Supporting information

Synthesis of novel ferrocene-benzofuran hybrids via palladium and copper catalyzed reactions

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NMR spectra of products

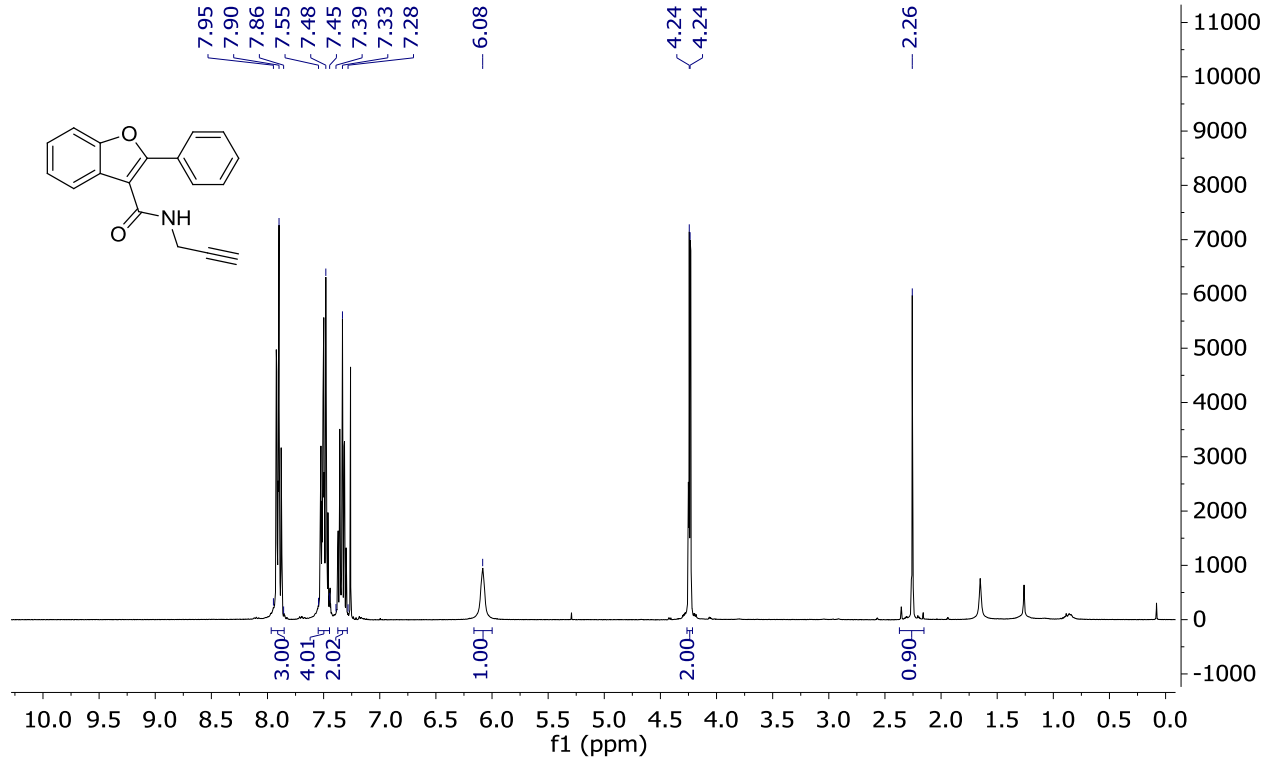

Figure S1. ^{1}H-NMR spectrum of compound **2** (400.13 MHz, $CDCl_3$)

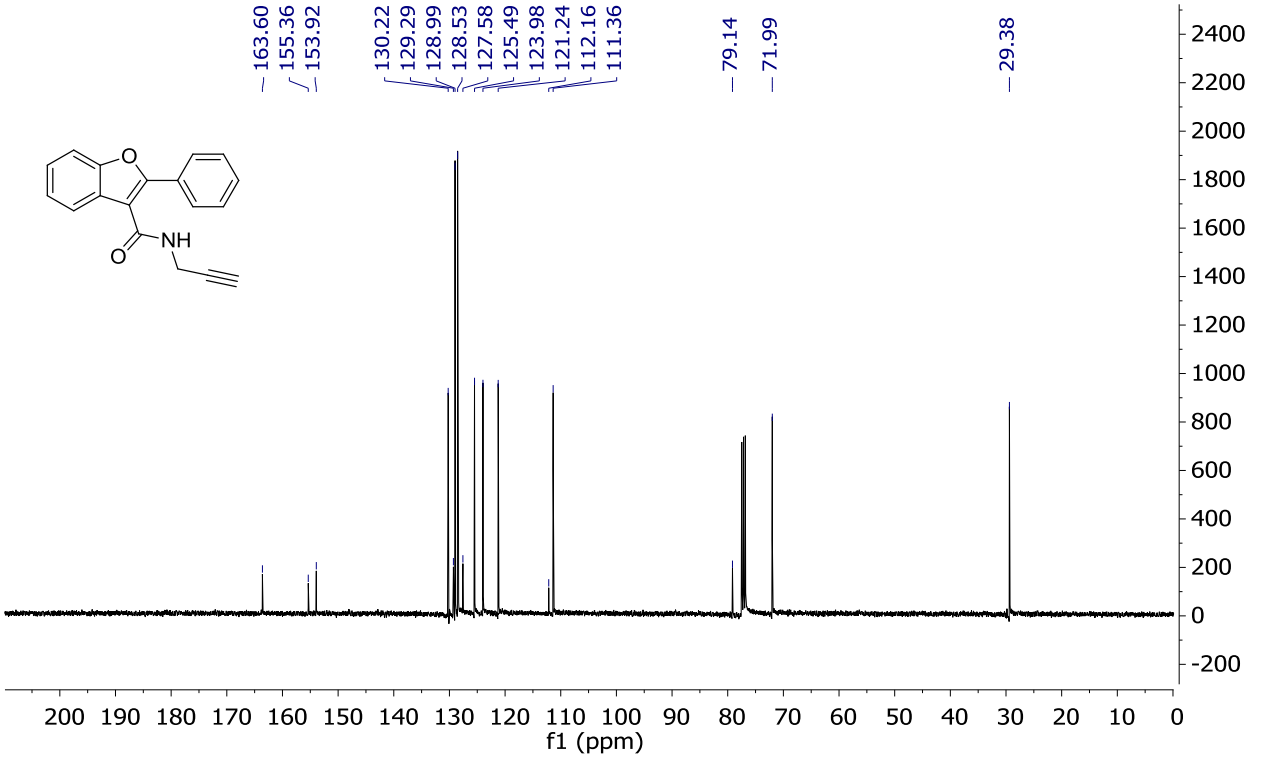

Figure S2. $^{13}C\{^{1}H\}$-NMR spectrum of compound **2** (100.62 MHz, $CDCl_3$)

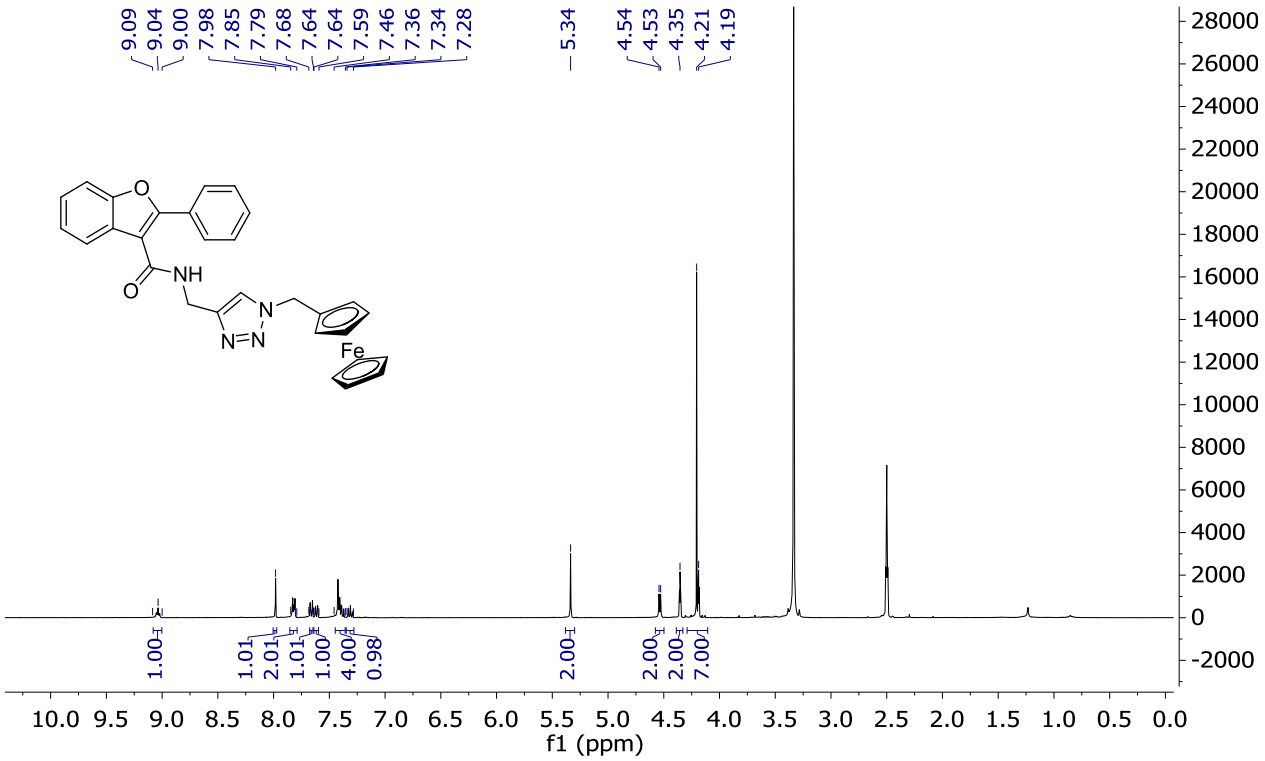

Figure S3. ^{1}H-NMR spectrum of compound **3** (400.13 MHz, DMSO-d_6)

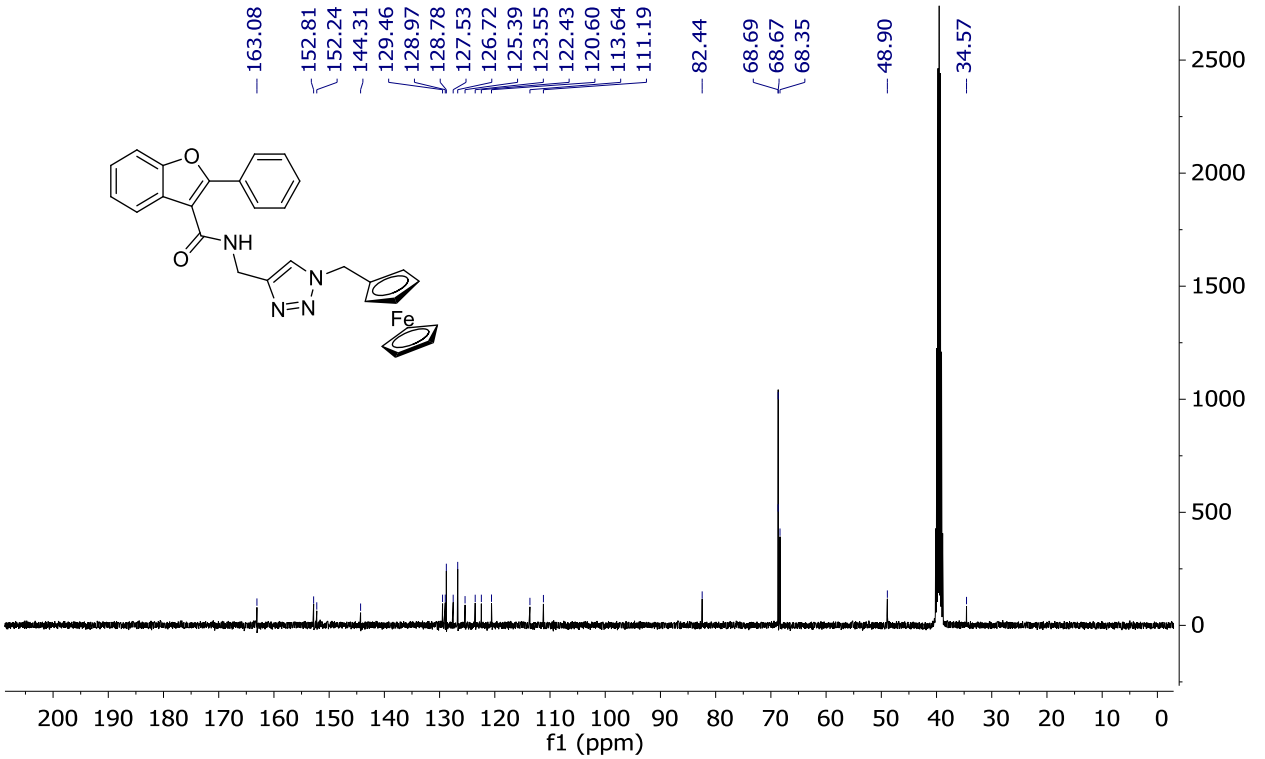

Figure S4. ^{13}C{^{1}H}-NMR spectrum of compound **3** (100.62 MHz, DMSO-d_6)

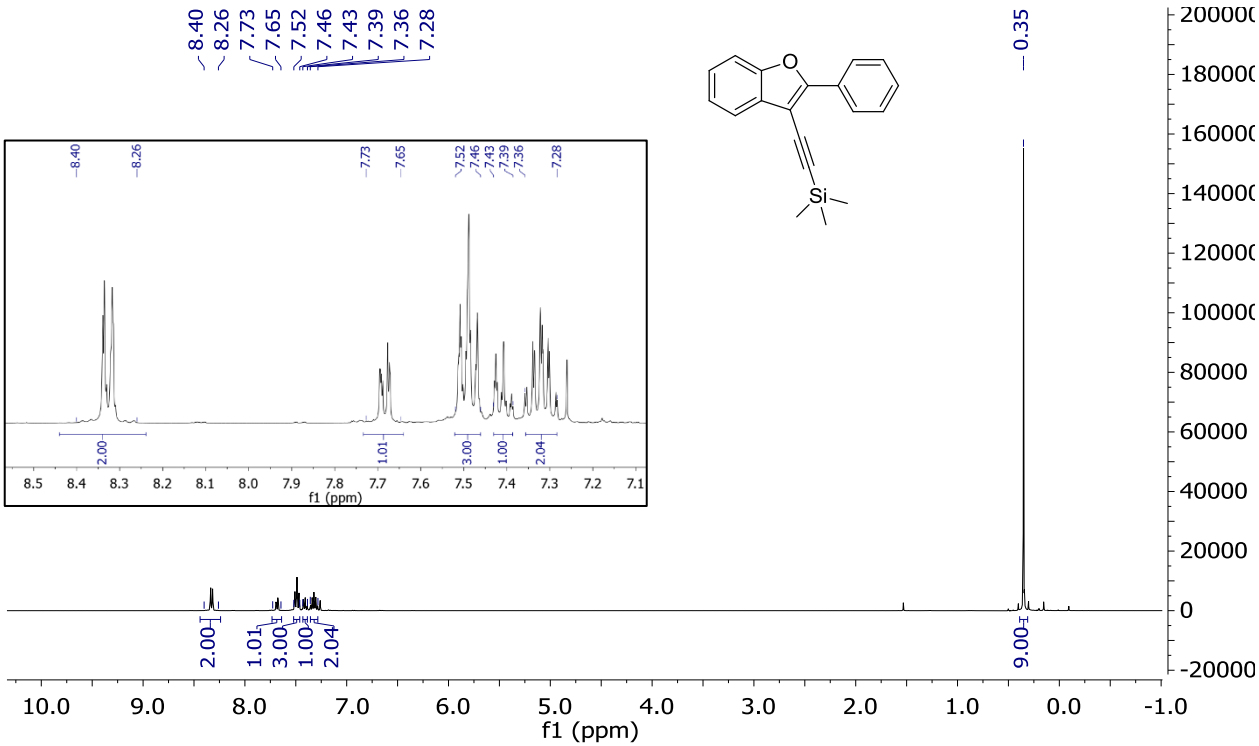

Figure S5. ^{1}H-NMR spectrum of compound **4** (400.13 MHz, $CDCl_3$)

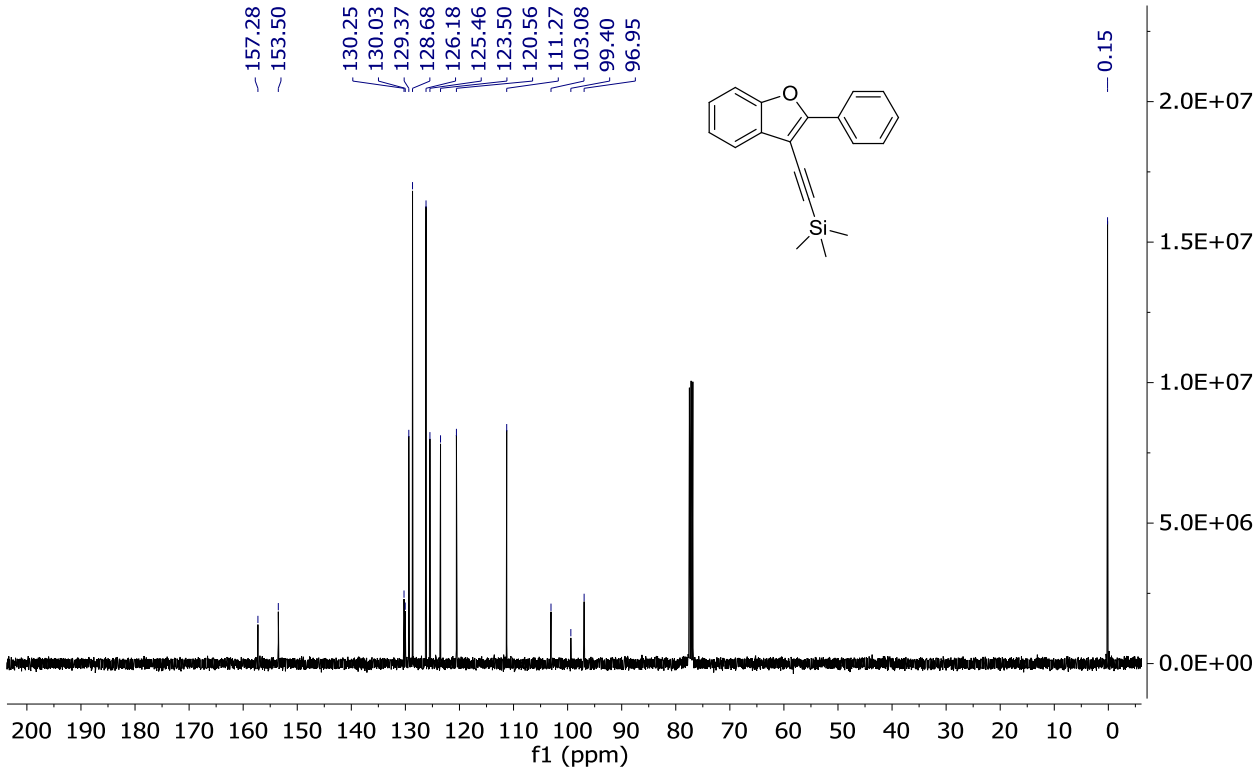

Figure S6. $^{13}C\{^{1}H\}$-NMR spectrum of compound **4** (100.62 MHz, $CDCl_3$)

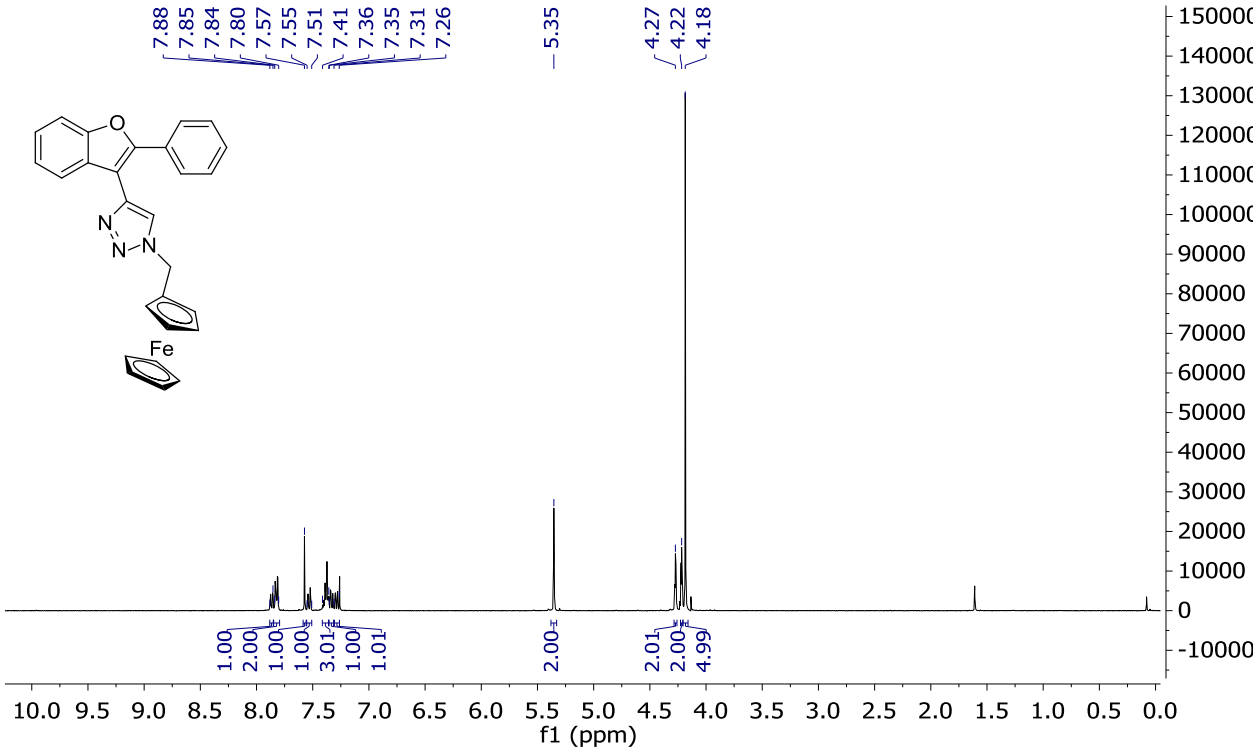

Figure S7. ^{1}H-NMR spectrum of compound **6a** (400.13 MHz, $CDCl_3$)

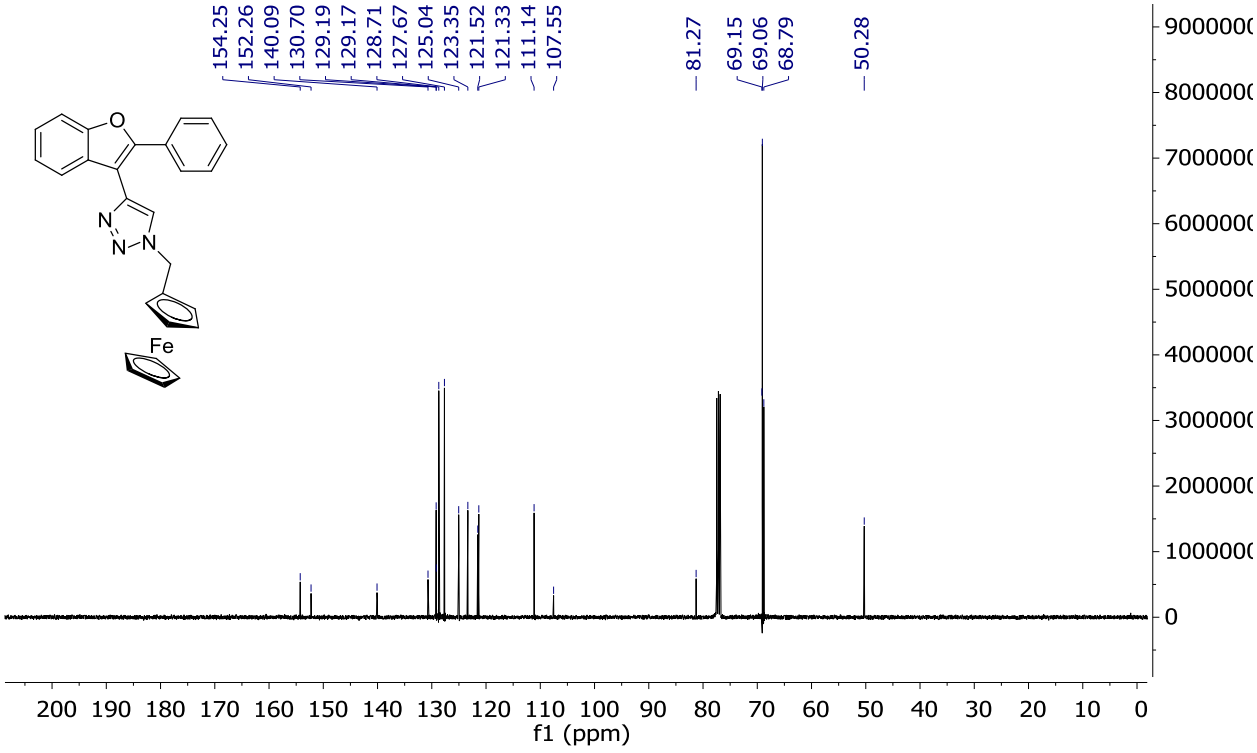

Figure S8. ^{13}C{^{1}H}-NMR spectrum of compound **6a** (100.62 MHz, $CDCl_3$)

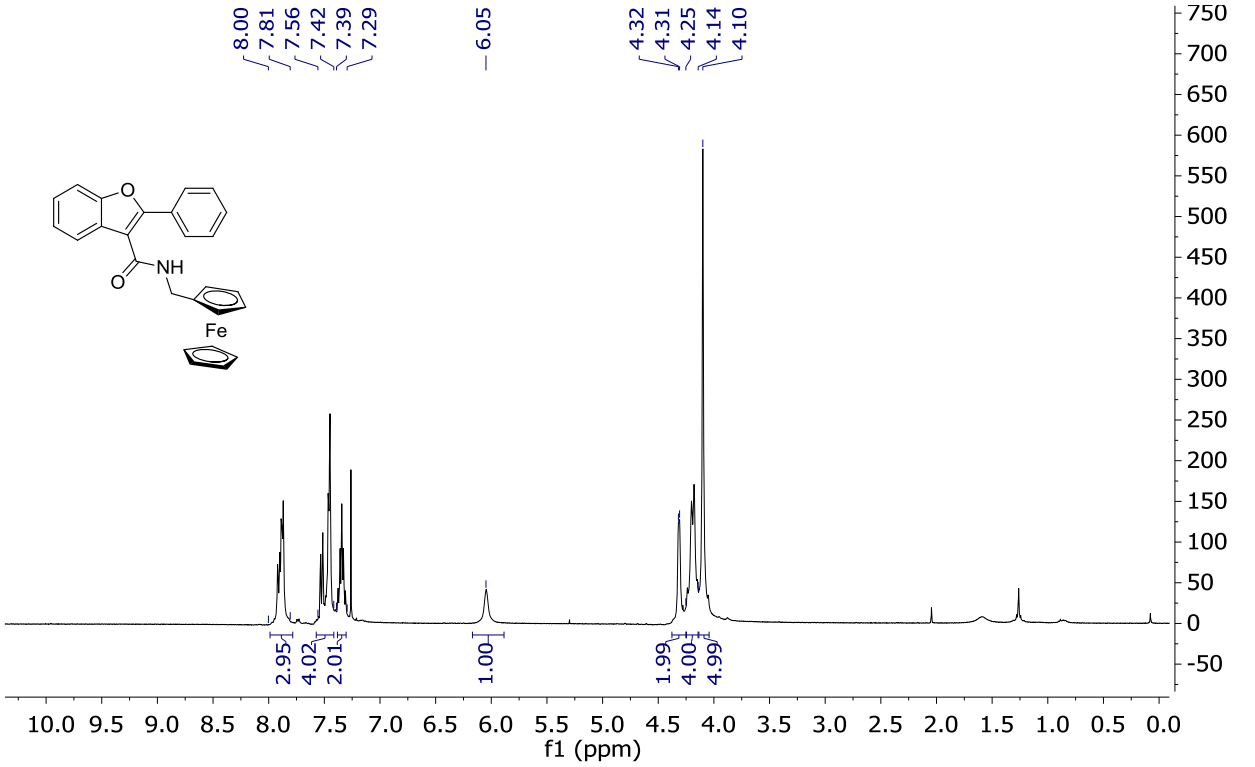

Figure S9. ^{1}H-NMR spectrum of compound **7** (400.13 MHz, $CDCl_3$)

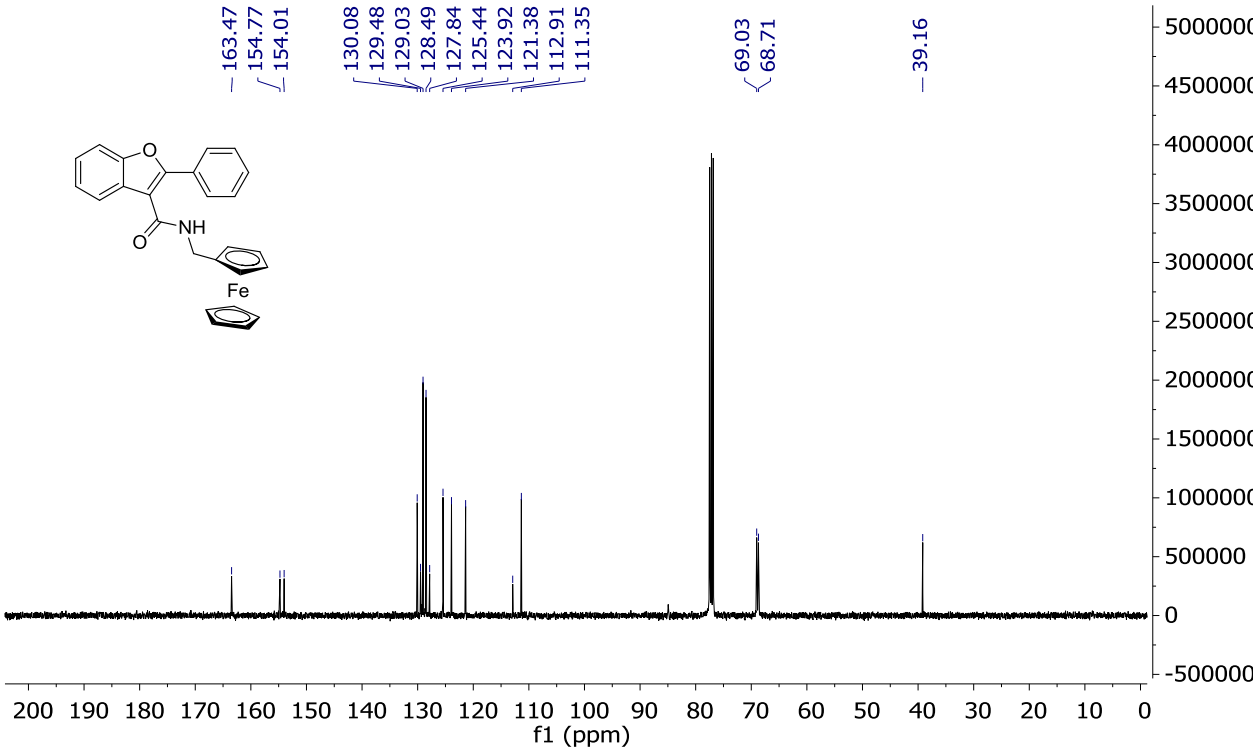

Figure S10. ^{13}C{^{1}H}-NMR spectrum of compound **7** (100.62 MHz, $CDCl_3$)

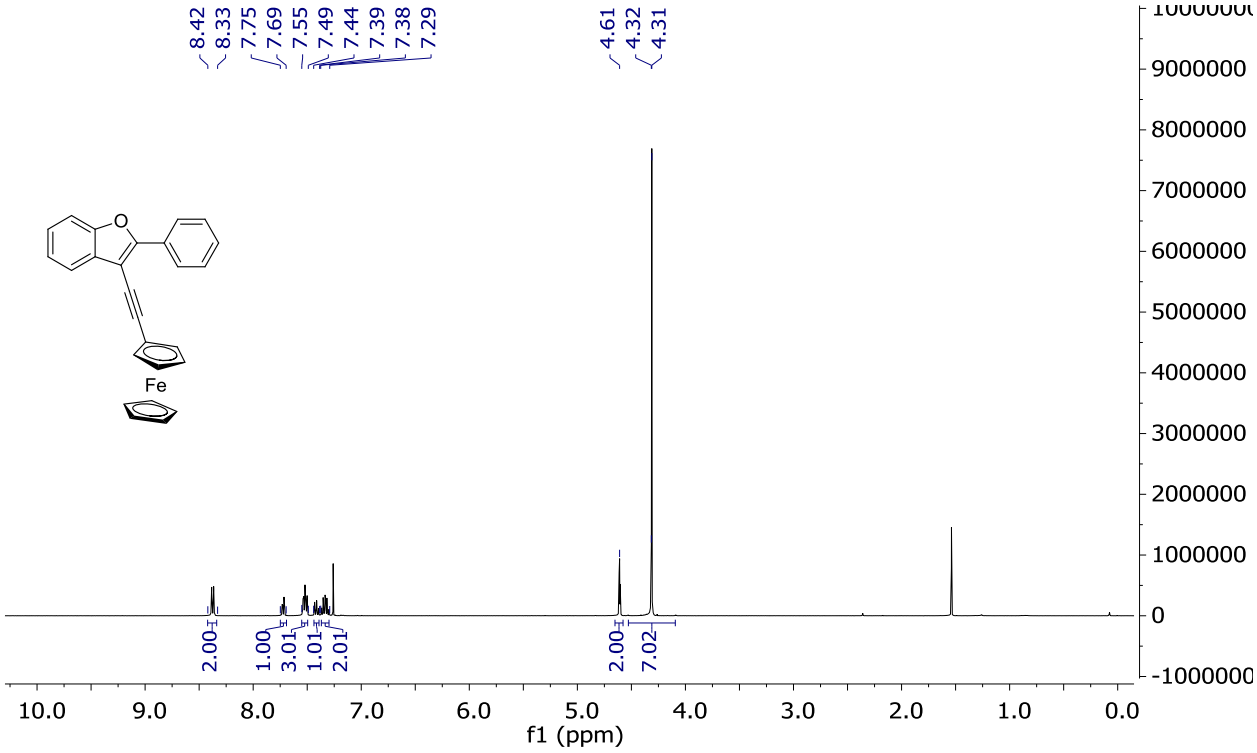

Figure S11. ^{1}H-NMR spectrum of compound **9** (400.13 MHz, $CDCl_3$)

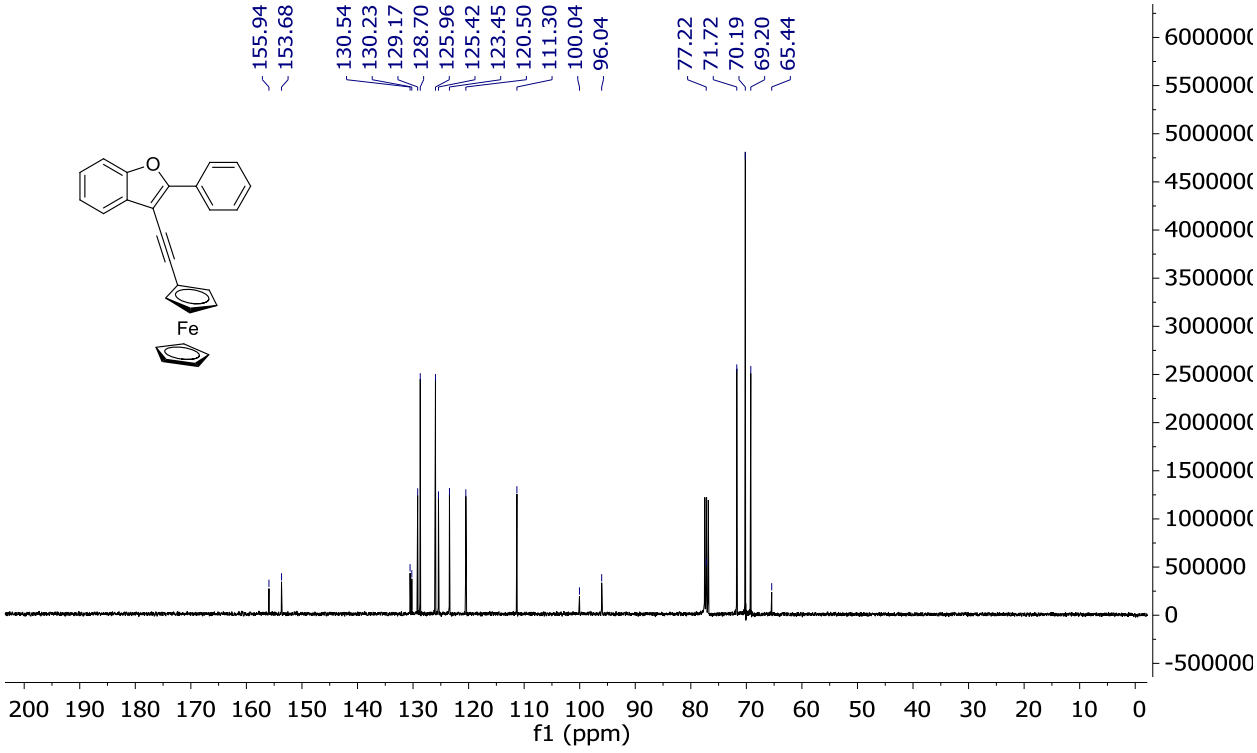

Figure S12. $^{13}C\{^{1}H\}$-NMR spectrum of compound **9** (100.62 MHz, $CDCl_3$)

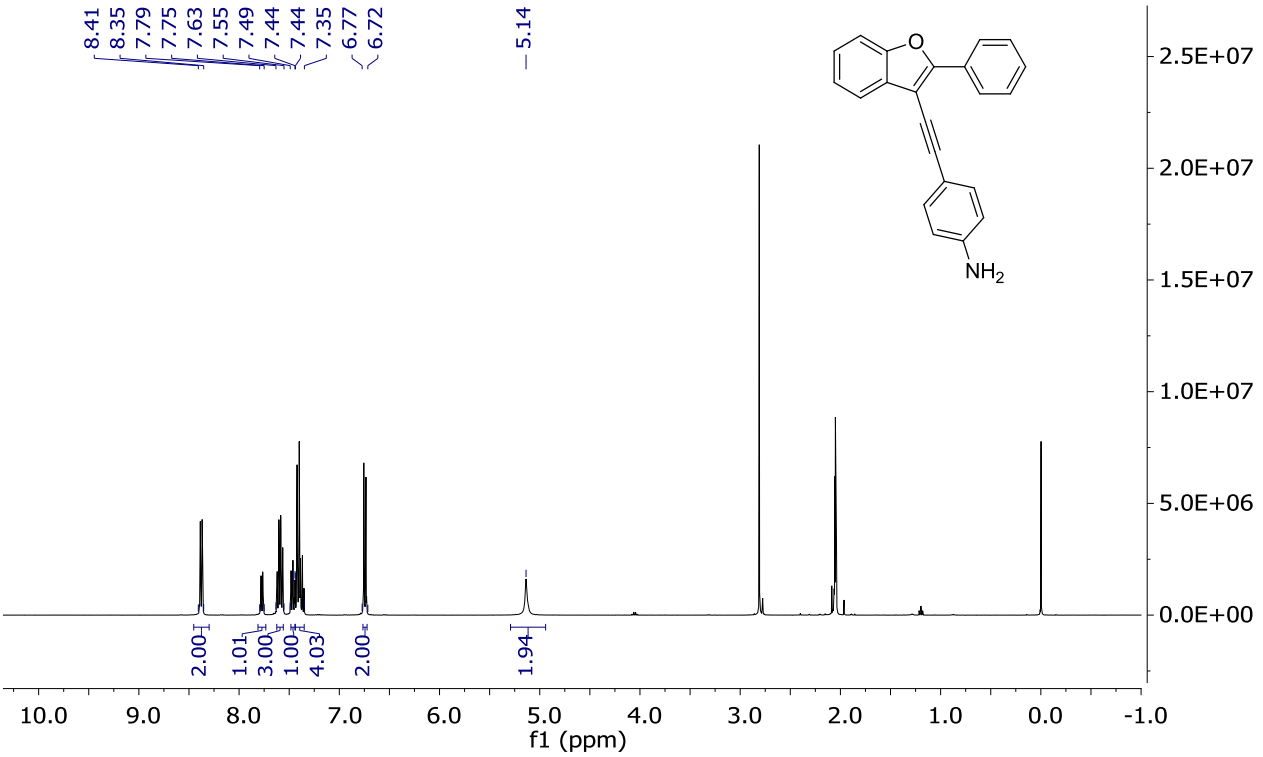

Figure S13. ^{1}H-NMR spectrum of compound **10** (400.13 MHz , Acetone-d_6)

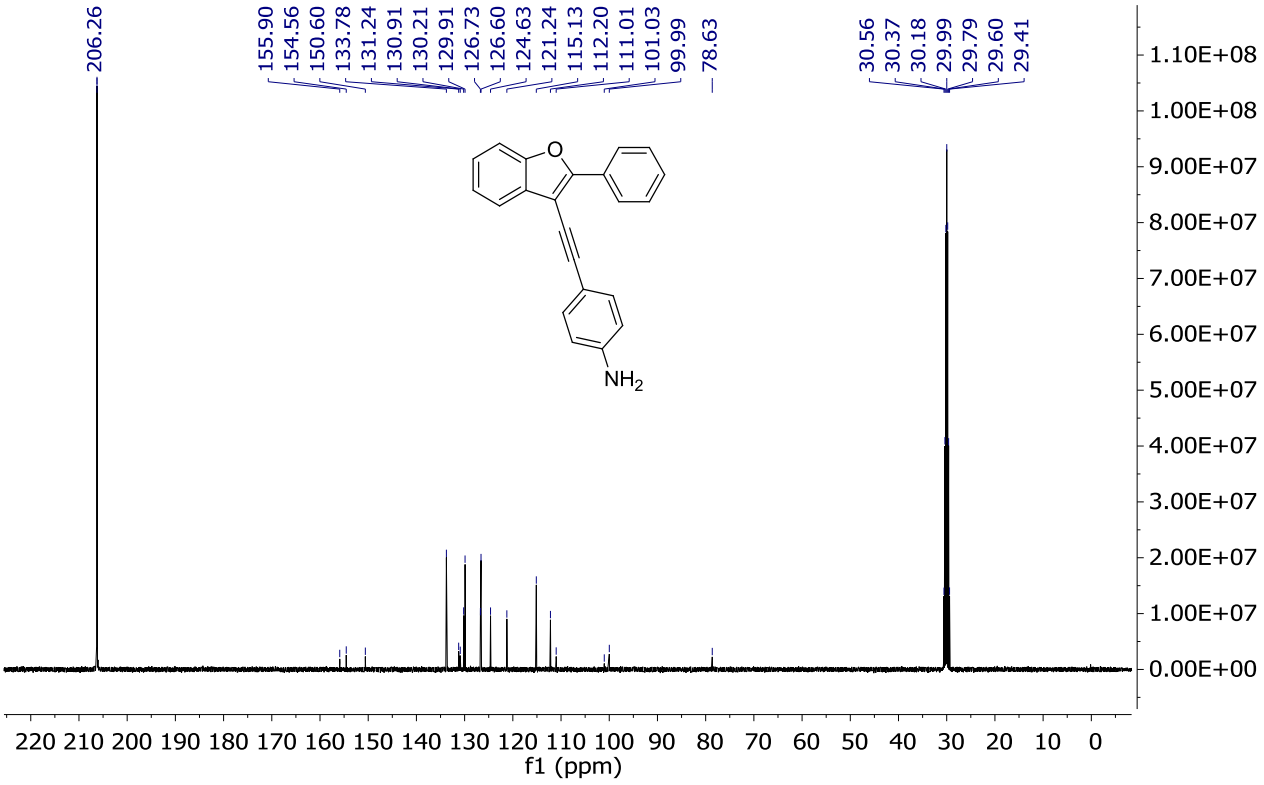

Figure S14. ^{13}C{^{1}H}-NMR spectrum of compound **10** (100.62 MHz, Acetone-d_6)

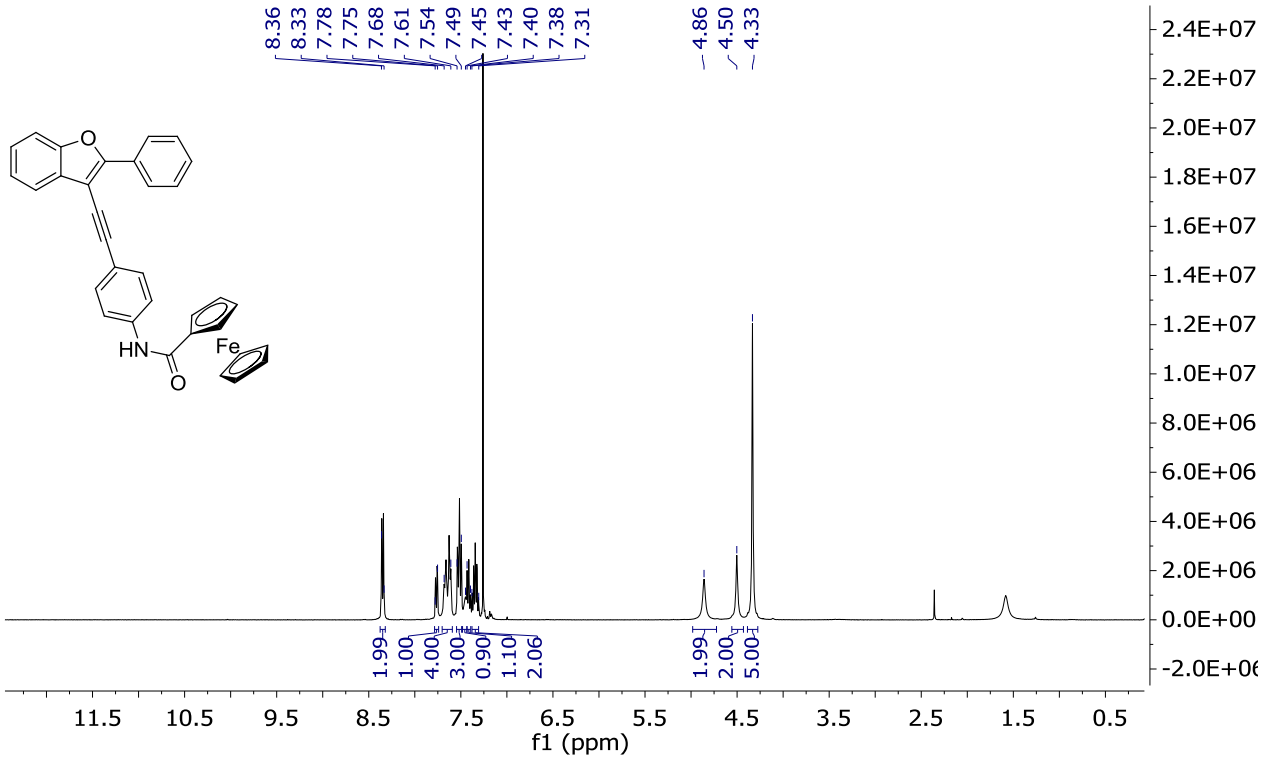

Figure S15. ^{1}H-NMR spectrum of compound **11** (400.13 MHz, $CDCl_3$)

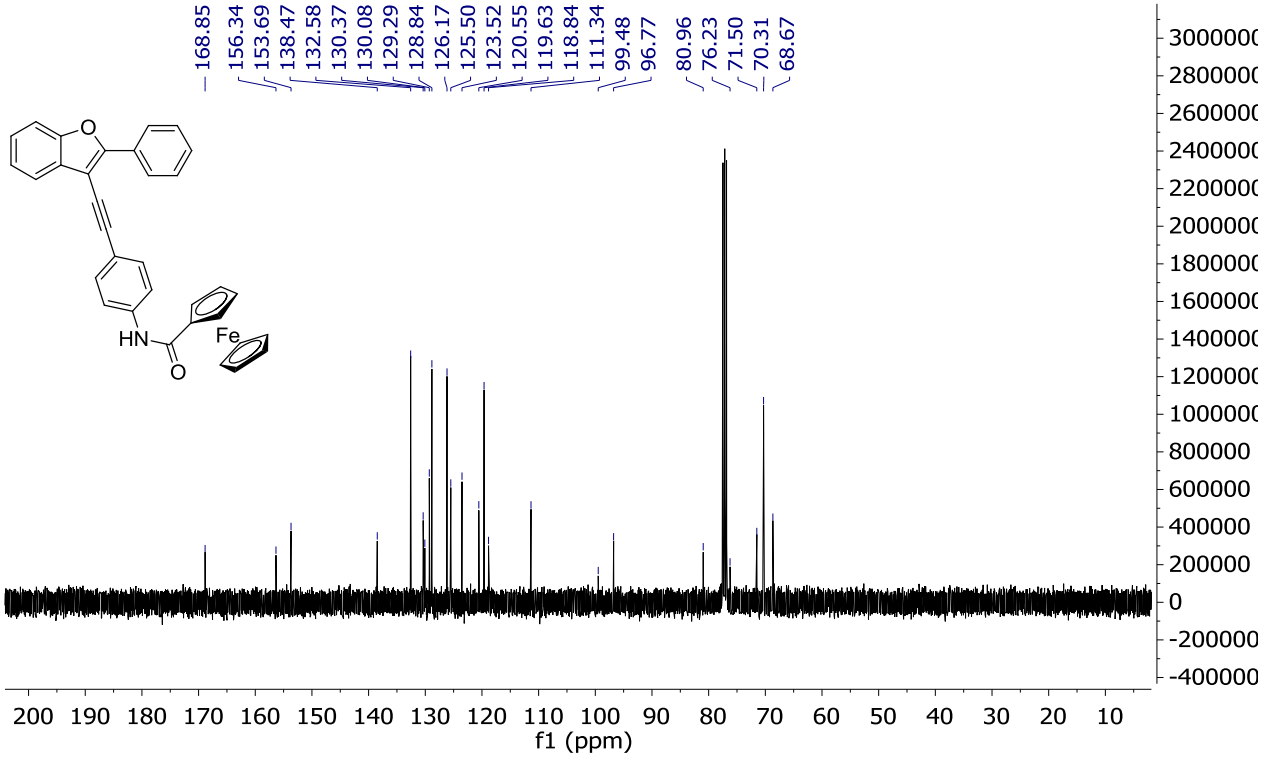

Figure S16. ^{13}C{^{1}H}-NMR spectrum of compound **11** (100.62 MHz, $CDCl_3$)

SWV measurements of ferrocene-benzofuran hybrids

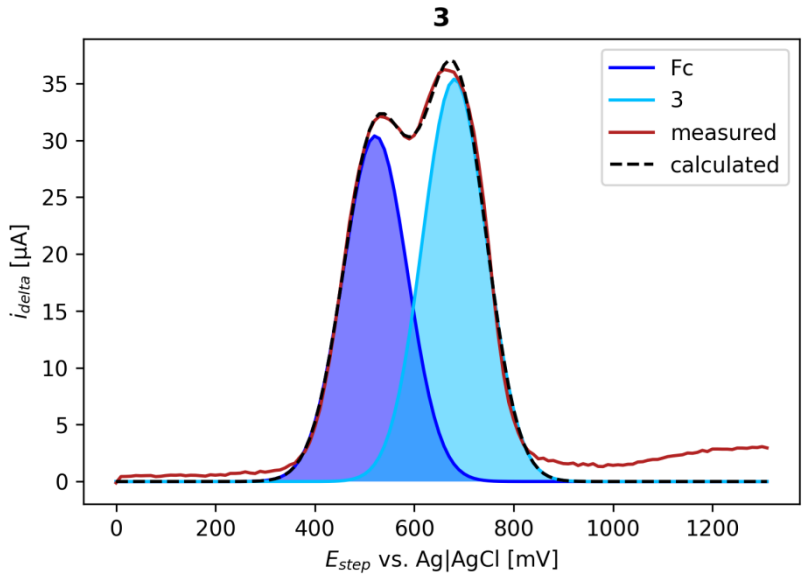

Figure S17. Measured and calculated SWV curves of ferrocene-benzofuran hybrid **3** (setup: 2.5×10^{-3} M in CH_2Cl_2, supporting electrolyte: 0.1 M *n*-Bu_4NPF_6, in the presence of ferrocene (Fc) (1.25×10^{-3} M), working electrode: glassy carbon, reference electrode: Ag/AgCl (H_2O), auxiliary electrode: Pt wire) and calculated curves for individual components.

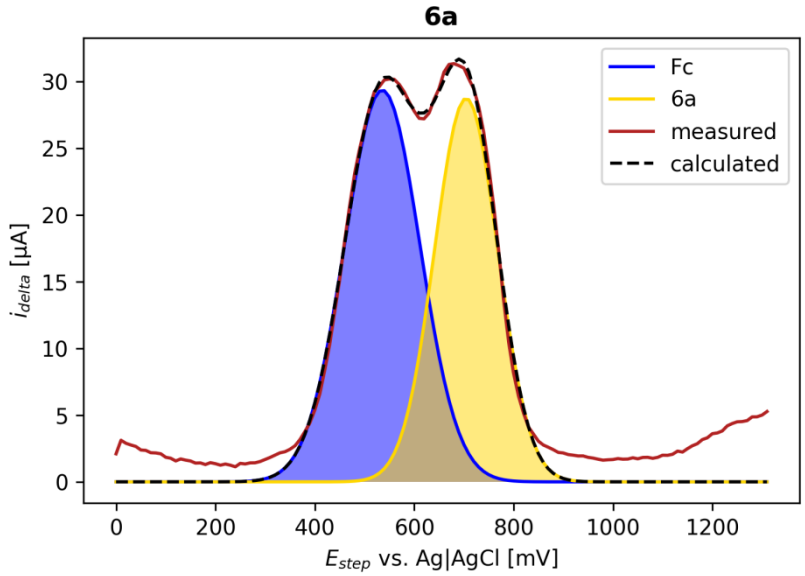

Figure S18. Measured and calculated SWV curves of ferrocene-benzofuran hybrid **6a** (setup: 2.5×10^{-3} M in CH_2Cl_2, supporting electrolyte: 0.1 M *n*-Bu_4NPF_6, in the presence of ferrocene (Fc) (1.25×10^{-3} M), working electrode: glassy carbon, reference electrode: Ag/AgCl (H_2O), auxiliary electrode: Pt wire) and calculated curves for individual components.

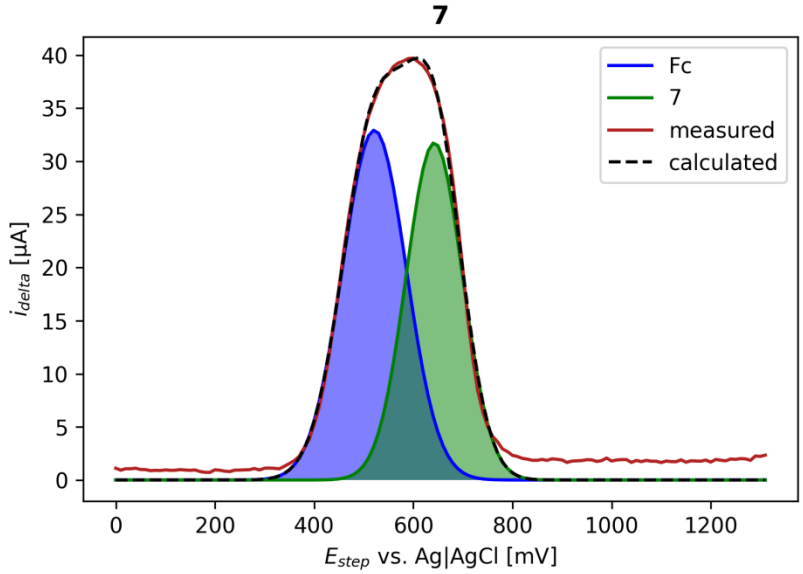

Figure S19. Measured and calculated SWV curves of ferrocene-benzofuran hybrid **7** (setup: 2.5×10^{-3} M in CH_2Cl_2, supporting electrolyte: 0.1 M *n*-Bu_4NPF_6, in the presence of ferrocene (Fc) (1.25×10^{-3} M), working electrode: glassy carbon, reference electrode: Ag/AgCl (H_2O), auxiliary electrode: Pt wire) and calculated curves for individual components.

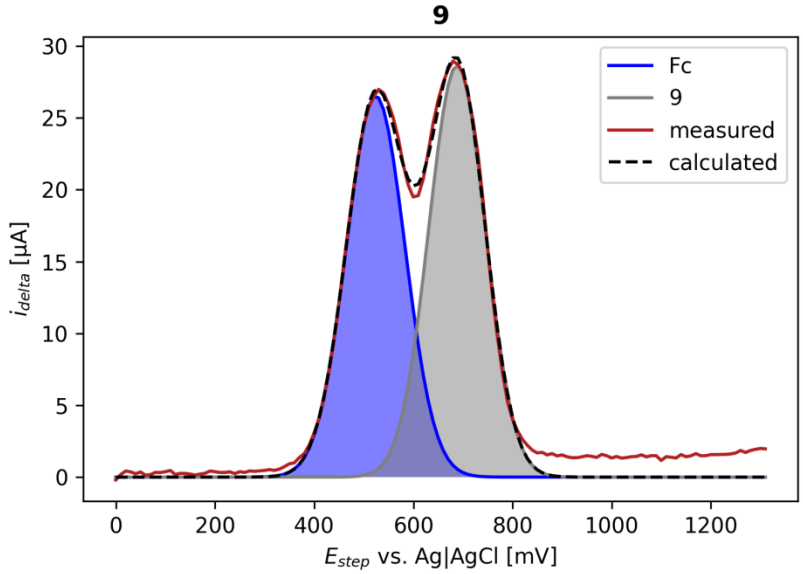

Figure S20. Measured and calculated SWV curves of ferrocene-benzofuran hybrid **9** (setup: 2.5×10^{-3} M in CH_2Cl_2, supporting electrolyte: 0.1 M *n*-Bu_4NPF_6, in the presence of ferrocene (Fc) (1.25×10^{-3} M), working electrode: glassy carbon, reference electrode: Ag/AgCl (H_2O), auxiliary electrode: Pt wire) and calculated curves for individual components.

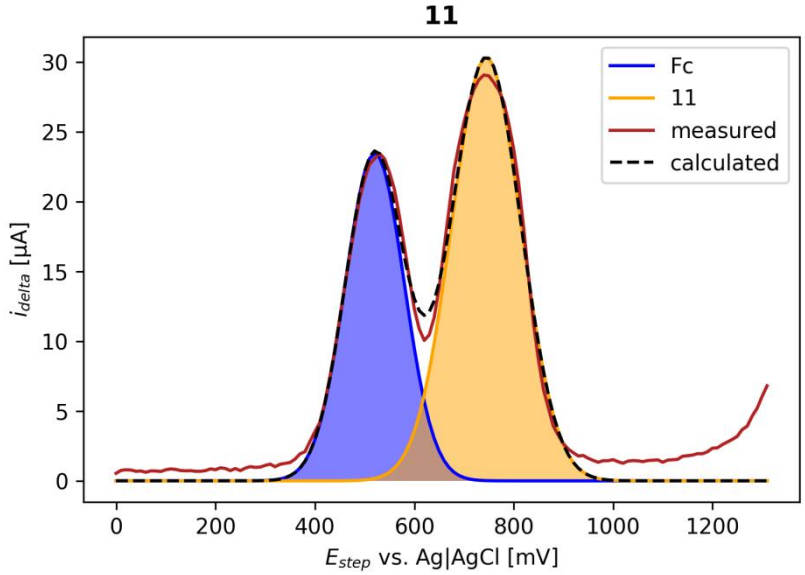

Figure S21. Measured and calculated SWV curves of ferrocene-benzofuran hybrid **11** (setup: 2.5×10^{-3} M in CH_2Cl_2, supporting electrolyte: 0.1 M *n*-Bu_4NPF_6, in the presence of ferrocene (Fc) (1.25×10^{-3} M), working electrode: glassy carbon, reference electrode: Ag/AgCl (H_2O), auxiliary electrode: Pt wire) and calculated curves for individual components.

Cytotoxicity measurements

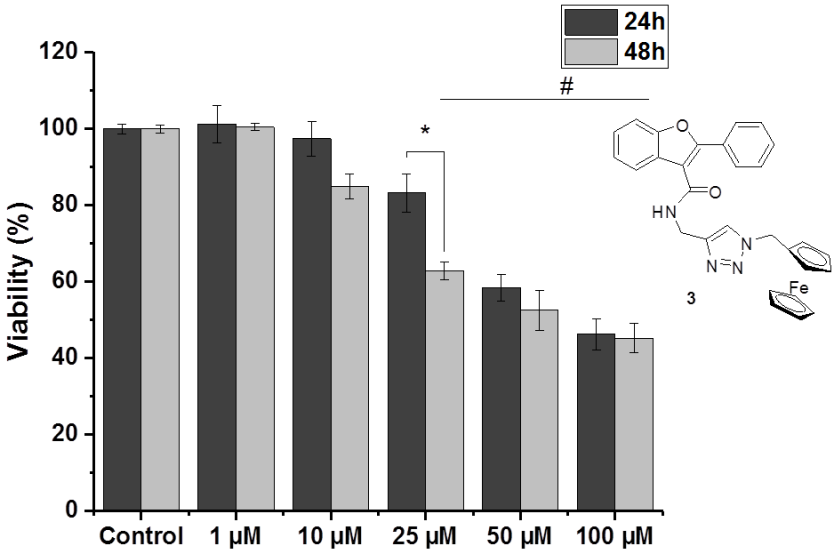

Figure S22. The effects of compound **3** on the viability of MCF7 cells, evaluated by MTT assay. Cells were treated with 1 µM, 10 µM, 25 µM, 50 µM and 100 µM for 24 h or 48h. Data are shown as mean ± SEM of at least three separate experiments. * $p < 0.05$ compared with the untreated cells. # : $p < 0.05$ compared with the cells treated with the 10 µM solution

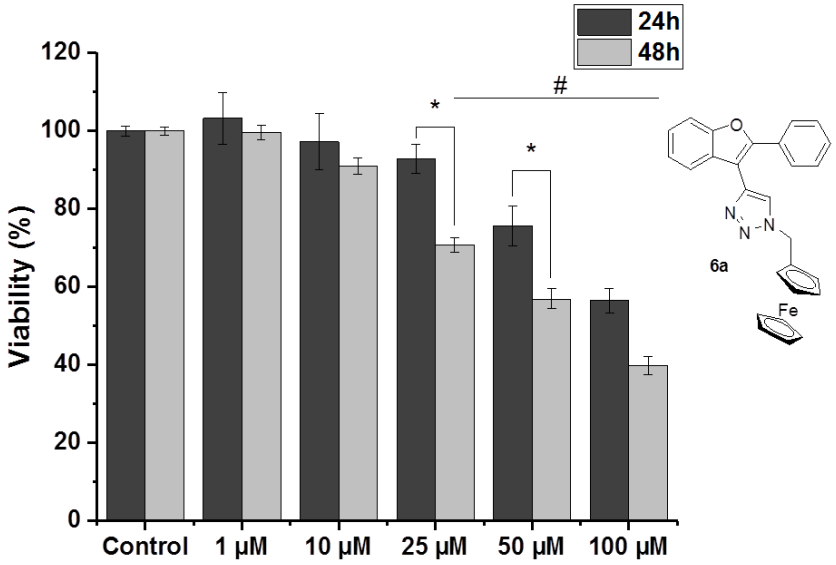

Figure S23. The effects of compound **6a** on the viability of MCF7 cells, evaluated by MTT assay. Cells were treated with 1 µM, 10 µM, 25 µM, 50 µM and 100 µM for 24 h or 48h. Data are shown as mean ± SEM of at least three separate experiments. * $p < 0.05$ compared with the untreated cells. # : $p < 0.05$ compared with the cells treated with the 10 µM solution

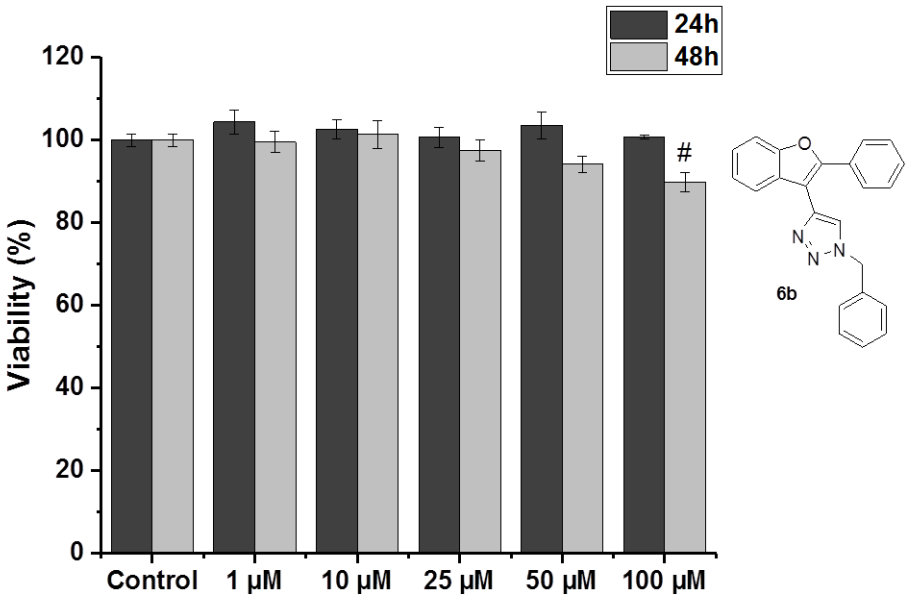

Figure S24. The effects of compound **6b** on the viability of MCF7 cells, evaluated by MTT assay. Cells were treated with 1 µM, 10 µM, 25 µM, 50 µM and 100 µM for 24 h or 48h. Data are shown as mean ± SEM of at least three separate experiments. # : $p < 0.05$ compared with the cells treated with the 10 µM solution

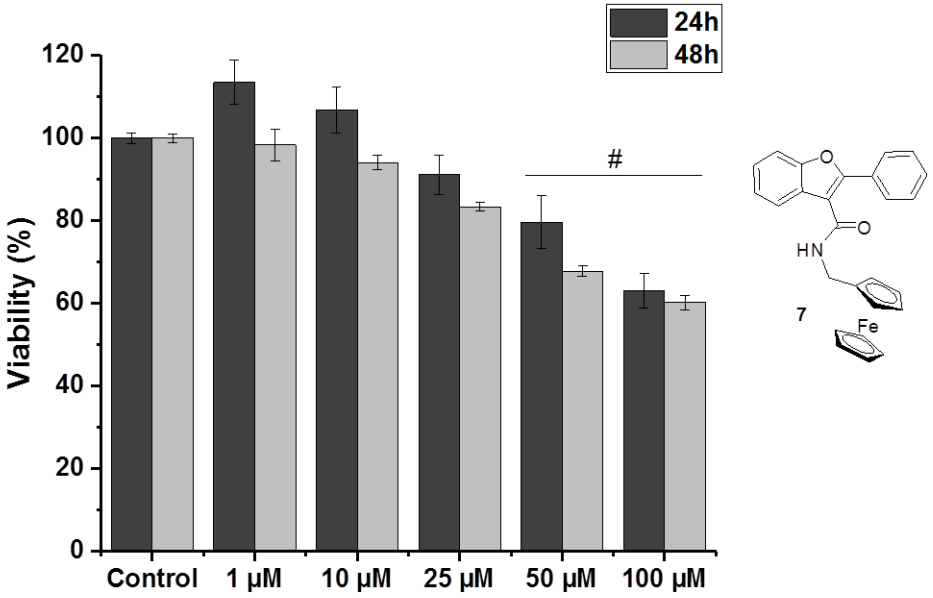

Figure S25. The effects of compound **7** on the viability of MCF7 cells, evaluated by MTT assay. Cells were treated with 1 µM, 10 µM, 25 µM, 50 µM and 100 µM for 24 h or 48h. Data are shown as mean ± SEM of at least three separate experiments. # : $p < 0.05$ compared with the cells treated with the 10 µM solution

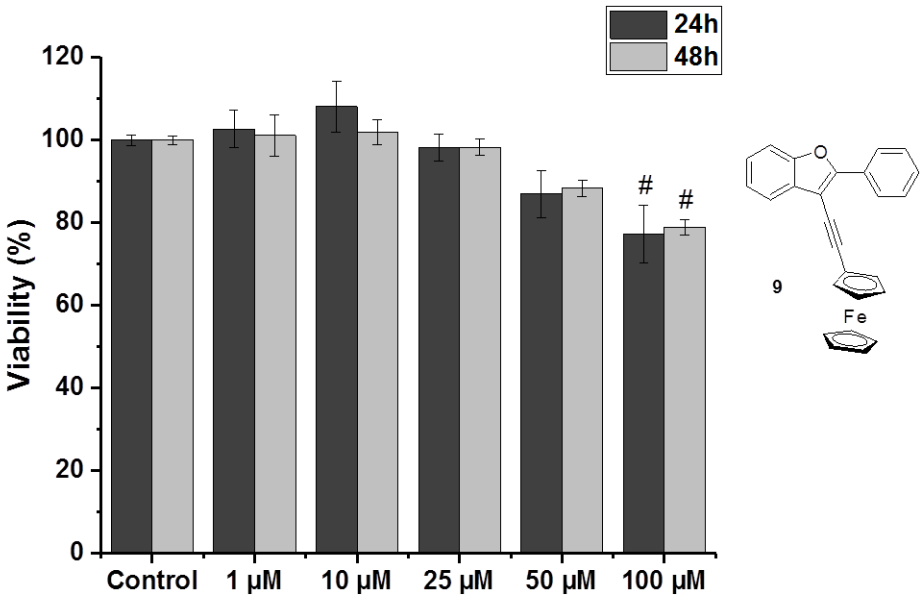

Figure S26. The effects of compound **9** on the viability of MCF7 cells, evaluated by MTT assay. Cells were treated with 1 µM, 10 µM, 25 µM, 50 µM and 100 µM for 24 h or 48h. Data are shown as mean ± SEM of at least three separate experiments. # : $p < 0.05$ compared with the cells treated with the 10 µM solution

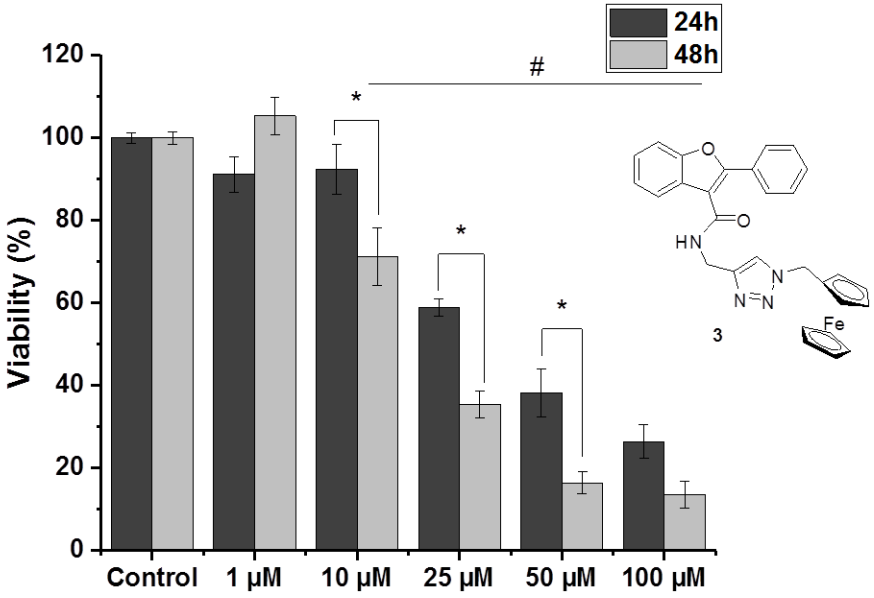

Figure S27. The effects of compound **3** on the viability of MDA-MB-231 cells, evaluated by MTT assay. Cells were treated with 1 µM, 10 µM, 25 µM, 50 µM and 100 µM for 24 h or 48h. Data are shown as mean ± SEM of at least three separate experiments. * $p < 0.05$ compared with the untreated cells. # : $p < 0.05$ compared with the cells treated with the 10 µM solution

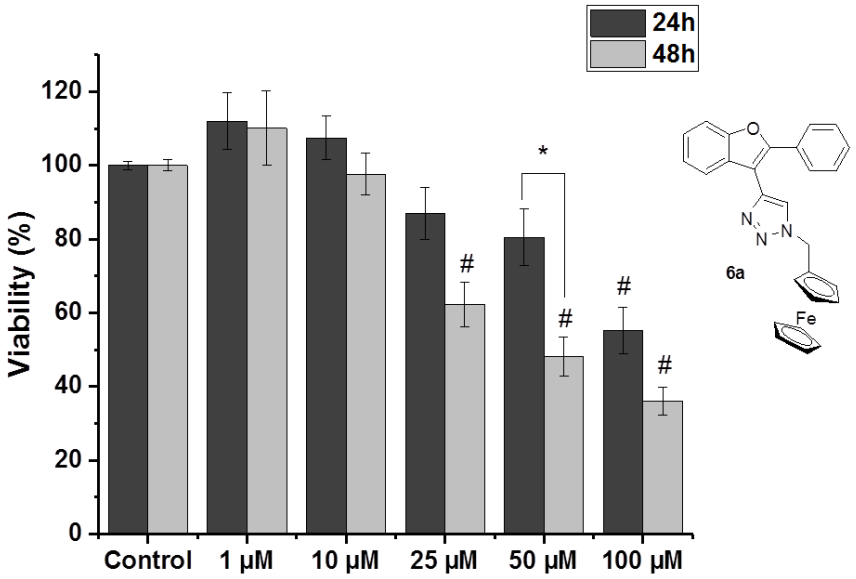

Figure S28. The effects of compound **6a** on the viability of MDA-MB-231 cells, evaluated by MTT assay. Cells were treated with 1 μM, 10 μM, 25 μM, 50 μM and 100 μM for 24 h or 48h. Data are shown as mean ± SEM of at least three separate experiments. * $p < 0.05$ compared with the untreated cells. # : $p < 0.05$ compared with the cells treated with the 10 μM solution

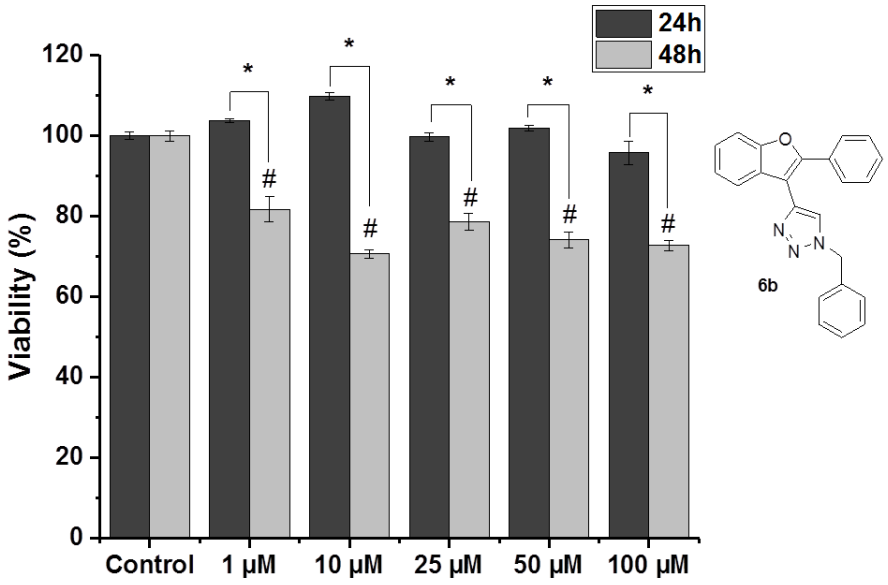

Figure S29. The effects of compound **6b** on the viability of MDA-MB-231 cells, evaluated by MTT assay. Cells were treated with 1 μM, 10 μM, 25 μM, 50 μM and 100 μM for 24 h or 48h. Data are shown as mean ± SEM of at least three separate experiments. * $p < 0.05$ compared with the untreated cells. # : $p < 0.05$ compared with the cells treated with the 10 μM solution

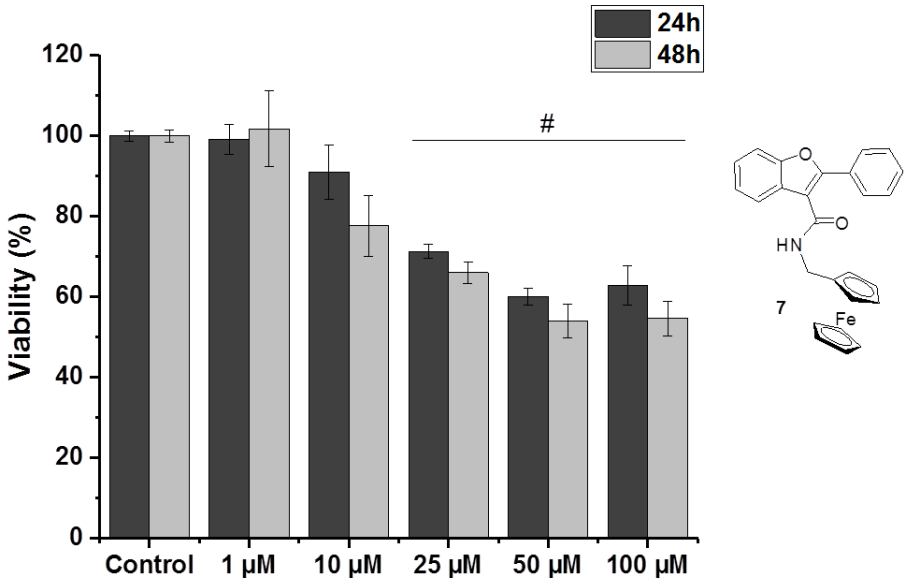

Figure S30. The effects of compound **7** on the viability of MDA-MB-231 cells, evaluated by MTT assay. Cells were treated with 1 µM, 10 µM, 25 µM, 50 µM and 100 µM for 24 h or 48h. Data are shown as mean ± SEM of at least three separate experiments. # : $p < 0.05$ compared with the cells treated with the 10 µM solution

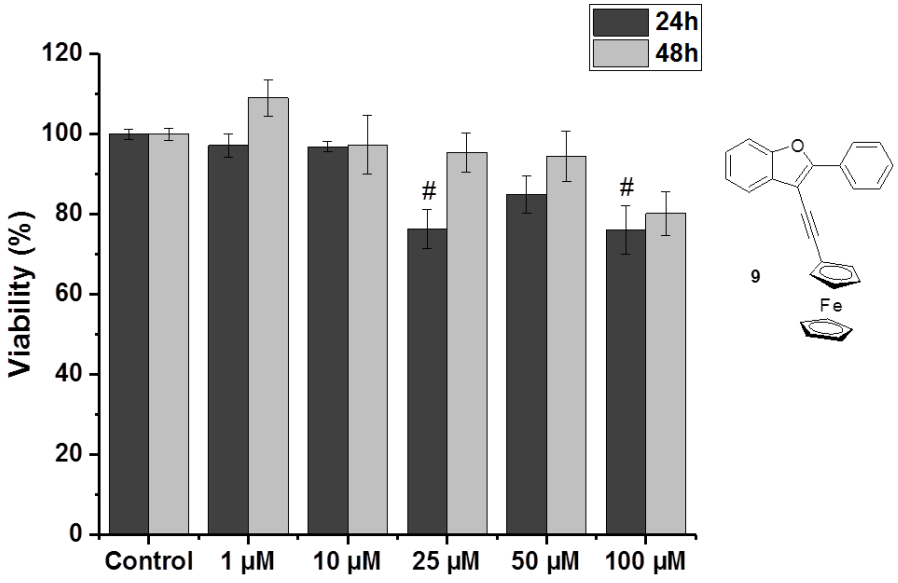

Figure S31. The effects of compound **9** on the viability of MDA-MB-231 cells, evaluated by MTT assay. Cells were treated with 1 µM, 10 µM, 25 µM, 50 µM and 100 µM for 24 h or 48h. Data are shown as mean ± SEM of at least three separate experiments. # : $p < 0.05$ compared with the cells treated with the 10 µM solution

Crystallography

Table S1. Crystallographic data of compound **9**

Crystal data	
Chemical formula	$C_{26}H_{18}FeO$
M_r	402.25
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	295
a, *b*, *c* (Å)	7.7793(2), 10.3553(2), 23.3552(6)
b (°)	90.692 (2)
V (Å^3)	1881.29 (8)
Z	4
Radiation type	Mo *K*a
m (mm^{-1})	0.82
Crystal size (mm)	0.39 × 0.29 × 0.07
Data collection	
Diffractometer	Oxford Diffraction Xcalibur Gemini Ultra R
Absorption correction	Analytical
T_{min}, T_{max}	0.794, 0.945
No. of measured, independent and observed [$I > 2s(I)$] reflections	26238, 4138, 3240
R_{int}	0.035
(sin q/l)$_{max}$ (Å^{-1})	0.641
Refinement	
$R[F^2 > 2s(F^2)]$, $wR(F^2)$, S	0.037, 0.103, 1.03
No. of reflections	4138
No. of parameters	298
H-atom treatment	mixed
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e·Å^{-3})	0.29, -0.18