_3$), $^{13}C$ (in $CDCl_3$) NMR, HR-MS and IR data for compound **14**






Erreur = 0.4 ppm (erreur calculée pour l'ion expérimental 343.06553 par rapport à la valeur théorique de 343.06541)

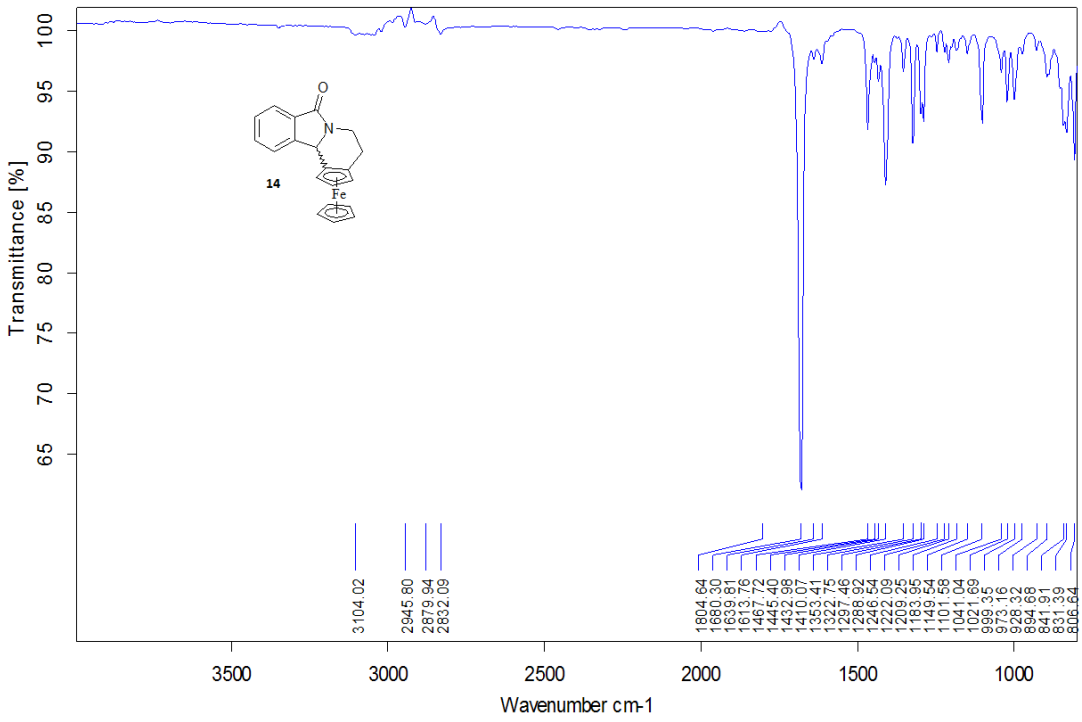
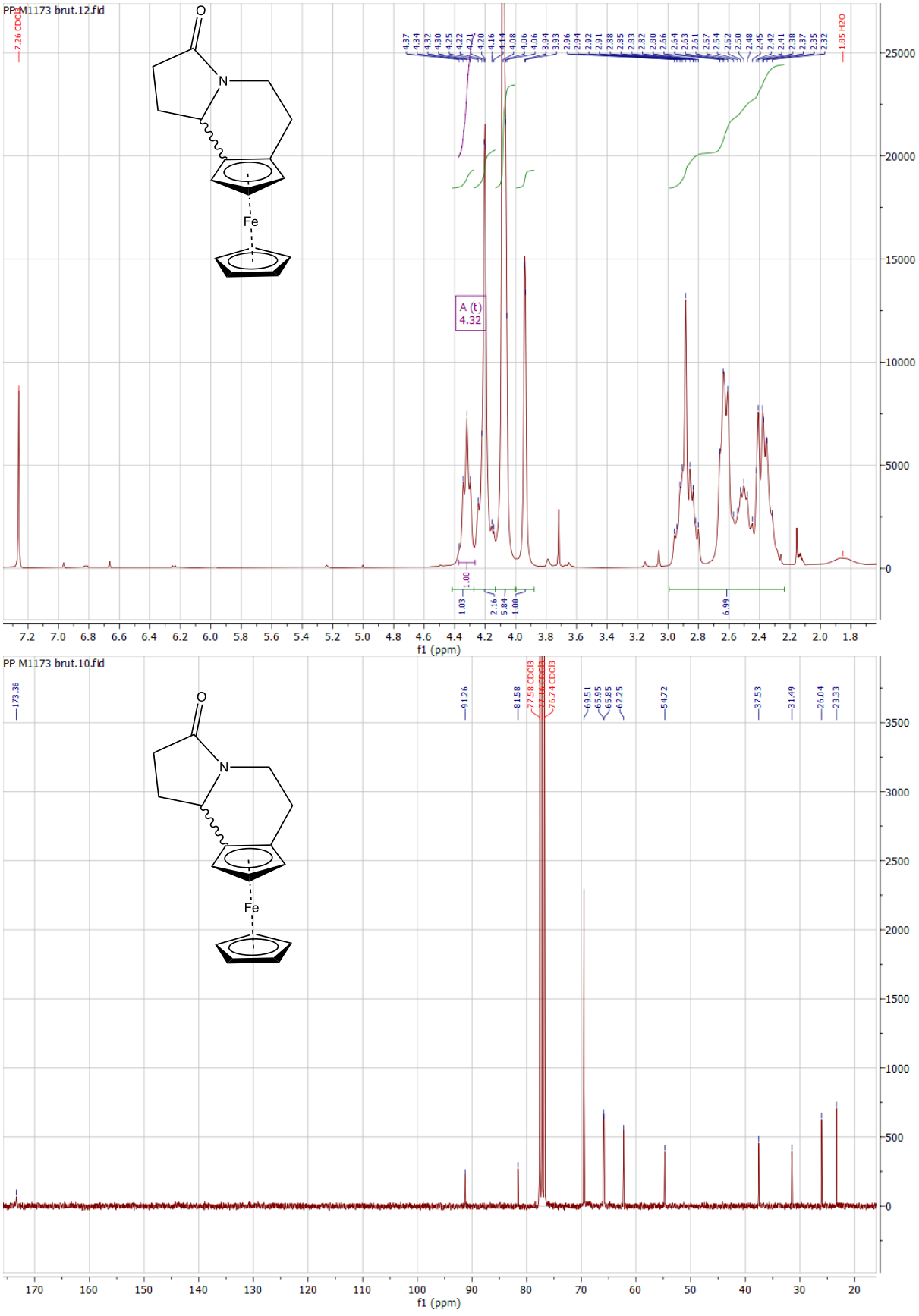
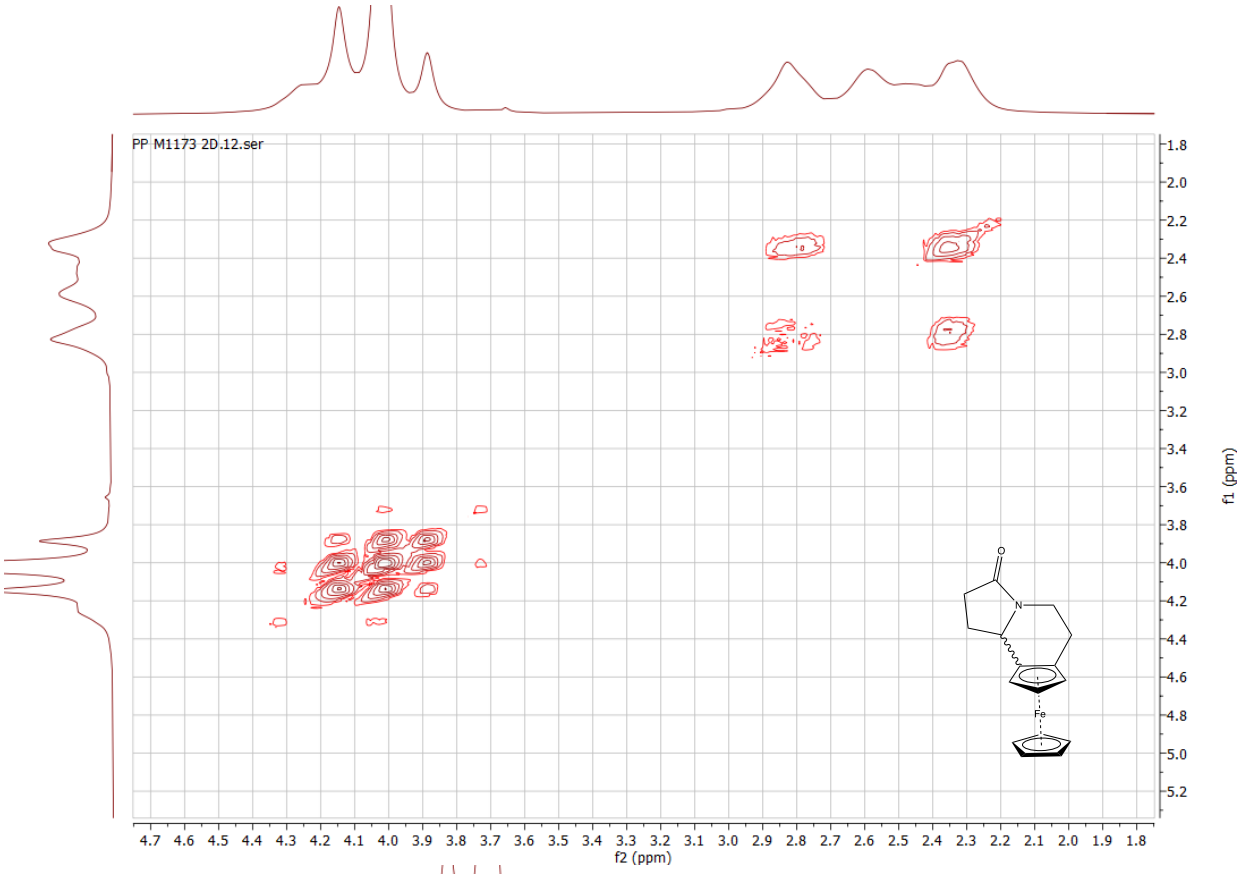
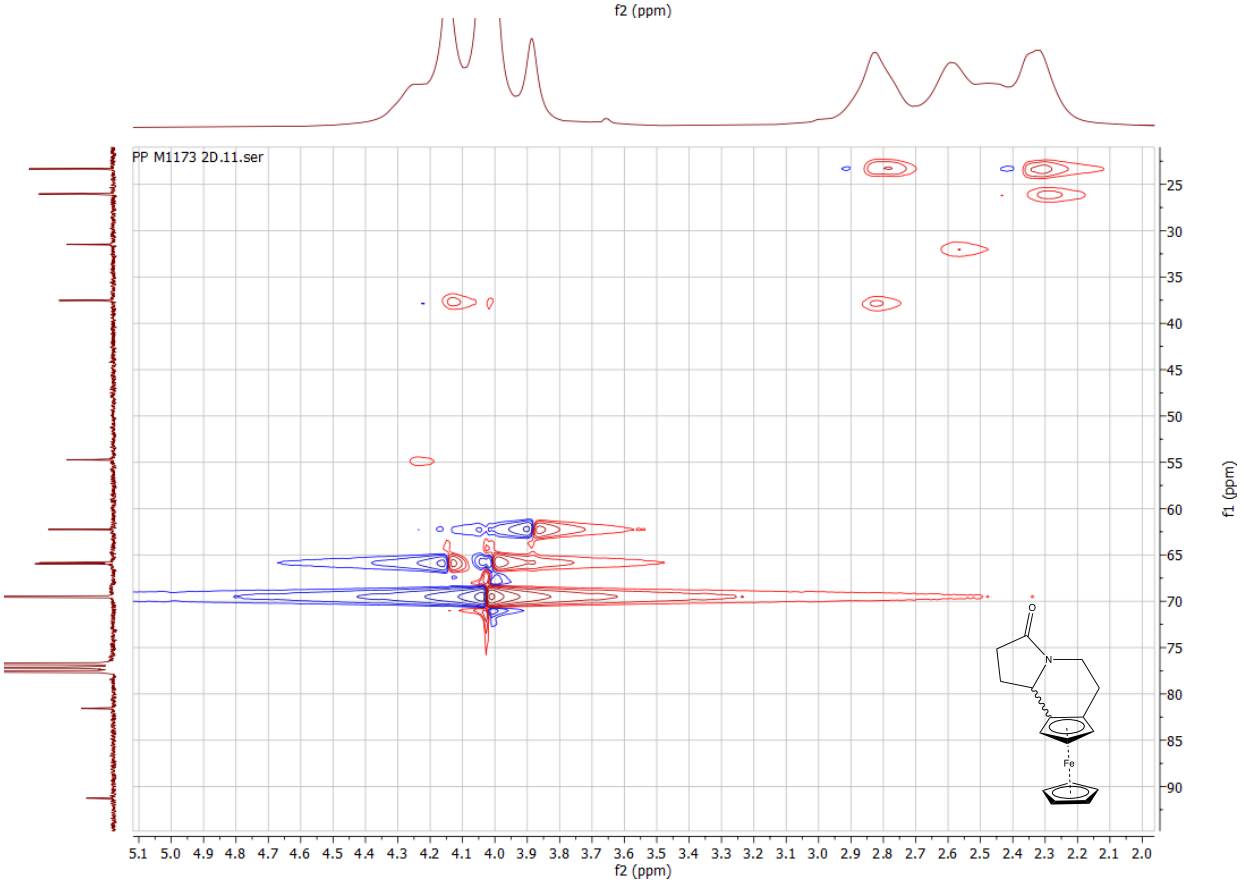
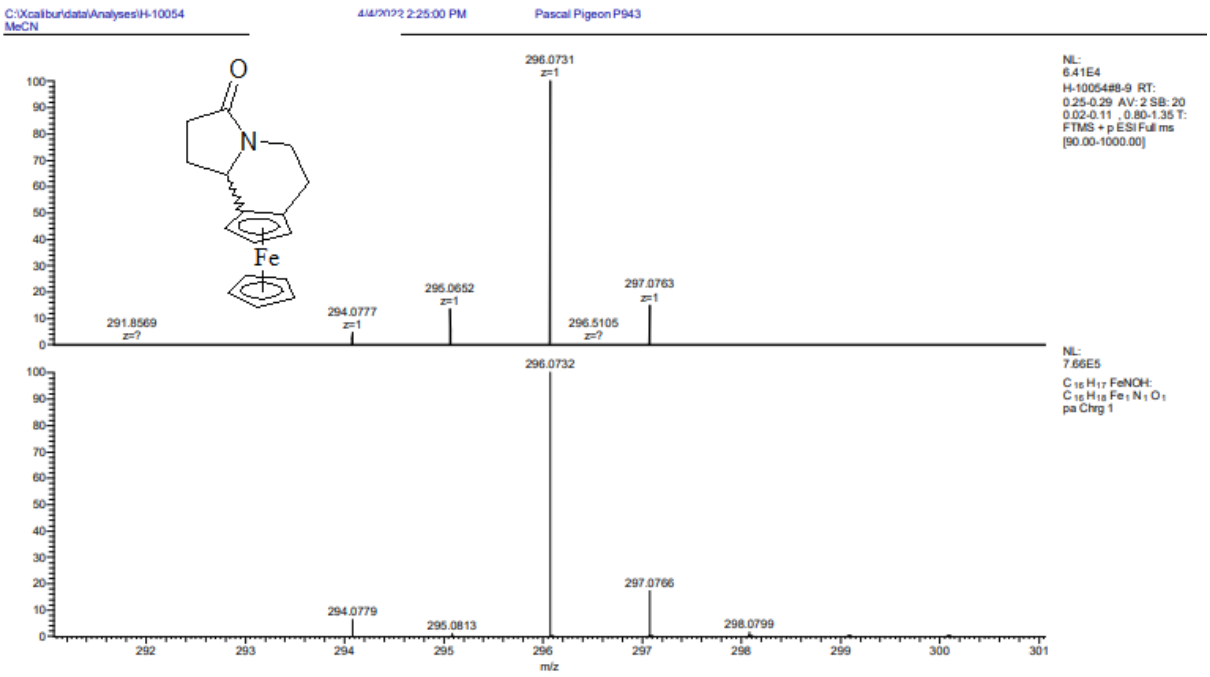


**Figure S39**: $^{1}H$ (in $CDCl_3$), $^{13}C$ (in $CDCl_3$), COSY (in $CDCl_3$), HMQC (in $CDCl_3$) NMR, HR-MS and IR data for compound **15**




PP M1173 2D.12.ser
f2 (ppm)
f1 (ppm)
O
N
Fe


PP M1173 2D.11.ser
f2 (ppm)
f1 (ppm)
O
N
Fe




# Experimental/theoretical isotopic pattern MS spectrum

**Error = -0.4 ppm; Relative Intensity (%) 100**

**HRMS (ESI) m/z: [M+H]+ Calcd for C16H17FeNOH 296.0732. Found 296.0731; (Error: -0.4 ppm).**

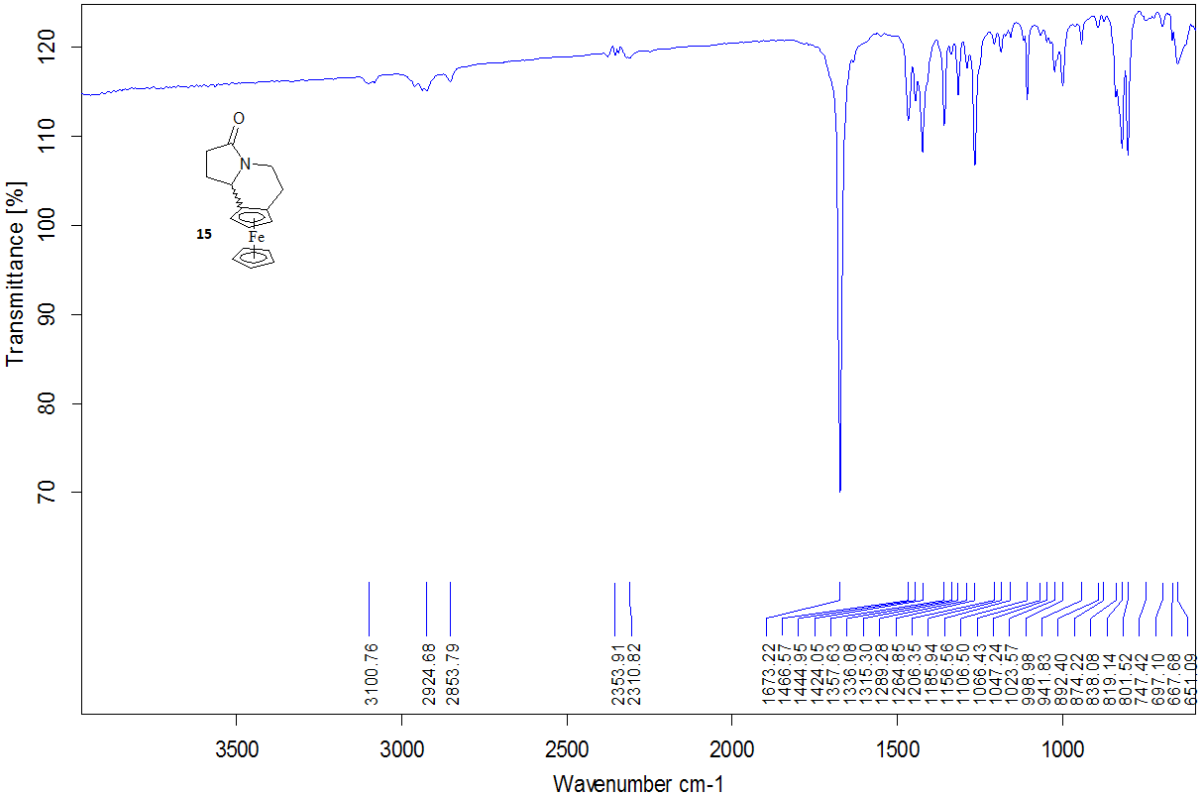
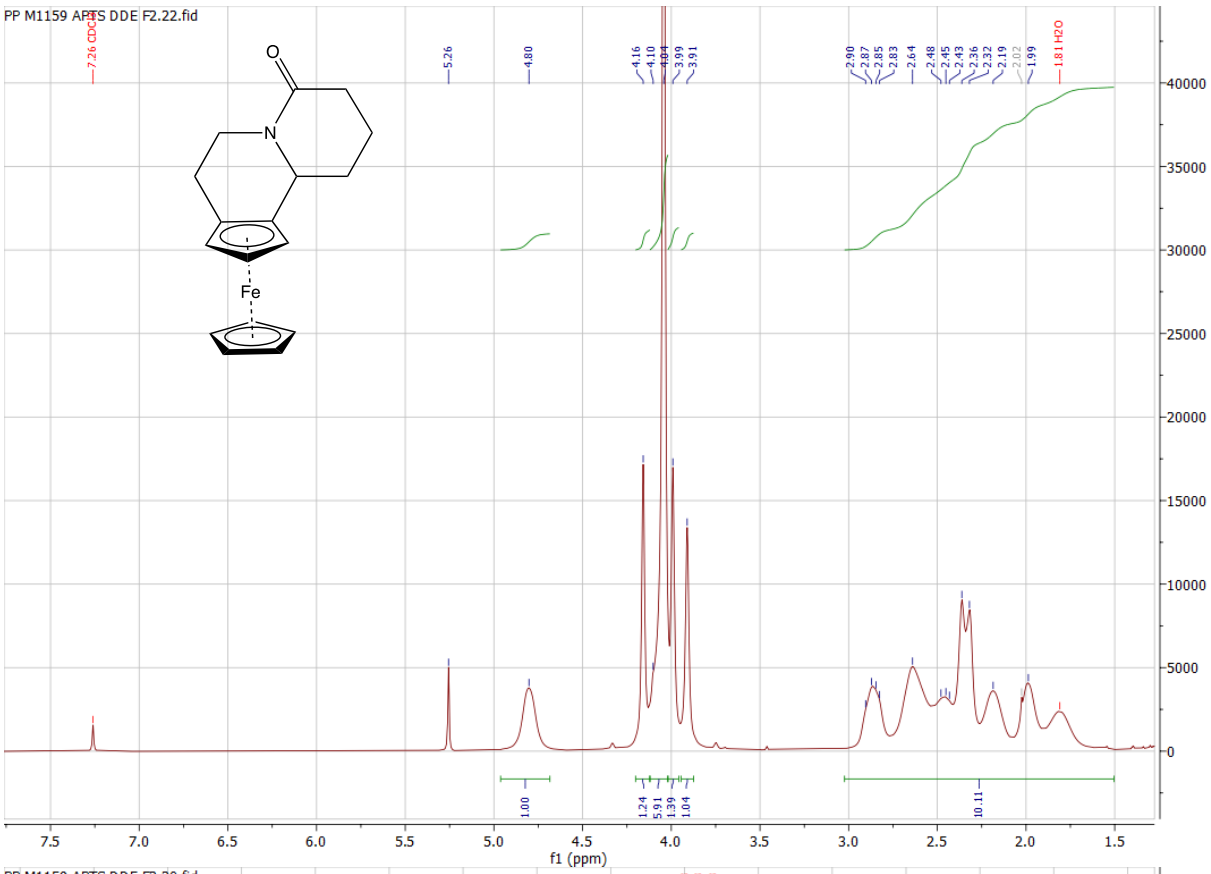
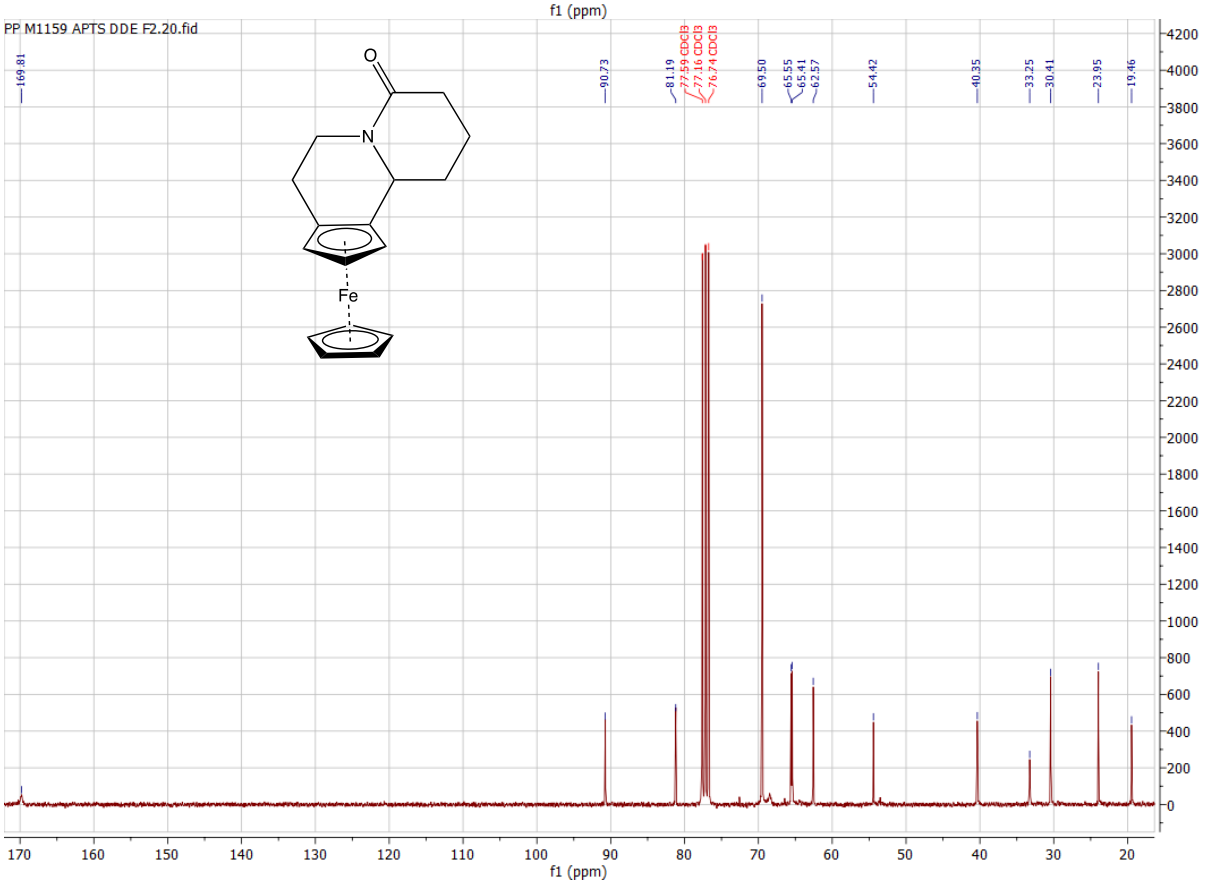
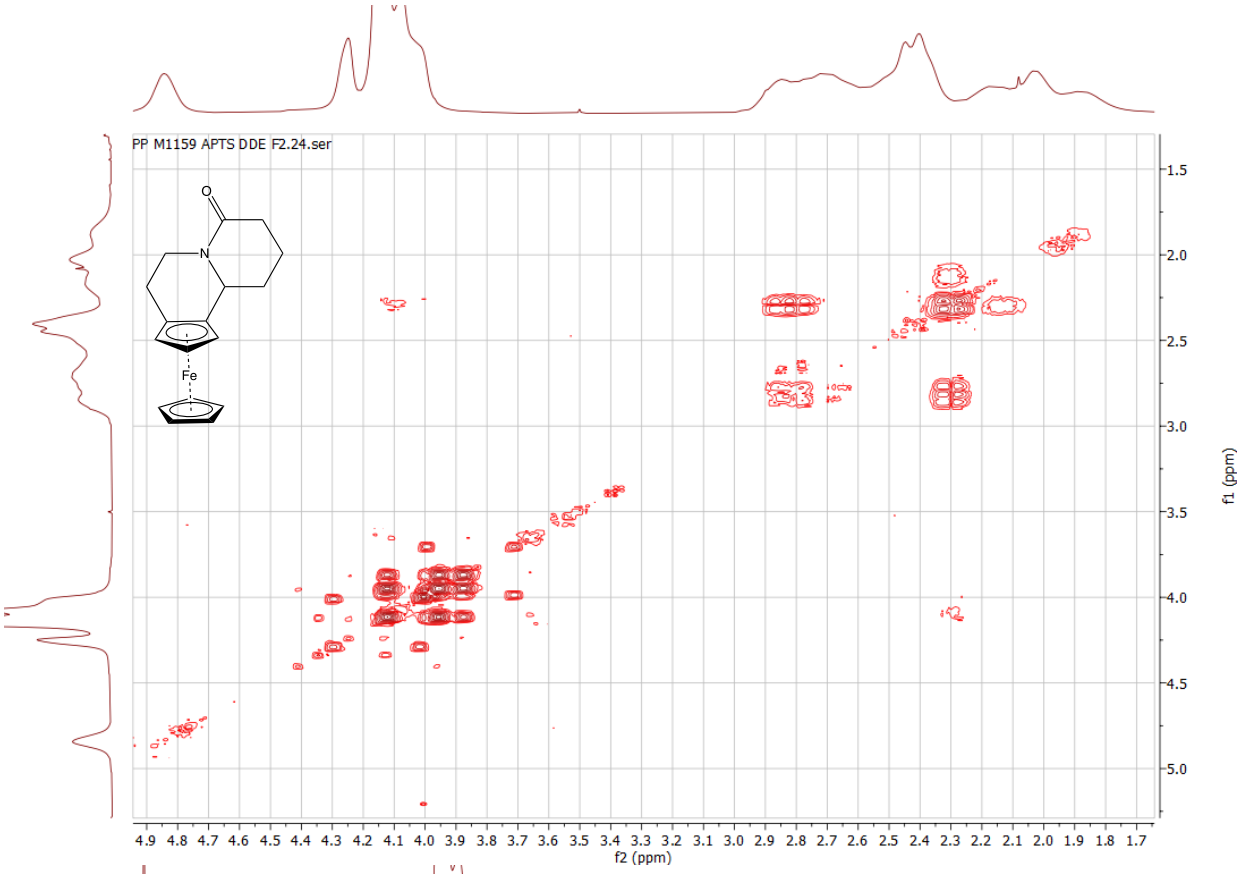
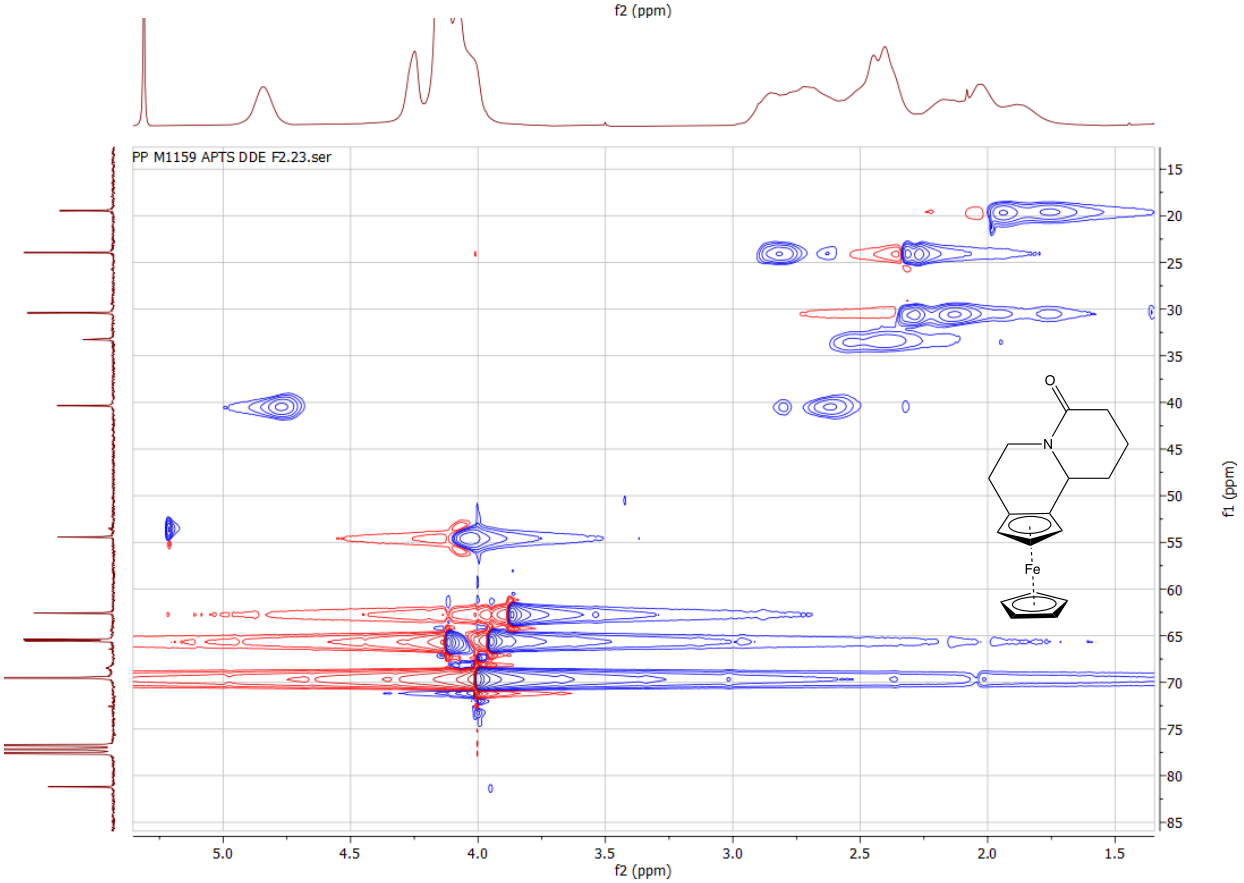


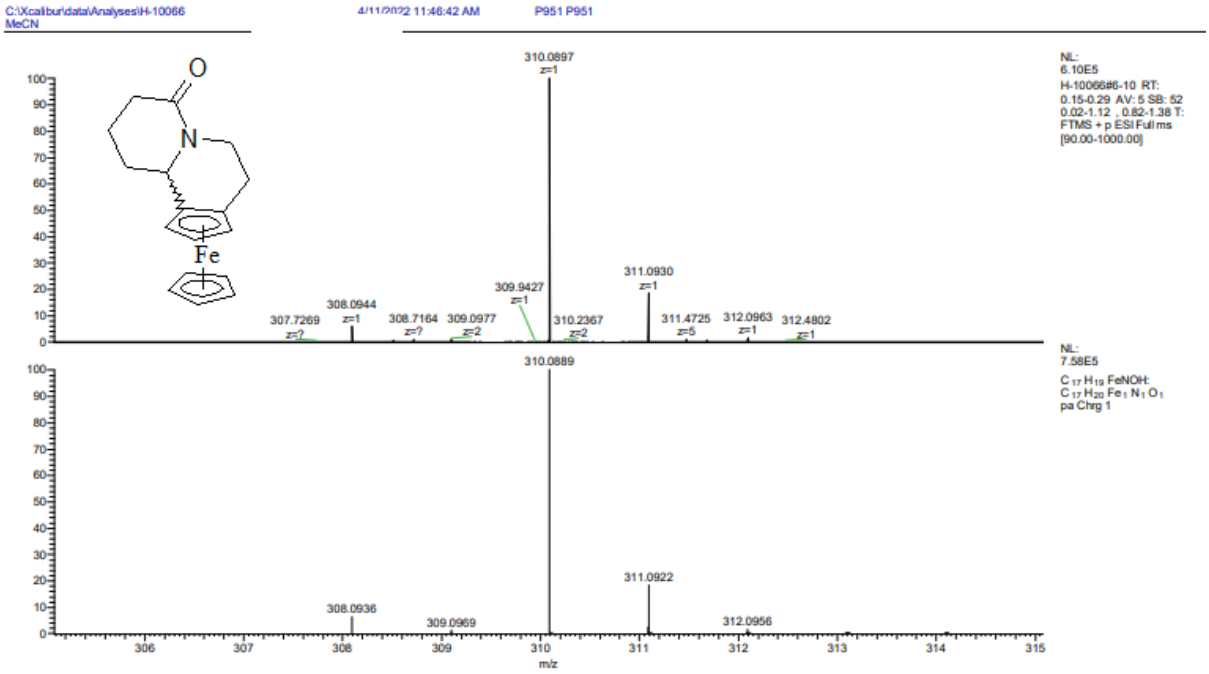
**Figure S40**: $^{1}H$ (in $CDCl_3$), $^{13}C$ (in $CDCl_3$), COSY (in $CDCl_3$), HMQC (in $CDCl_3$) NMR, HR-MS and IR data for compound **16**




PP M1159 APTS DDE F2.24.ser
O
N
Fe
f2 (ppm)
f1 (ppm)


PP M1159 APTS DDE F2.23.ser
O
N
Fe
f2 (ppm)
f1 (ppm)




# Experimental/theoretical isotopic pattern MS spectrum

**Error = 2.7 ppm; Relative Intensity (%) 100**

**HRMS (ESI) m/z: [M+H]+ Calcd for C17H19FeNOH 310.0889. Found 310.0897; (Error: 2.7 ppm).**

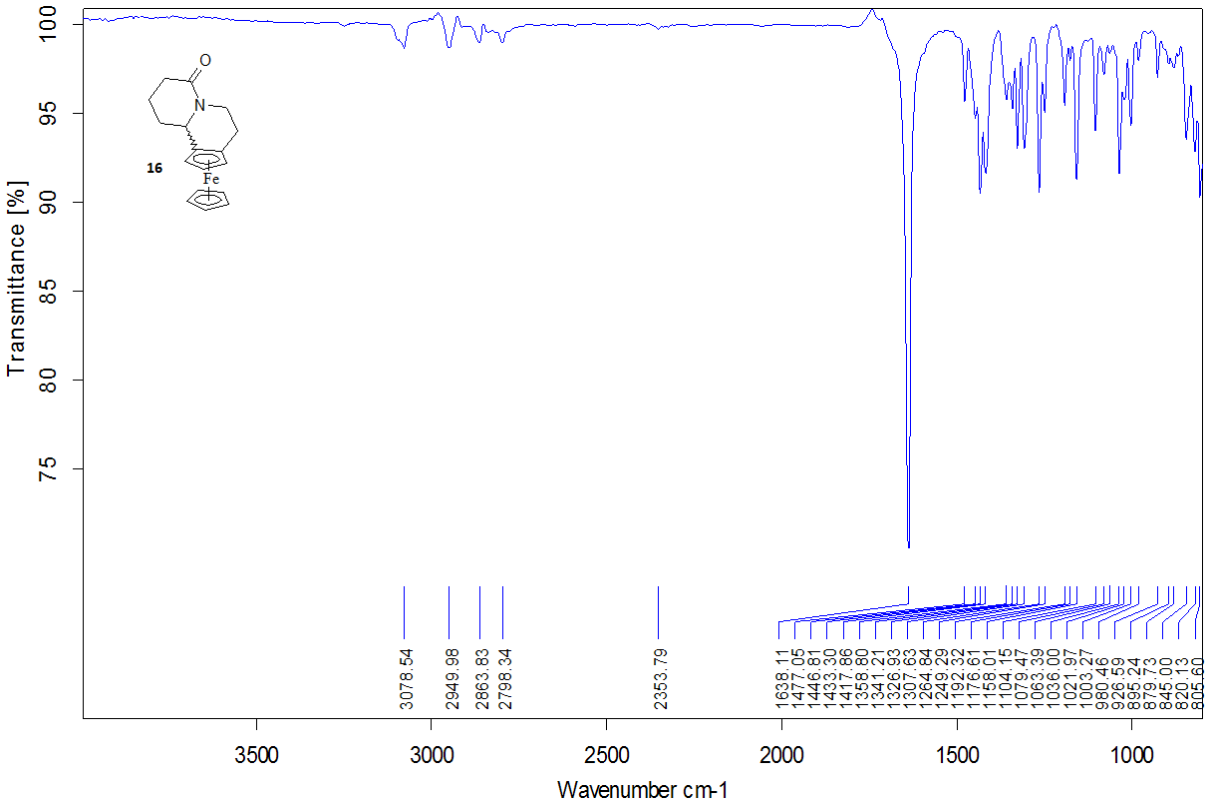
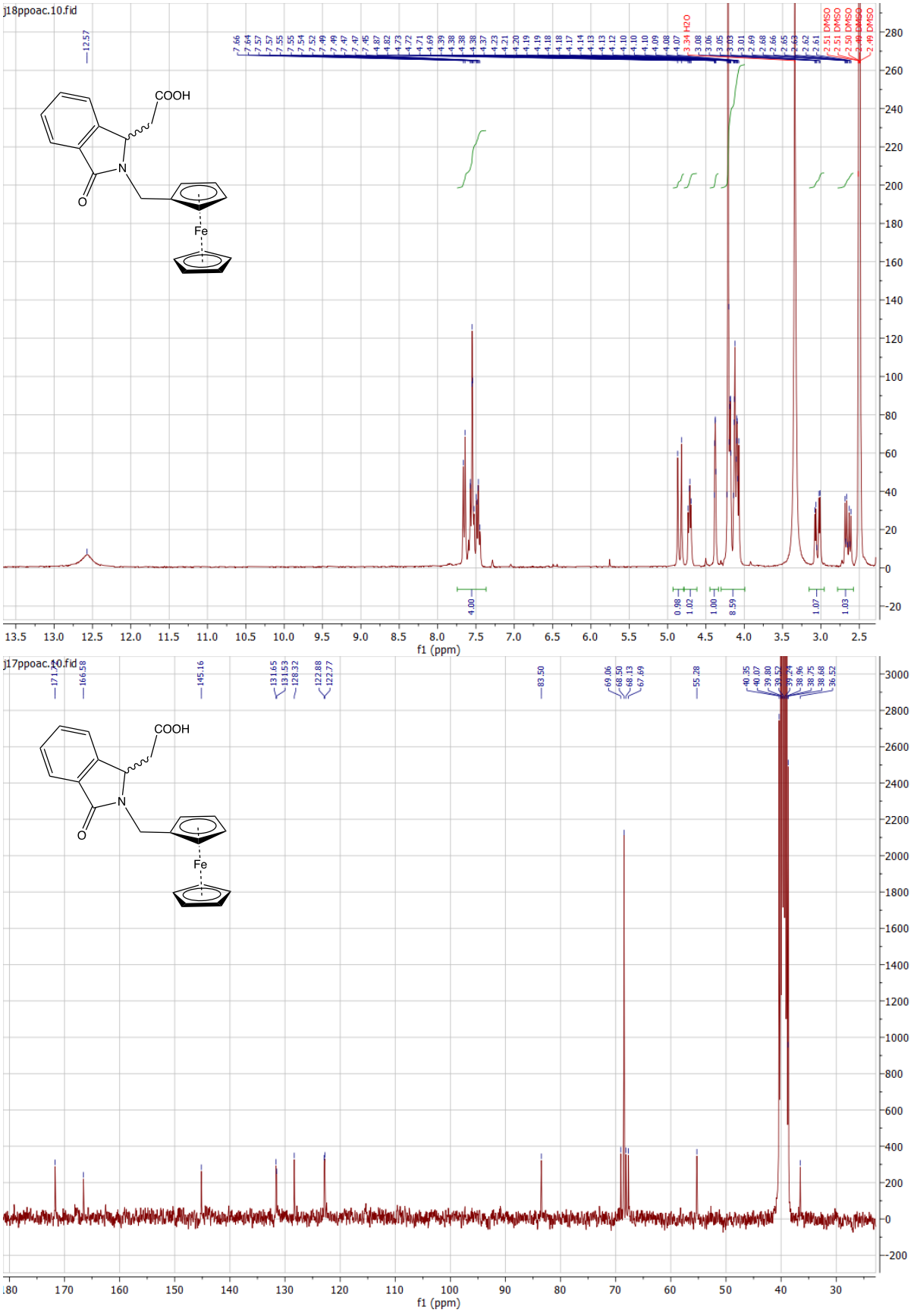


**Figure S41**: $^{1}H$ (in DMSO-$d_6$), $^{13}C$ (in DMSO-$d_6$) and COSY (in DMSO-$d_6$) NMR and IR data for compound **17**



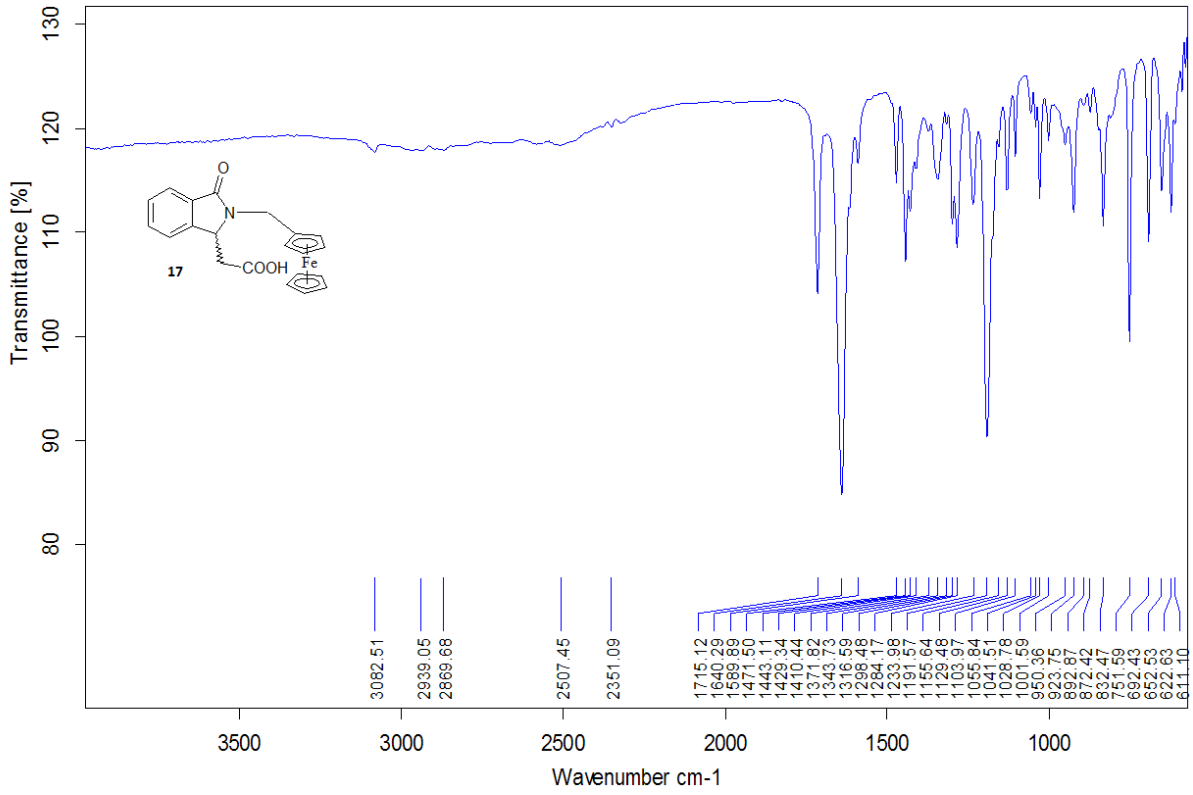
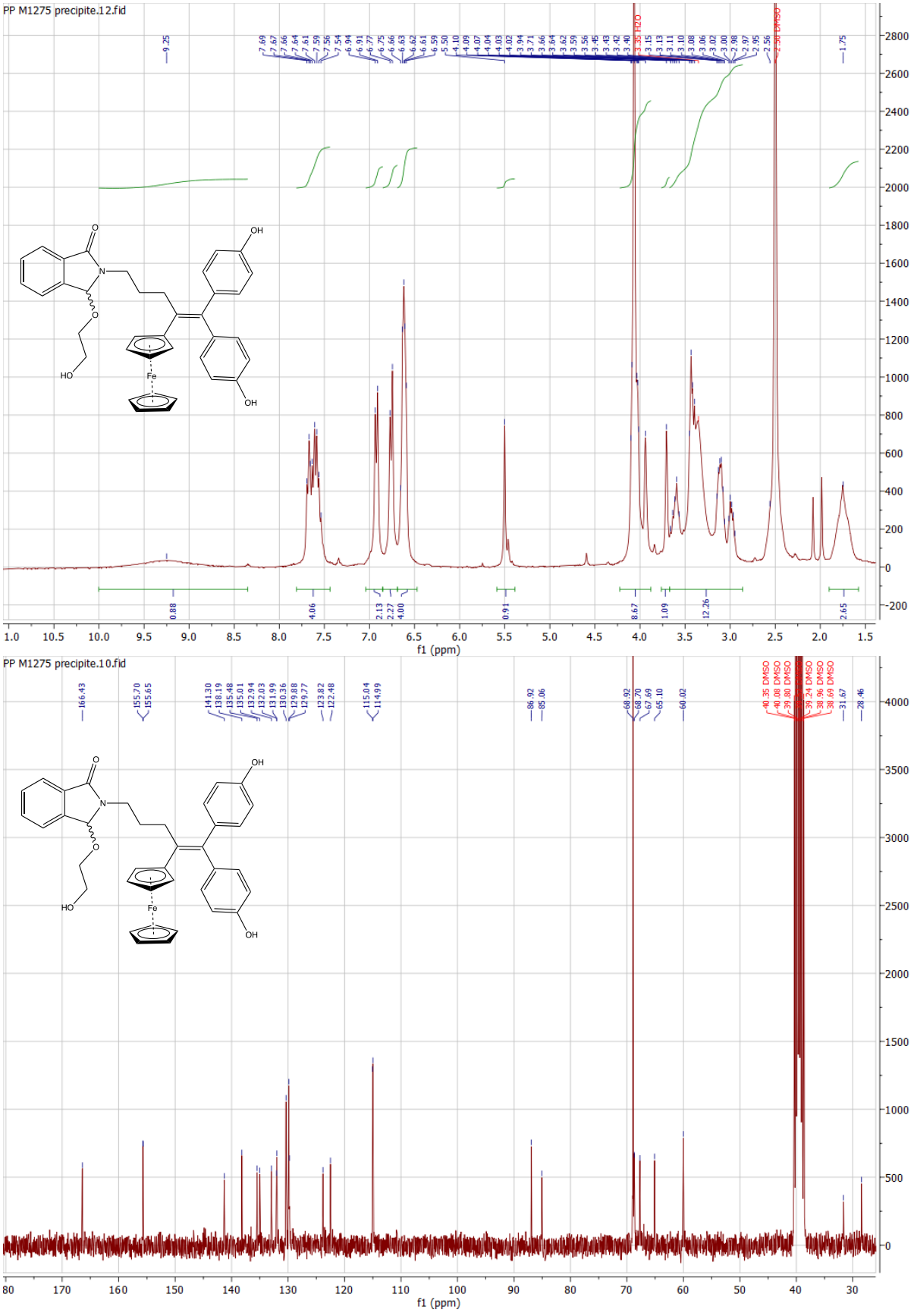
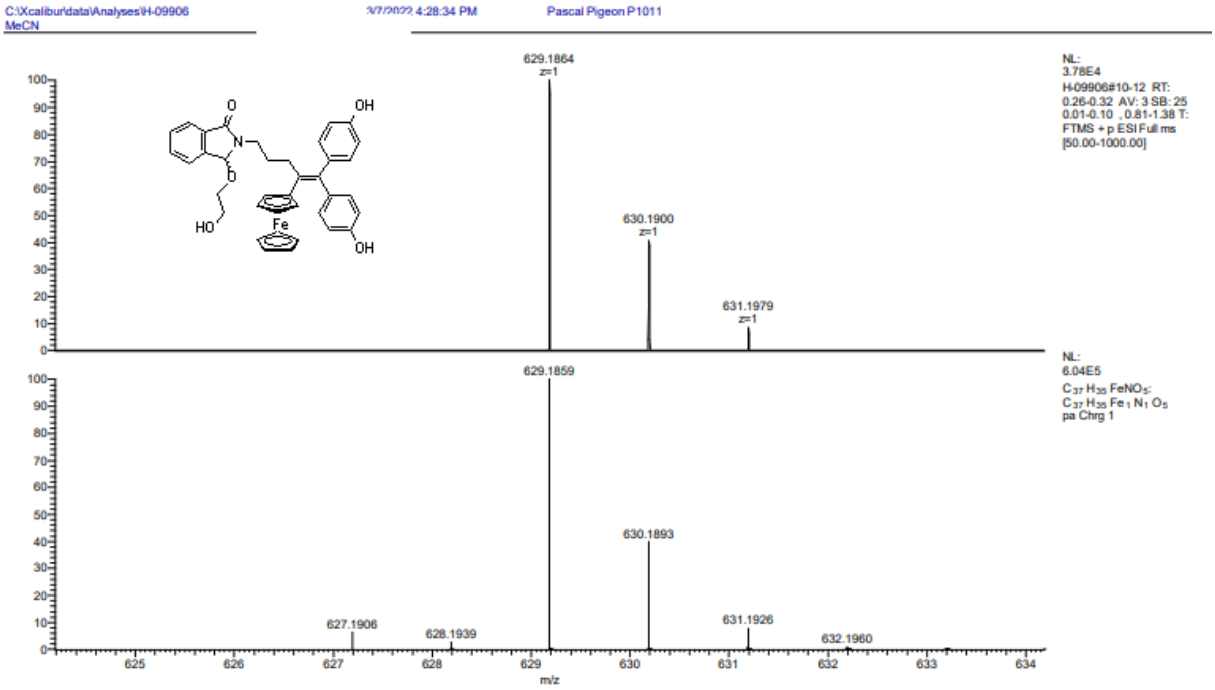

Transmittance [%]
130
120
110
100
90
80
O
N
COOH
Fe
17
3082.51
2939.05
2869.68
2507.45
2351.09
1715.12
1640.29
1589.89
1471.50
1443.11
1429.34
1410.44
1371.82
1343.73
1316.59
1298.48
1284.17
1233.98
1191.57
1155.64
1129.48
1103.97
1055.84
1041.51
1028.78
1001.59
950.36
923.75
892.87
872.42
832.47
751.59
692.43
652.53
622.63
611.10
3500
3000
2500
2000
1500
1000
Wavenumber cm-1

**Figure S42**: $^{1}H$ (in DMSO-$d_6$) and $^{13}C$ (in DMSO-$d_6$) NMR, HR-MS and IR data for compound **20**






# Experimental/theoretical isotopic pattern MS spectrum

**Error = 0.8 ppm; Relative Intensity (%) 100**

**HRMS (ESI) m/z: [M]+ Calcd for C37H35FeNO5 629.1859 . Found 629.1864; (Error: 0.8 ppm).**

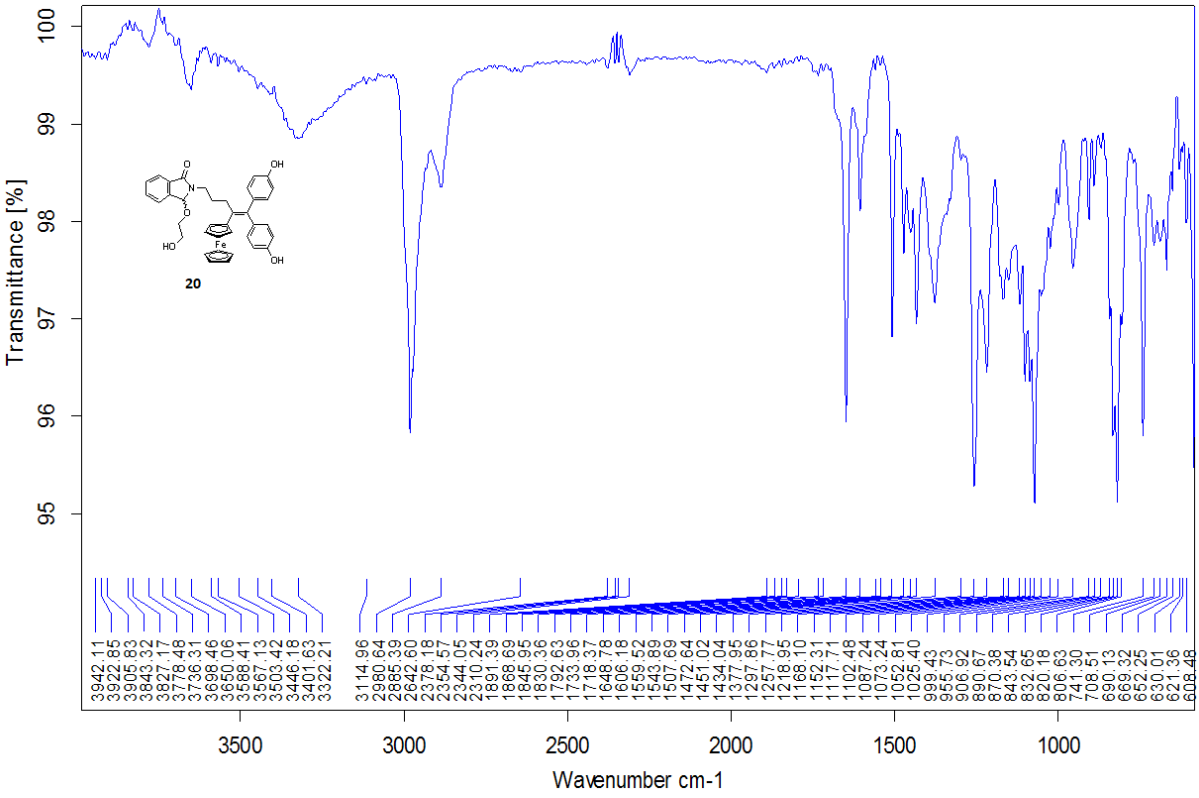
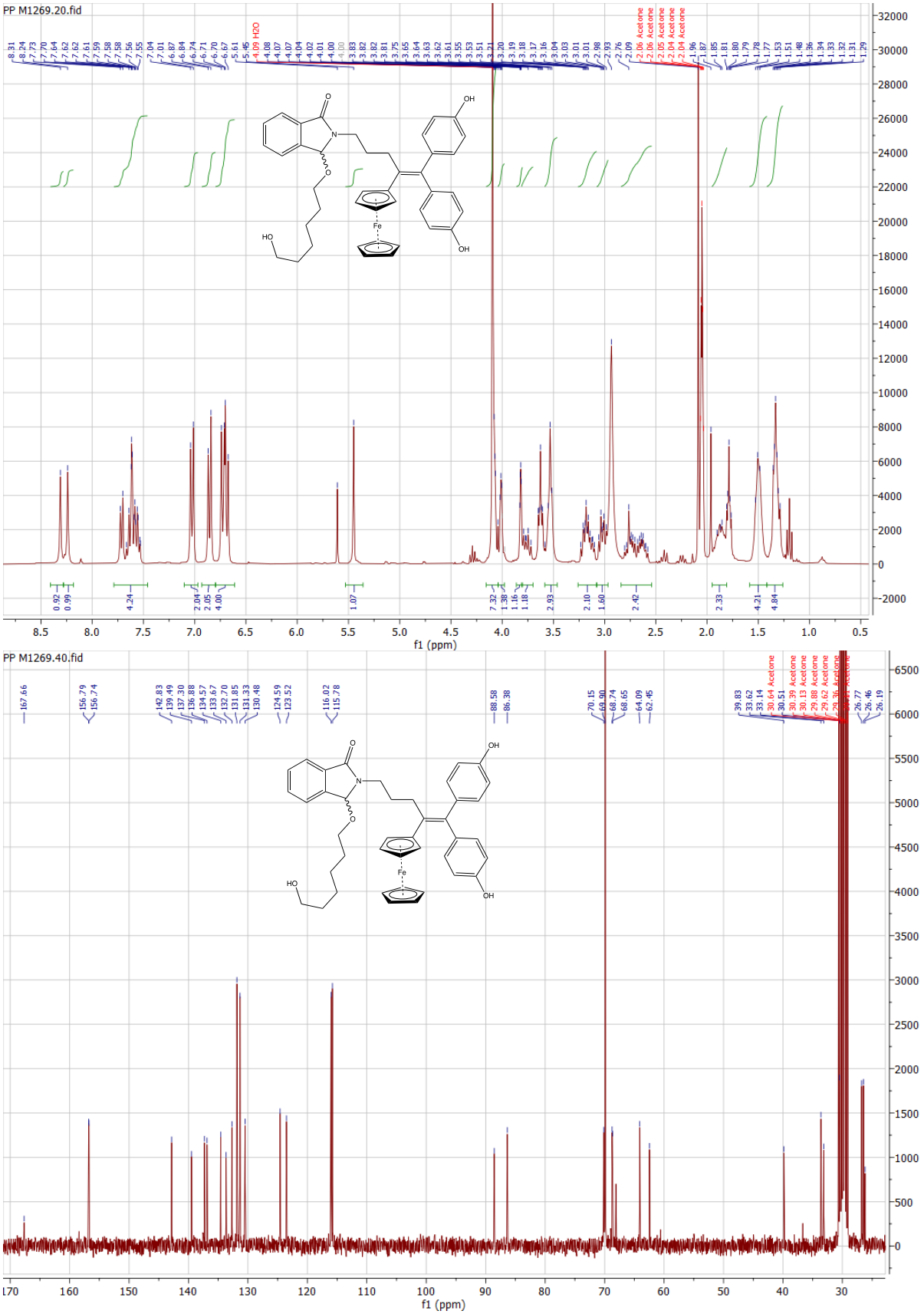
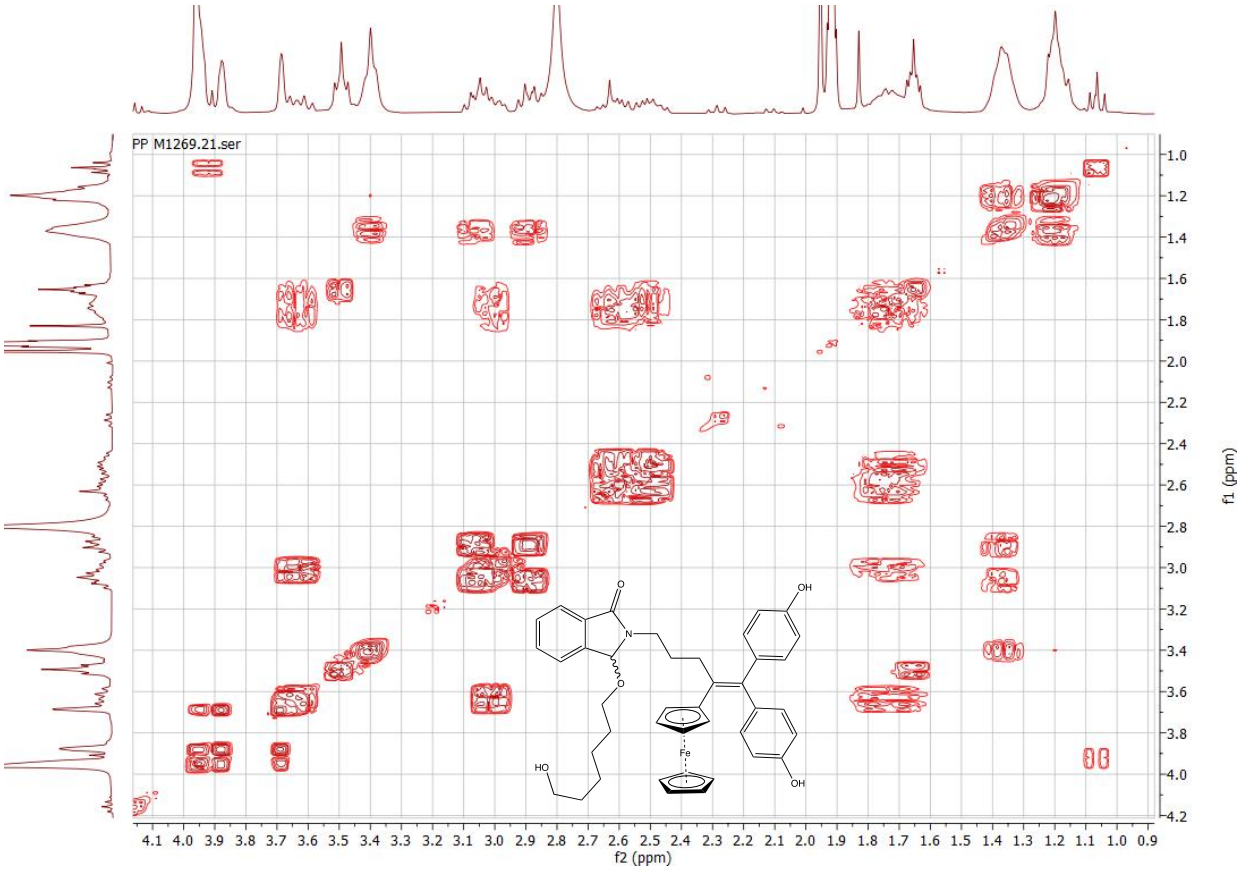
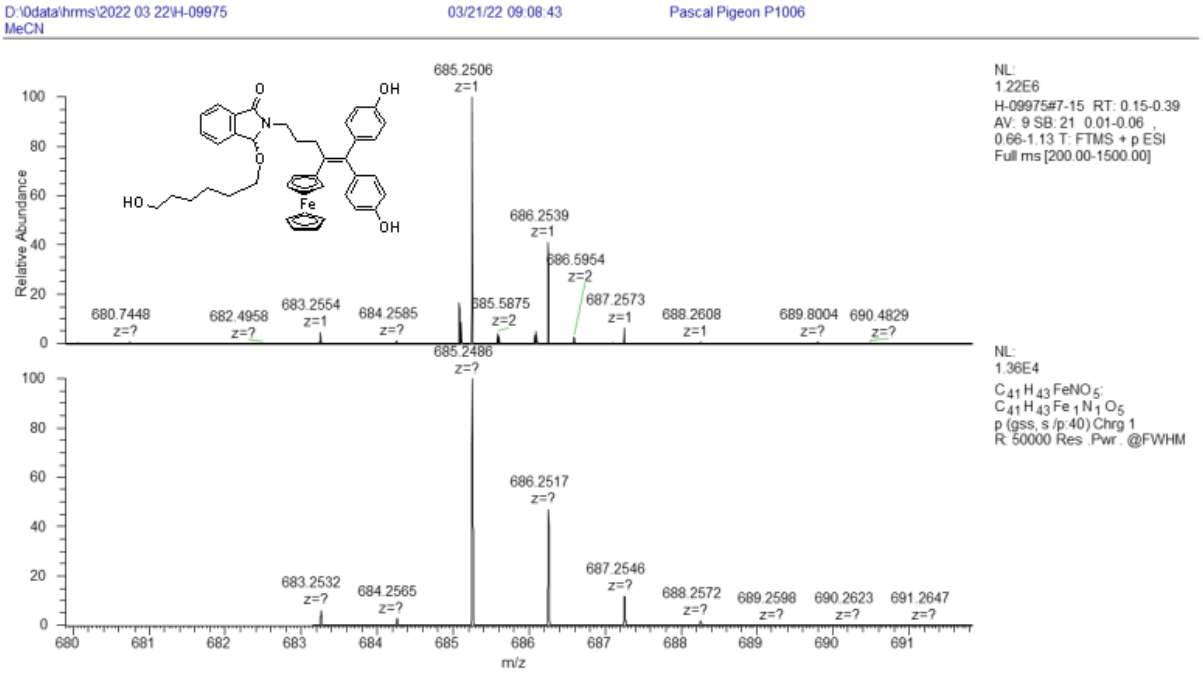


**Figure S43**: $^{1}H$ (in acetone-$d_6$), $^{13}C$ (in acetone-$d_6$) and COSY (in acetone-$d_6$) NMR, HR-MS and IR data for compound **21**






# Experimental/theoretical isotopic pattern MS spectrum

**Error = 2.9 ppm; Relative Intensity (%) 100**

**HRMS (ESI) m/z: [M]+ Calcd for C41H43FeNO5 685.2486 . Found 685.2506; (Error: 2.9 ppm).**

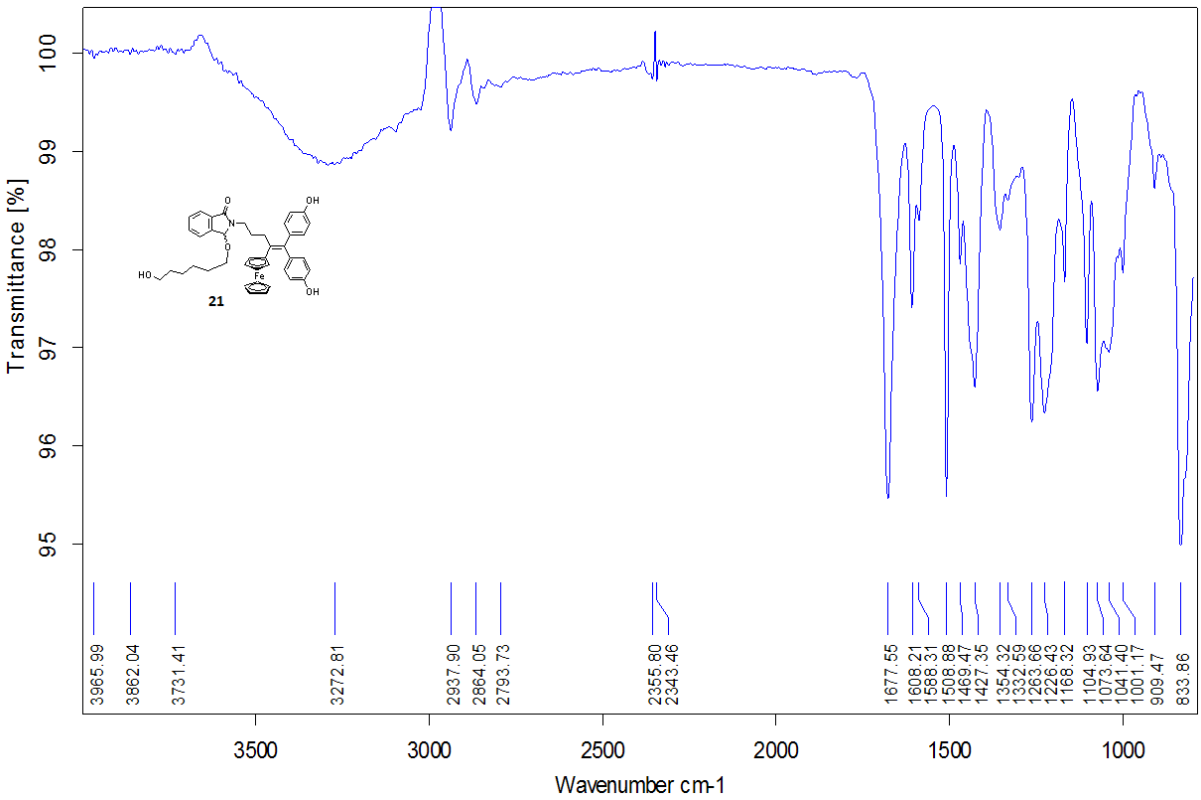
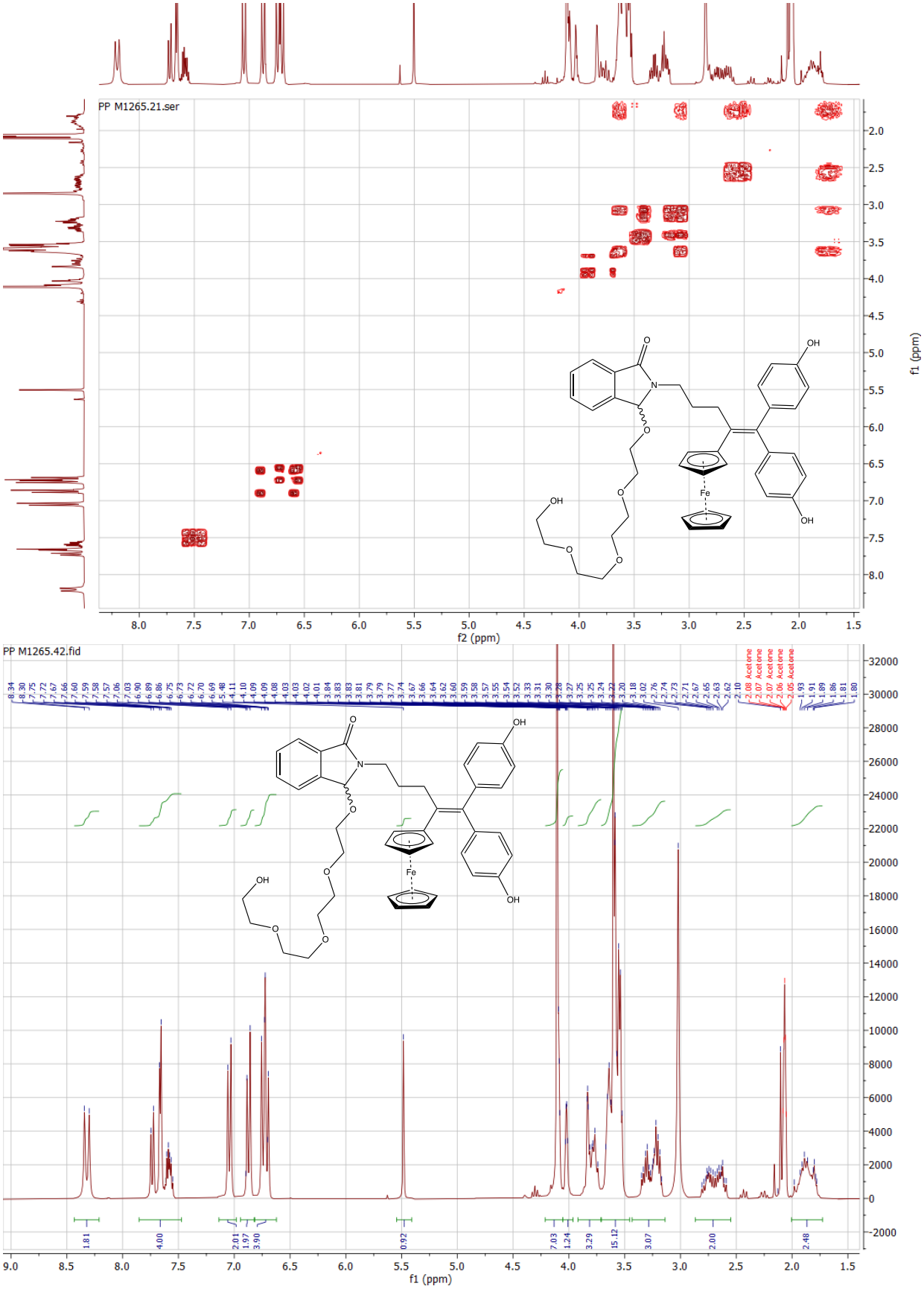
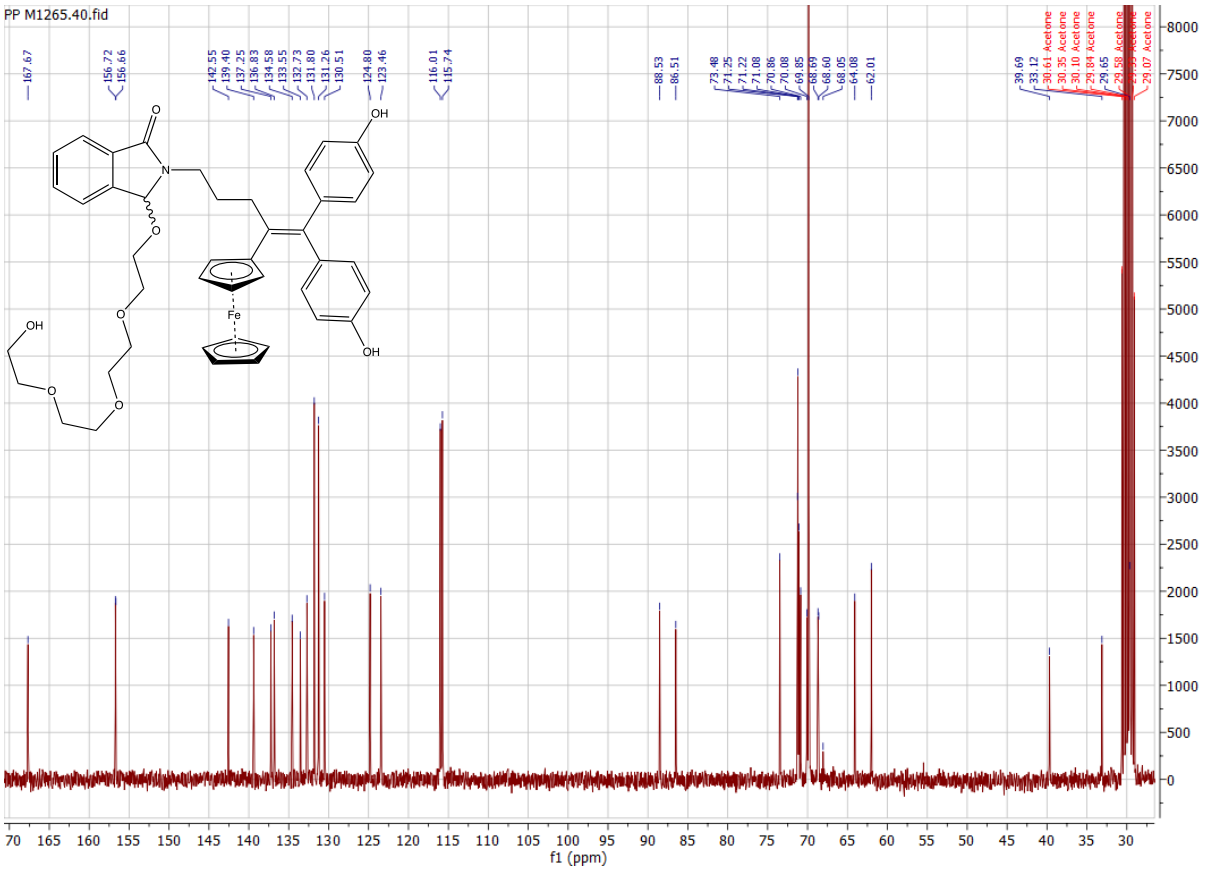
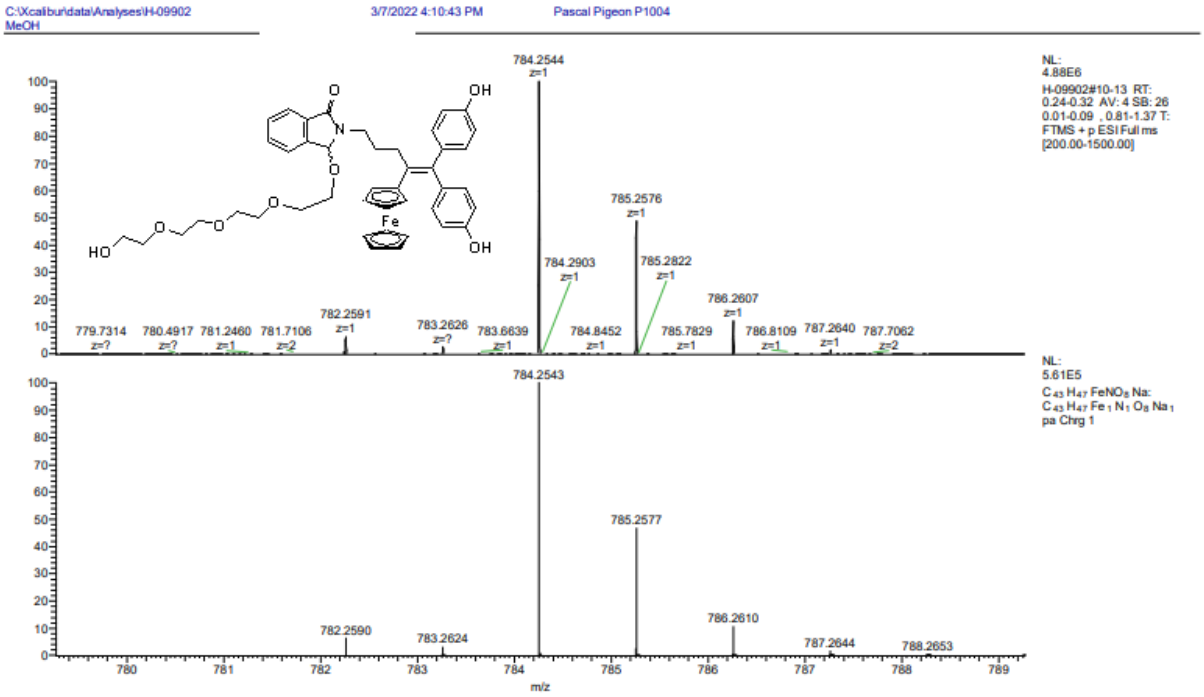

Transmittance [%]
100
99
98
97
96
95
21
3965.99
3862.04
3731.41
3272.81
2937.90
2864.05
2793.73
2355.80
2343.46
1677.55
1608.21
1588.31
1508.88
1469.47
1427.35
1354.32
1332.59
1263.66
1226.43
1168.32
1104.93
1073.64
1041.40
1001.17
909.47
833.86
3500
3000
2500
2000
1500
1000
Wavenumber cm-1

**Figure 44**: COSY (in acetone-$d_6$), $^{1}H$ (in acetone-$d_6$), $^{13}C$ (in acetone-$d_6$) NMR, HR-MS and IR data for compound **22**






# Experimental/theoretical isotopic pattern MS spectrum

**Error = 0.1 ppm; Relative Intensity (%) 100**

**HRMS (ESI) m/z: [M+Na]+ Calcd for C43H47FeNO8Na 784.2543. Found 784.2544; (Error: 0.1 ppm).**

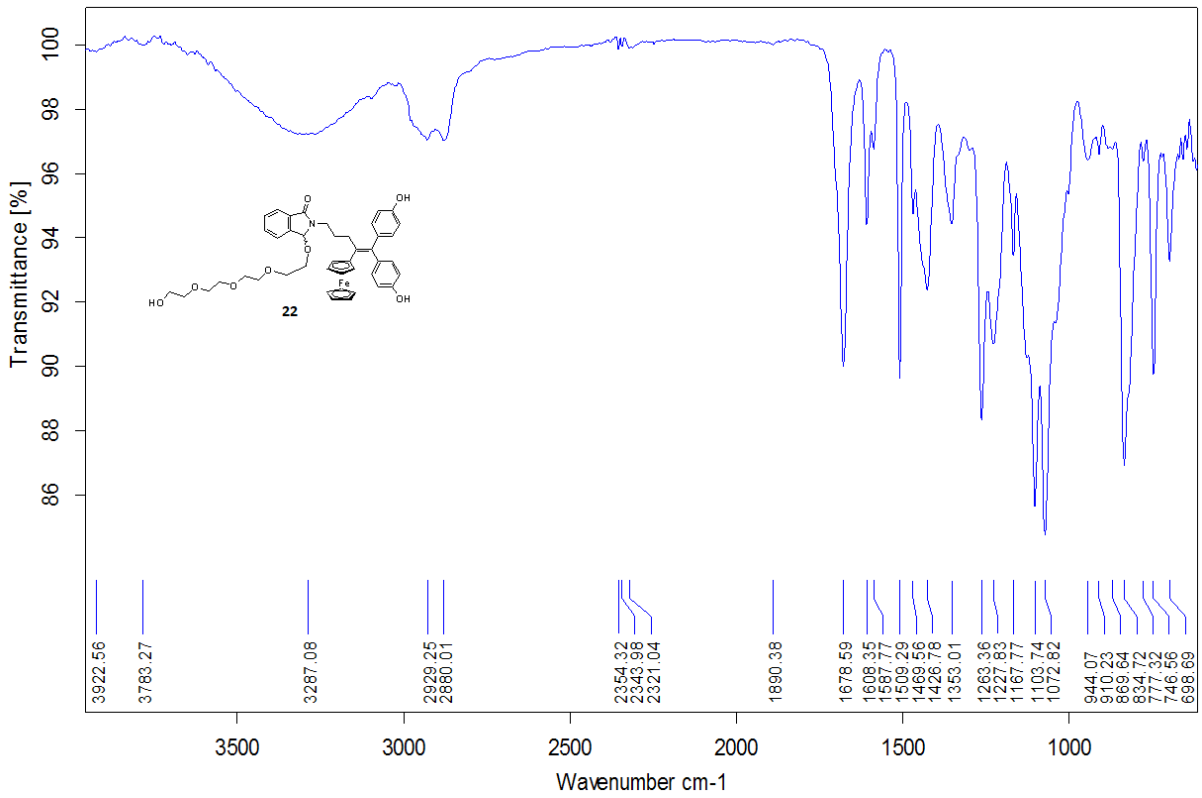
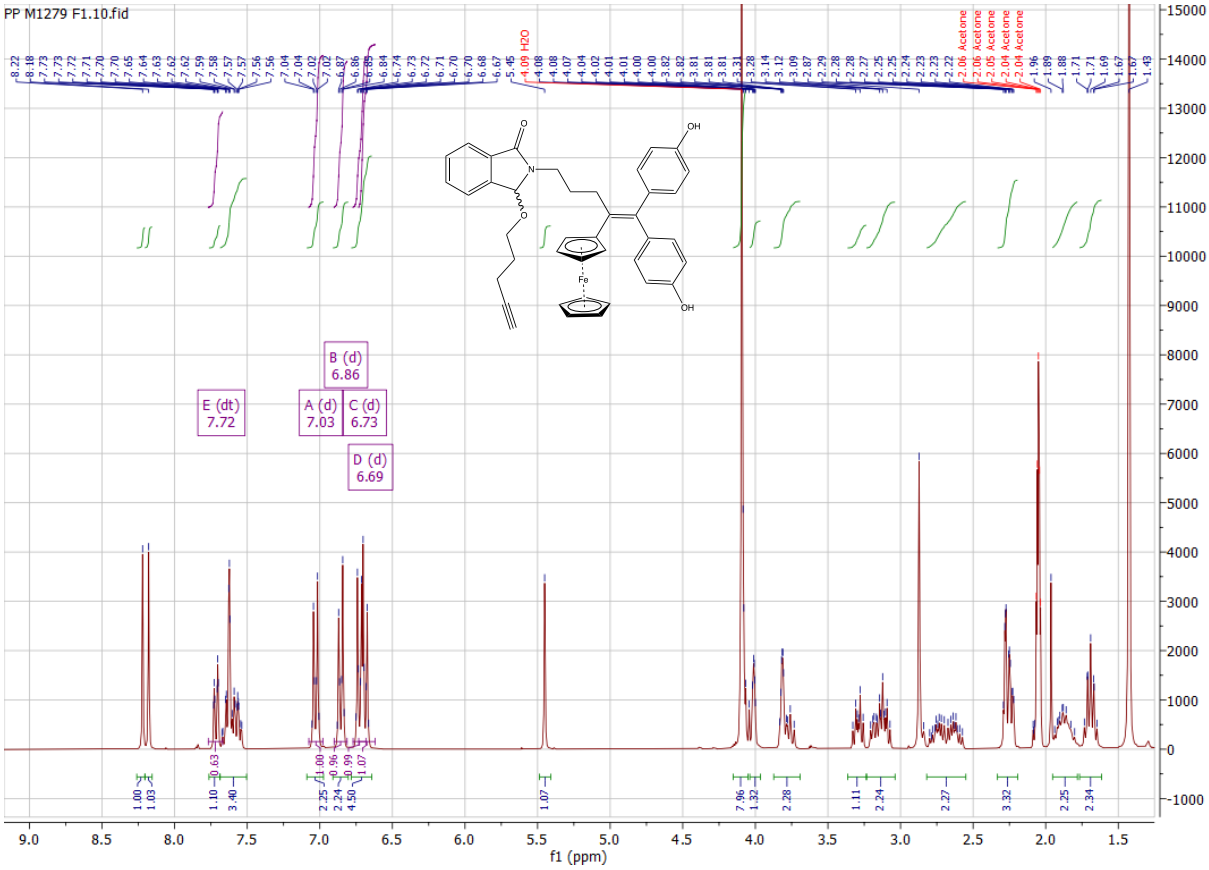
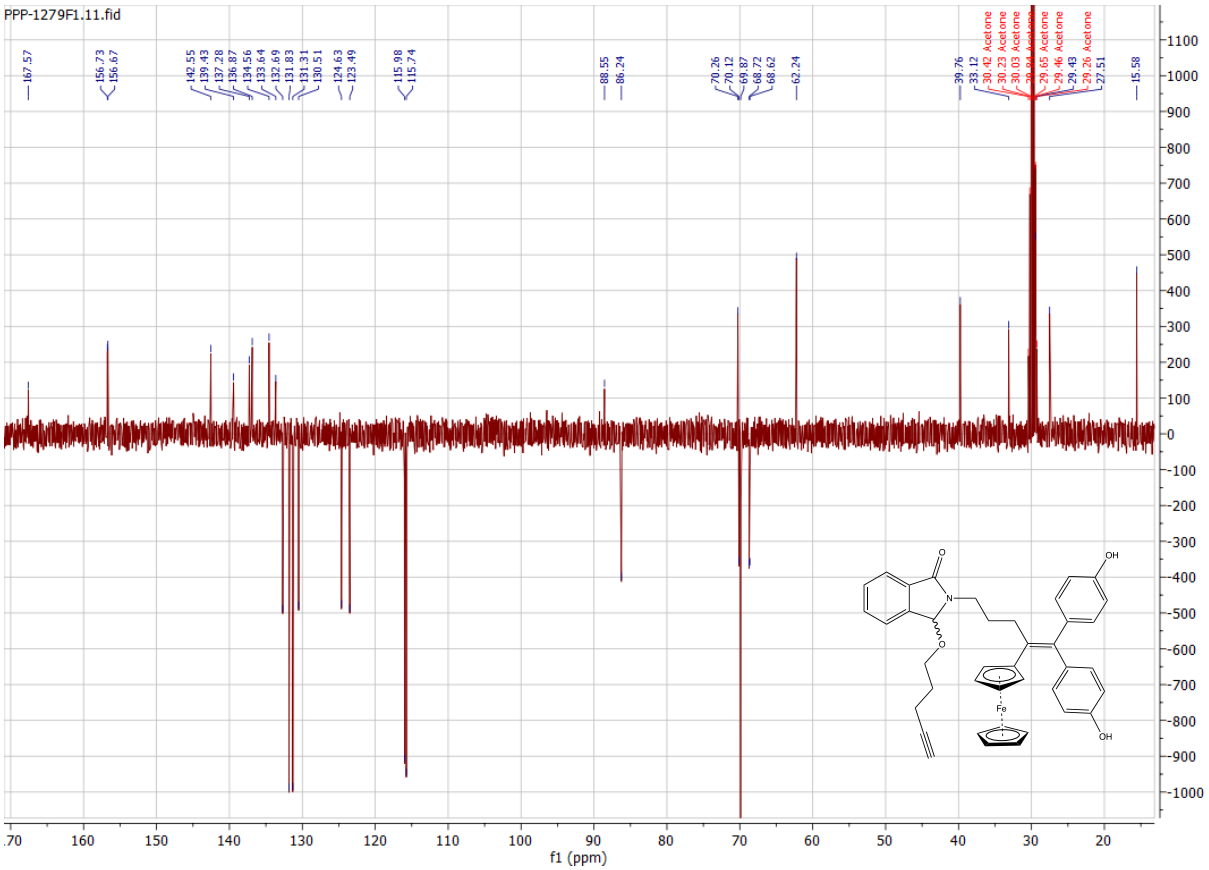
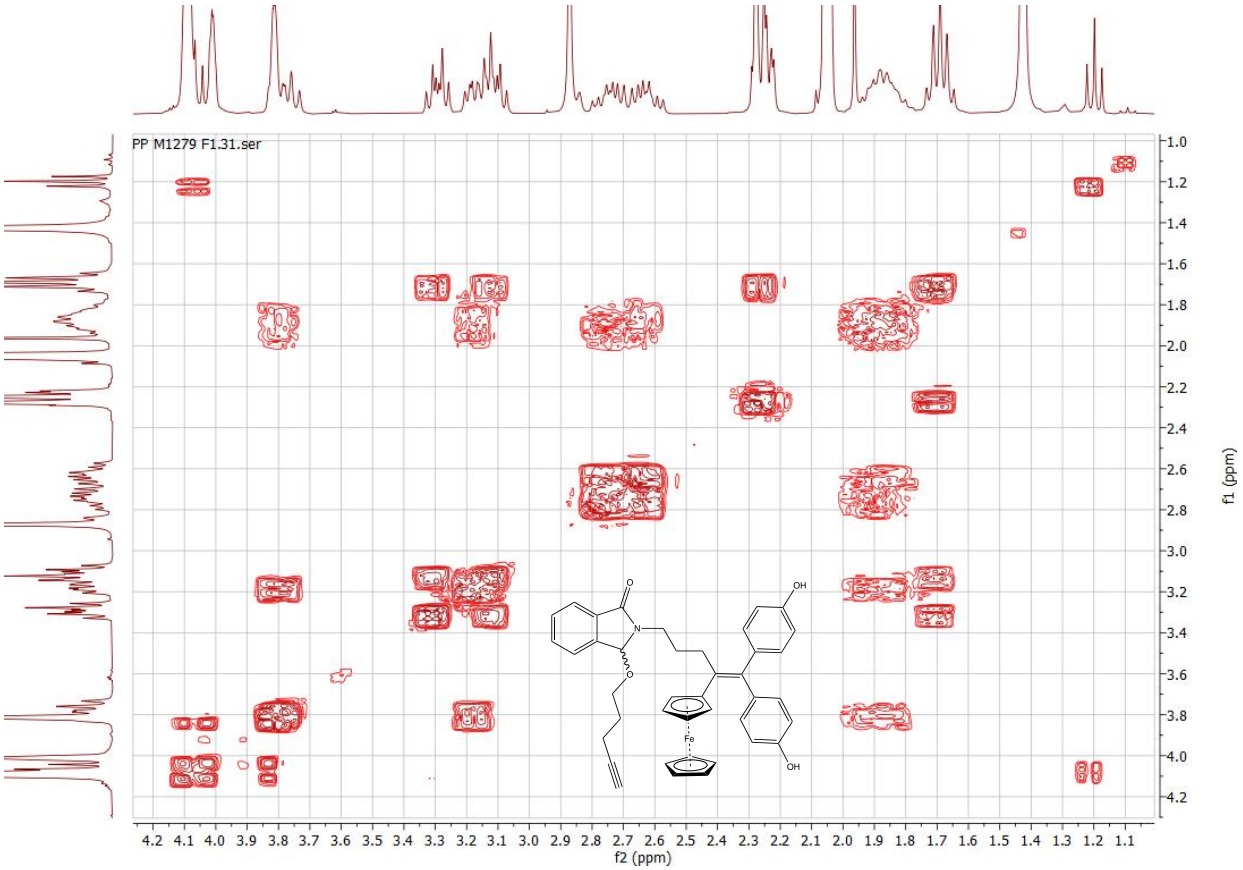
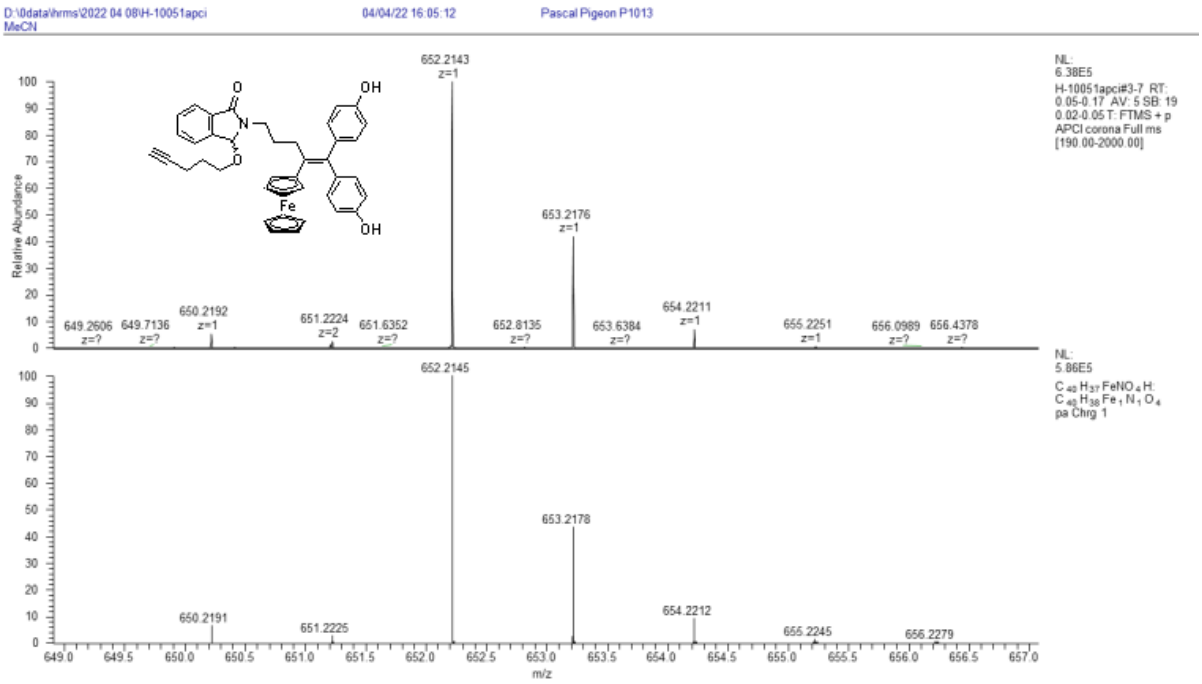

Transmittance [%]
100
98
96
94
92
90
88
86
22
3922.56
3783.27
3287.08
2929.25
2880.01
2354.32
2343.98
2321.04
1890.38
1678.59
1608.35
1587.77
1509.29
1469.56
1426.78
1353.01
1263.36
1227.83
1167.77
1103.74
1072.82
944.07
910.23
869.64
834.72
777.32
746.56
698.69
3500
3000
2500
2000
1500
1000
Wavenumber cm-1

**Figure S45**: $^{1}$H (in acetone-d$_6$), JMOD (in acetone-d$_6$), COSY (in acetone-d$_6$) NMR, HR-MS and IR data for compound **23**






# Experimental/theoretical isotopic pattern MS spectrum

**Error = -0.3 ppm; Relative Intensity (%) 100**

**HRMS (APCI) m/z: [M+H]+ Calcd for C40H37FeNO4H 652.2145. Found 652.2143; (Error: -0.3 ppm).**

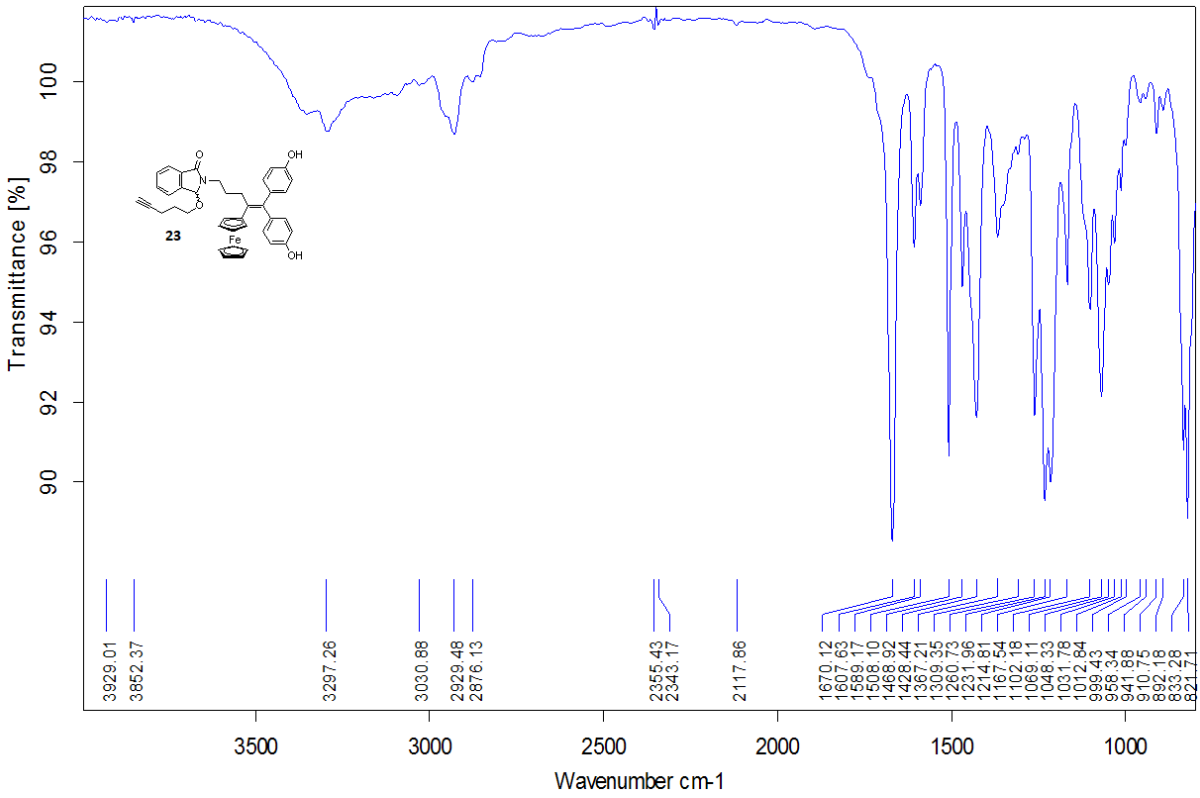
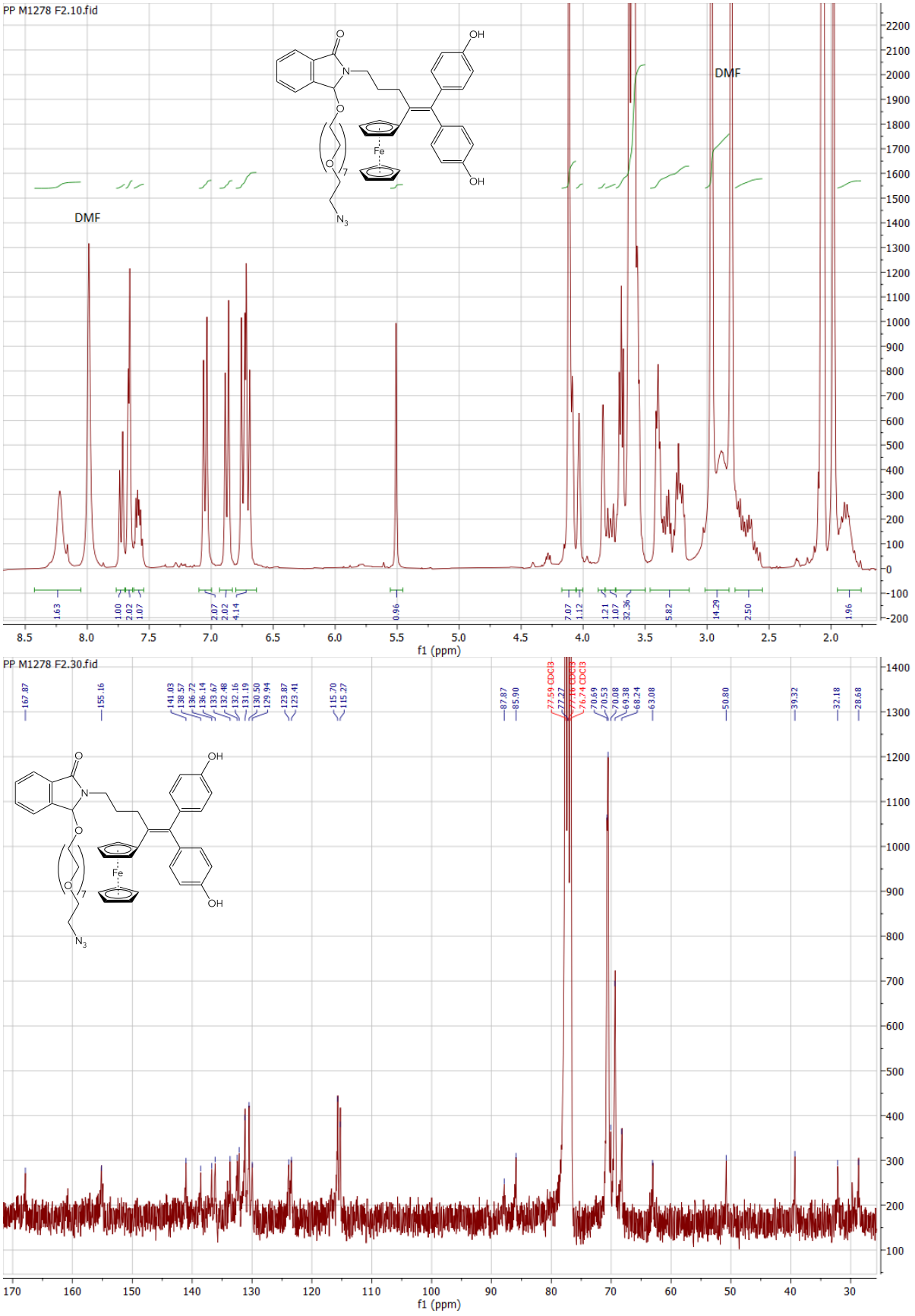
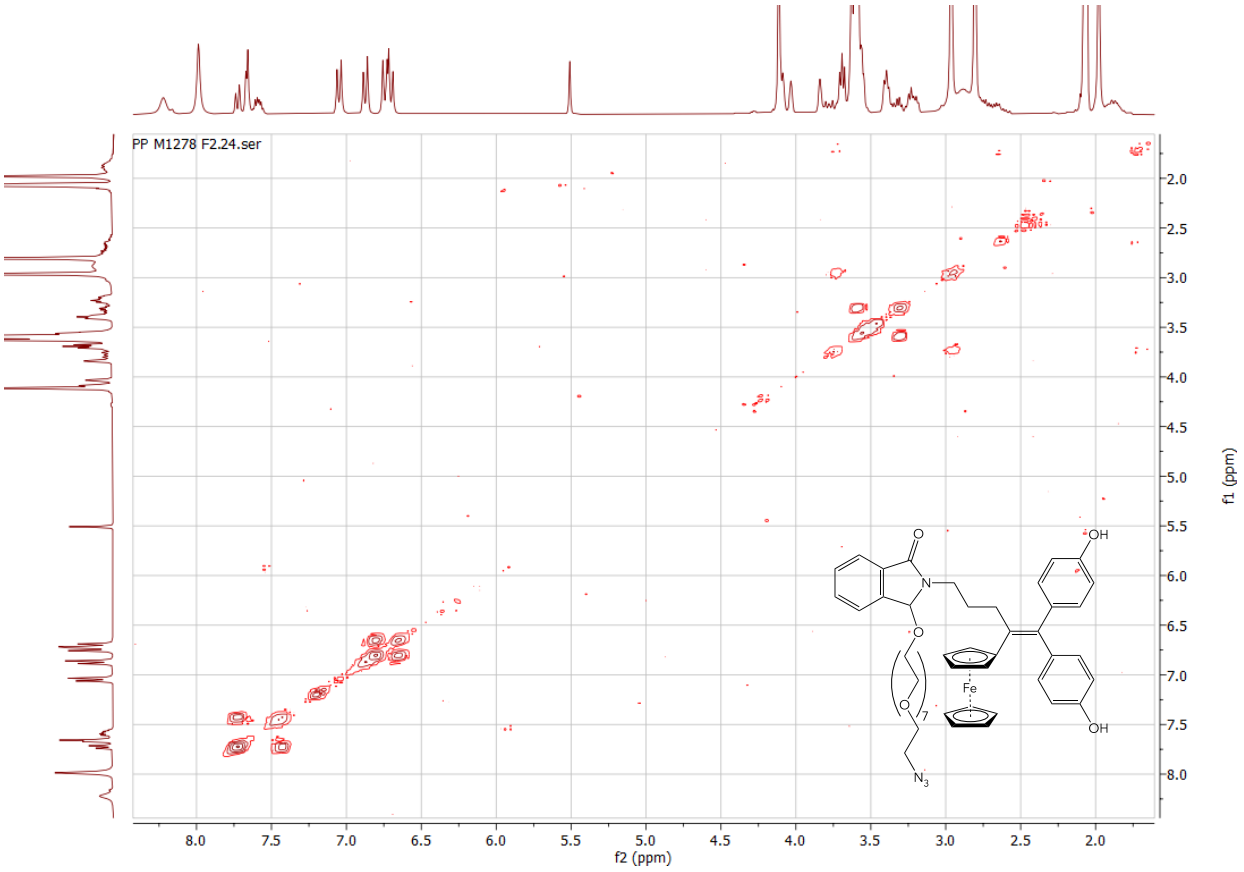
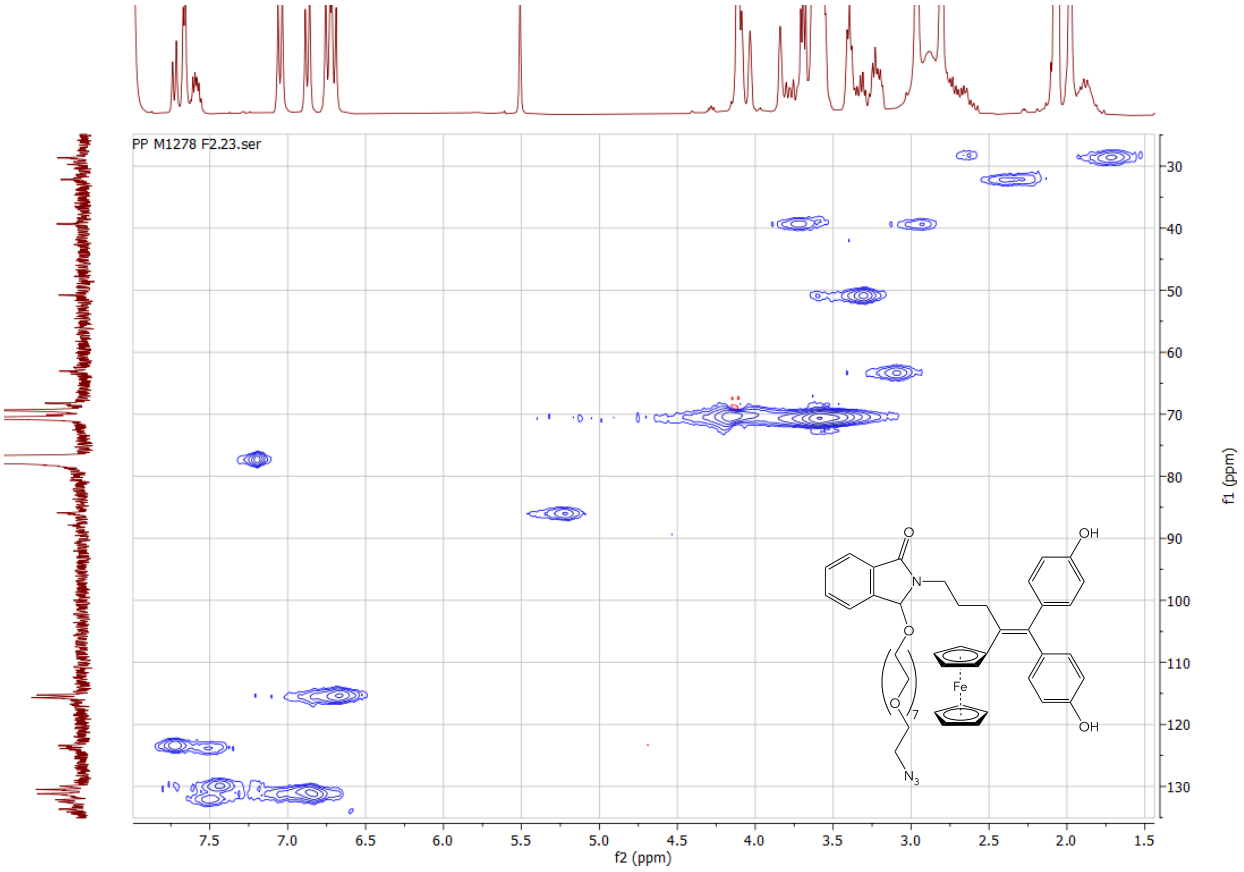
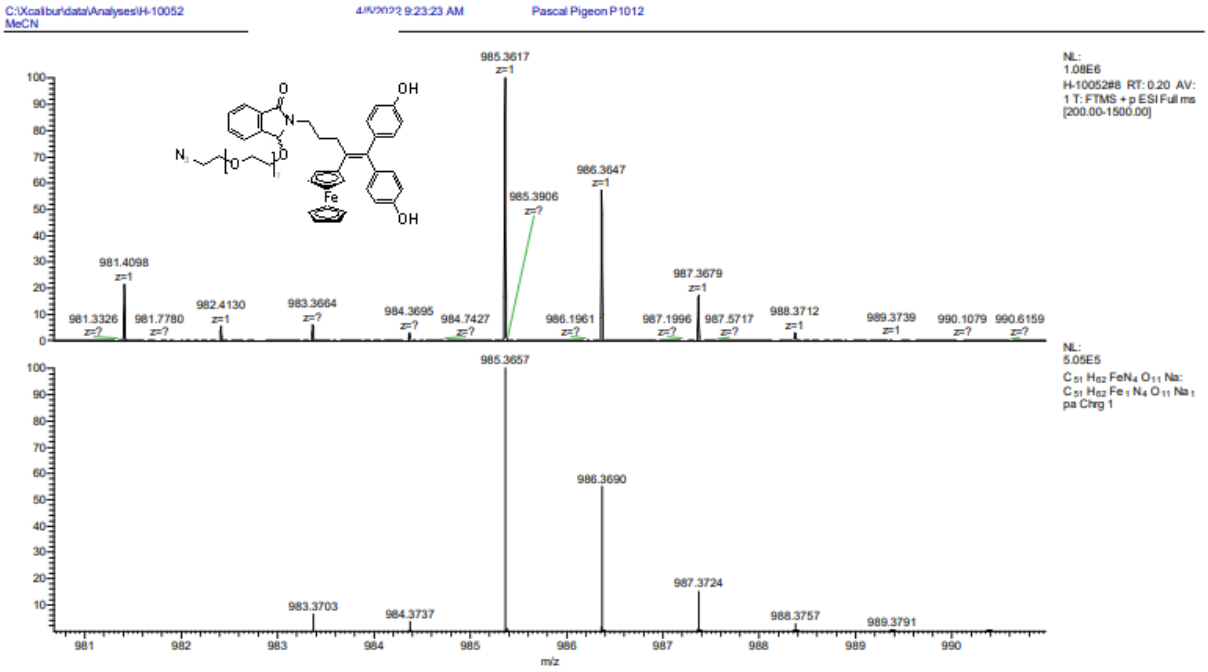

Transmittance [%]
90
92
94
96
98
100
23
Fe
OH
OH
3929.01
3852.37
3297.26
3030.88
2929.48
2876.13
2355.43
2343.17
2117.86
1670.12
1607.63
1589.17
1508.10
1468.92
1428.44
1367.21
1309.55
1260.73
1231.96
1214.81
1167.54
1102.18
1069.11
1048.33
1031.78
1012.84
999.43
958.34
941.88
910.75
892.18
833.28
821.71
3500
3000
2500
2000
1500
1000
Wavenumber cm-1

**Figure S46**: $^{1}H$ (in $CDCl_3$), $^{13}C$ (in $CDCl_3$), COSY (in $CDCl_3$), HMQC (in $CDCl_3$) NMR, HR-MS and IR data for compound **24**




PP M1278 F2.24.ser
f2 (ppm)
f1 (ppm)
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
OH
OH
Fe
N3


PP M1278 F2.23.ser
f2 (ppm)
f1 (ppm)
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
30
40
50
60
70
80
90
100
110
120
130
OH
OH
Fe
N3




# Experimental/theoretical isotopic pattern MS spectrum

**Error = -4.0 ppm; Relative Intensity (%) 100**

**HRMS m/z: [M+Na]+ Calcd for C51H62FeN4O11Na 983.3703 Found 983.3664 ; (Error: -4.0 ppm).**

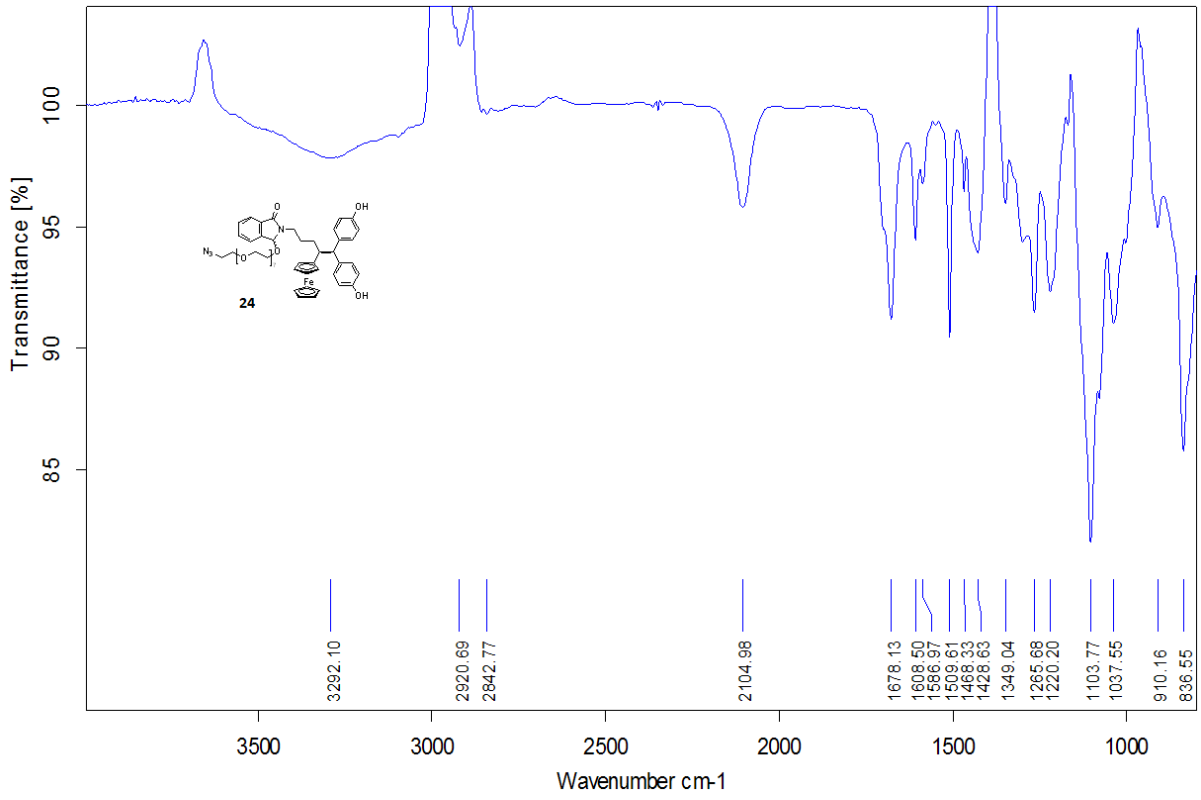
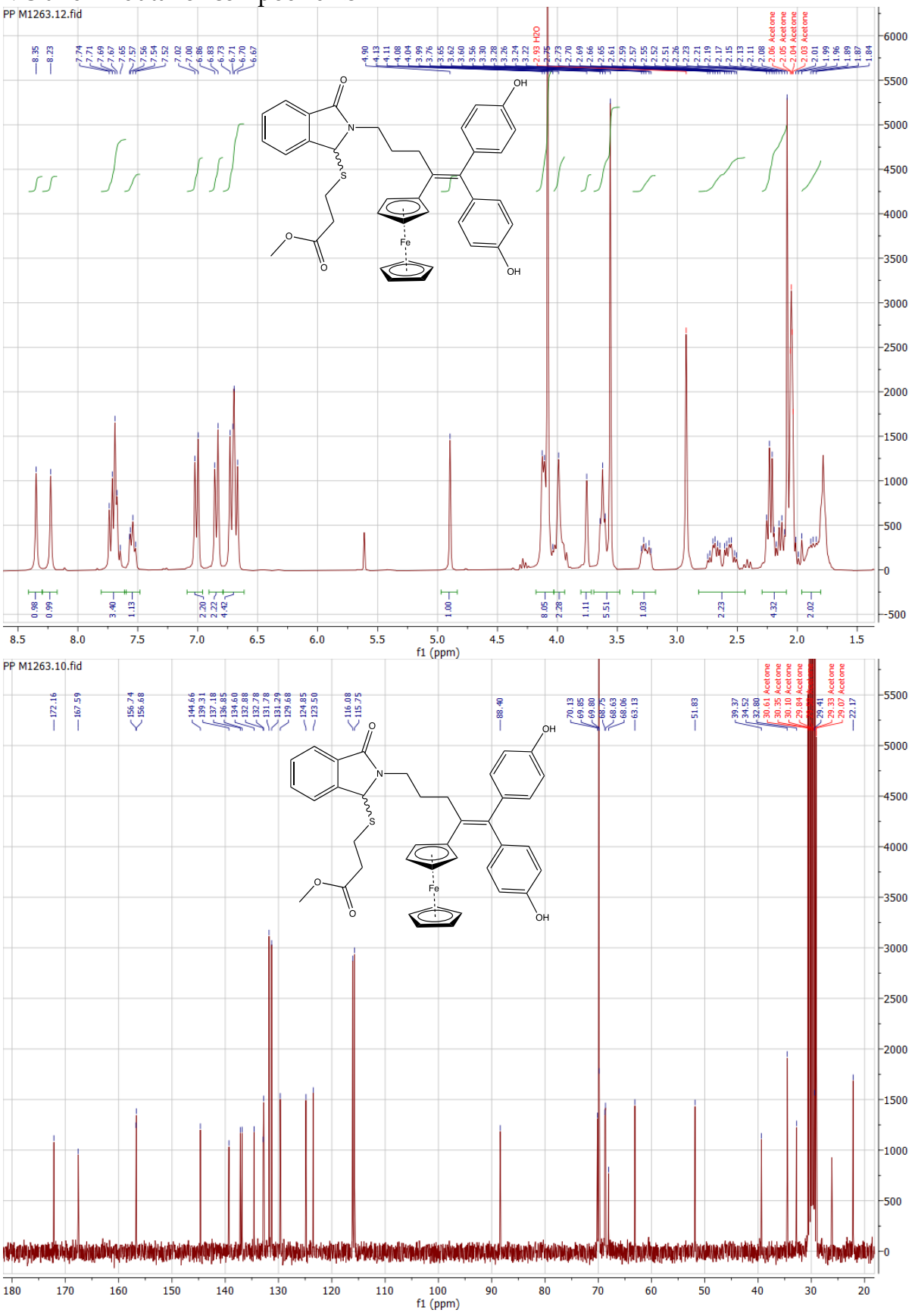
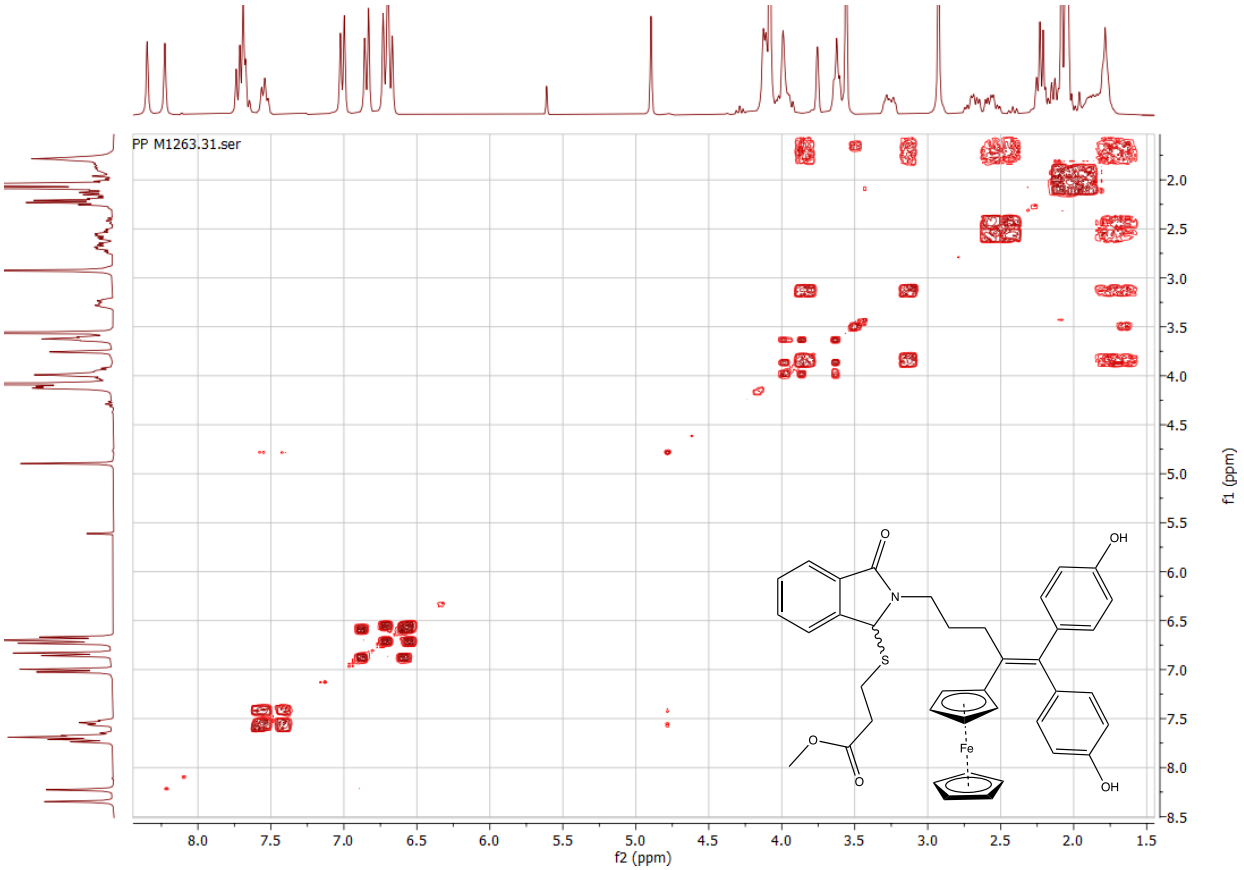
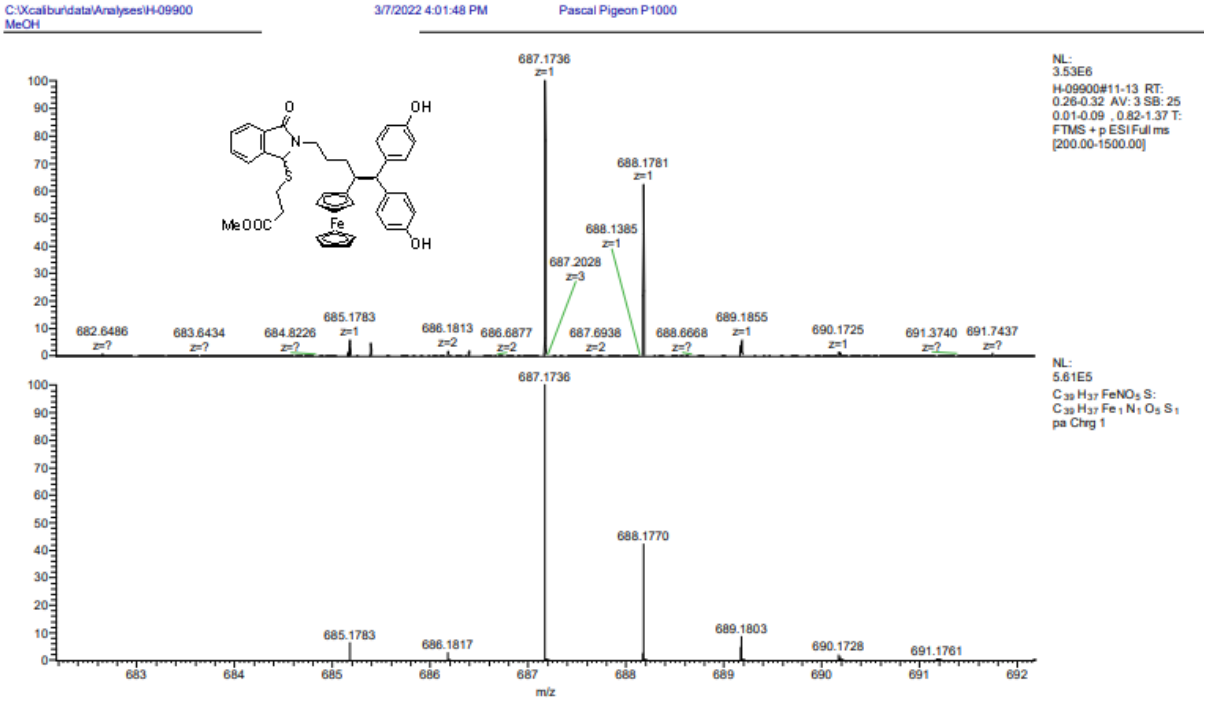


**Figure S47**: $^{1}H$ (in acetone-$d_6$), $^{13}C$ (in acetone-$d_6$), COSY (in acetone-$d_6$) NMR, HR-MS and IR data for compound **25**






# Experimental/theoretical isotopic pattern MS spectrum

**Error = 0.0 ppm; Relative Intensity (%) 100**

**HRMS (ESI) m/z: [M]+ Calcd for C39H37FeNO5S 687.1736 . Found 687.1736; (Error: 0.0 ppm).**

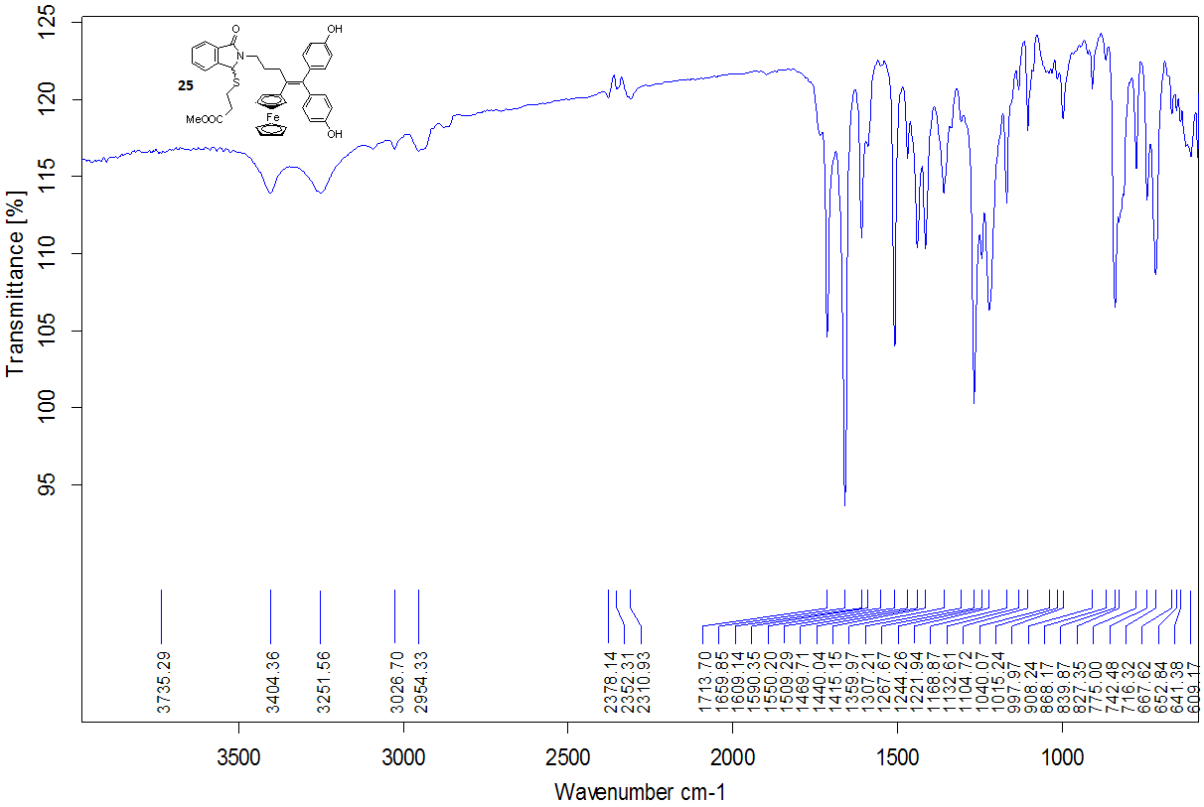
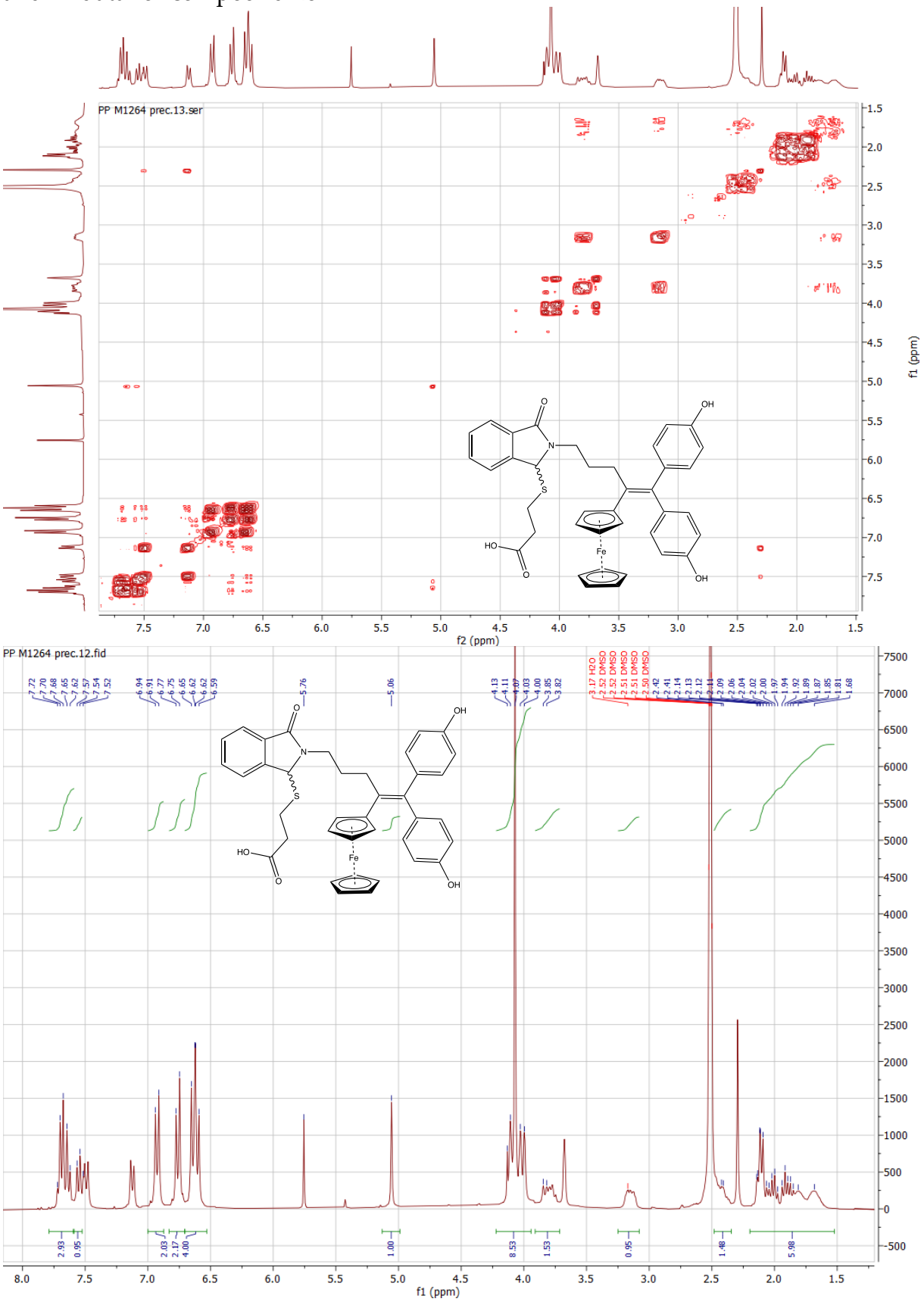
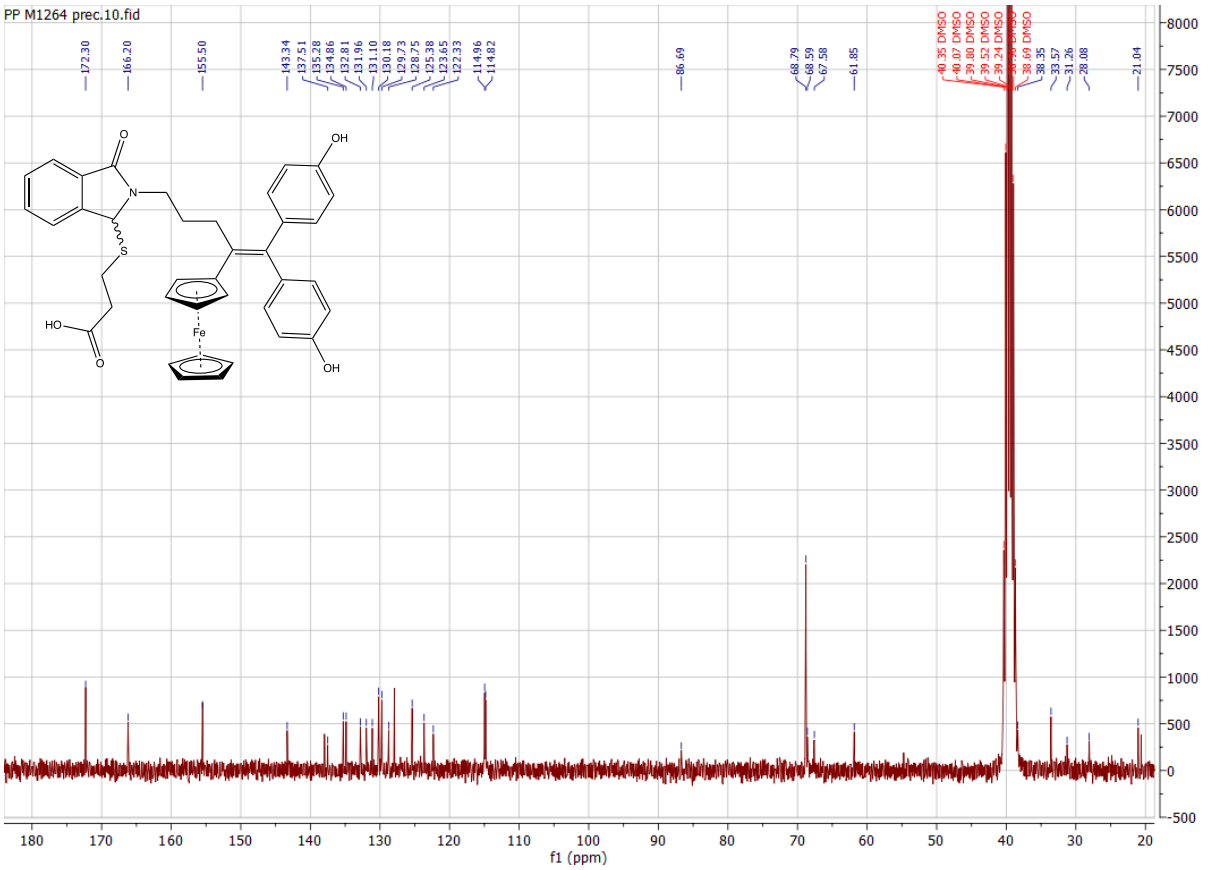
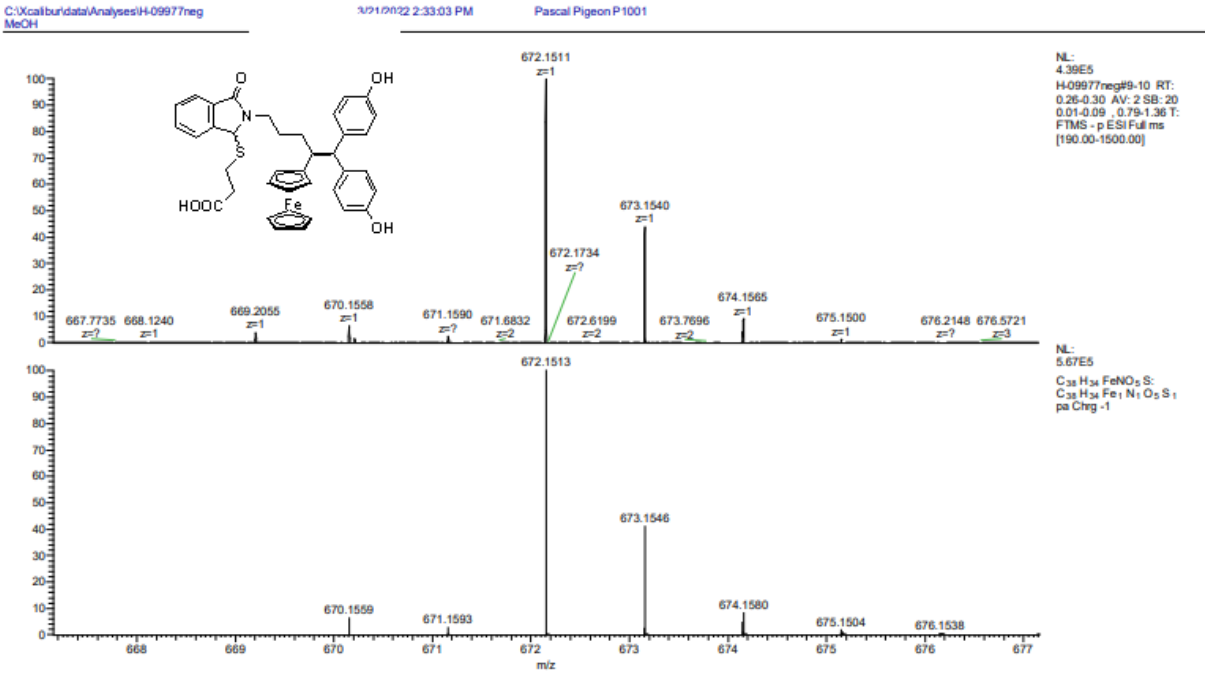

Transmittance [%]
125
120
115
110
105
100
95
3735.29
3404.36
3251.56
3026.70
2954.33
2378.14
2352.31
2310.93
1713.70
1659.85
1609.14
1590.35
1550.20
1509.29
1469.71
1440.04
1415.15
1359.97
1307.21
1267.67
1244.26
1221.94
1168.87
1132.61
1104.72
1040.07
1015.24
997.97
908.24
868.17
839.87
827.35
775.00
742.48
716.32
667.62
652.84
641.38
609.17
3500
3000
2500
2000
1500
1000
Wavenumber cm-1
25
MeOOC
Fe
OH
OH

**Figure S48**: COSY (in DMSO-$d_6$), $^{1}H$ (in DMSO-$d_6$), $^{13}C$ (in DMSO-$d_6$) NMR, HR-MS and IR data for compound **26**






# Experimental/theoretical isotopic pattern MS spectrum

**Error = -0.2 ppm; Relative Intensity (%) 100**

**HRMS (ESI) m/z: [M] 1- Calcd for C38H34FeNO5S672.1513 . Found 672.1511; (Error: -0.2 ppm).**

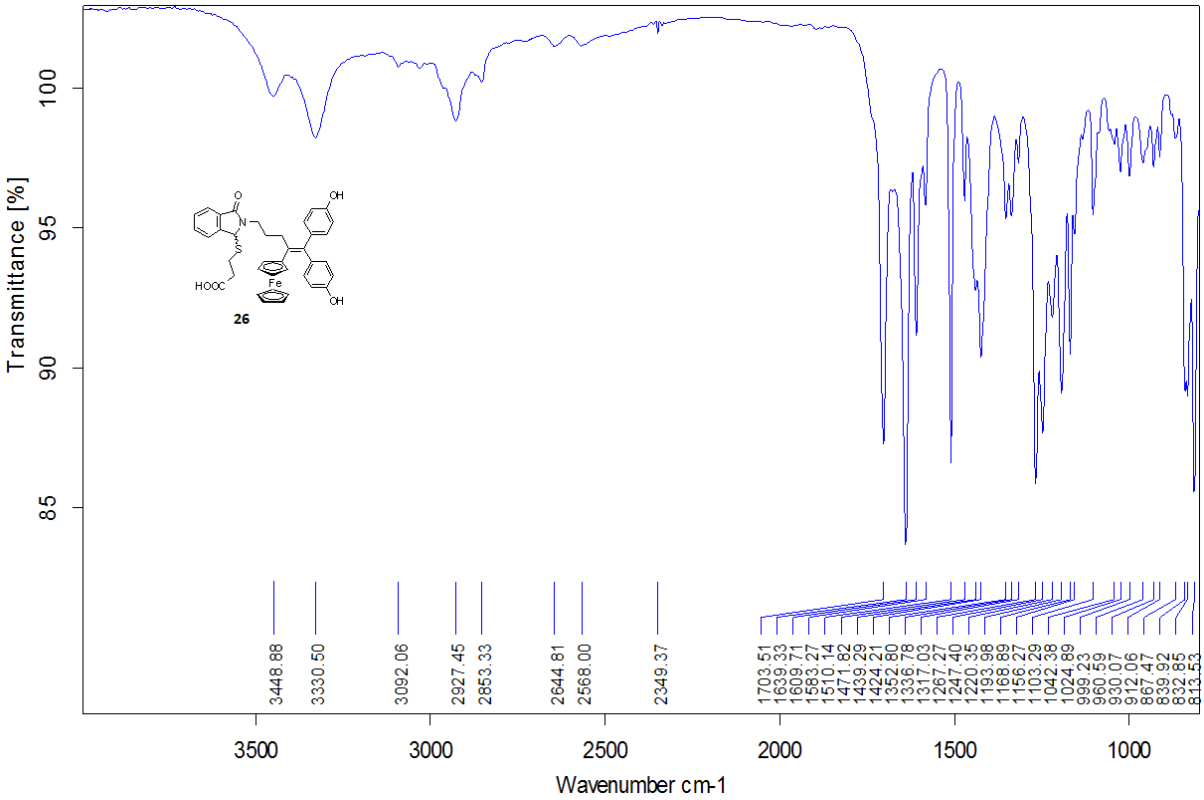
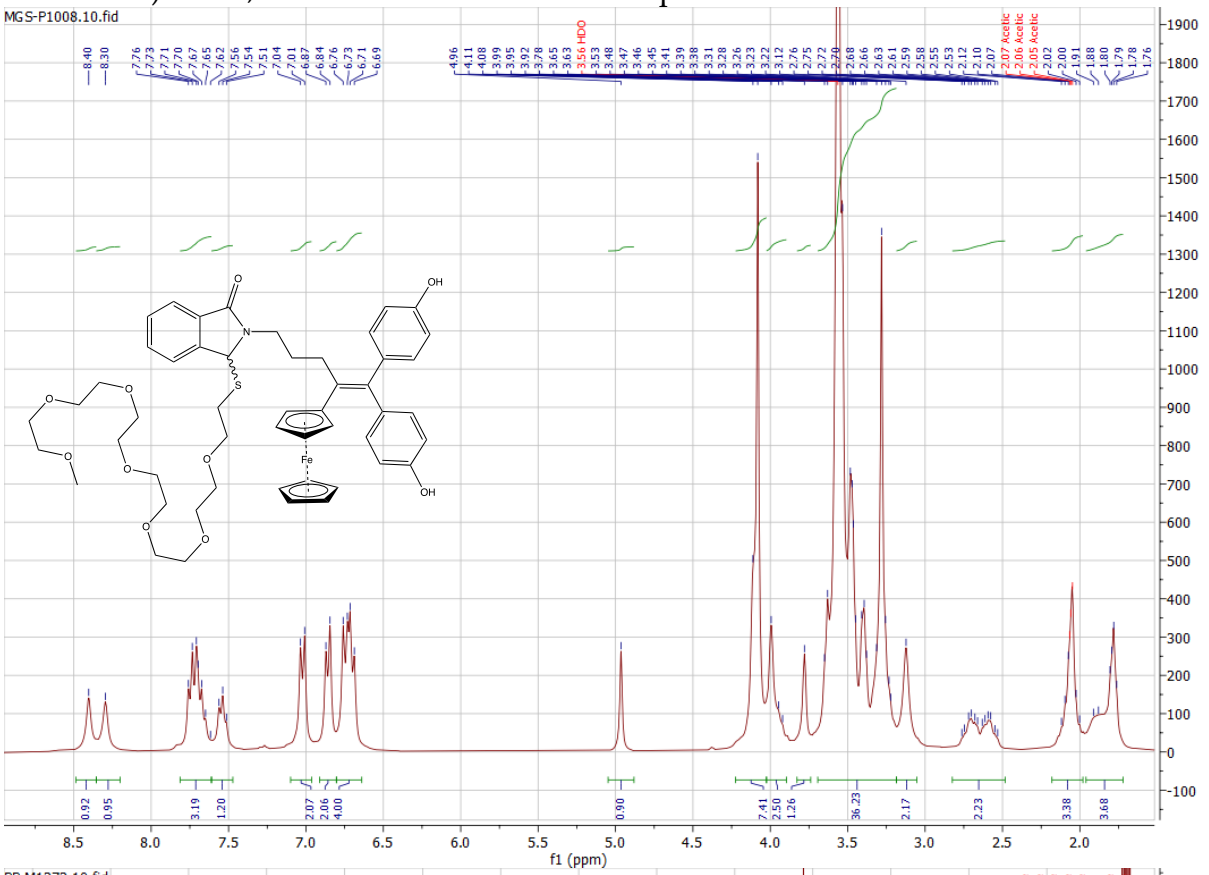
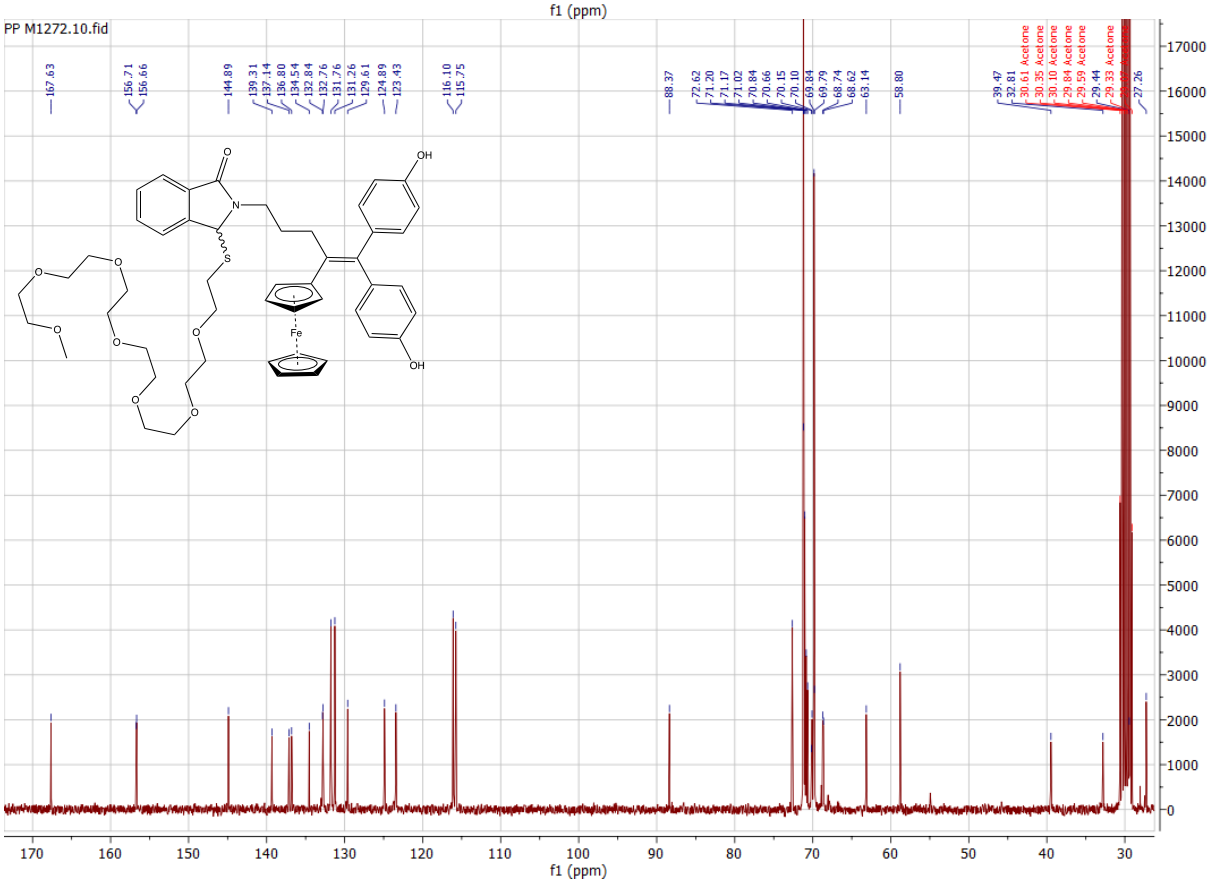
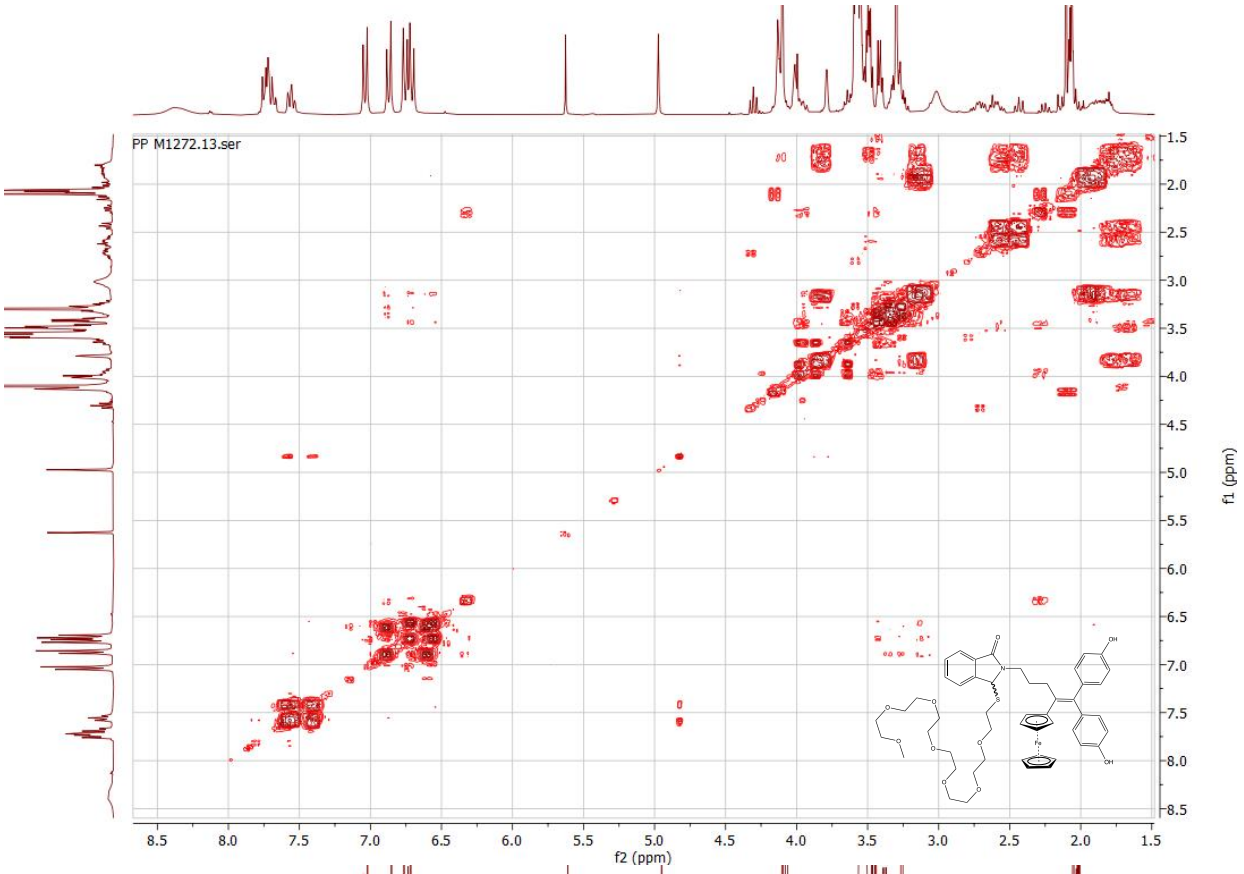
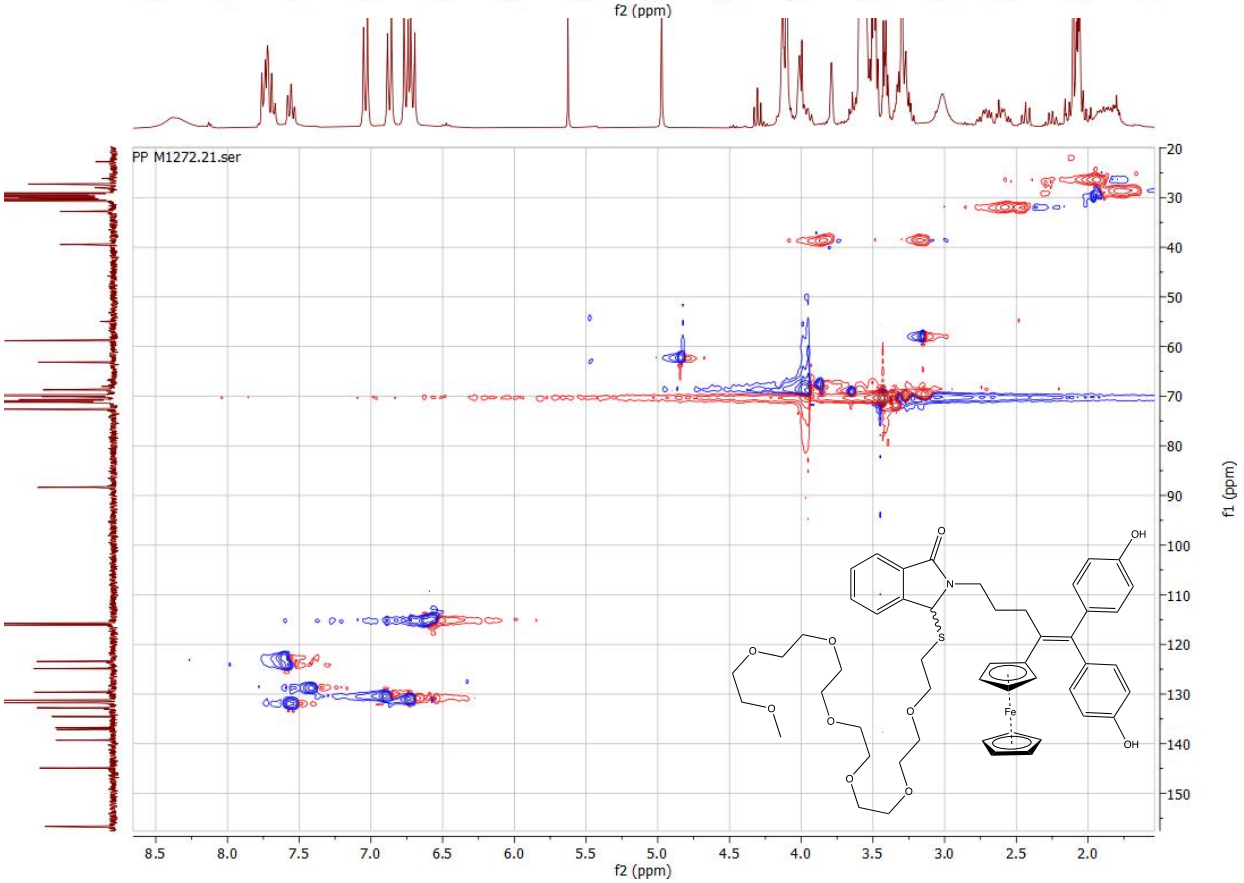

Transmittance [%]
100
95
90
85
HOOC
Fe
OH
OH
O
N
26
3448.88
3330.50
3092.06
2927.45
2853.33
2644.81
2568.00
2349.37
1703.51
1639.33
1609.71
1583.27
1510.14
1471.82
1439.29
1424.21
1352.80
1336.78
1317.03
1267.27
1247.40
1220.35
1193.98
1168.89
1156.27
1103.29
1042.38
1024.89
999.23
960.59
930.07
912.06
867.47
839.92
832.85
813.53
3500
3000
2500
2000
1500
1000
Wavenumber cm-1

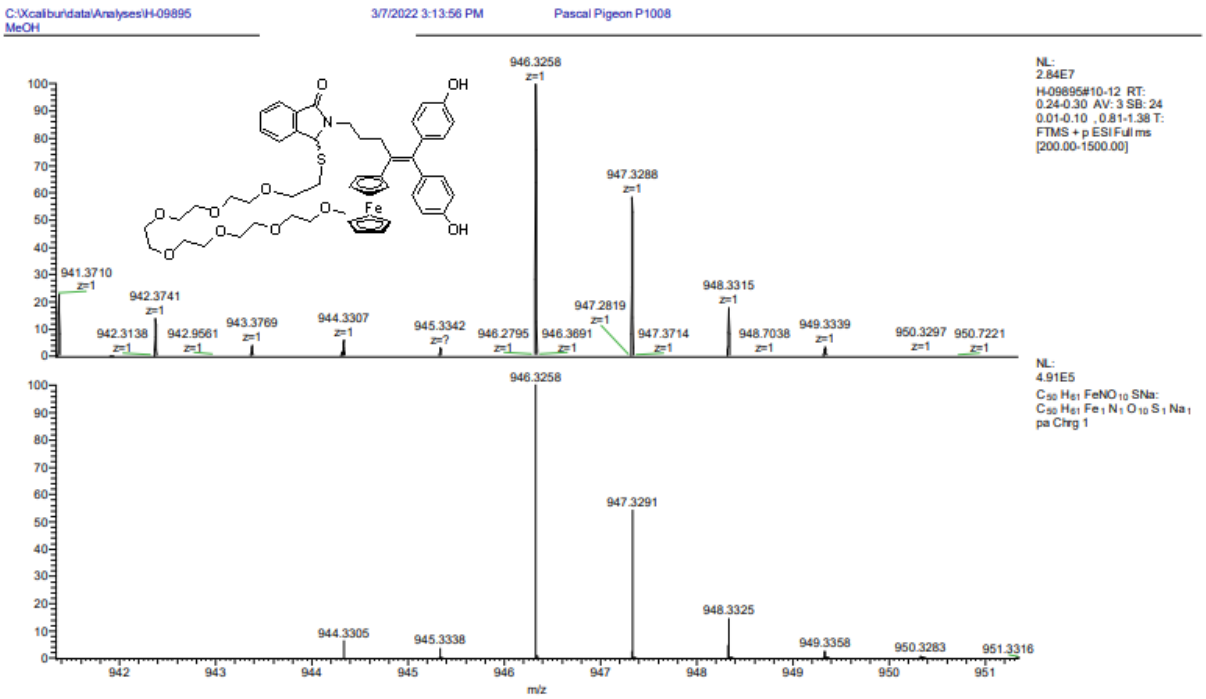
**Figure S49**: $^{1}H$ (in acetone-$d_6$), $^{13}C$ (in acetone-$d_6$), COSY (in acetone-$d_6$), HMQC (in acetone-$d_6$) NMR, HR-MS and IR data for compound **27**




PP M1272.13.ser
f2 (ppm)
f1 (ppm)


PP M1272.21.ser
f2 (ppm)
f1 (ppm)




# Experimental/theoretical isotopic pattern MS spectrum

**Error = 0.0 ppm; Relative Intensity (%) 100**

**HRMS (ESI) m/z: [M+Na]+ Calcd for C50H61FeNO10SNa 946.3258. Found 946.3258; (Error: 0.0 ppm).**

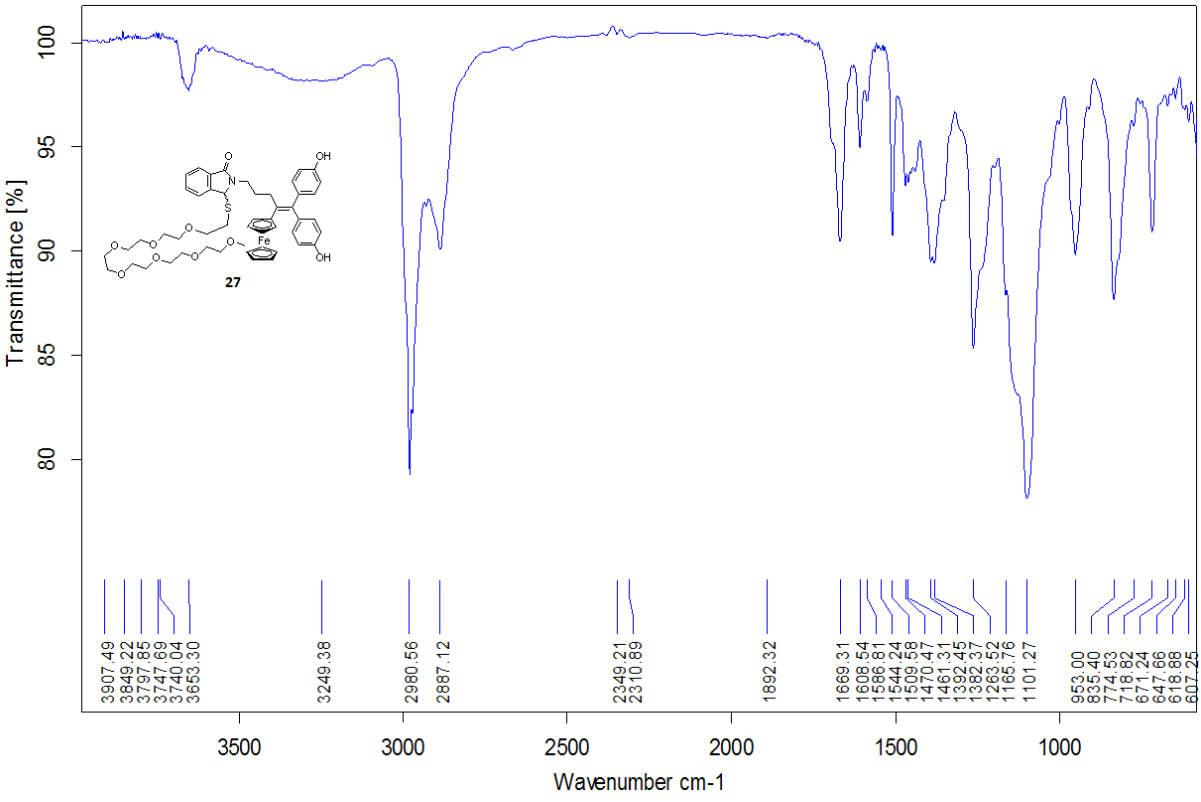
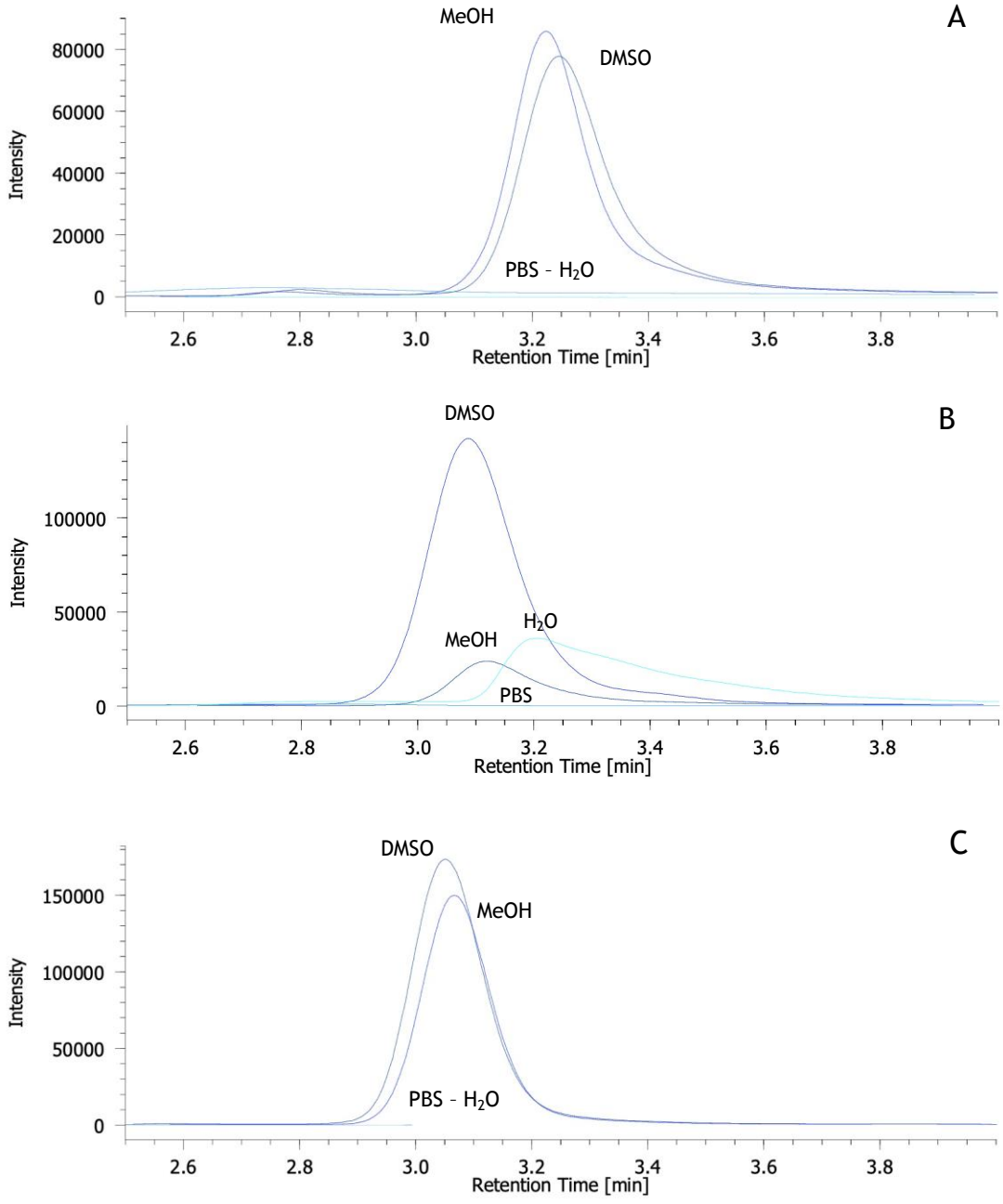


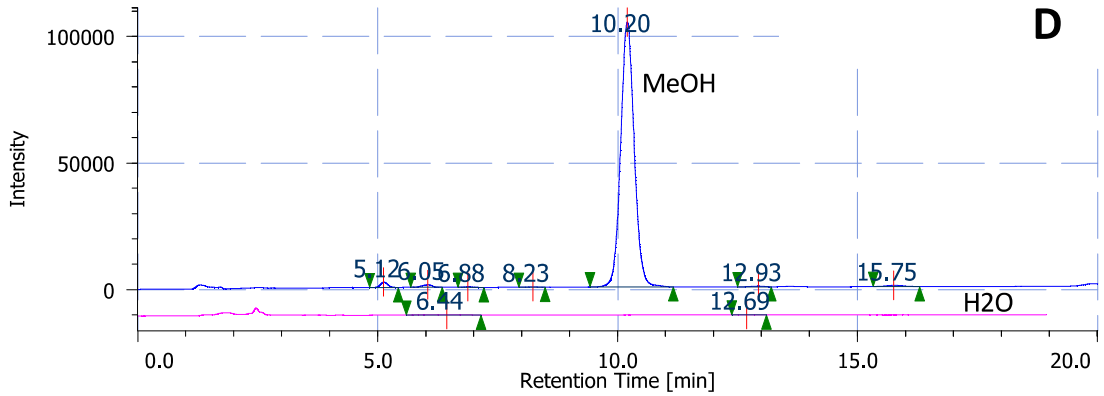
**Table S1**. Crystallographic data and structure refinement parameters for **15**, **23•acetone** and **25•acetone**.

| **Parameters** | **15** | **23•0.5acetone** | **25•acetone** |
|---|---|---|---|
| Chemical formula | $C_{16}H_{17}FeNO$ | $C_{41.5}H_{40}FeNO_{4.5}$ | $C_{42}H_{43}FeNO_6S$ |
| Formula weight (g.mol$^{-1}$) | 295.15 | 680.59 | 745.68 |
| Crystal system | monoclinic | monoclinic | triclinic |
| Space group | $P2_1/c$ | $P2_1/n$ | P-1 |
| Crystal size (mm$^3$) | 0.37 x 0.27 x 0.06 | 0.2 x 0.1 x 0.05 | 0.3 x 0.2 x 0.1 |
| Crystal color and shape | Yellow prism | Orange prism | Orange plate |
| a (Å) | 14.6466(7) | 9.8118(3) | 10.7220(5) |
| b (Å) | 7.1923(3) | 17.2893(6) | 13.2436(6) |
| c (Å) | 12.0545(6) | 20.2760(6) | 15.3329(6) |
| $\alpha$ (Å) | 90 | 90 | 97.196(3) |
| $\beta$ (Å) | 94.662(4) | 91.557(2) | 103.916(4) |
| $\gamma$ (Å) | 90 | 90 | 113.797(4) |
| Cell volume (Å$^3$) | 1265.65(10) | 3438.33(19) | 1872.10(16) |
| T (k) | 200(1) | 200(1) | 200 |
| Wavelength | 1.54178 | 1.54178 | 0.71073 |
| Z | 4 | 4 | 2 |
| $\varrho_{calcd}$ (g.cm-$^3$) | 1.549 | 1.315 | 1.323 |
| $\mu$ (mm$^{-1}$) | 9.458 | 3.874 | 0.507 |
| Scan rage (°) | $6.063 < \theta < 66.571$ | $4.37 < \theta < 66.47$ | $1.9360 < \theta < 32.2830$ |
| Index ranges | $-17 \le h \le 16$ | $-11 \le h \le 10$ | $-14 \le h \le 14$ |
| | $-5 \le k \le 8$ | $-20 \le k \le 20$ | $-17 \le k \le 17$ |
| | $-14 \le l \le 14$ | $-24 \le l \le 21$ | $-20 \le l \le 20$ |
| Reflections (all / independent) | 9310 / 2242 | 26640 / 6066 | 25312 / 9219 |
| Completeness (%) | 99.9 | 99.8 | 99.3 |
| $R_{int}$ | 0.0471 | 0.0505 | 0.0892 |
| Data / parameters / restraints | 2242 / 173 / 0 | 6066 / 455 / 27 | 9219 / 471 / 0 |
| Goodness-of-fit on $F^2$ | 1.025 | 1.031 | 1.102 |
| *R1* [$I>2\sigma(I)$] (%) | 3.50 | 3.82 | 6.30 |
| wR2 (all data) (%) | 9.04 | 9.82 | 16.76 |
| Largest difference peak and hole (Å$^{-3}$) | 0.247, -0.290 | 0.265, -0.341 | 1.517, -0.588 |

**Figure S50**: Solubility studies by RP-HPLC analysis of compounds **18** (A), **20** (B) and **22** (C), **24** (D) and **27** (E)

A given amount of compounds **18**, **20** and **22** was weighted and suspended in a given volume of tested solvent (DMSO, MeOH, PBS and $H_2O$) to reach a theoretical concentration of 1 mM. Suspensions were sonicated for 1 min and shaken at R.T. for 18 h. The resulting solutions were filtrated (pore size 0.2 µm) and diluted to 100 µM in MeCN (for the solutions in organic solvents). HPLC analysis was performed on Nucleodur C18 column, (100 Å, 5 µm, 4.6 x 150 mm, Macherey-Nagel) using MeCN/$H_2O$ 65:35 at 1 mL/min with detection at 302 nm (**18**, **20** and **22**) or MeCN/$H_2O$ 55:45 at 1 mL/min with detection at 254 nm (**24** and **27**).




D
100000
50000
0
Intensity
10.20
MeOH
5.12
6.05
6.88
8.23
12.93
15.75
6.44
12.69
H2O
0.0
5.0
10.0
15.0
20.0
Retention Time [min]

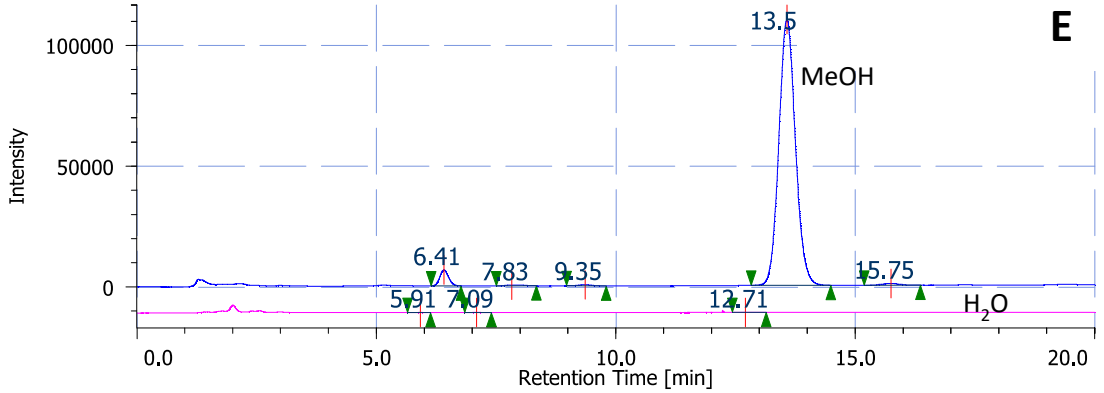

E
100000
50000
0
Intensity
13.5
MeOH
6.41
7.83
9.35
15.75
5.91
7.09
12.71
H2O
0.0
5.0
10.0
15.0
20.0
Retention Time [min]

**Figure S51**. UV-vis spectra of compounds **19**, **20, 22**, **23** and **25** (50 μM) treated by HRP (46 nM) and $H_2O_2$ (200 μM) in 0.2 M TRIS buffer pH 8.1. Conversion to the phenolate form of the quinone methides is assessed by the appearance of the characteristic bands at ca. 570 and 360 nm.

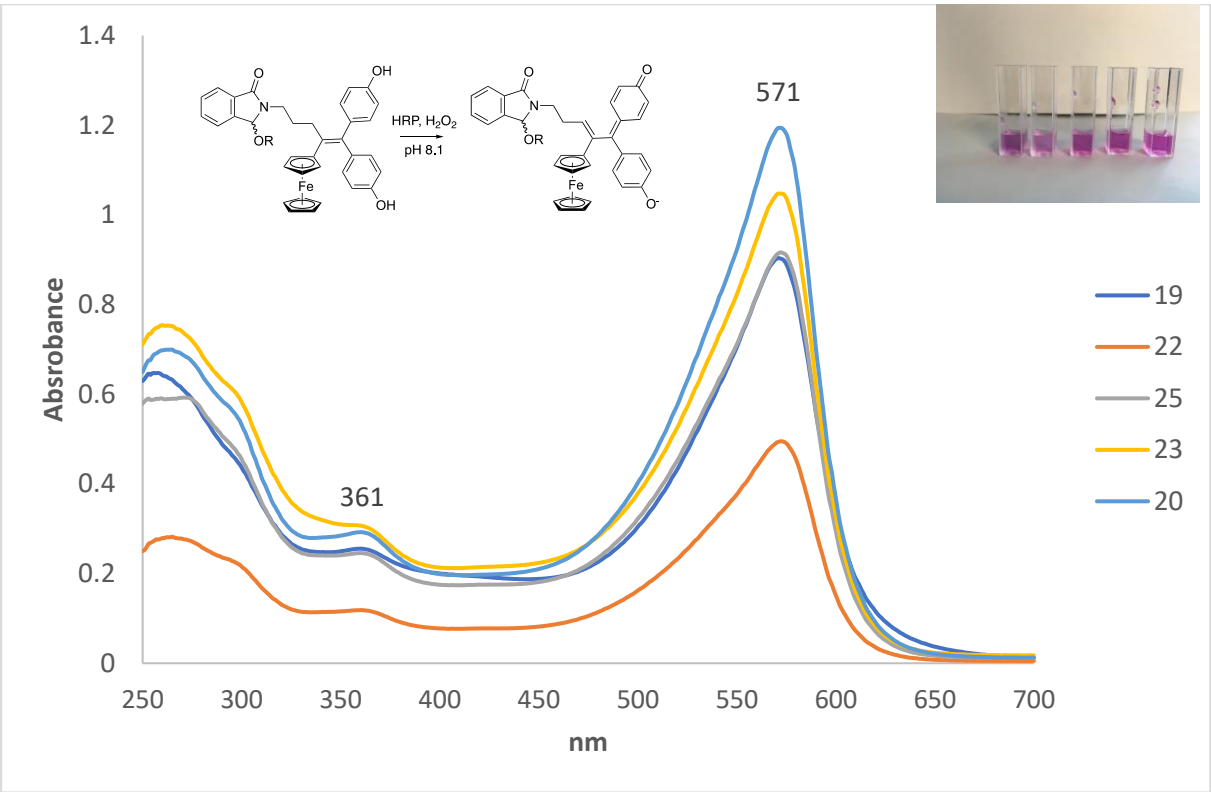
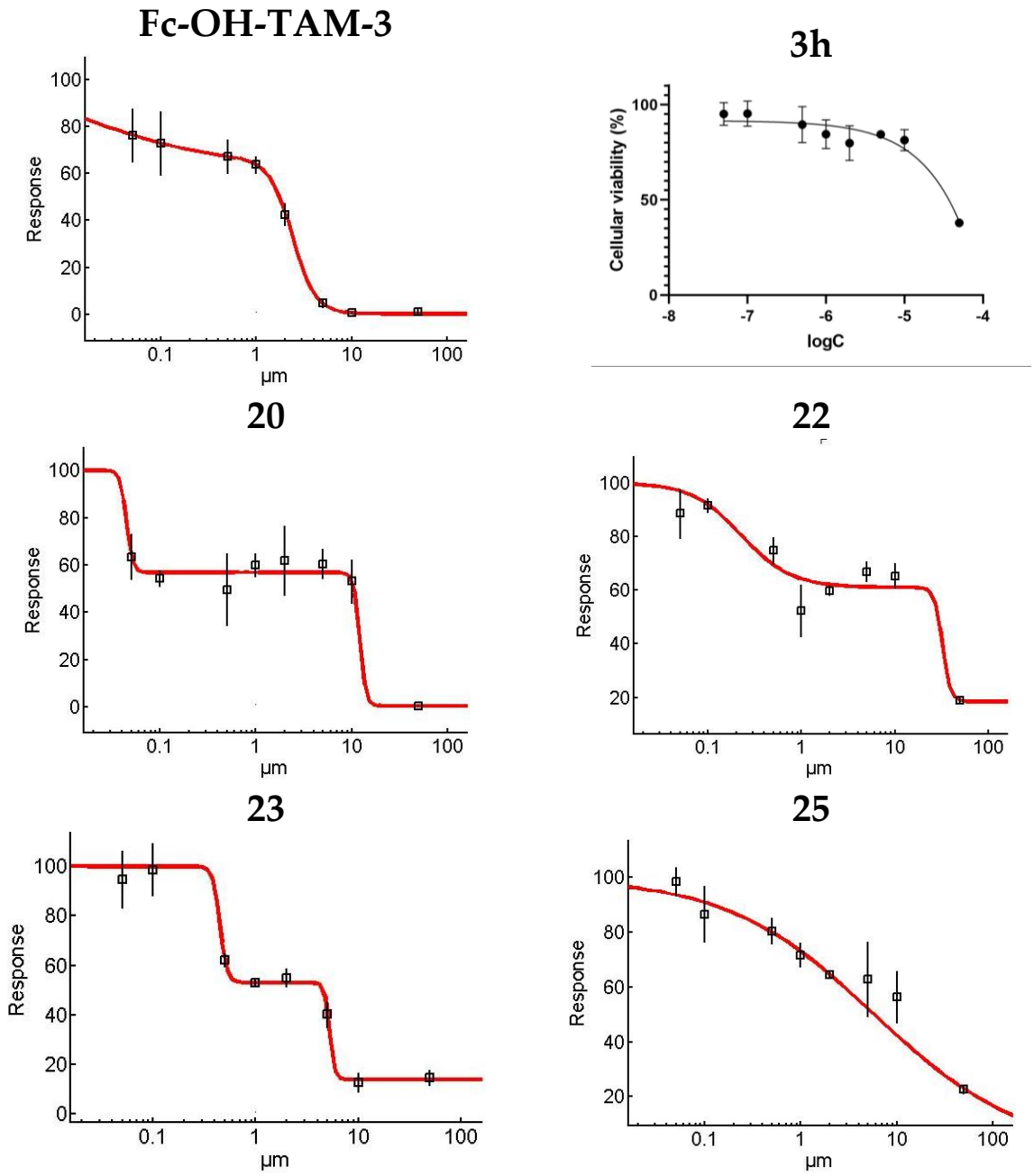
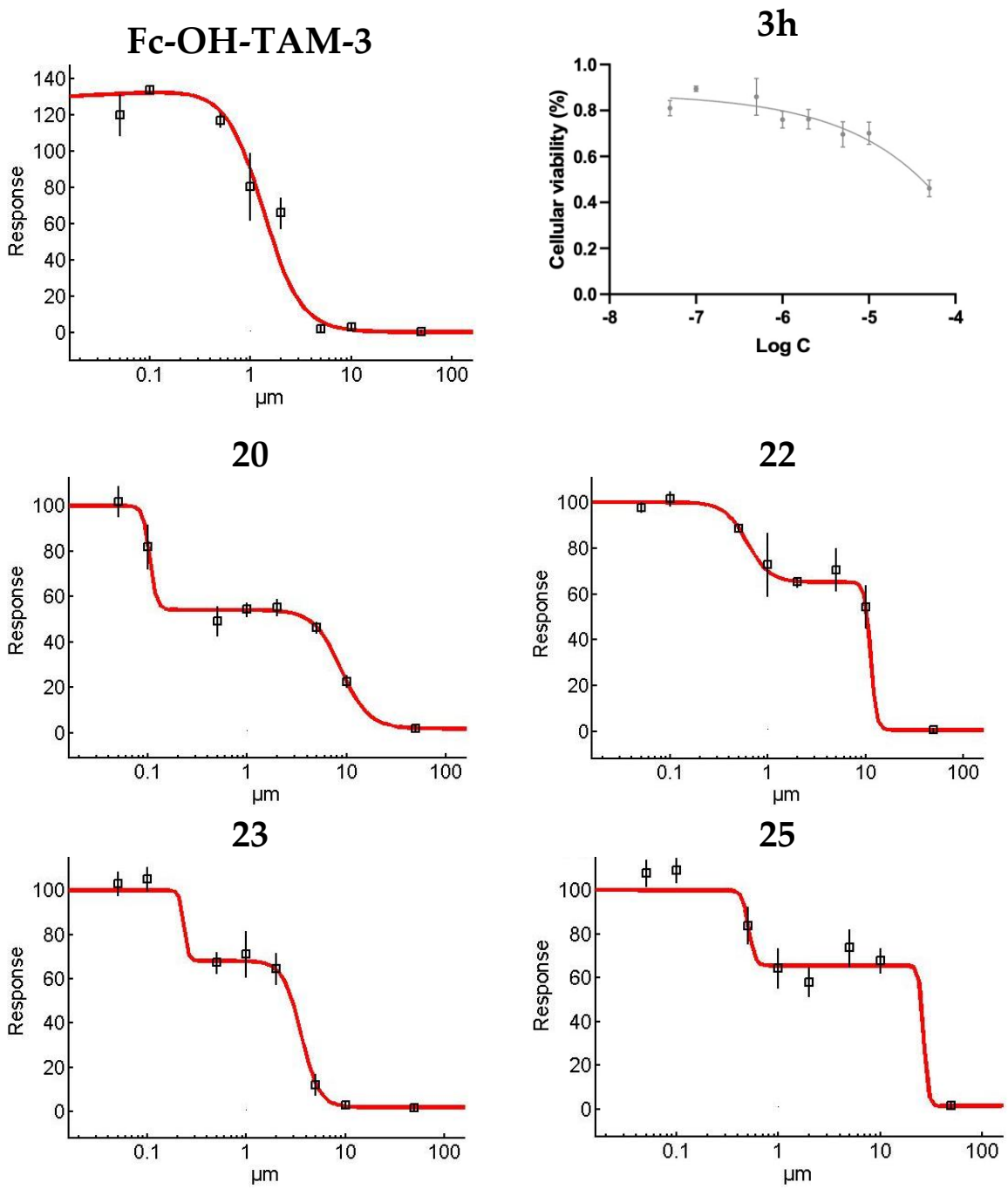


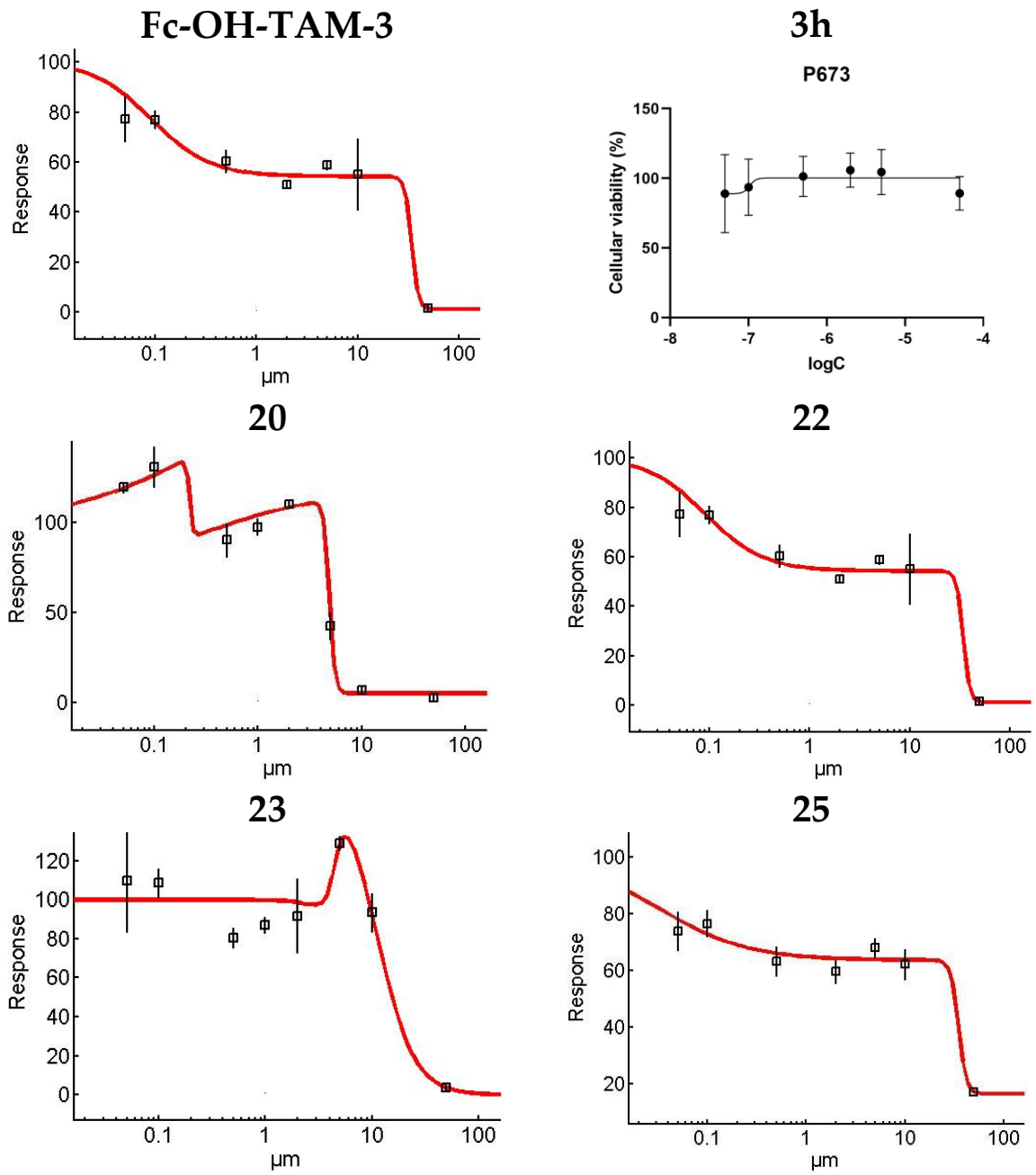
**Figure S52**: MTT cell viability assay for compounds **Fc-OH-TAM-3**, **3h**, **20**, **22**, **23** and **25**.




**A:** Fitting of dose-response curves for compounds **Fc-OH-TAM-3**, **3h**, **20**, **22**, **23**, **25** on MCF-7 cells using Dr-Fit Software (Di Veroli et al. Sci. Rep. 2015, 5, 14701) or GraphPad Prism.

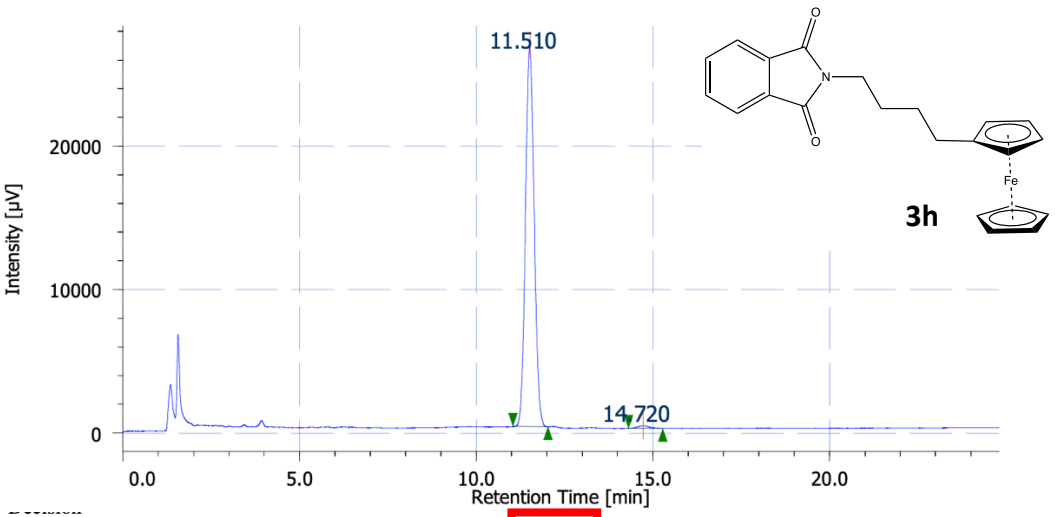



**B:** Fitting of dose-response curves for compounds **Fc-OH-TAM-3**, **3h**, **20**, **22**, **23**, **25** on MDA-MB-231 cells using Dr-Fit Software (Di Veroli et al. Sci. Rep. 2015, 5, 14701) or GraphPad Prism.

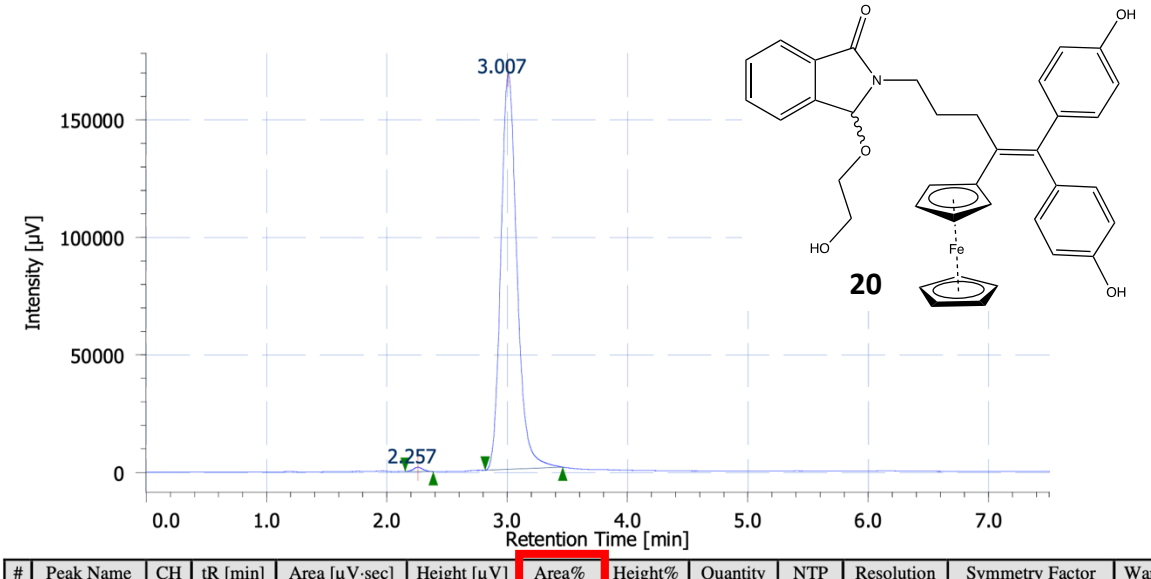



**B:** Fitting of dose-response curves for compounds **Fc-OH-TAM-3**, **3h**, **20**, **22**, **23**, **25** on hTERT-RPE1 cells using Dr-Fit Software (Di Veroli et al. Sci. Rep. 2015, 5, 14701) or GraphPad Prism.

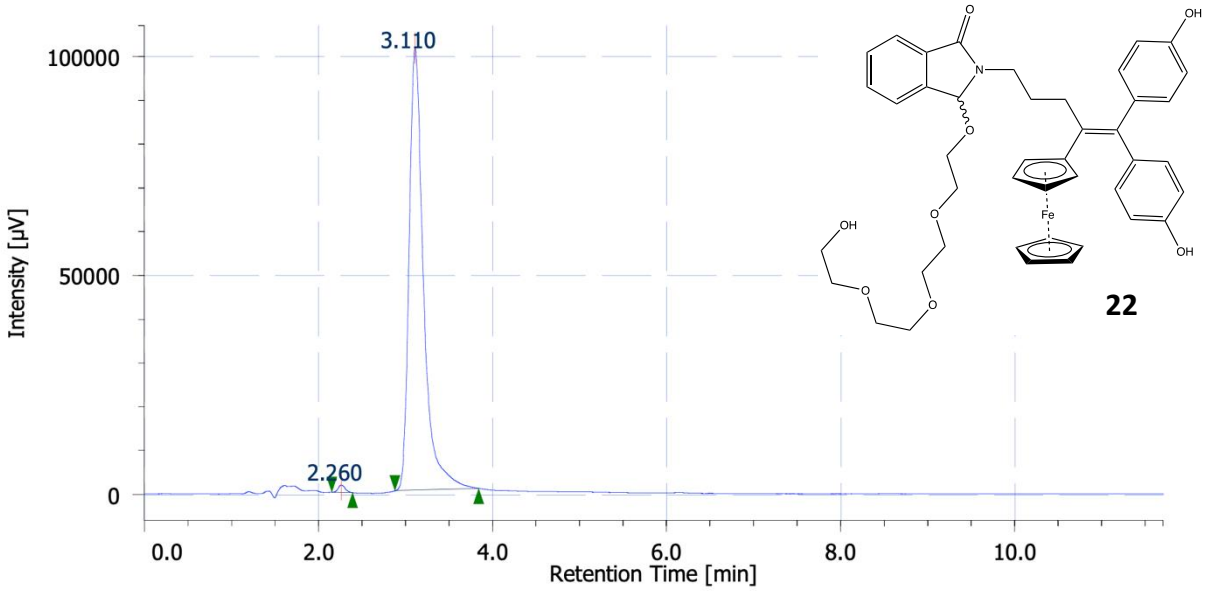
**Figure S53**: HPLC traces for compounds **3h**, **20**, **22**, **23** and **25** (100 µM, acetonitrile, DMSO 1%; method loaded for all with acetonitrile/$H_2O$ = 65/35, except **3h** with acetonitrile/$H_2O$ = 75/25)



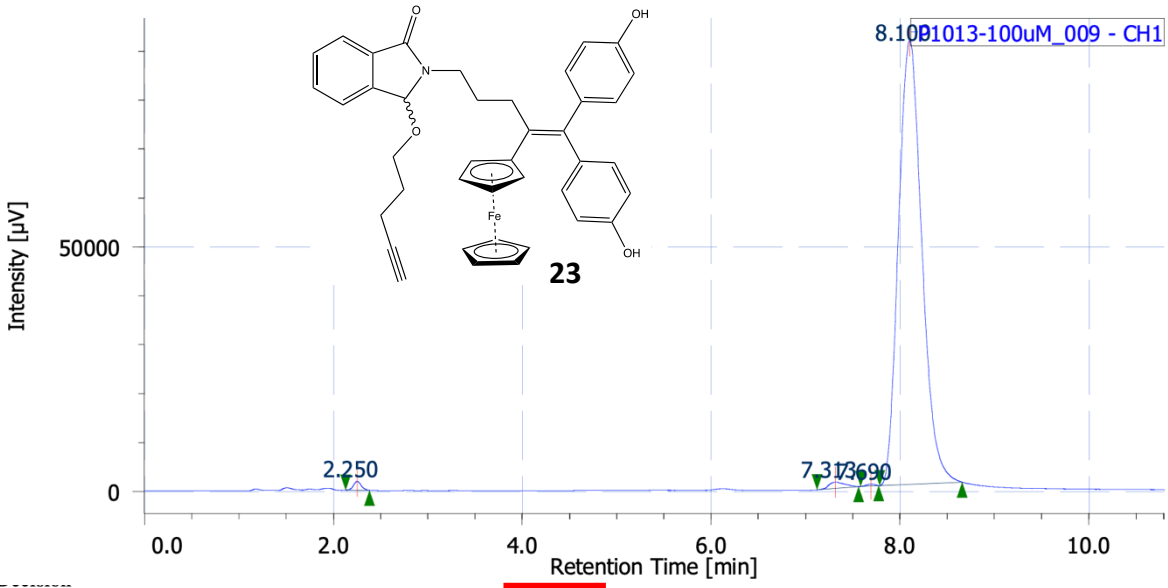

| # | Peak Name | CH | tR [min] | Area [µV·sec] | Height [µV] | Area% | Height% | Quantity | NTP | Resolution | Symmetry Factor | Warning |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | Unknown | 1 | 11.510 | 453536 | 26579 | 99.109 | 99.339 | N/A | 10397 | 6.062 | 1.063 | |
| 2 | Unknown | 1 | 14.720 | 4076 | 177 | 0.891 | 0.661 | N/A | 9308 | N/A | 1.158 | |



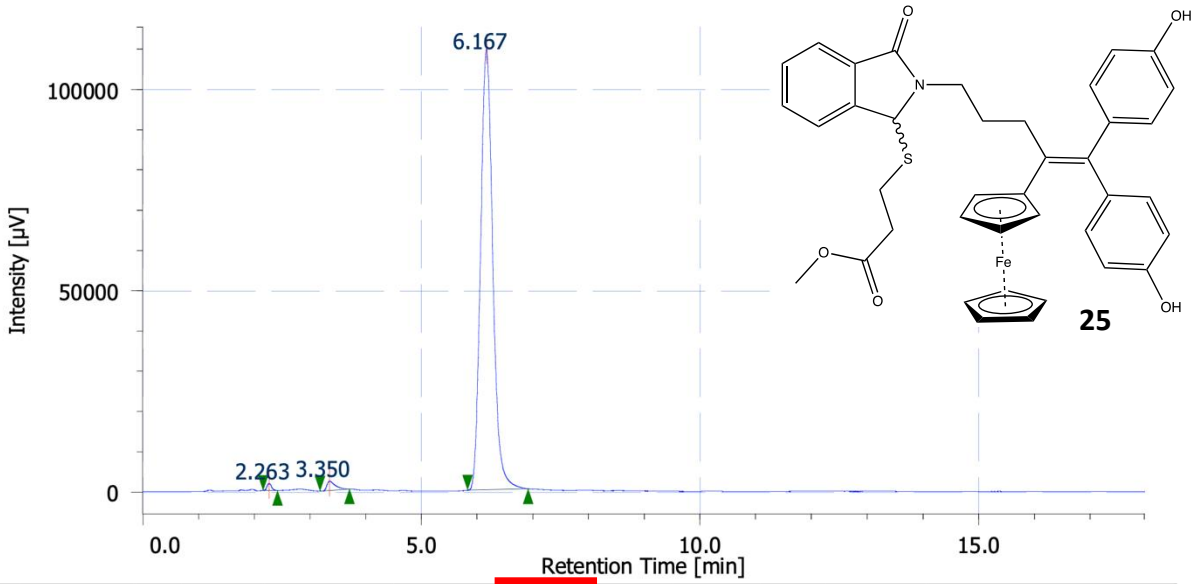

| # | Peak Name | CH | tR [min] | Area [µV·sec] | Height [µV] | Area% | Height% | Quantity | NTP | Resolution | Symmetry Factor | Warning |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | Unknown | 1 | 2.257 | 9980 | 1797 | 0.633 | 1.056 | N/A | 3683 | 3.896 | 1.148 | |
| 2 | Unknown | 1 | 3.007 | 1565580 | 168465 | 99.367 | 98.944 | N/A | 2570 | N/A | 1.215 | |




| # | Peak Name | CH | tR [min] | Area [μV·sec] | Height [μV] | Area% | Height% | Quantity | NTP | Resolution | Symmetry Factor | Warning |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | Unknown | 1 | 2.260 | 9469 | 1713 | 0.810 | 1.668 | N/A | 3750 | 4.004 | 1.192 | |
| 2 | Unknown | 1 | 3.110 | 1159459 | 100965 | 99.190 | 98.332 | N/A | 2002 | N/A | 1.539 | |




| # | Peak Name | CH | tR [min] | Area [μV·sec] | Height [μV] | Area% | Height% | Quantity | NTP | Resolution | Symmetry Factor | Warning |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | Unknown | 1 | 2.250 | 10286 | 1824 | 0.648 | 1.937 | N/A | 3652 | 21.801 | 1.126 | |
| 2 | Unknown | 1 | 7.313 | 15061 | 1291 | 0.948 | 1.370 | N/A | 8525 | 1.527 | 1.298 | |
| 3 | Unknown | 1 | 7.690 | 2309 | 373 | 0.145 | 0.396 | N/A | 29899 | 1.299 | 0.922 | |
| 4 | Unknown | 1 | 8.100 | 1560587 | 90692 | 98.259 | 96.297 | N/A | 5075 | N/A | 1.192 | |




25

| # | Peak Name | CH | tR [min] | Area [µV·sec] | Height [µV] | Area% | Height% | Quantity | NTP | Resolution | Symmetry Factor | Warning |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | Unknown | 1 | 2.263 | 10131 | 180 | 0.594 | 1.588 | N/A | 3633 | 5.208 | 1.143 | |
| 2 | Unknown | 1 | 3.350 | 24972 | 232 | 1.465 | 2.046 | N/A | 2496 | 8.525 | 2.107 | |
| 3 | Unknown | 1 | 6.167 | 1669127 | 10942 | 97.940 | 96.366 | N/A | 3912 | N/A | 1.148 | |