Supplementary Information (SI) for Dalton Transactions.

New redox-active Cu complexes with tridentate chelating ligands based on 2-thioimidazol-4-ones as potential antiproliferative agents

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Supporting Information

Content

NMR Spectra and structure assignment

Spectra of organic compounds

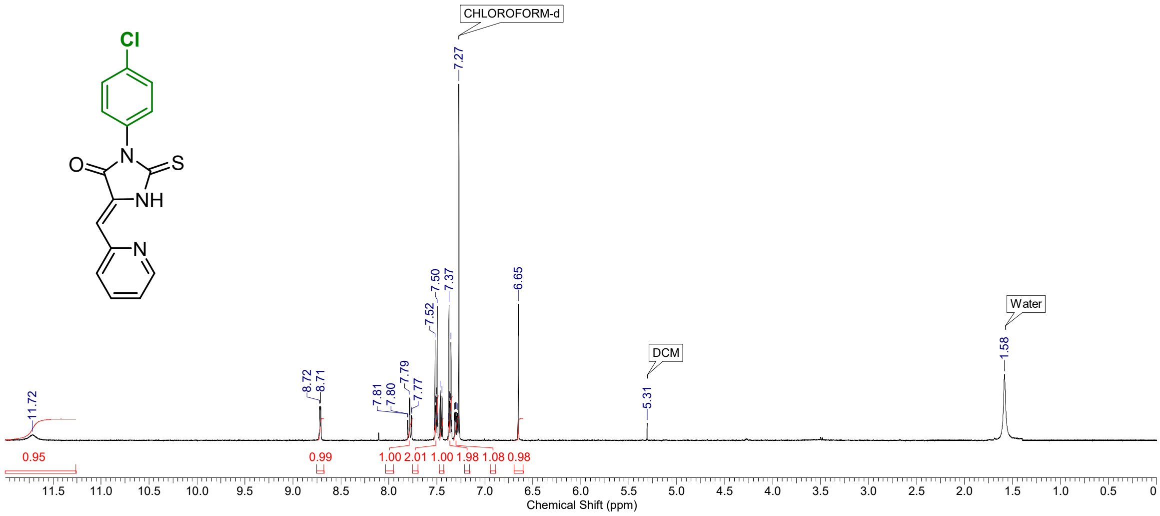


Figure S1. [1]H NMR spectrum of (Z)-3-(4-chlorophenyl)-5-(pyridin-2-ylmethylene)-2-thioxoimidazolidin-4-one **2**.

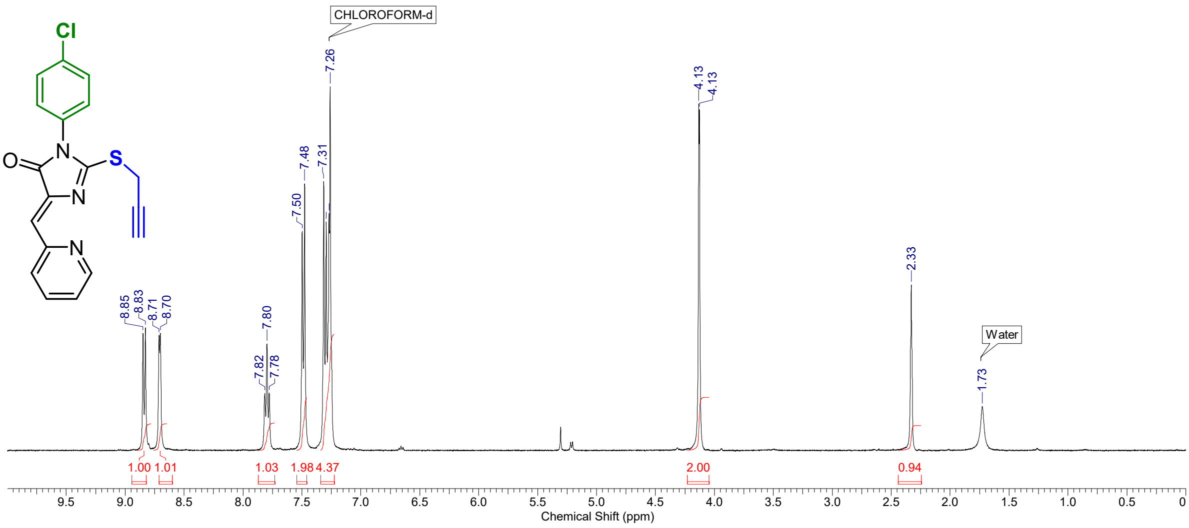


Figure S2. [1]H NMR spectrum of (Z)-3-(4-chlorophenyl)-2-(prop-2-yn-1-ylthio)-5-(pyridin-2-ylmethylene)-3,5-dihydro-4H-imidazol-4-one **3**.

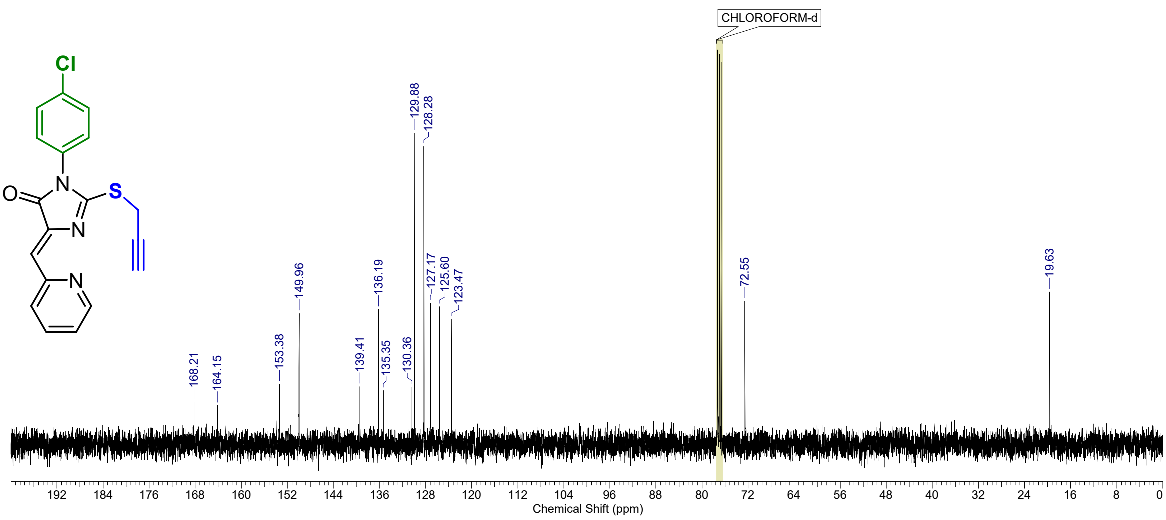


Figure S3. [13]C NMR spectrum of (Z)-3-(4-chlorophenyl)-2-(prop-2-yn-1-ylthio)-5-(pyridin-2-ylmethylene)-3,5-dihydro-4H-imidazol-4-one **3**.

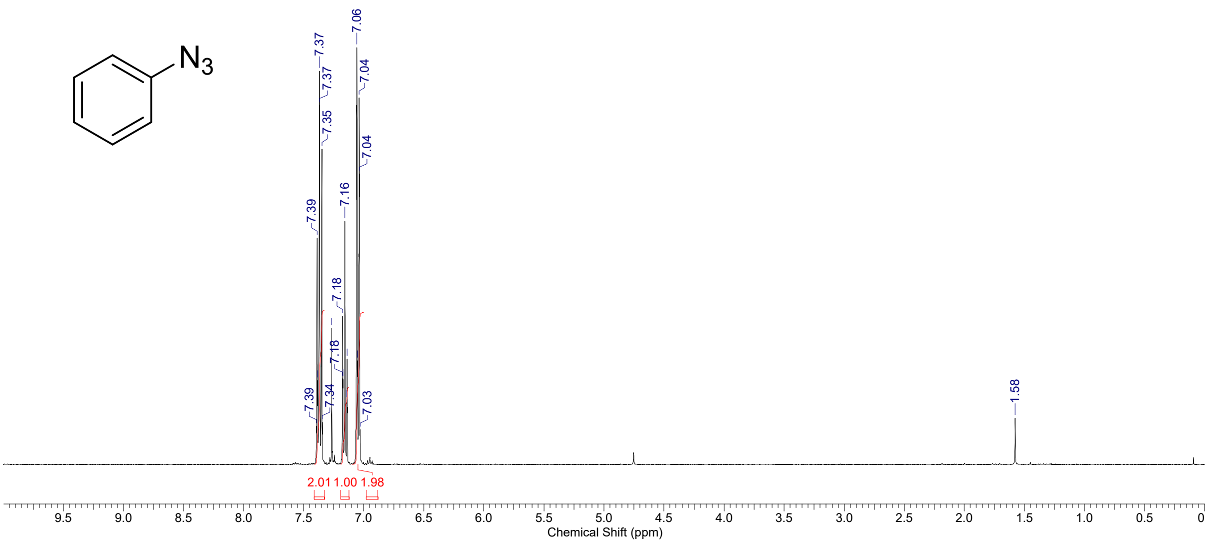


Figure S4. ^{1}H NMR spectrum of Phenyl azide **4**.

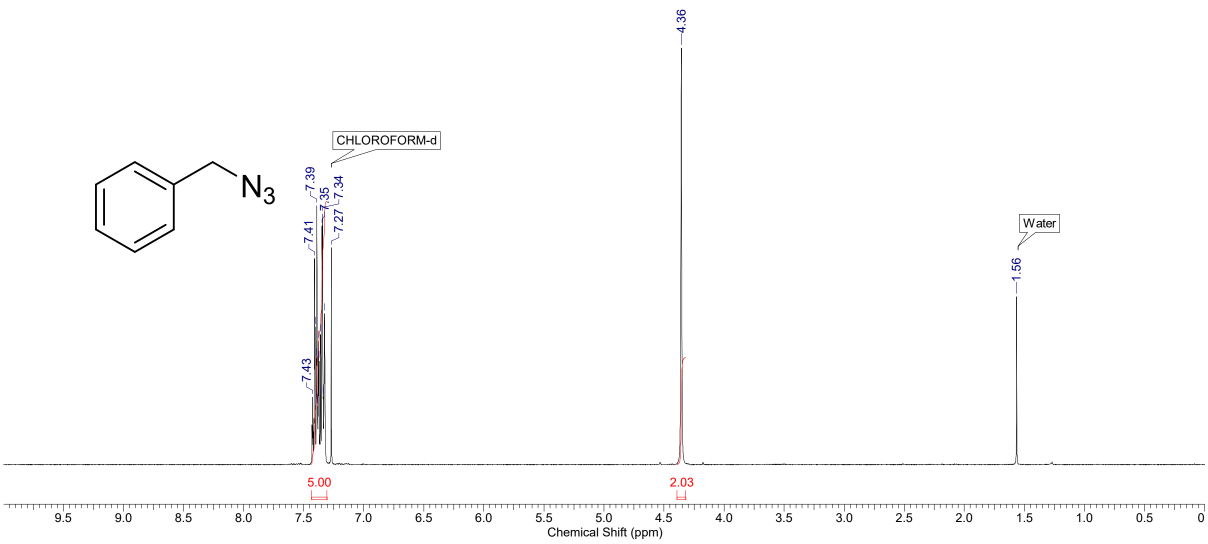


Figure S5. ^{1}H NMR spectrum of Benzyl azide **5**.

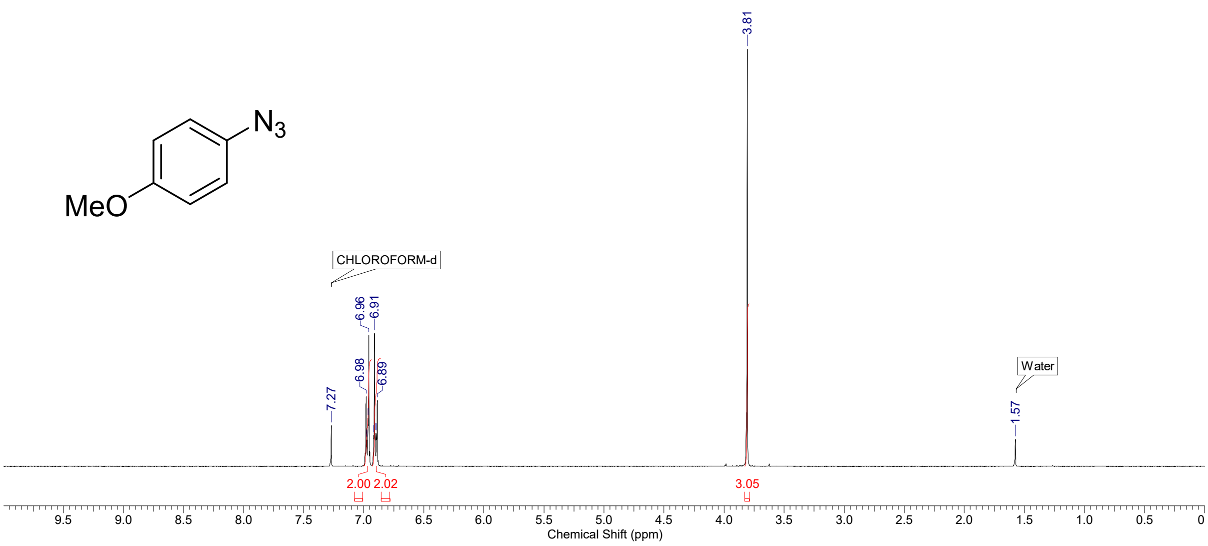


Figure S6. ^{1}H NMR spectrum of 4-methoxyphenyl azide **6**.

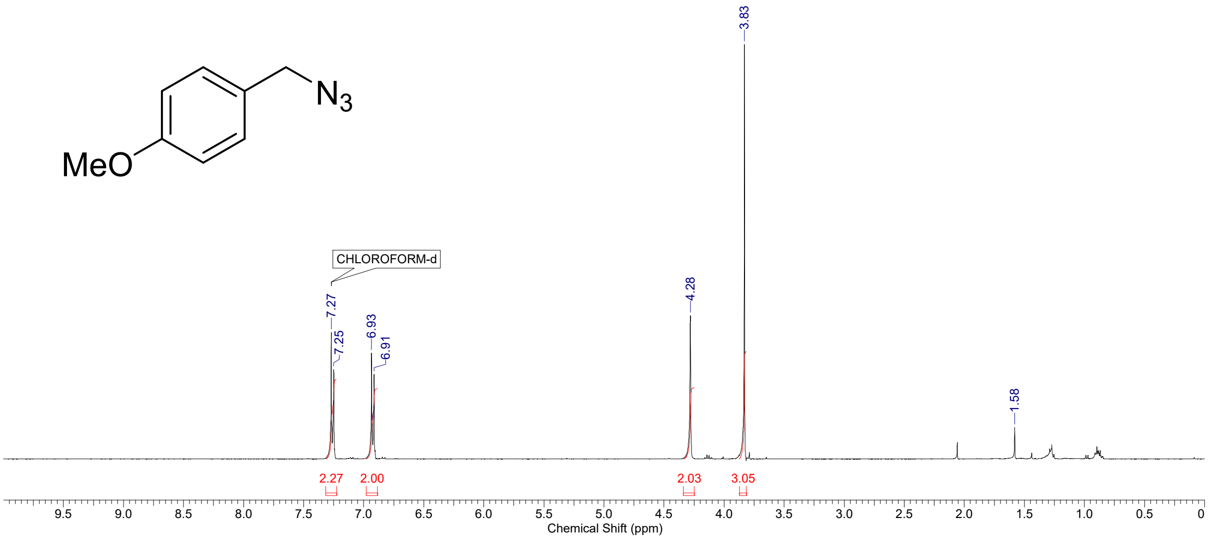


Figure S7. ^{1}H NMR spectrum of 4-methoxybenzyl azide **7**.

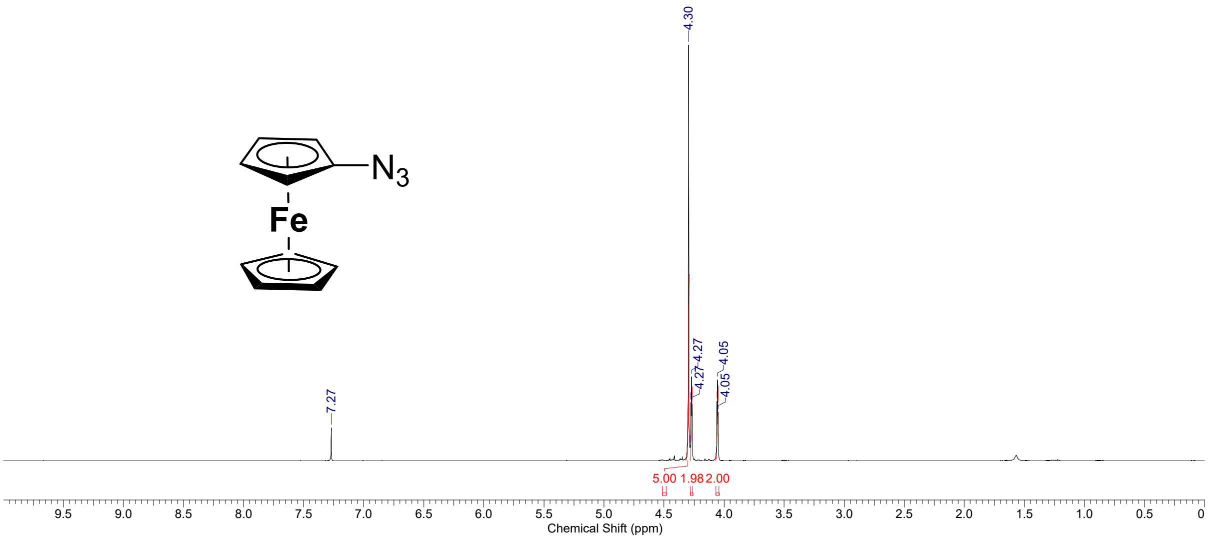


Figure S8. ^{1}H NMR spectra of Ferrocenyl azide **8**.

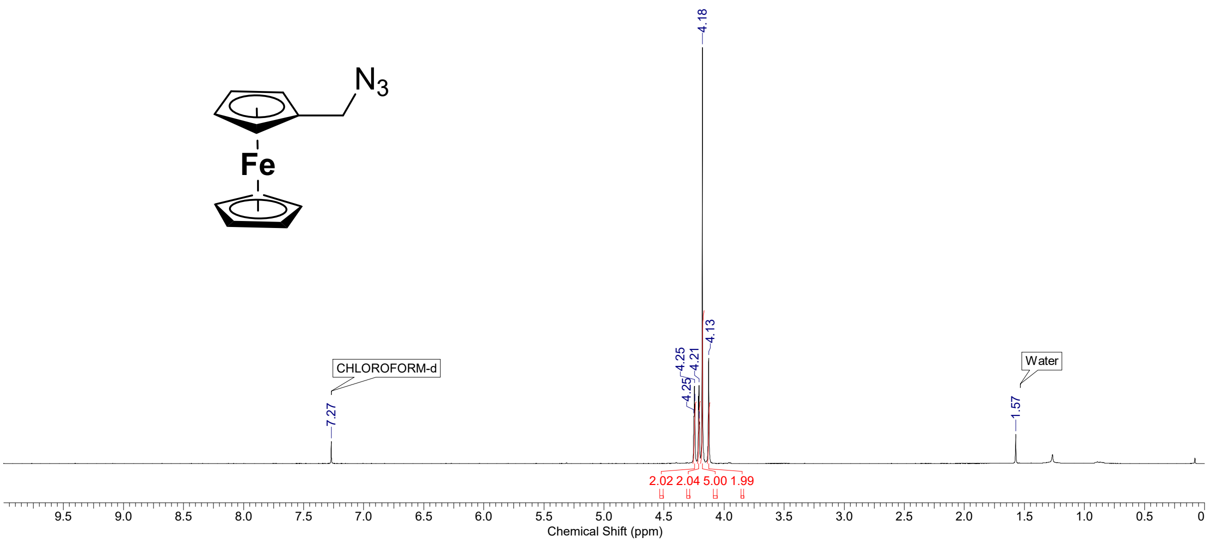


Figure S9. ^{1}H NMR spectra of Azidomethylferrocene **9**.

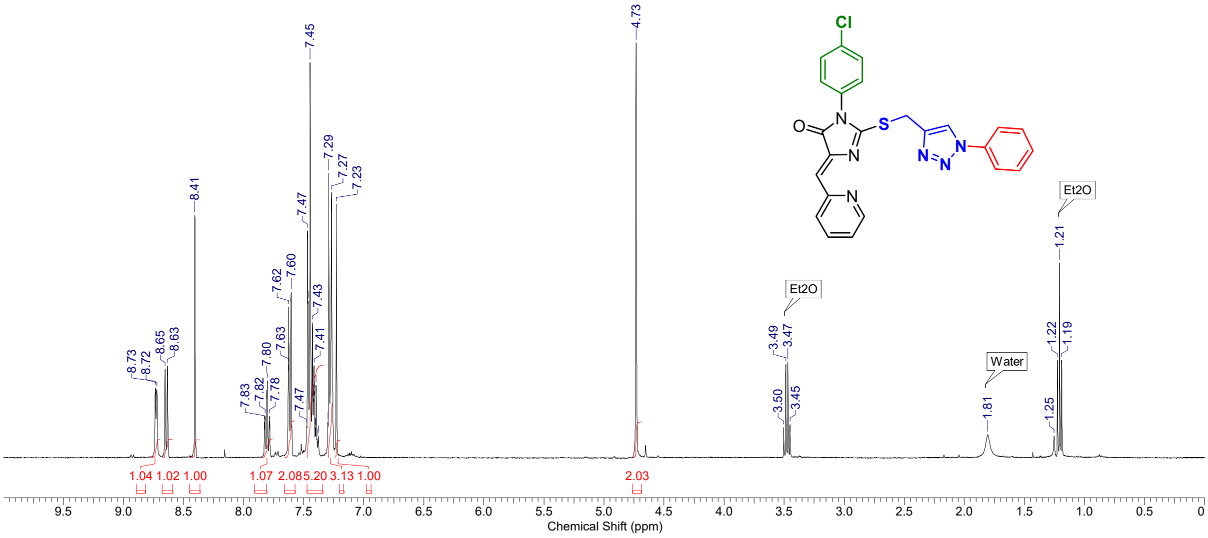


Figure S10. ^{1}H NMR spectra of (Z)-3-(4-chlorophenyl)-2-(((1-phenyl-1H-1,2,3-triazol-4-yl)methyl)thio)-5-(pyridin-2-ylmethylene)-3,5-dihydro-4H-imidazol-4-one **10**.

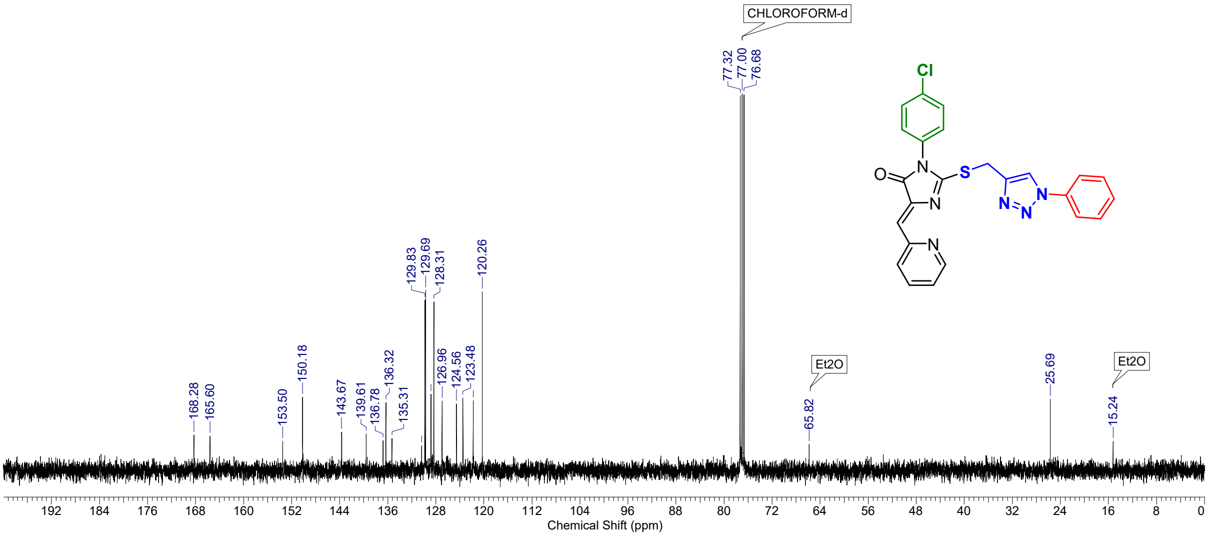


Figure S11. ^{13}C NMR spectra of (Z)-3-(4-chlorophenyl)-2-(((1-phenyl-1H-1,2,3-triazol-4-yl)methyl)thio)-5-(pyridin-2-ylmethylene)-3,5-dihydro-4H-imidazol-4-one **10**.

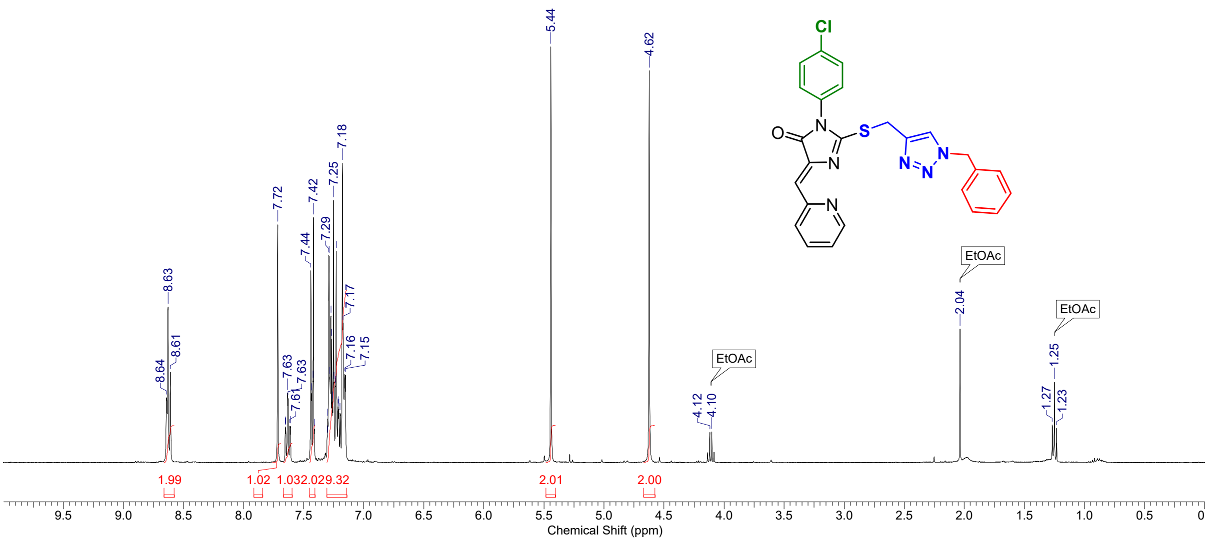


Figure S12. ^{1}H NMR spectra of (Z)-2-(((1-benzyl-1H-1,2,3-triazol-4-yl)methyl)thio)-3-(4-chlorophenyl)-5-(pyridin-2-ylmethylene)-3,5-dihydro-4H-imidazol-4-one **11**.

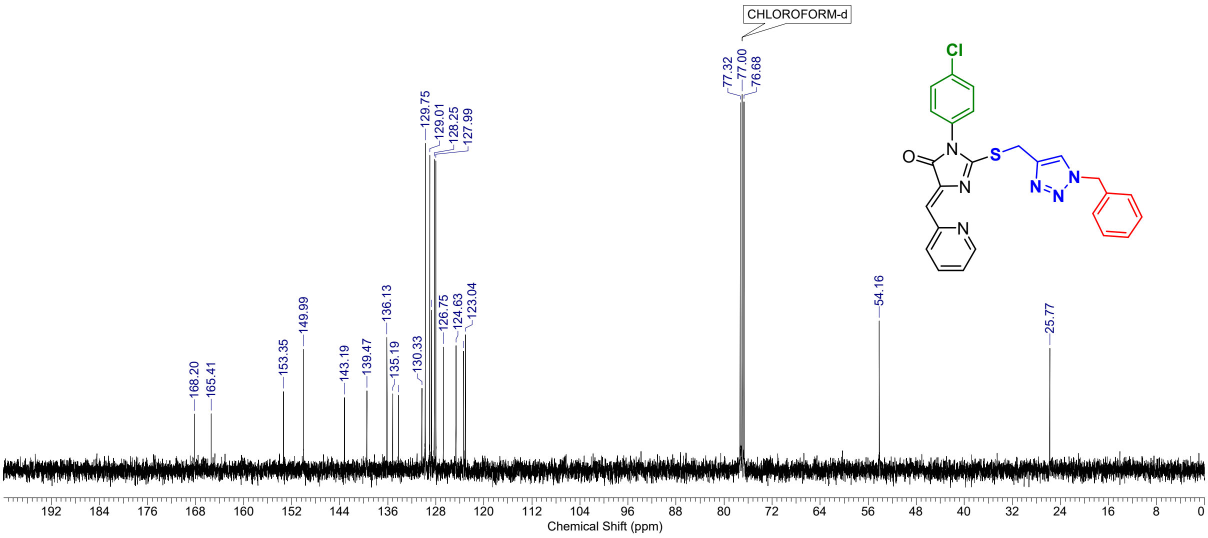


Figure S13. [13]C NMR spectra of (Z)-2-(((1-benzyl-1H-1,2,3-triazol-4-yl)methyl)thio)-3-(4-chlorophenyl)-5-(pyridin-2-ylmethylene)-3,5-dihydro-4H-imidazol-4-one **11**.

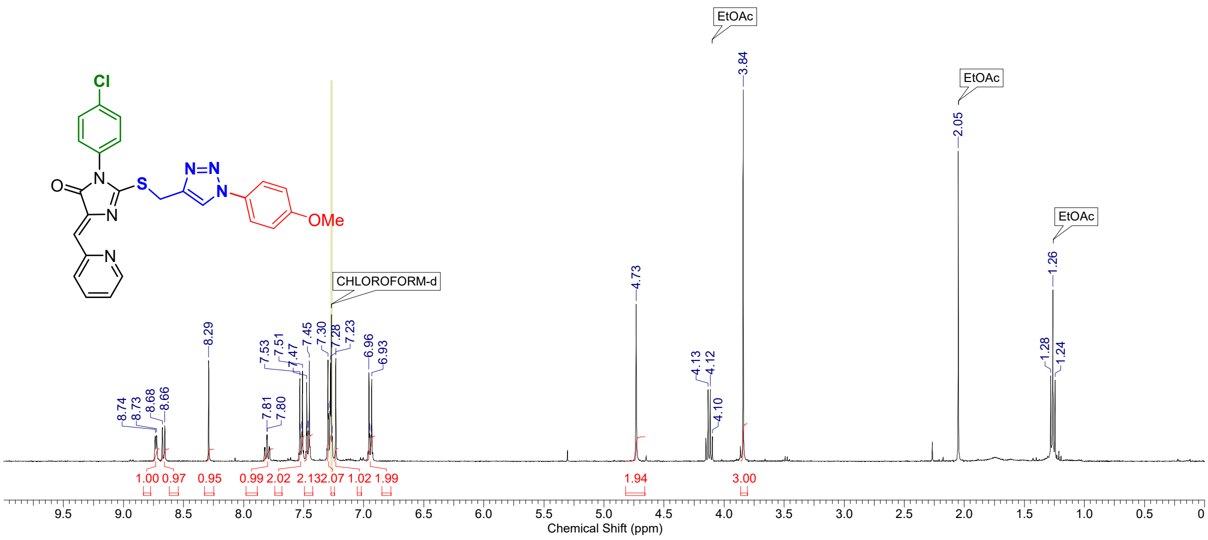


Figure S14. [1]H NMR spectra of (Z)-3-(4-chlorophenyl)-2-(((1-(4-methoxyphenyl)-1H-1,2,3-triazol-4-yl)methyl)thio)-5-(pyridin-2-ylmethylene)-3,5-dihydro-4H-imidazol-4-one **12**.

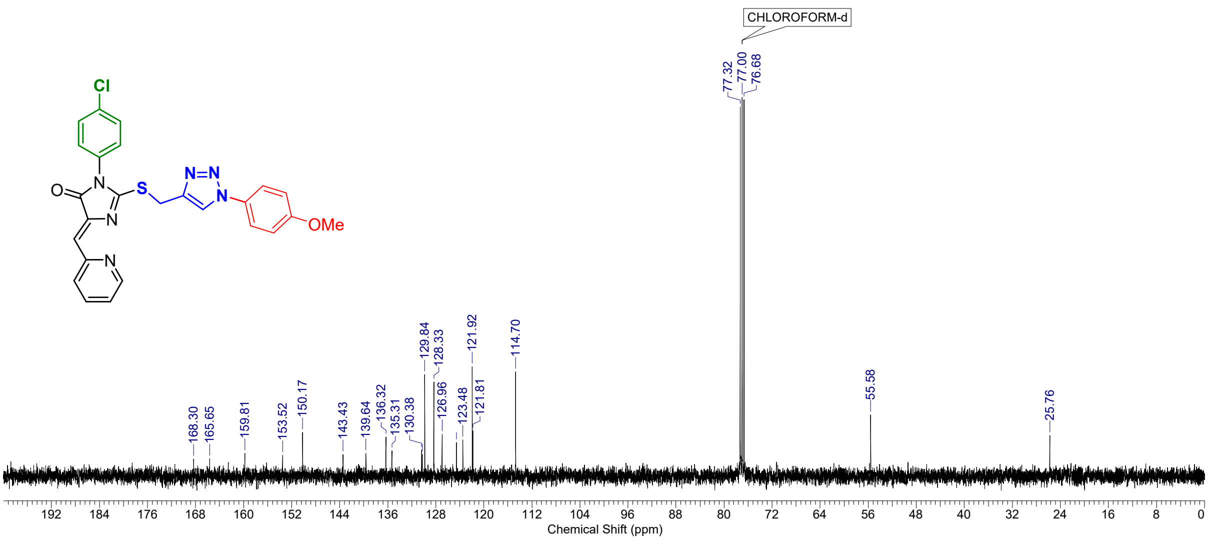


Figure S15. [13]C NMR spectra of (Z)-3-(4-chlorophenyl)-2-(((1-(4-methoxyphenyl)-1H-1,2,3-triazol-4-yl)methyl)thio)-5-(pyridin-2-ylmethylene)-3,5-dihydro-4H-imidazol-4-one **12**.

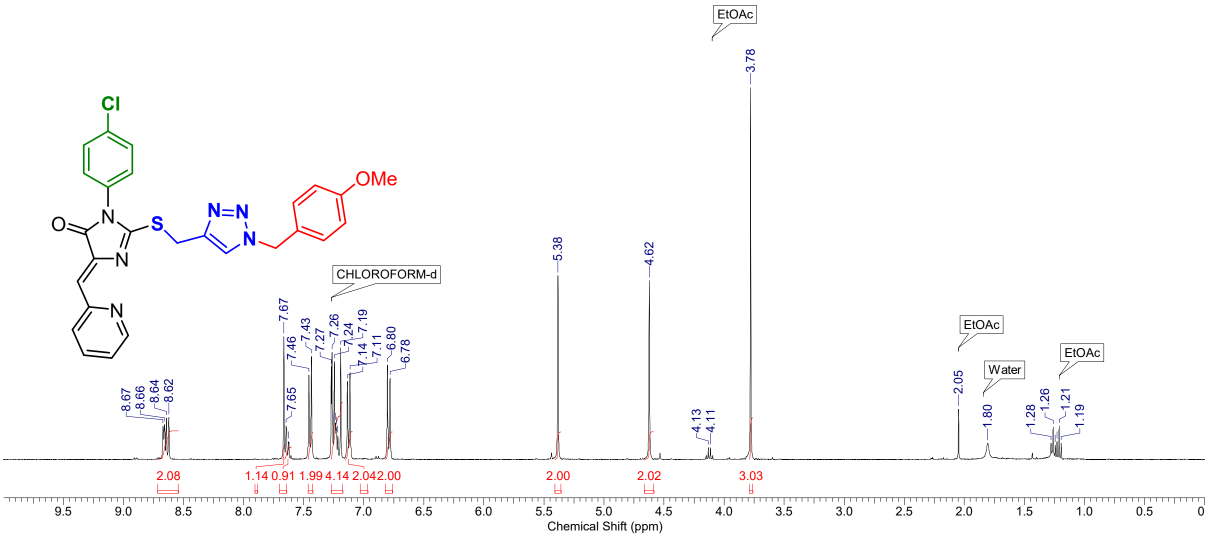


Figure S16. ^{1}H NMR spectra of (Z)-3-(4-chlorophenyl)-2-(((1-(4-methoxybenzyl)-1H-1,2,3-triazol-4-yl)methyl)thio)-5-(pyridin-2-ylmethylene)-3,5-dihydro-4H-imidazol-4-one **13**.

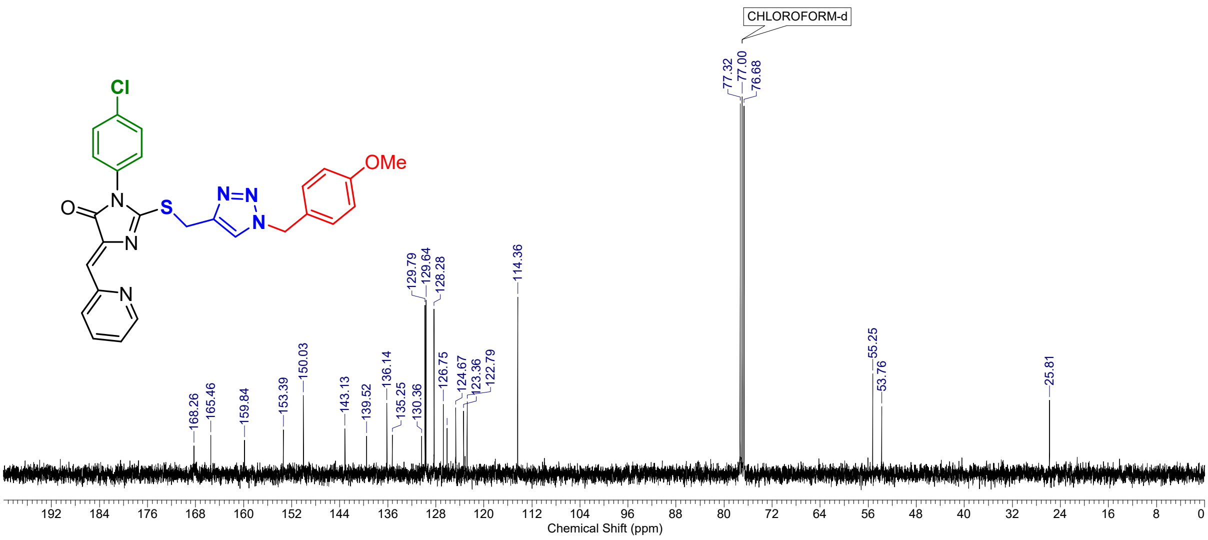


Figure S17. ^{13}C NMR spectra of (Z)-3-(4-chlorophenyl)-2-(((1-(4-methoxybenzyl)-1H-1,2,3-triazol-4-yl)methyl)thio)-5-(pyridin-2-ylmethylene)-3,5-dihydro-4H-imidazol-4-one **13**.

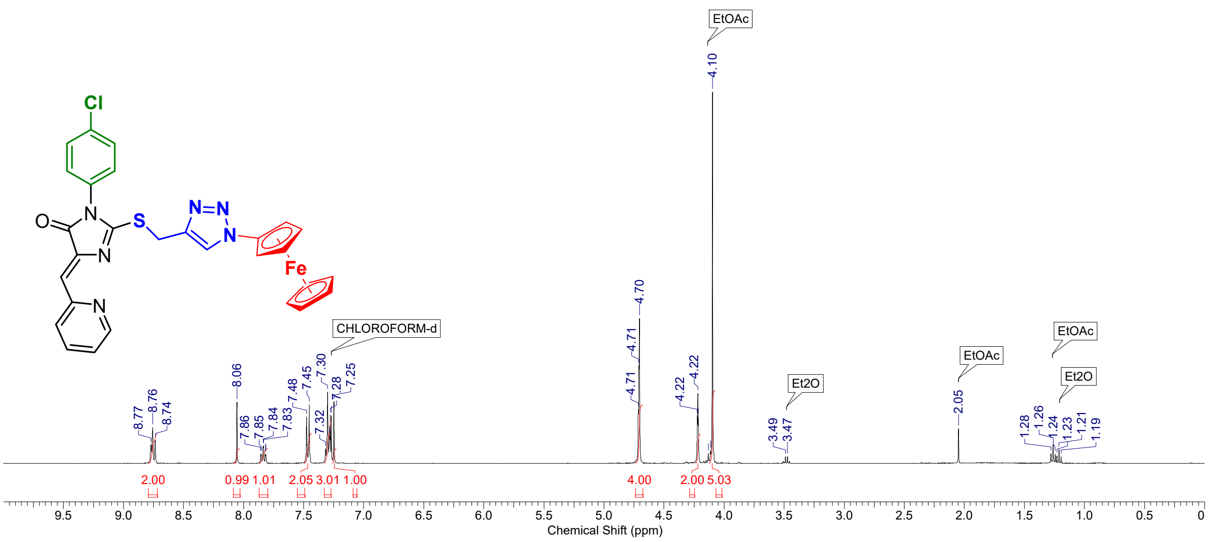


Figure S18. ^{1}H NMR spectra of (Z)-3-(4-chlorophenyl)-2-(((1-ferrocenyl-1H-1,2,3-triazol-4-yl)methyl)thio)-5-(pyridin-2-ylmethylene)-3,5-dihydro-4H-imidazol-4-one **14**.

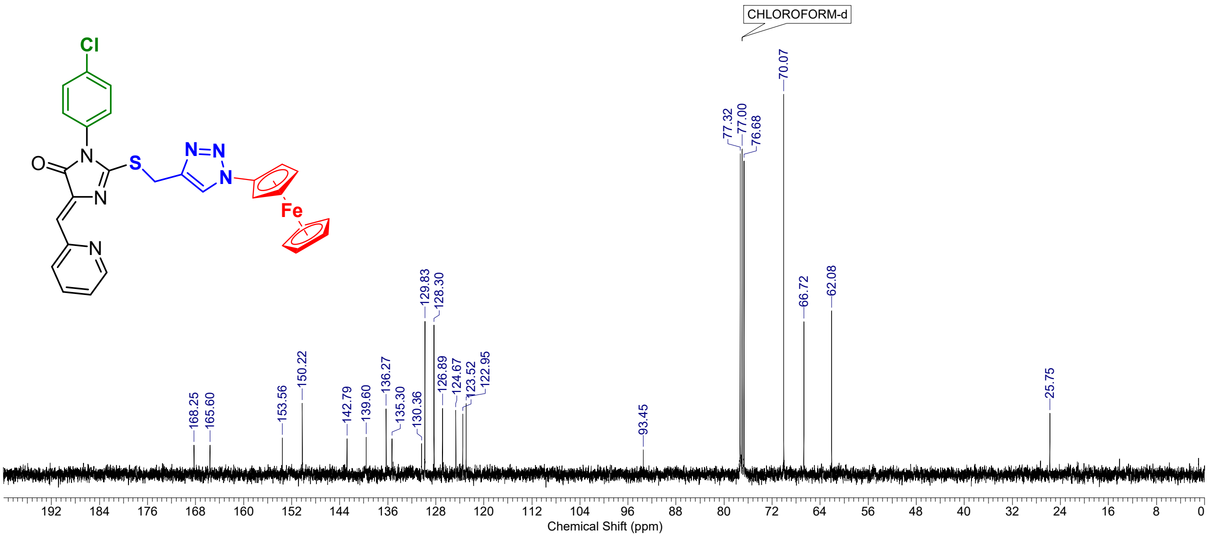


Figure S19. ^{13}C NMR spectra of (Z)-3-(4-chlorophenyl)-2-(((1-ferrocenyl-1H-1,2,3-triazol-4-yl)methyl)thio)-5-(pyridin-2-ylmethylene)-3,5-dihydro-4H-imidazol-4-one **14**.

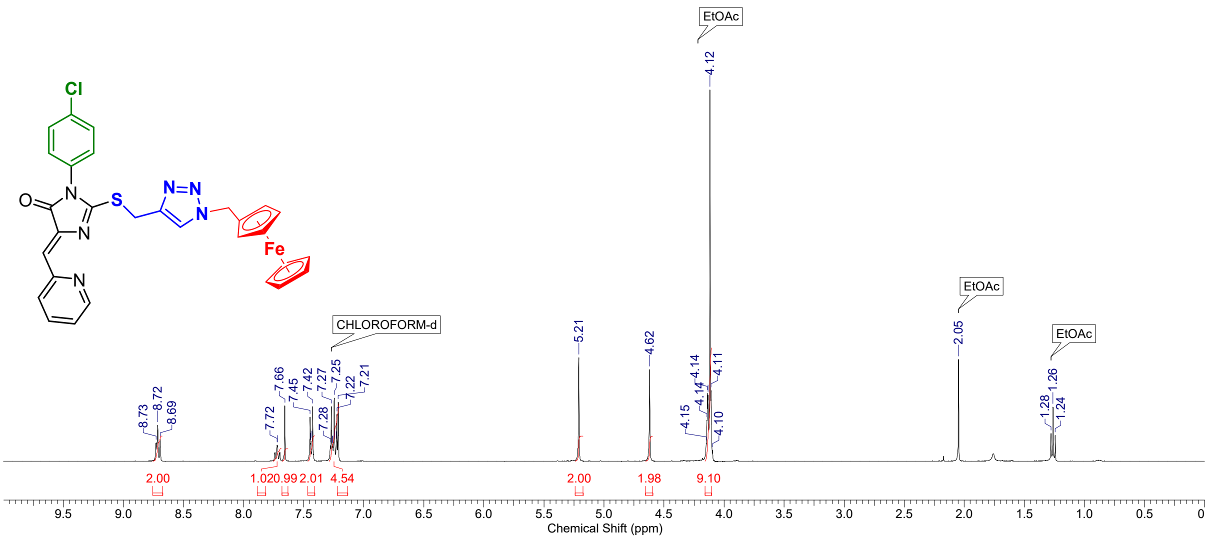


Figure S20. ^{1}H NMR spectra of (Z)-2-(((1-ferrocenylmethyl-1H-1,2,3-triazol-4-yl)methyl)thio)-3-(4-chlorophenyl)-5-(pyridin-2-ylmethylene)-3,5-dihydro-4H-imidazol-4-one **15**.

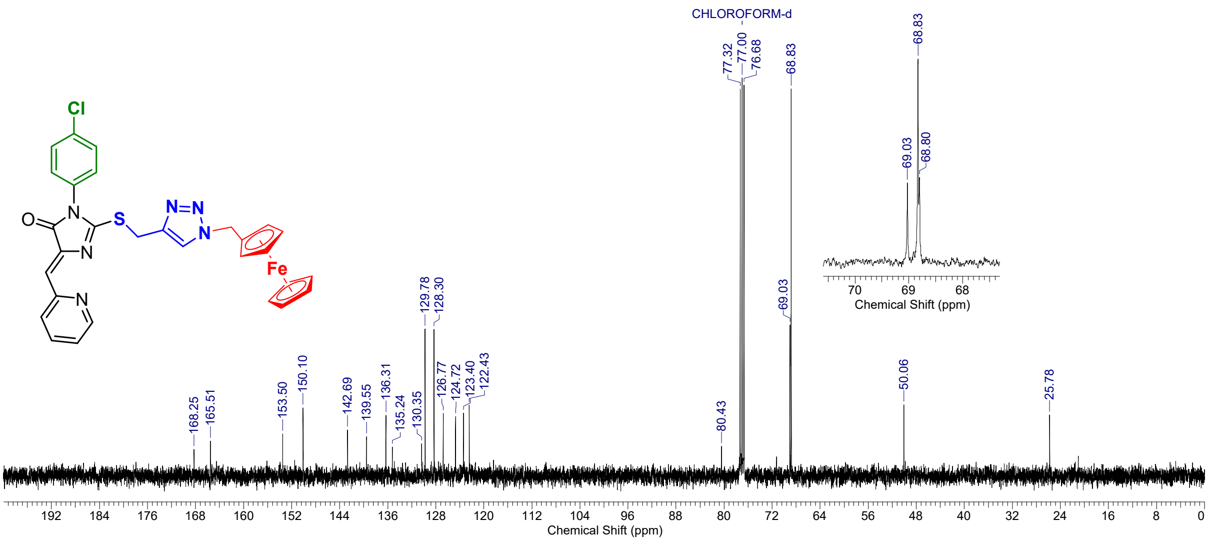


Figure S21. ^{1}H NMR spectra of (Z)-2-(((1-ferrocenylmethyl-1H-1,2,3-triazol-4-yl)methyl)thio)-3-(4-chlorophenyl)-5-(pyridin-2-ylmethylene)-3,5-dihydro-4H-imidazol-4-one **15**.

Elucidation of the ligands structure (2D NMR signal assignment)

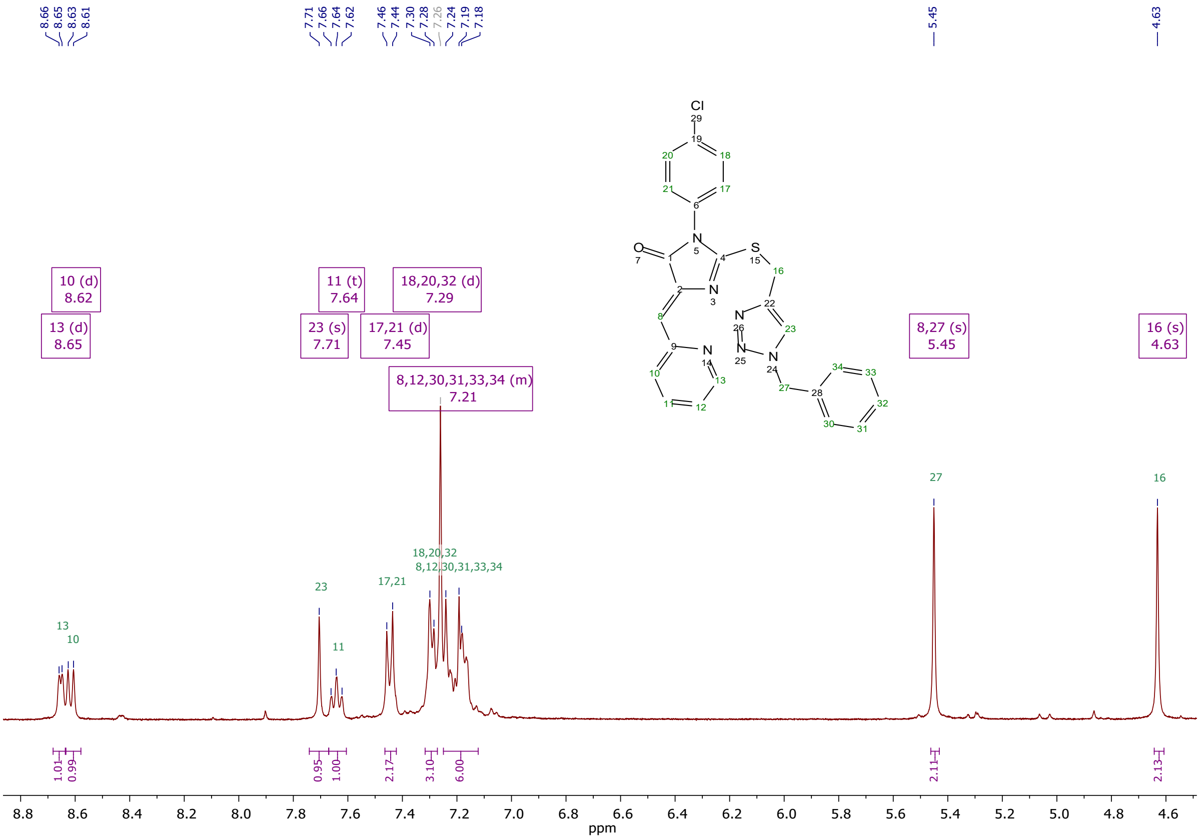


Figure S22. Signal assignment in ^{1}H NMR spectrum of compound **11**.

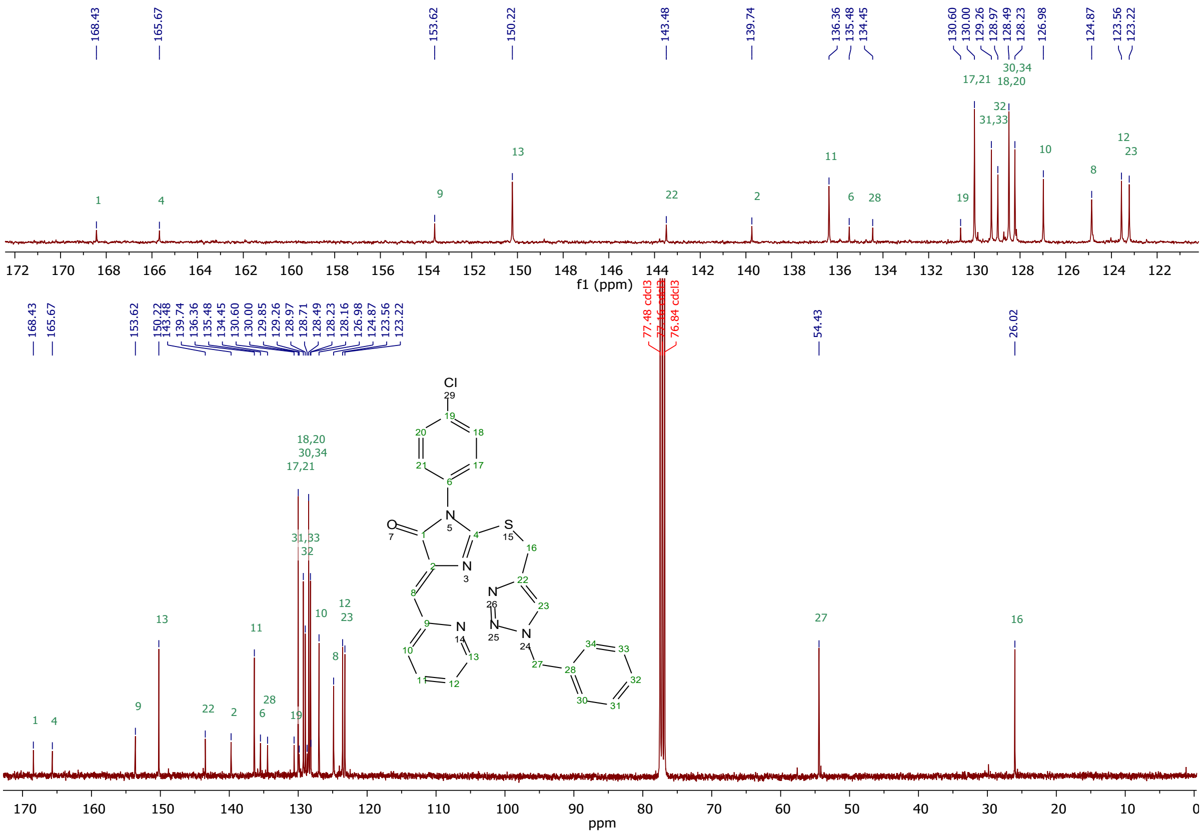


Figure S23. Signal assignment in ^{13}C NMR spectrum of compound **11**.

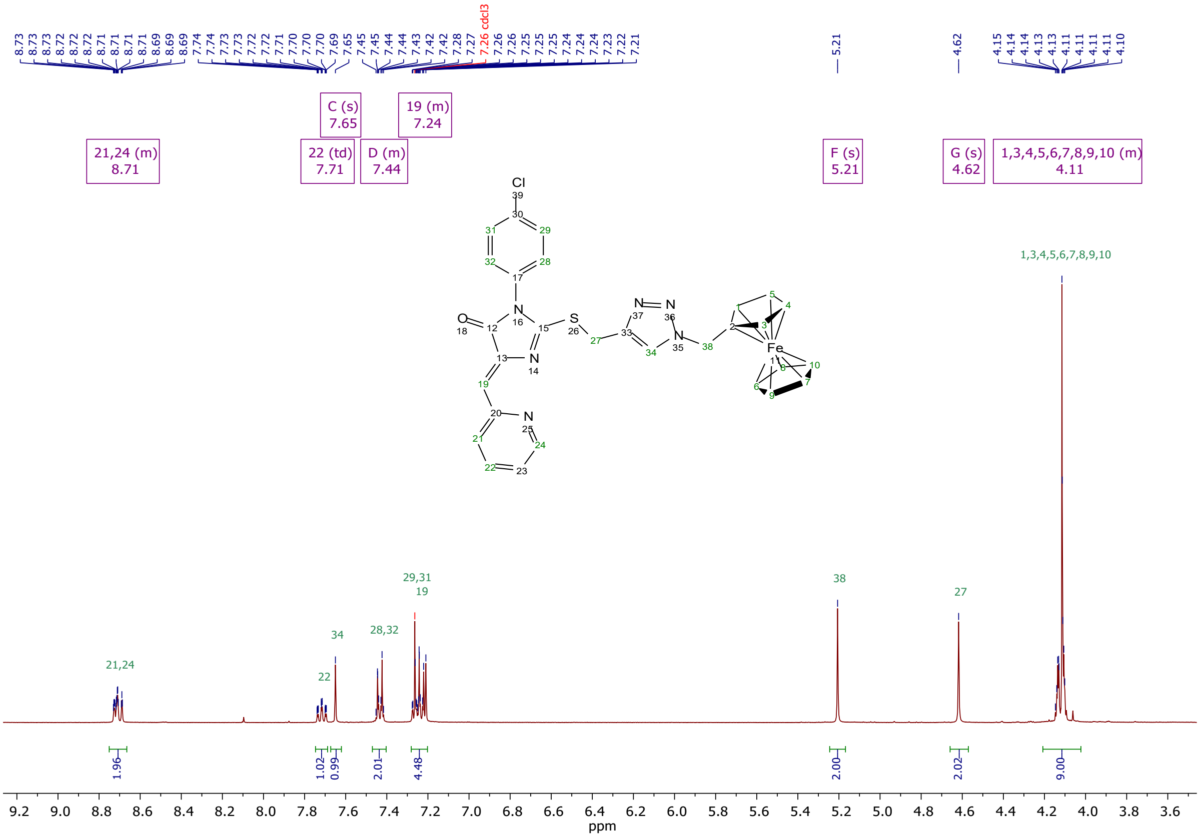


Figure S24. Signal assignment in ^{1}H NMR spectrum of compound **15**.

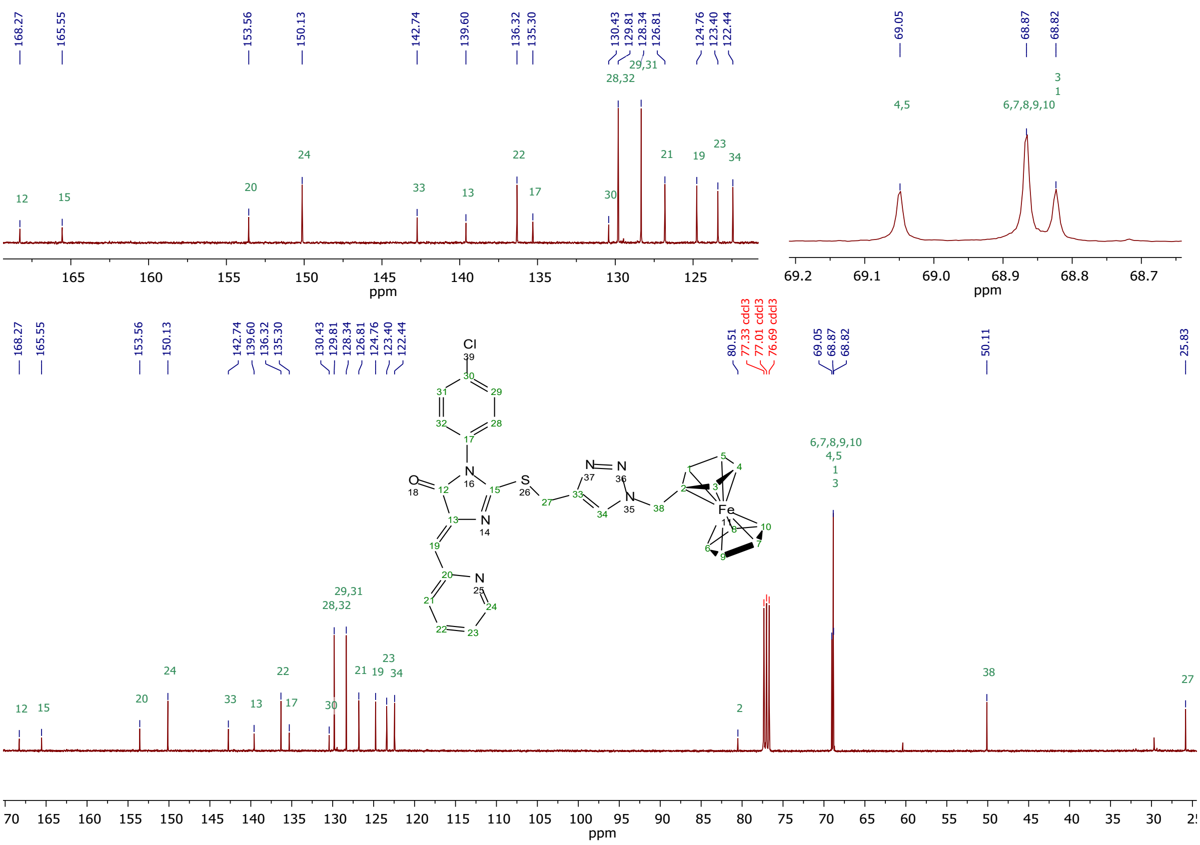


Figure S25. Signal assignment in ^{13}C NMR spectrum of compound **15.**

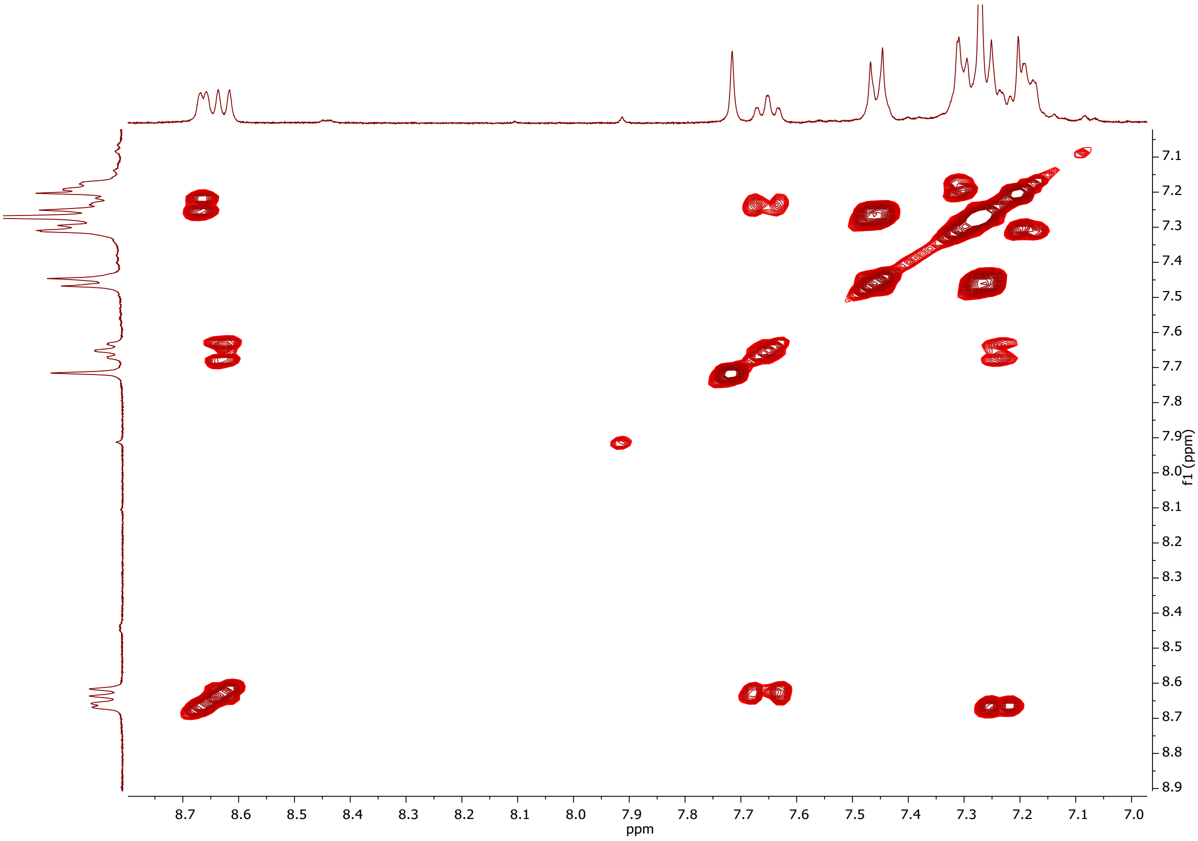


Figure S26. COSY [1]H NMR spectrum of **11** (Aromatic region).

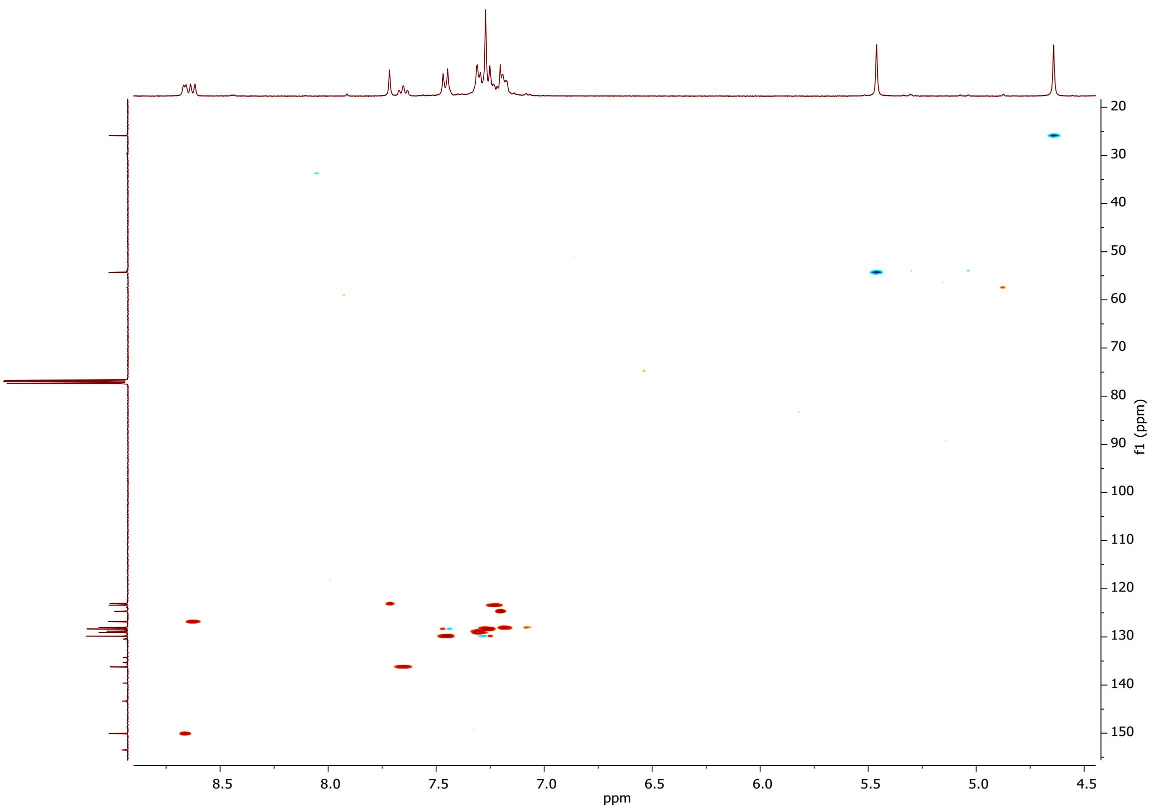


Figure S27. gHSQCAD spectrum of **11**.

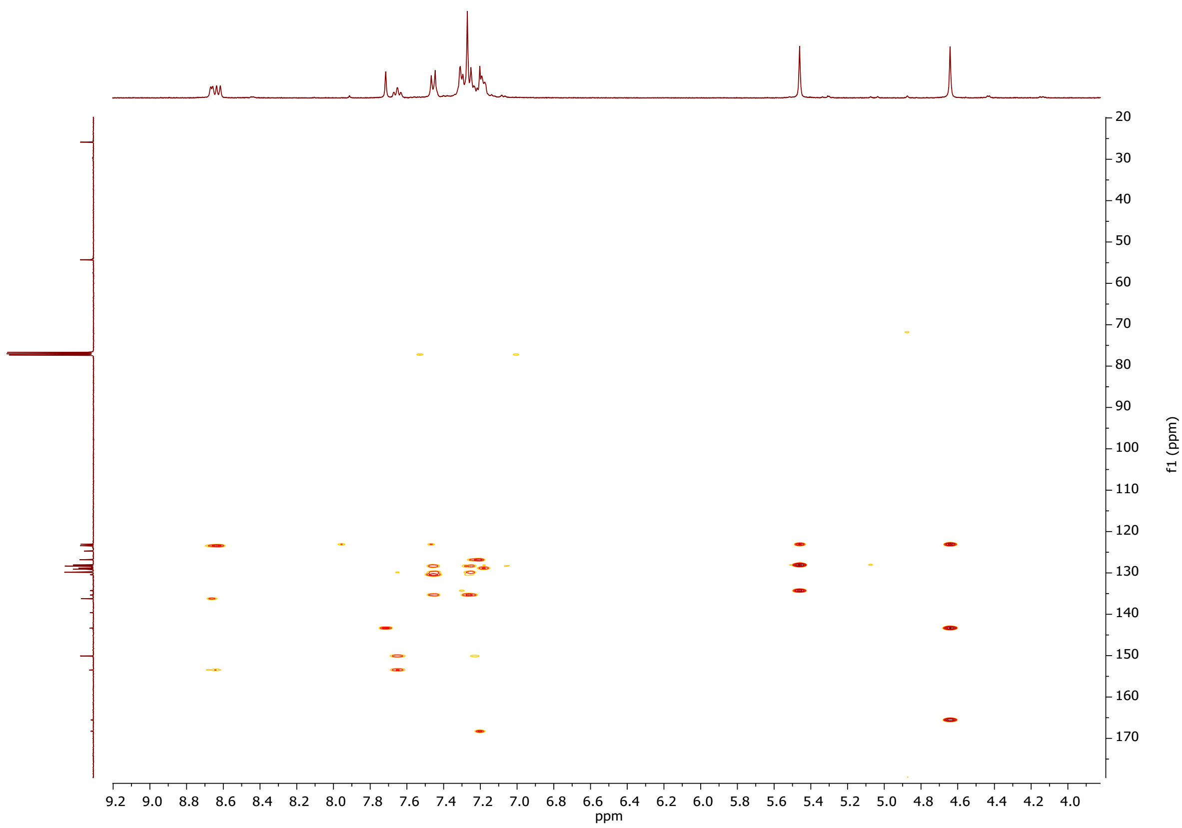


Figure S28. gHMBCAD spectrum of **11**.

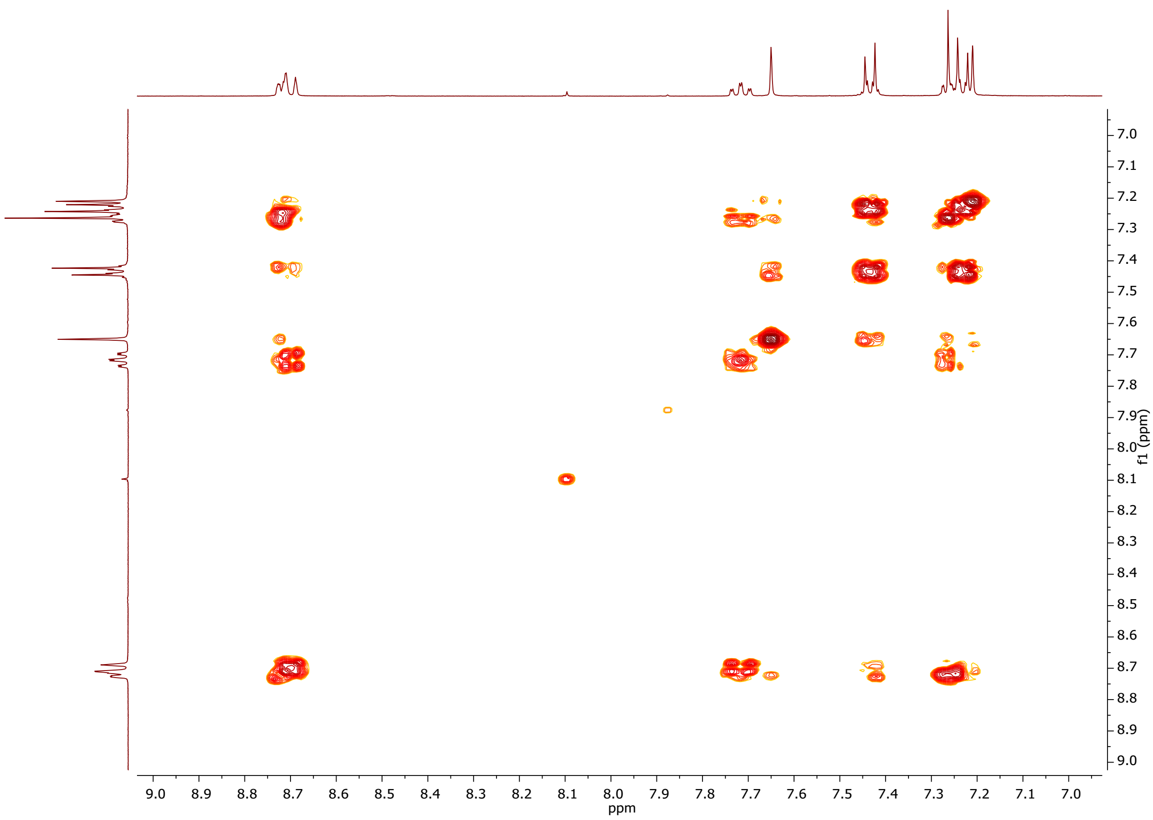


Figure S29. COSY ^{1}H NMR spectrum of **15** (Aromatic region).

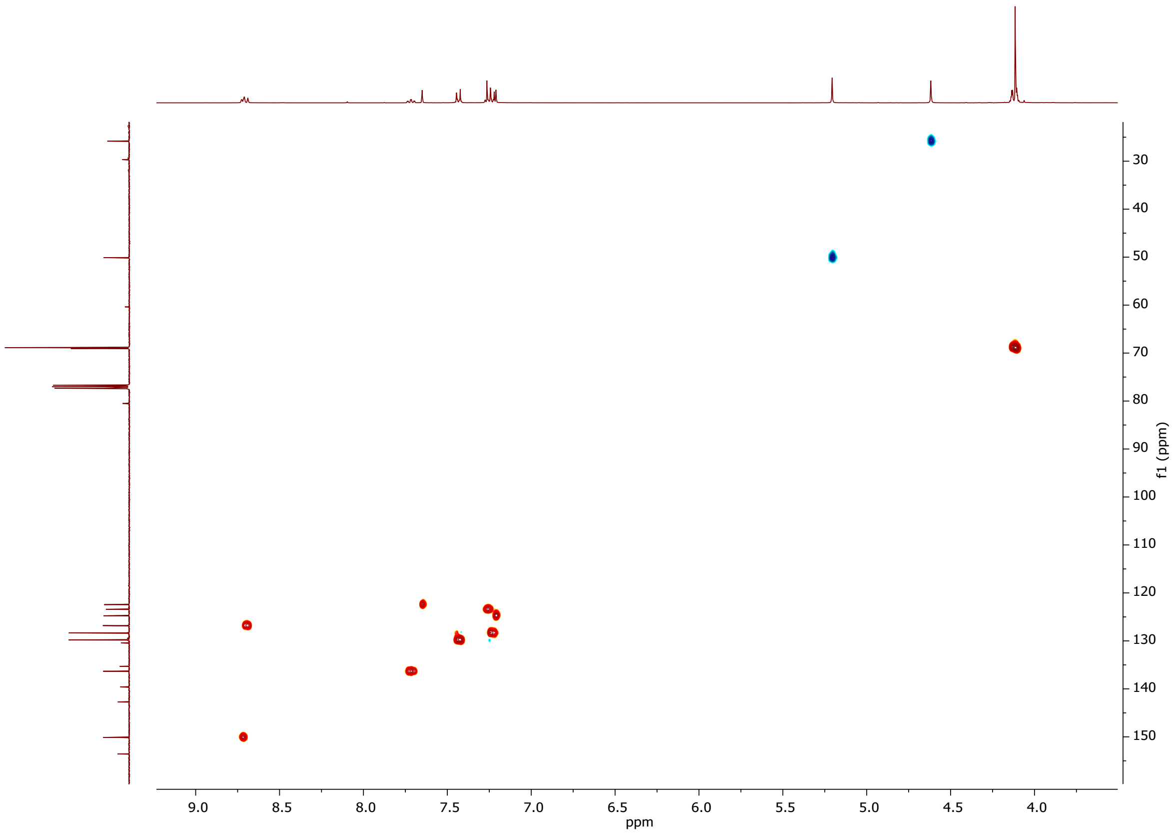


Figure S30. gHSQCAD spectrum of **15**.

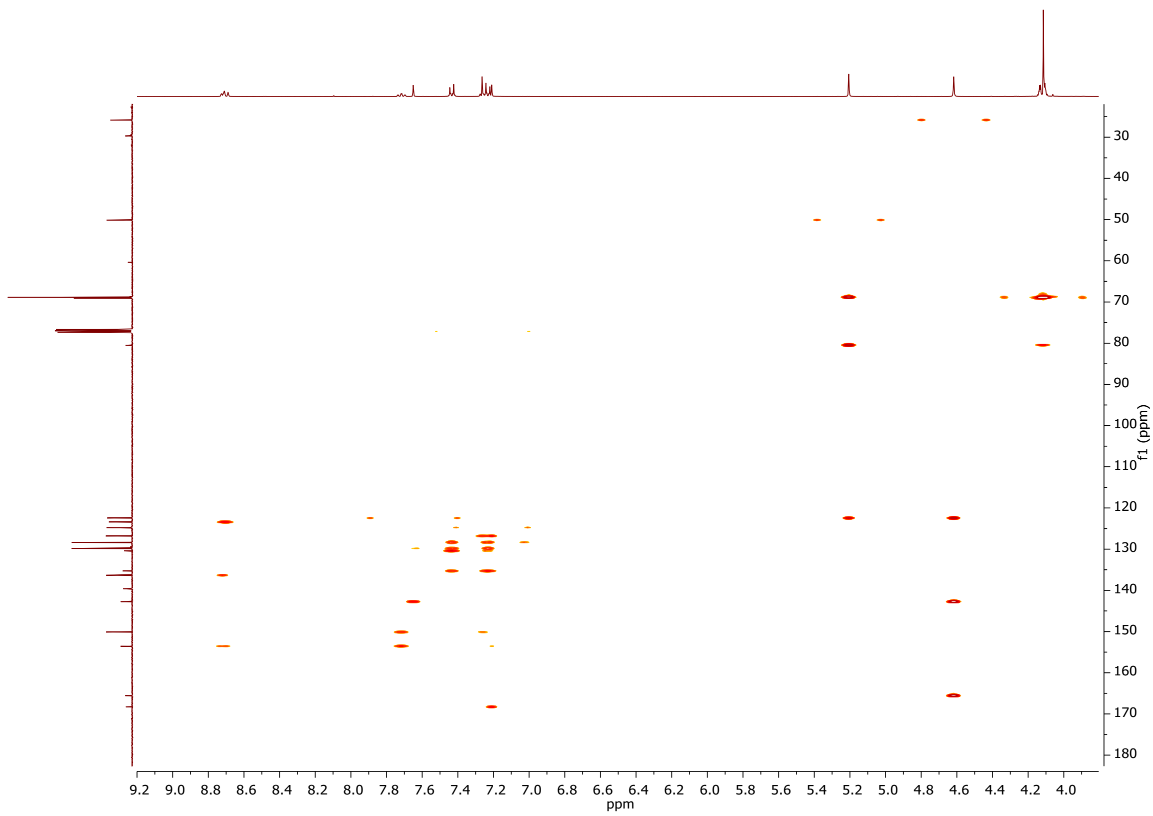


Figure S31. gHMBCAD spectrum of **15**.

Spectra of copper complexes

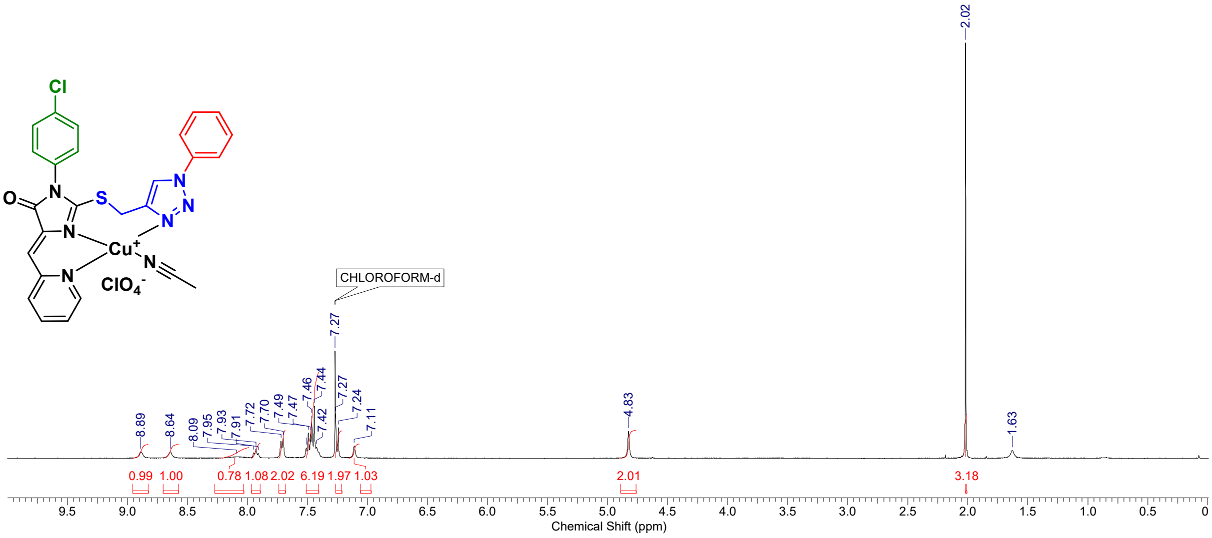


Figure S32. ¹H NMR spectra of (Z)-3-(4-chlorophenyl)-2-(((1-phenyl-1H-1,2,3-triazol-4-yl)methyl)thio)-5-(pyridin-2-ylmethylene)-3,5-dihydro-4H-imidazol-4-one copper (I) complex **10c**.

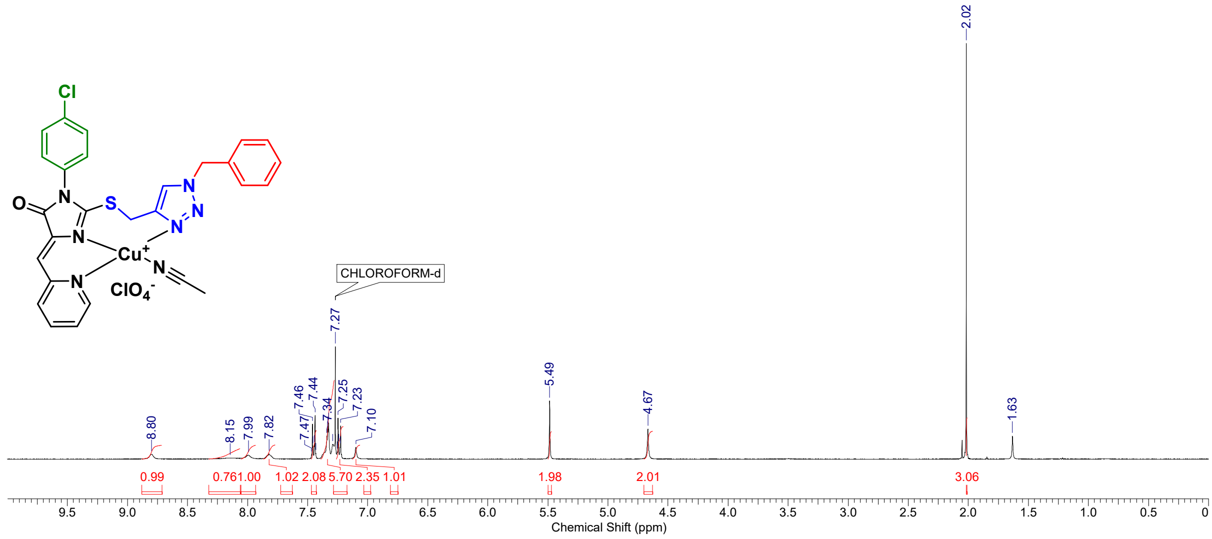


Figure S33. ¹H NMR spectra of (Z)-2-(((1-benzyl-1H-1,2,3-triazol-4-yl)methyl)thio)-3-(4-chlorophenyl)-5-(pyridin-2-ylmethylene)-3,5-dihydro-4H-imidazol-4-one copper (I) complex **11c**.

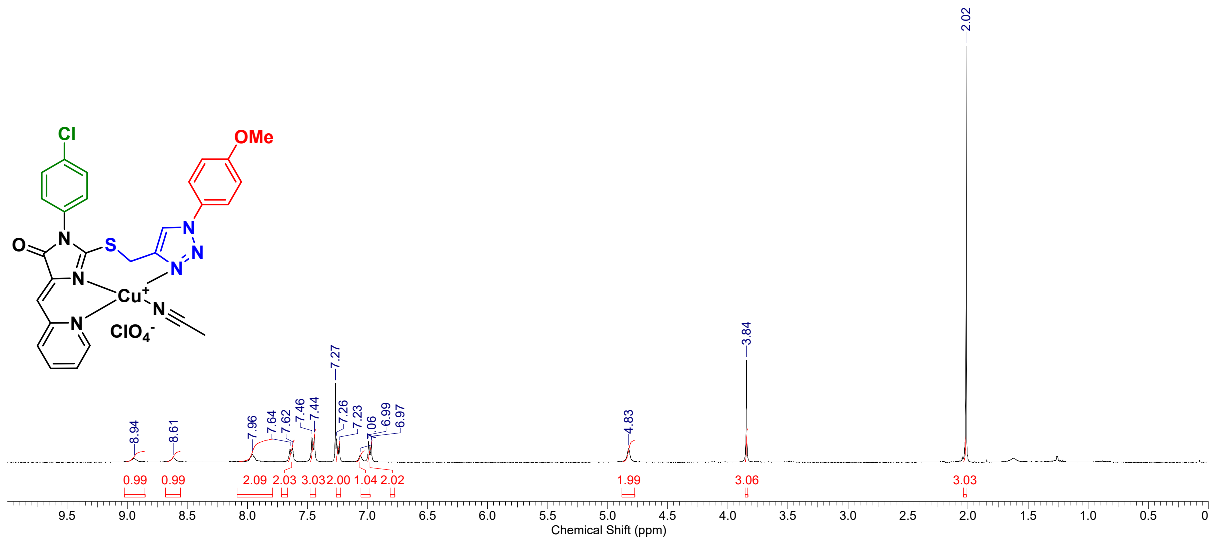


Figure S34. ¹H NMR spectra of (Z)-3-(4-chlorophenyl)-2-(((1-(4-methoxyphenyl)-1H-1,2,3-triazol-4-yl)methyl)thio)-5-(pyridin-2-ylmethylene)-3,5-dihydro-4H-imidazol-4-one copper (I) complex **12c**.

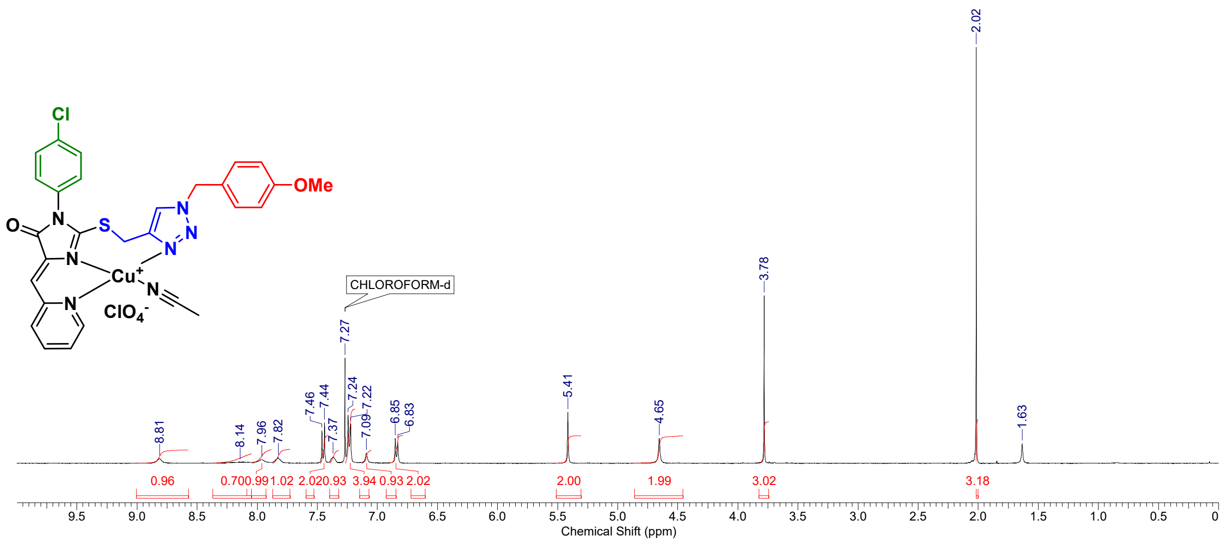


Figure S35. ^{1}H NMR spectra of (Z)-3-(4-chlorophenyl)-2-(((1-(4-methoxybenzyl)-1H-1,2,3-triazol-4-yl)methyl)thio)-5-(pyridin-2-ylmethylene)-3,5-dihydro-4H-imidazol-4-one copper (I) complex **13c**.

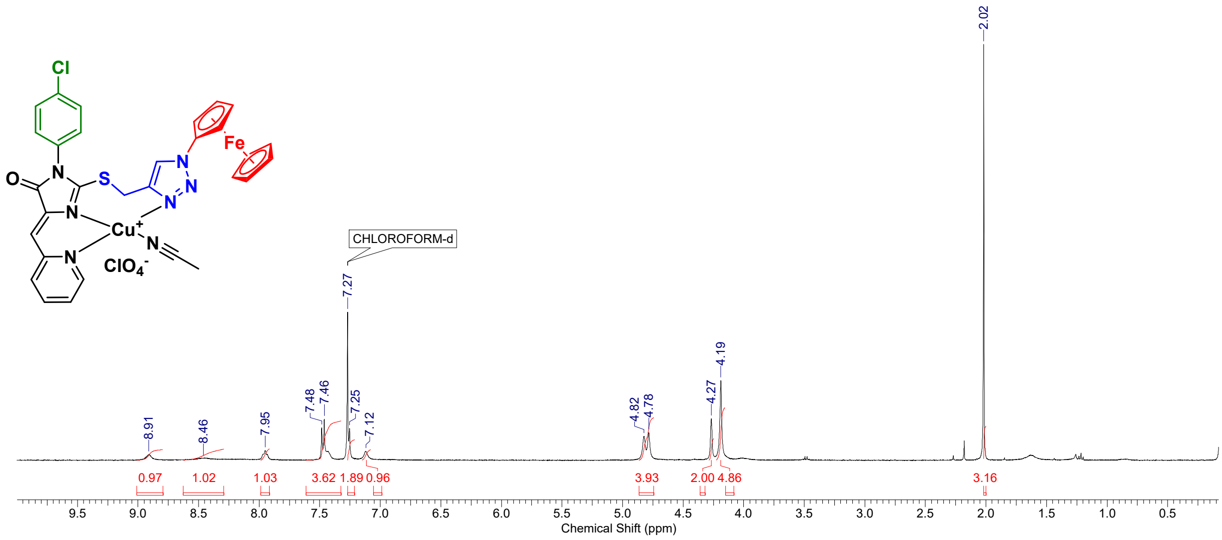


Figure S36. ^{1}H NMR spectra of (Z)-3-(4-chlorophenyl)-2-(((1-ferrocenyl-1H-1,2,3-triazol-4-yl)methyl)thio)-5-(pyridin-2-ylmethylene)-3,5-dihydro-4H-imidazol-4-one copper (I) complex **14c**.

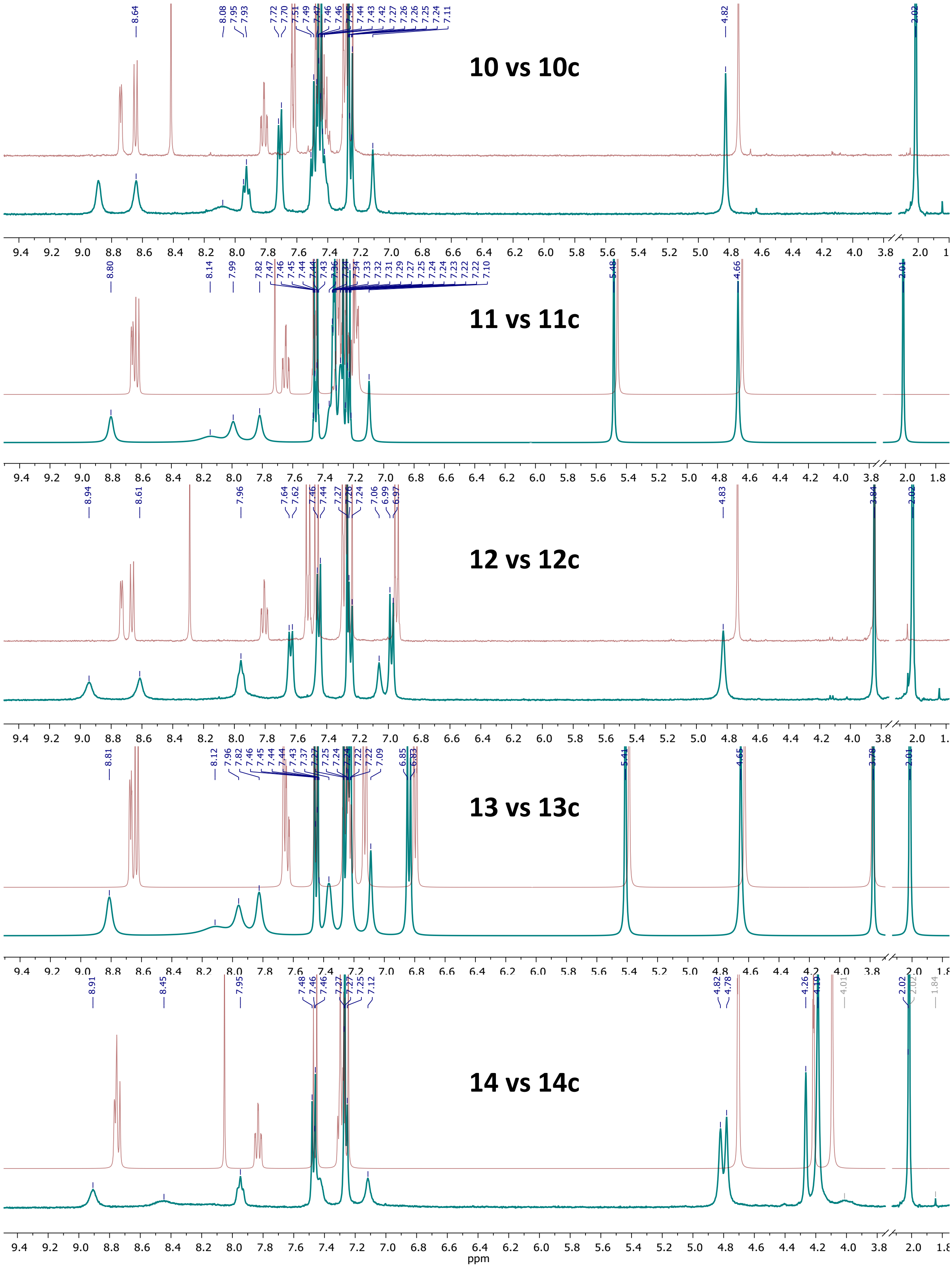


Figure S37. Comparison ^{1}H NMR spectra of ligands **10-14** (red) with corresponding complexes **10c-14c** (green).

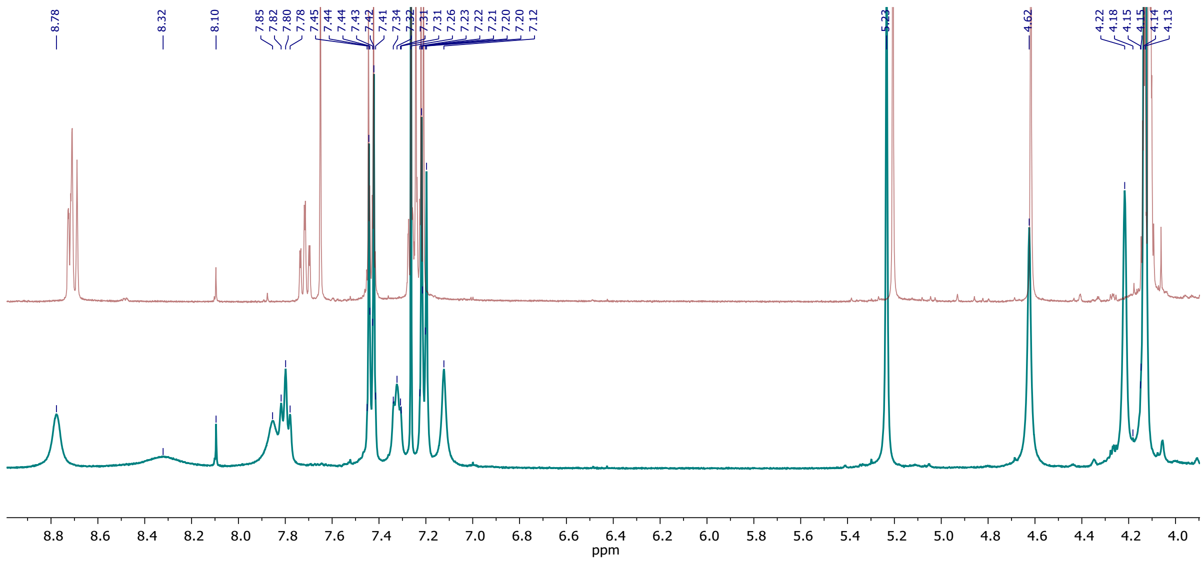
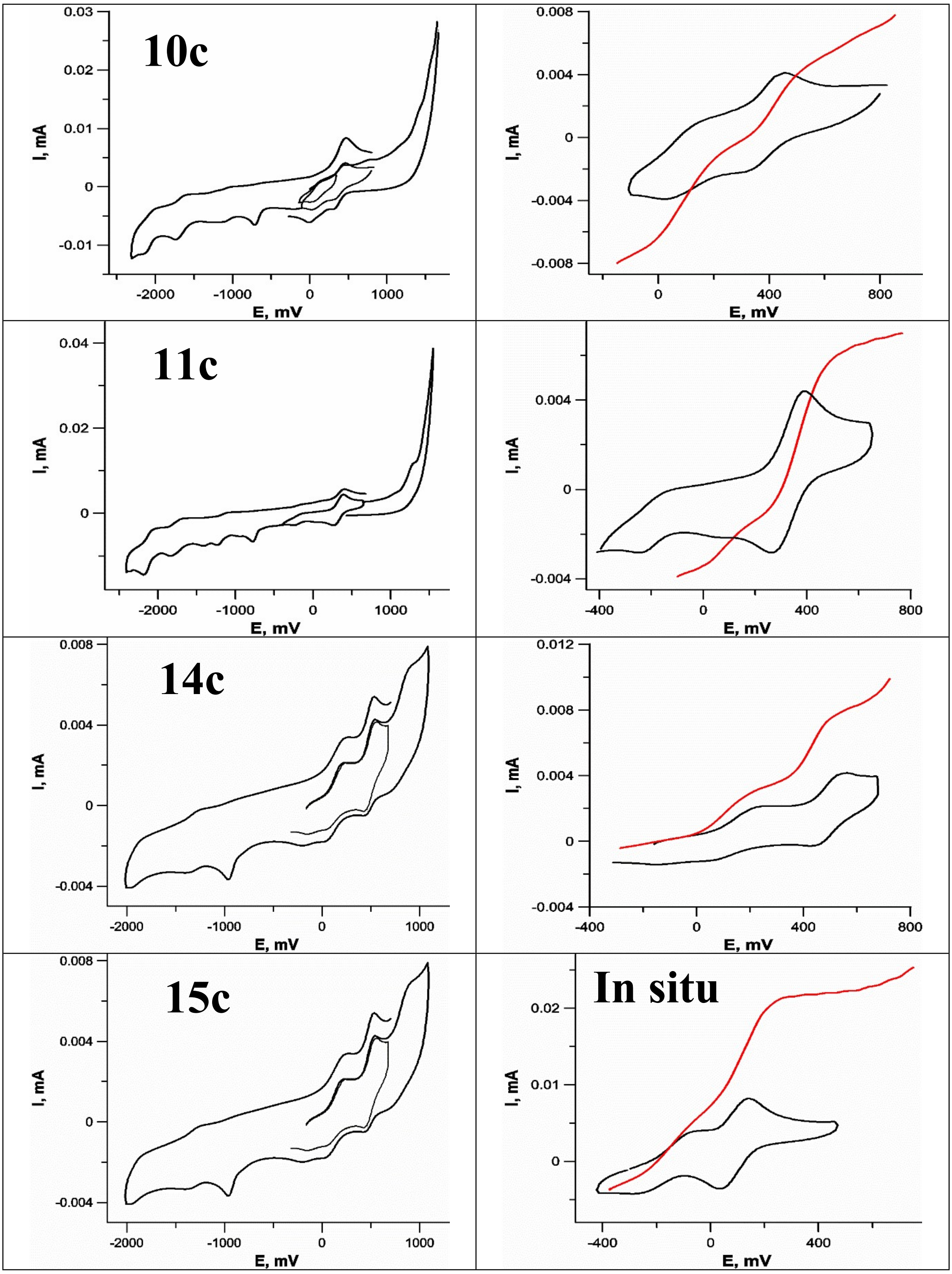


Figure S38. Comparison ^{1}H NMR spectra of ligands **15** (red) with mixture of **15** with equimolar amount of $Cu(CH_3CN)_4ClO_4$ in NMR tube (green).

Electrochemical studies



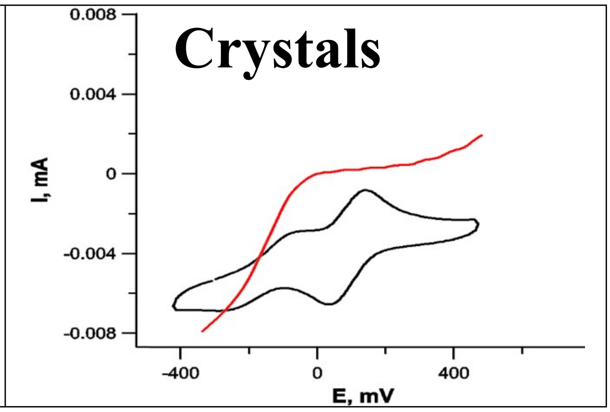


Figure S39. CV (left) and RDE (right) for complexes **10c**, **11c**, **14c**, **15c** (in situ) and (crystals).

Stability of complexes in aqueous media

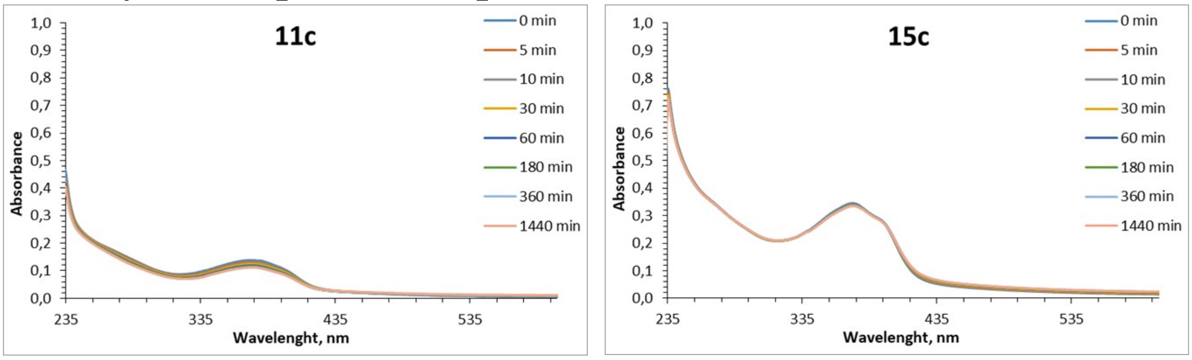


Figure S40. Optical absorption spectra of compounds **11c** and **15c** in 5% DMSO aqueous solution, C = 0.01 mM in time.

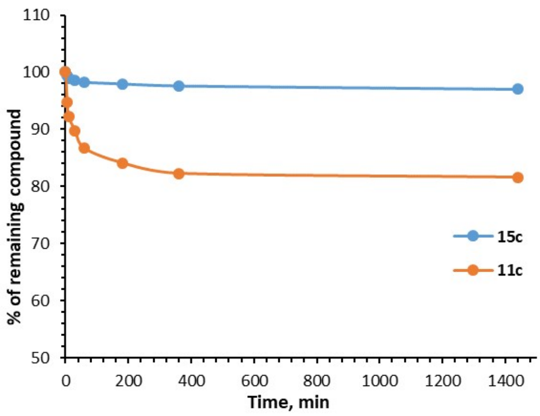
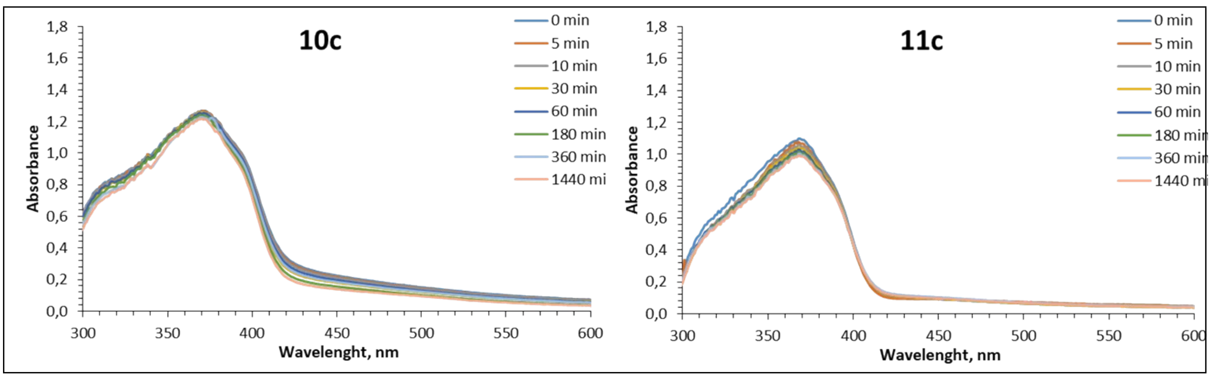


Figure S41. Kinetic curves of hydrolysis for compound **11c** and **15c** in 5% DMSO aqueous solution, C = 0.01 mM. λ = 375 nm, T = 25°C.



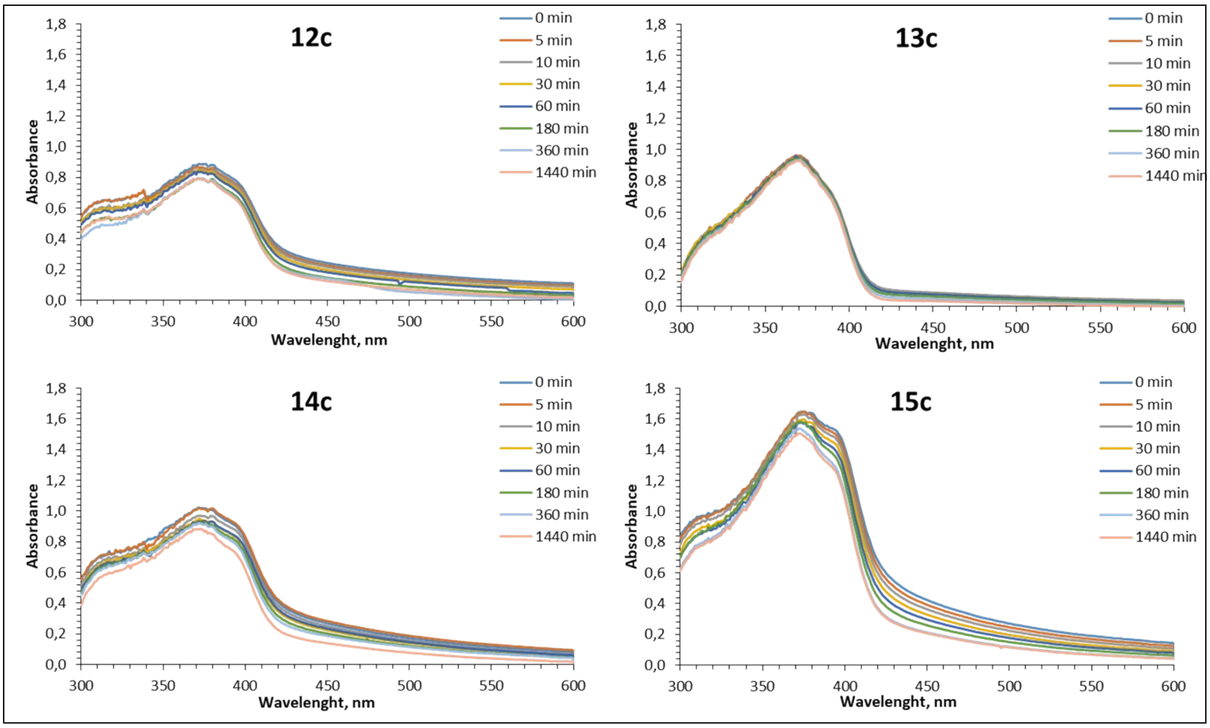


Figure S42. Optical absorption spectra of compounds **10c**-**15c** in DMEM cell culture media with 1% DMSO, C = 0.01 mM at T = 25^{o}C in time.

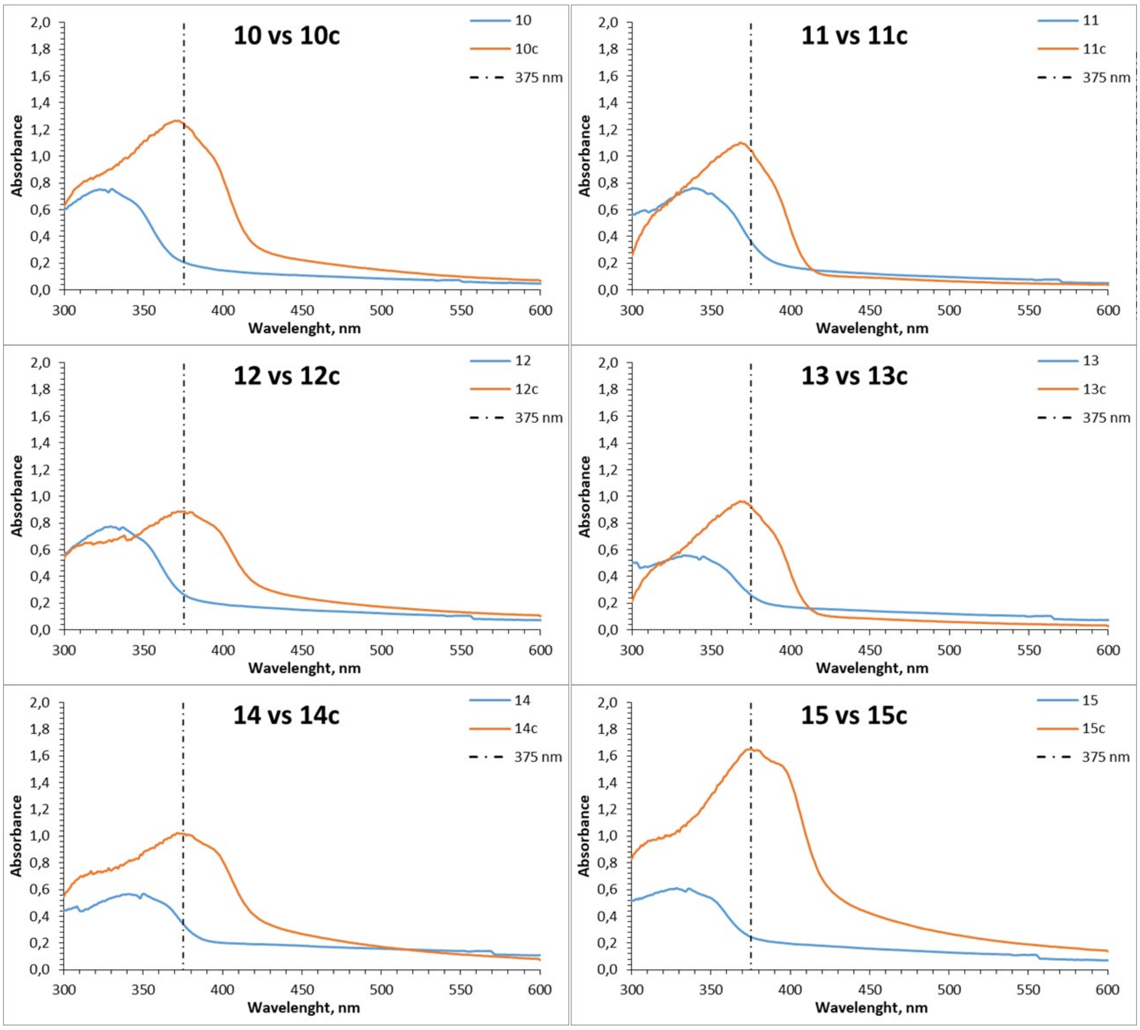


Figure S43. Optical absorption spectra of compounds **10c**-**15c** in comparison with corresponding ligands **10-15** in DMEM cell culture media with 1% DMSO, C = 0.01 mM at T = 25^{o}C. The vertical line shows the wavelength at which the kinetic curves were plotted.

In Vitro DNA intercalation test

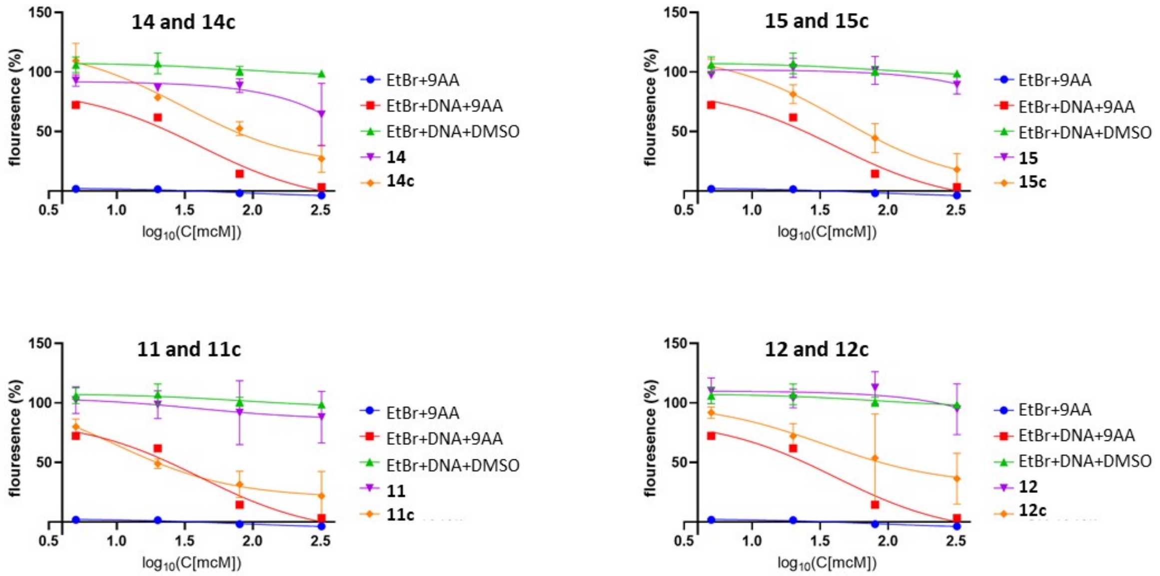
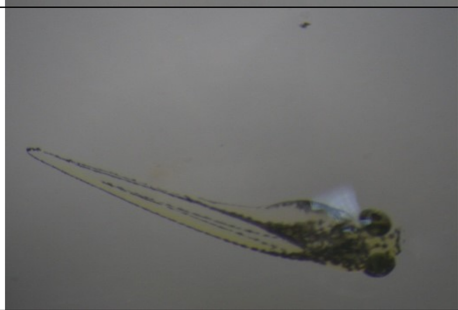
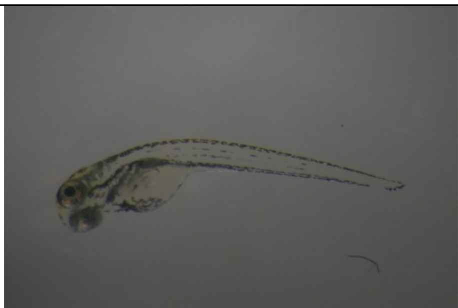


Figure S44. Decrease in the fluorescence of the EtBr-DNA complex under the influence of solutions of the coordination compound **11c**, **12c**, **14c**, **15c** and corresponding ligands. Positive control is acridine-9-amine (9AA).

In Vivo studies on zebrafish embryos

C, μM	**Ligand 15**
80	
27	
9	

3	
1	
control	

	Complex 15c	**Complex 11c**
10	X	X
5		X
2,5		
1,25		

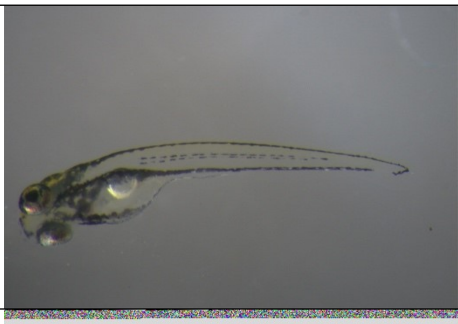
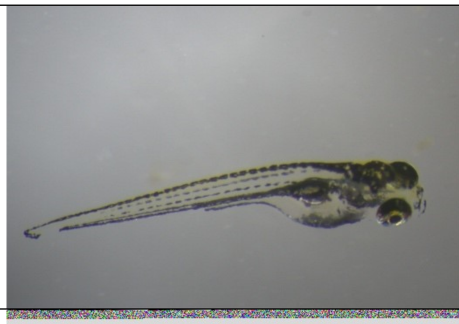
0,625		
control		

Figure S45. Photos of embryos after incubation with **15** and complexes **11c**, **15c** in concentrations 0-10/80 μM

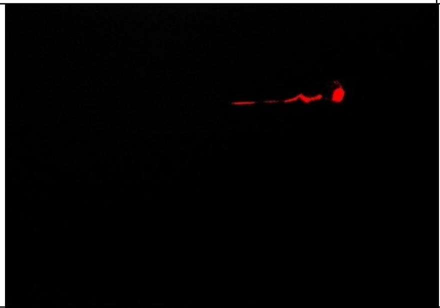
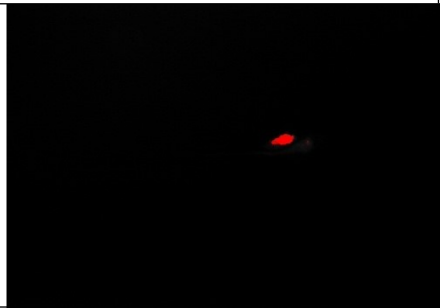
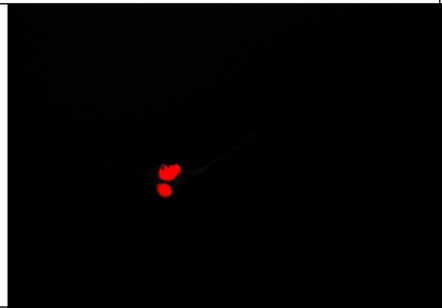
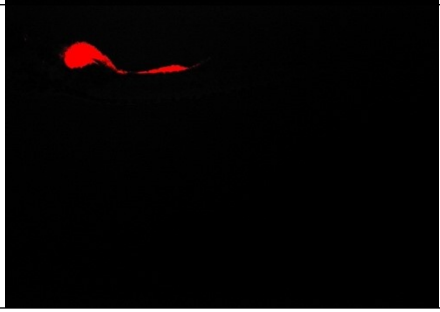
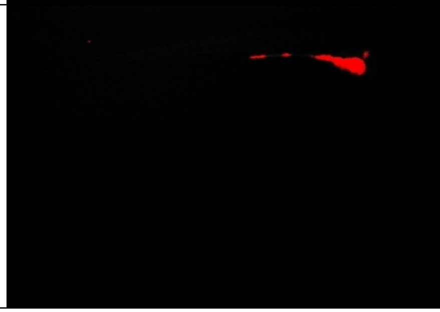
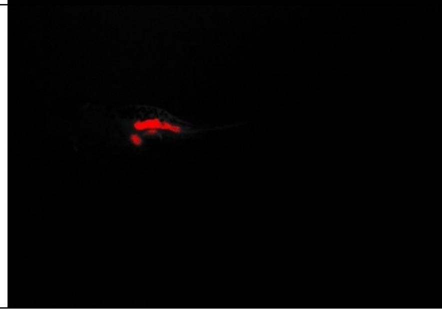
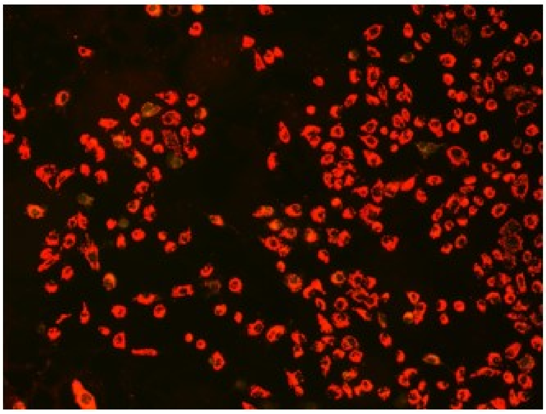
	15	15c	11c	control
The smallest				
medium				
The largest				

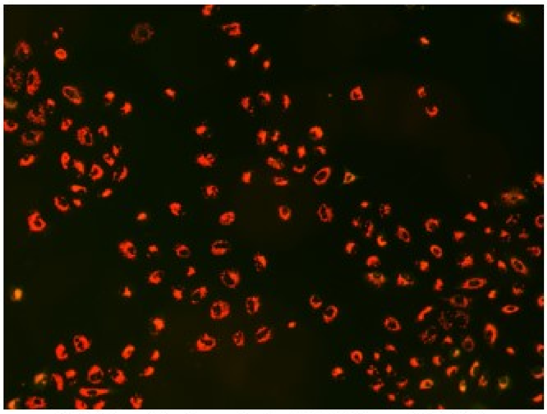
Figure S46. Tumor areas in zebrafish A549 xenograft model after incubation with DG-393 and complexes.

Membrane potential disruption studies

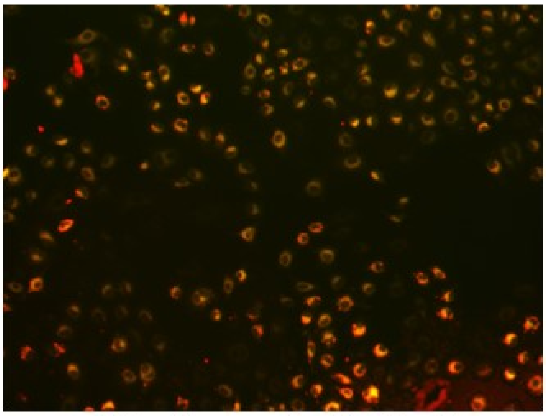
Cells A549 ($5x10^3$ cells/well) were plated out in 100 µl of DMEM/F12 media (PanEco LLC, Russia) in a 96-well plate and incubated at 37 °C, 5% CO2 for 18 h before treatment. Tested substances **15c** and **11c** were diluted in DMSO and added immediately to cells in final concentrations of 8 mcM and 10 mcM respectively. C10TPP (2 mcM) was used as a control drug. After 20 minutes of incubation, the media was changed to fresh and cationic carbocyanine dye JC1 (Lumiprobe RUS Ltd) was added up to 2 mcM and incubated for another 20 minutes. At the end of incubation cells were washed with PBS solution and analysed with CelenaX High Content Imaging System (provided by the Moscow State University Development Program).



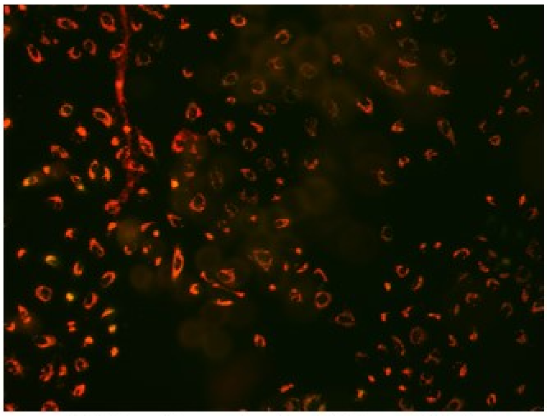
A549 cells, treated with 8 mcM **15c** and stained with 2 mcM JC1



A549 cells, treated with 10 mcM **11c** and stained with 2 mcM JC1



A549 cells, treated with 2,5 mcM C10TPP and stained with 2 mcM JC1



A549 cells, stained with 2 mcM JC1

Figure S47. Membrane potential disruption studies.

HRMS spectra of obtained compounds

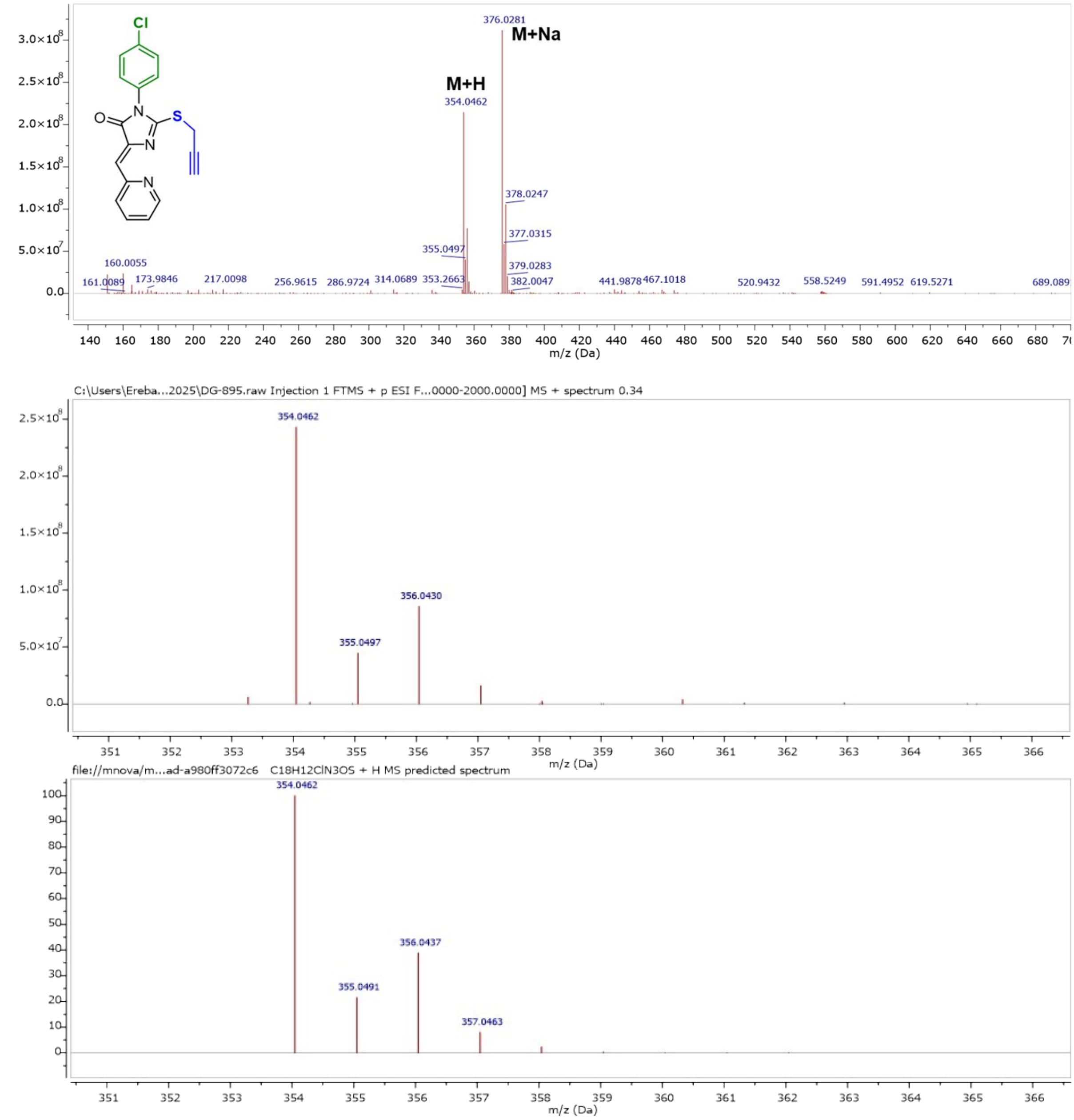


Fig. S48. Full (top), experimental [M+H] (middle) and predicted [M+H] (bottom) HRMS Spectra of compound **3**.

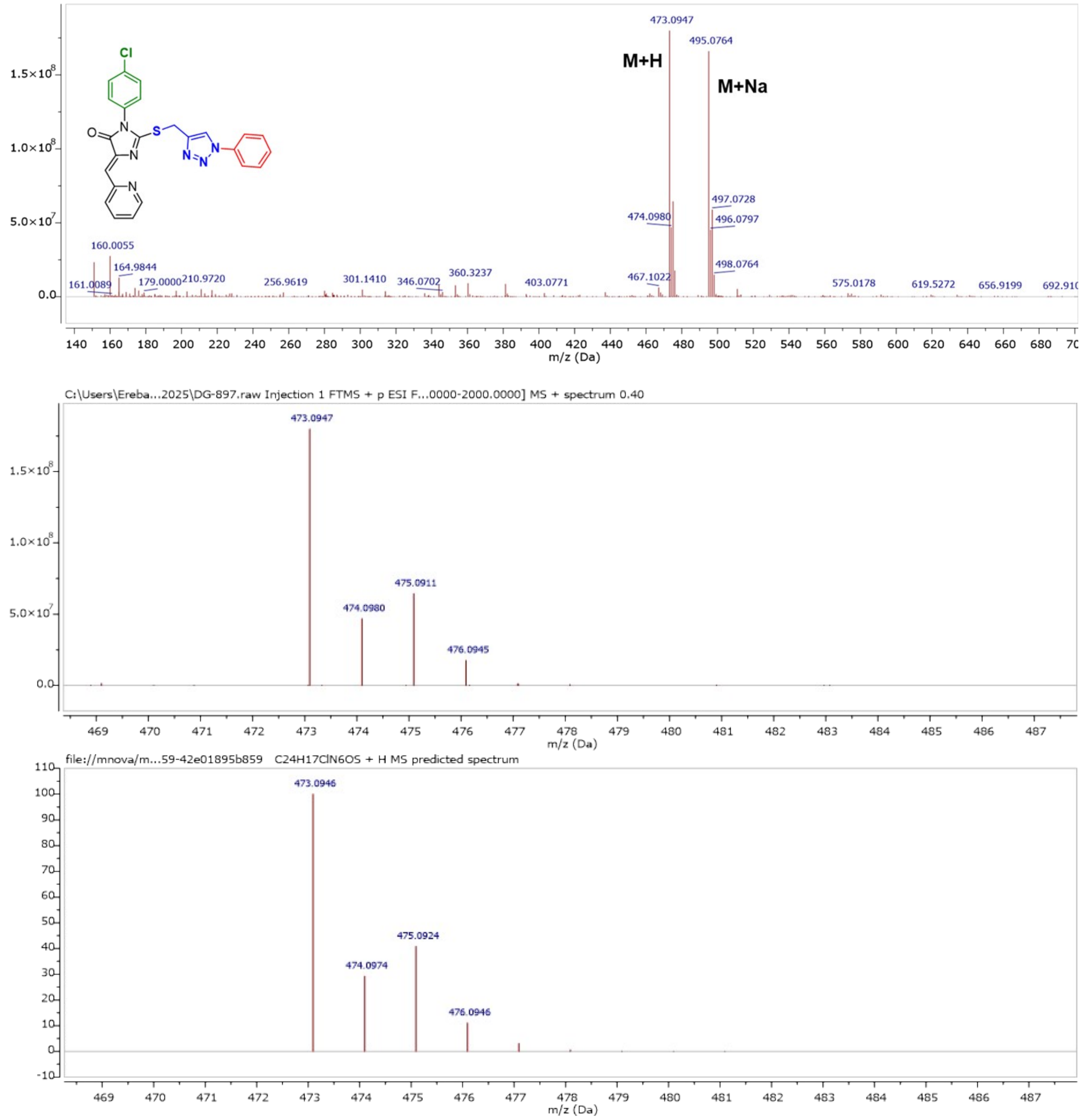


Fig. S49. Full (top), experimental [M+H] (middle) and predicted [M+H] (bottom) HRMS Spectra of compound **10**.

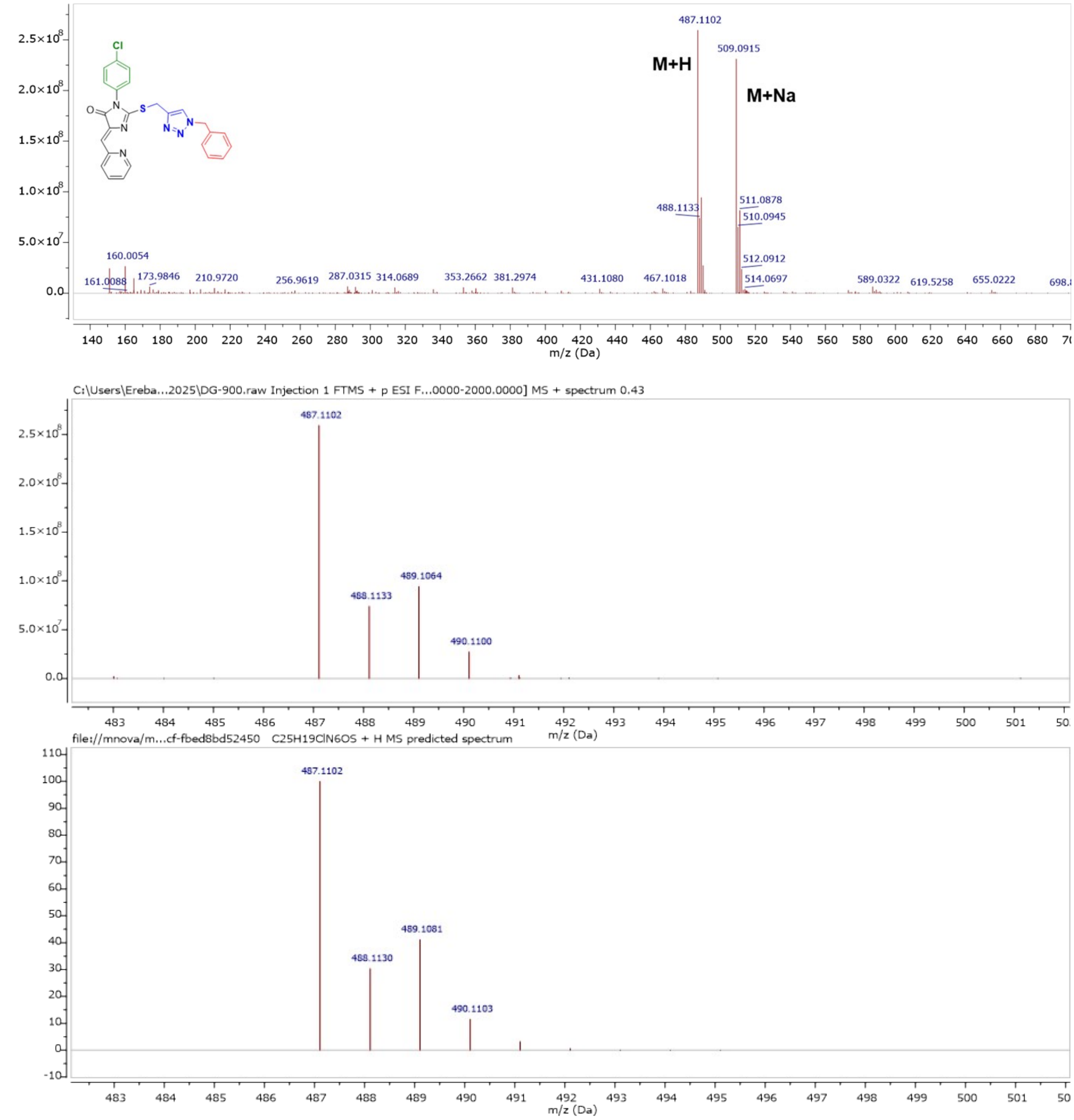


Fig. S50. Full (top), experimental [M+H] (middle) and predicted [M+H] (bottom) HRMS Spectra of compound **11**.

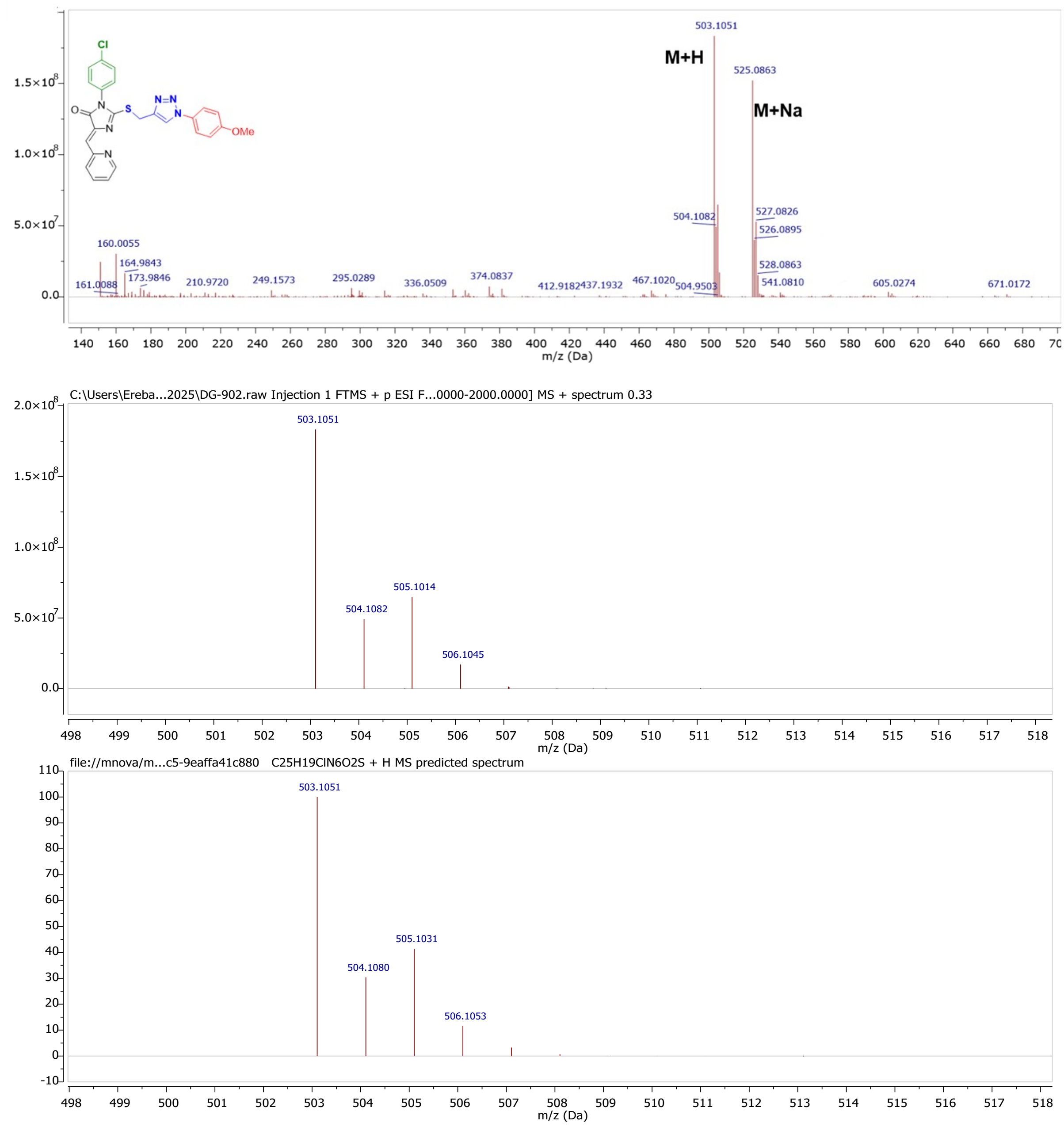


Fig. S51. Full (top), experimental [M+H] (middle) and predicted [M+H] (bottom) HRMS Spectra of compound **12**.

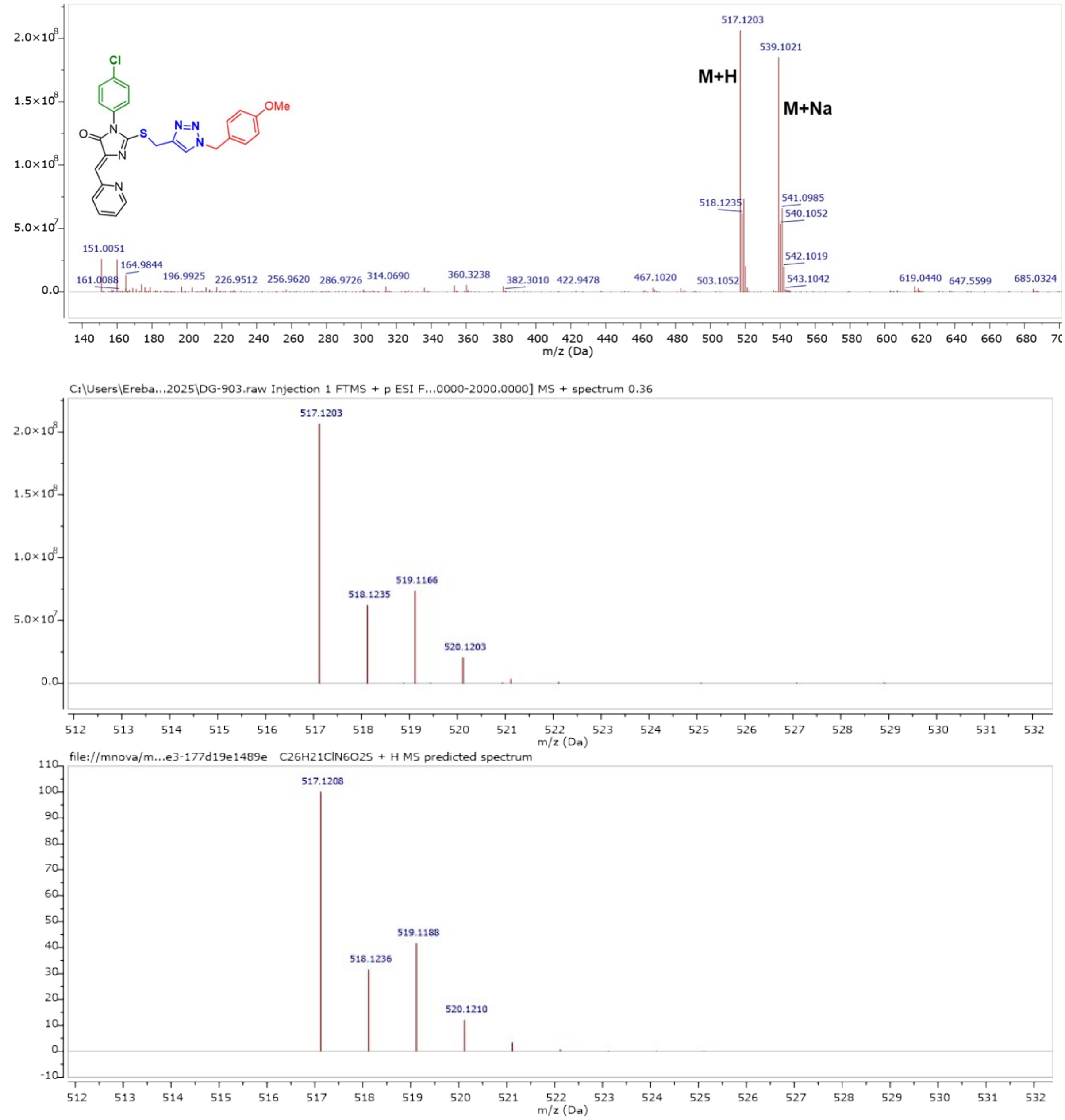


Fig. S52. Full (top), experimental [M+H] (middle) and predicted [M+H] (bottom) HRMS Spectra of compound **13**.

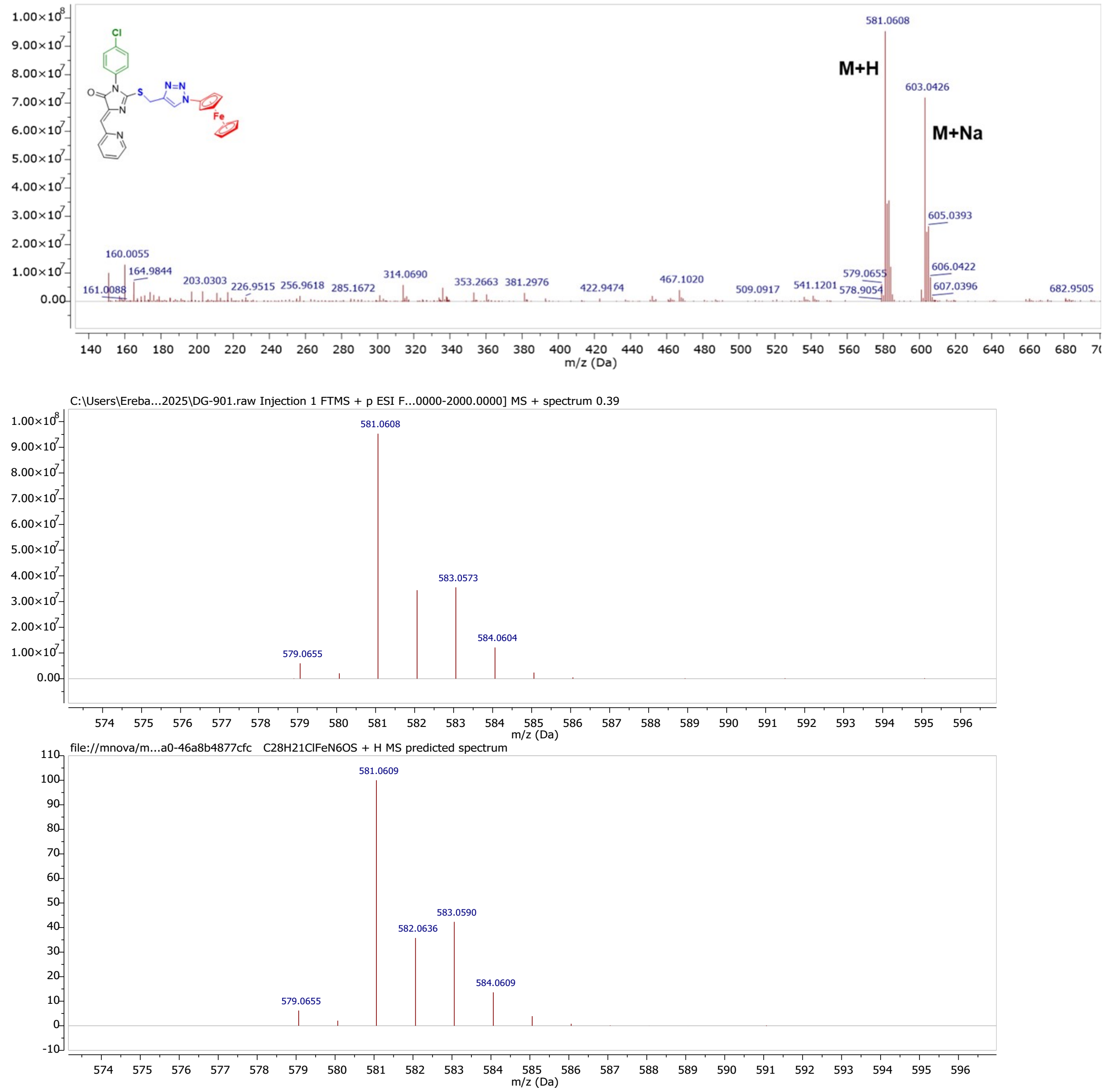


Fig. S53. Full (top), experimental [M+H] (middle) and predicted [M+H] (bottom) HRMS Spectra of compound **14**.

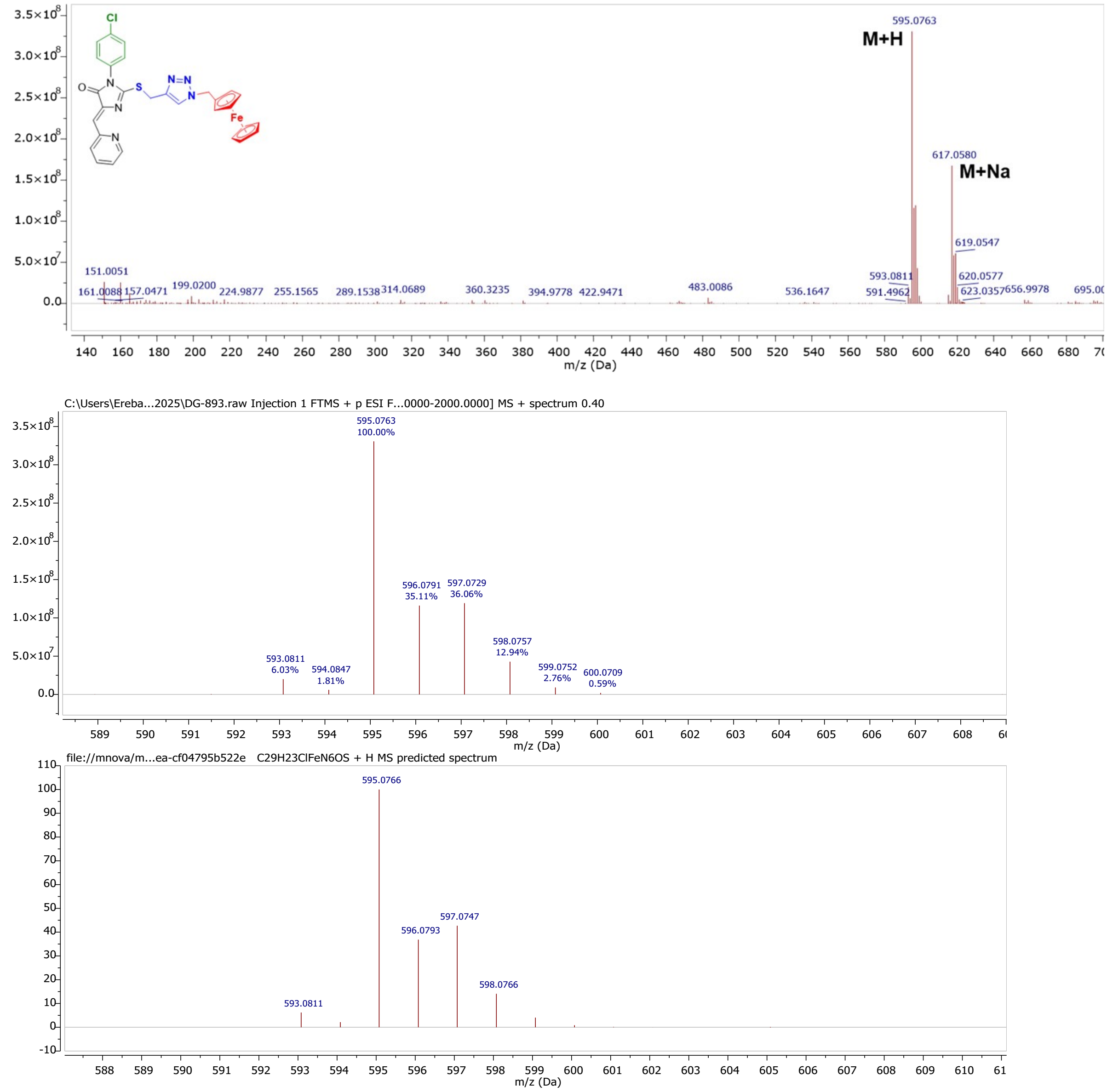


Fig. S54. Full (top), experimental [M+H] (middle) and predicted [M+H] (bottom) HRMS Spectra of compound **15**.

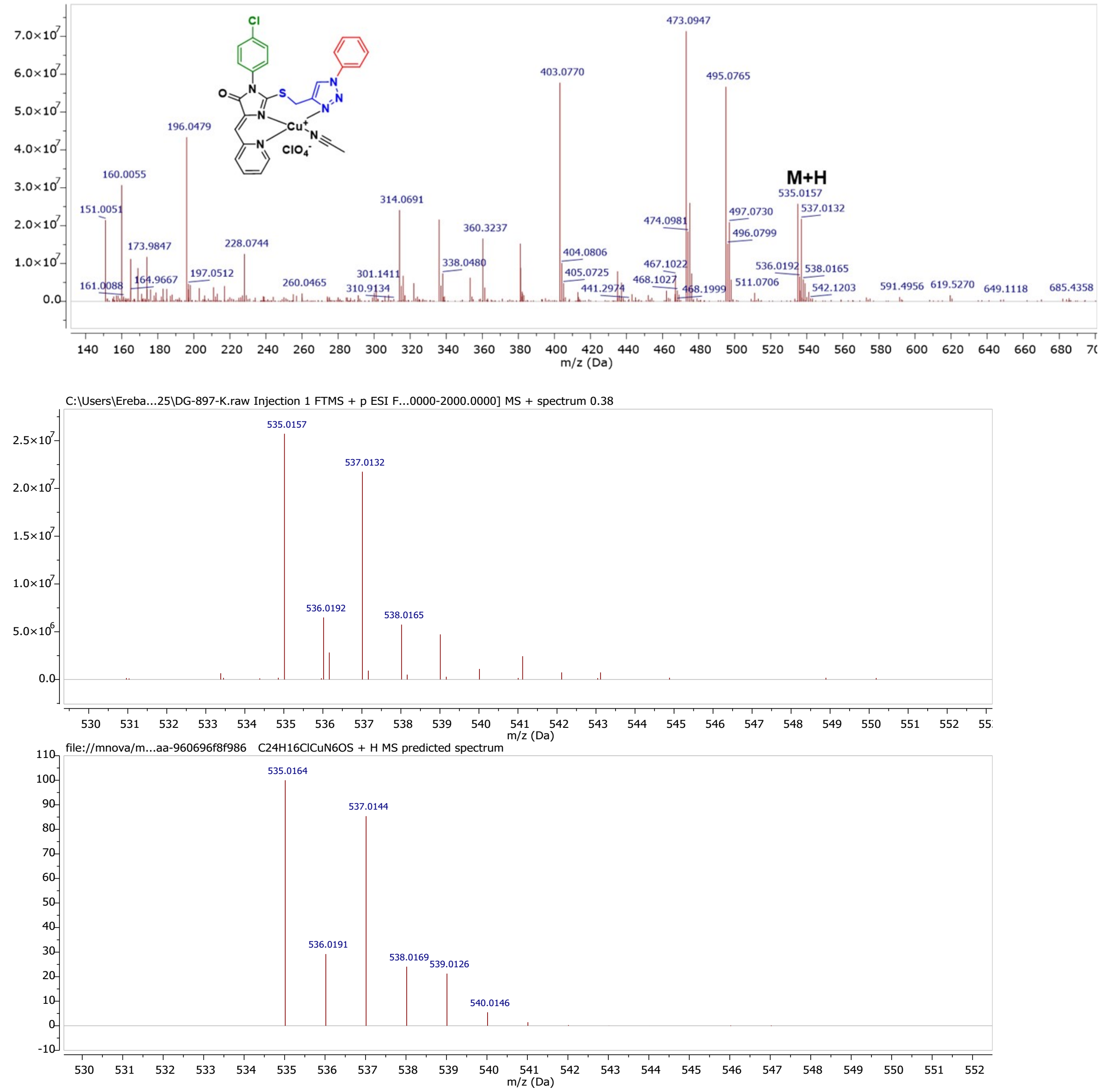


Fig. S55. Full (top), experimental [M+H] (middle) and predicted [M+H] (bottom) HRMS Spectra of compound **10c**.

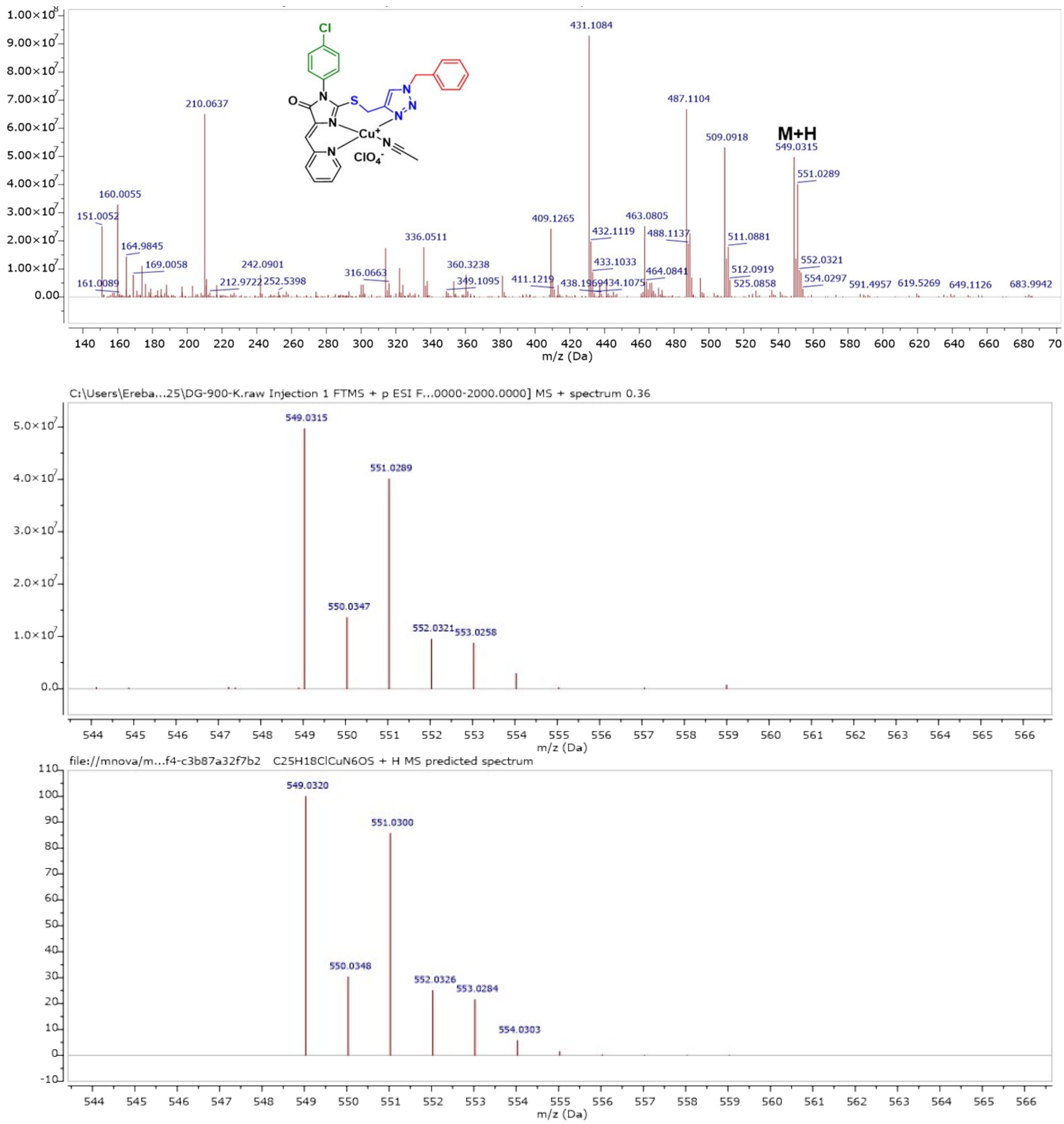


Fig. S56. Full (top), experimental [M+H] (middle) and predicted [M+H] (bottom) HRMS Spectra of compound **11c**.

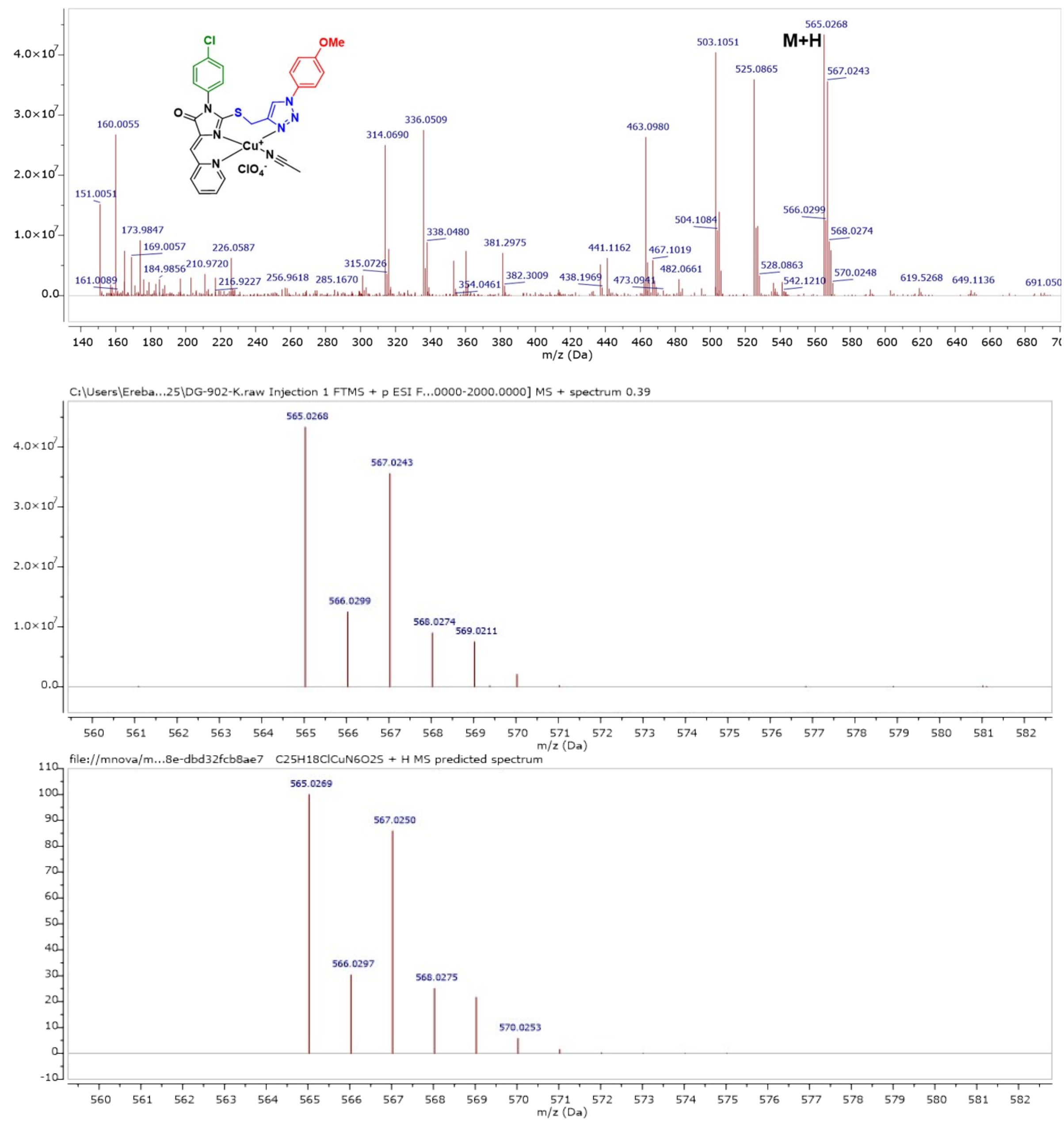


Fig. S57. Full (top), experimental [M+H] (middle) and predicted [M+H] (bottom) HRMS Spectra of compound **12c**.

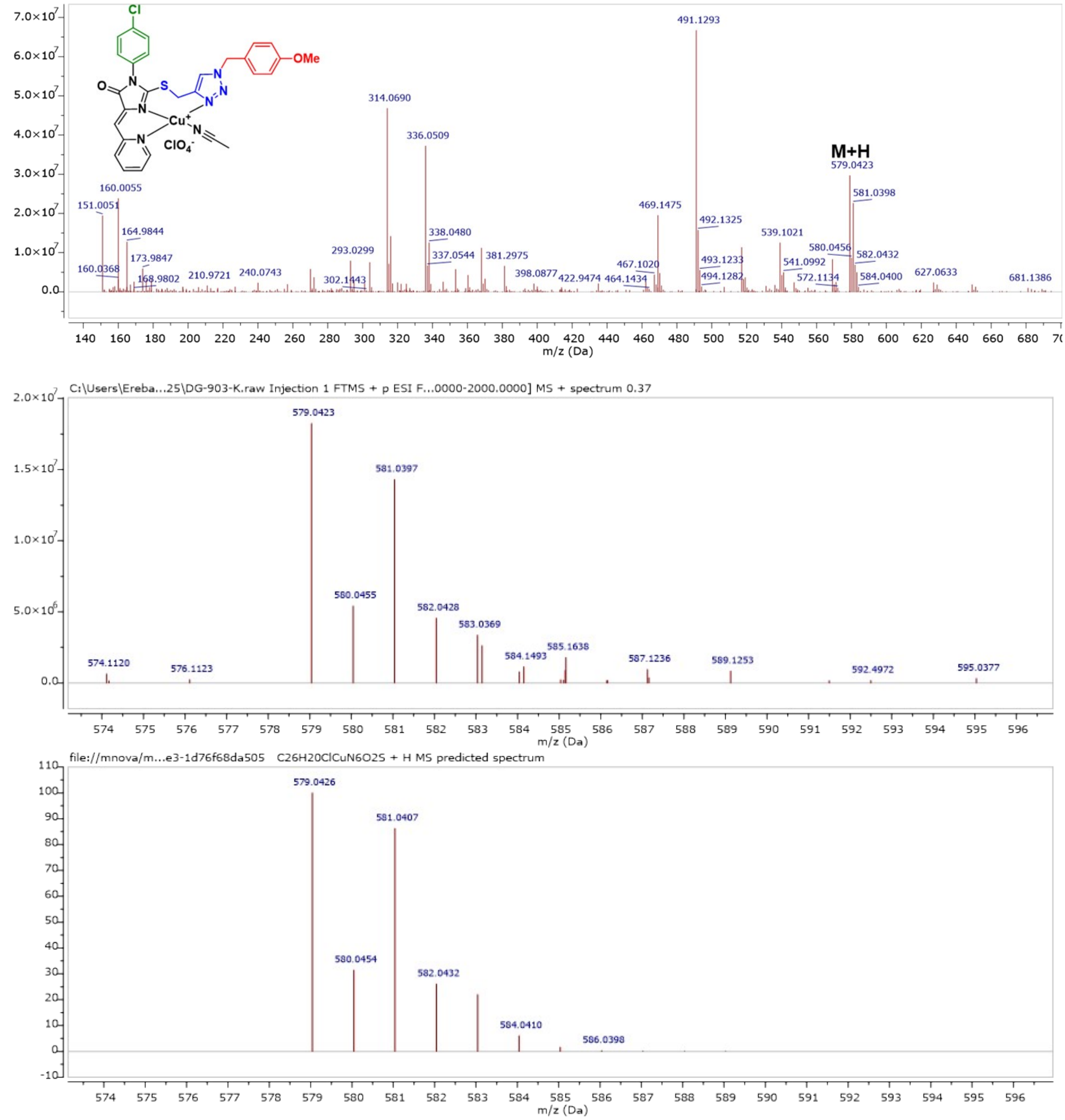


Fig. S58. Full (top), experimental [M+H] (middle) and predicted [M+H] (bottom) HRMS Spectra of compound **13c**.

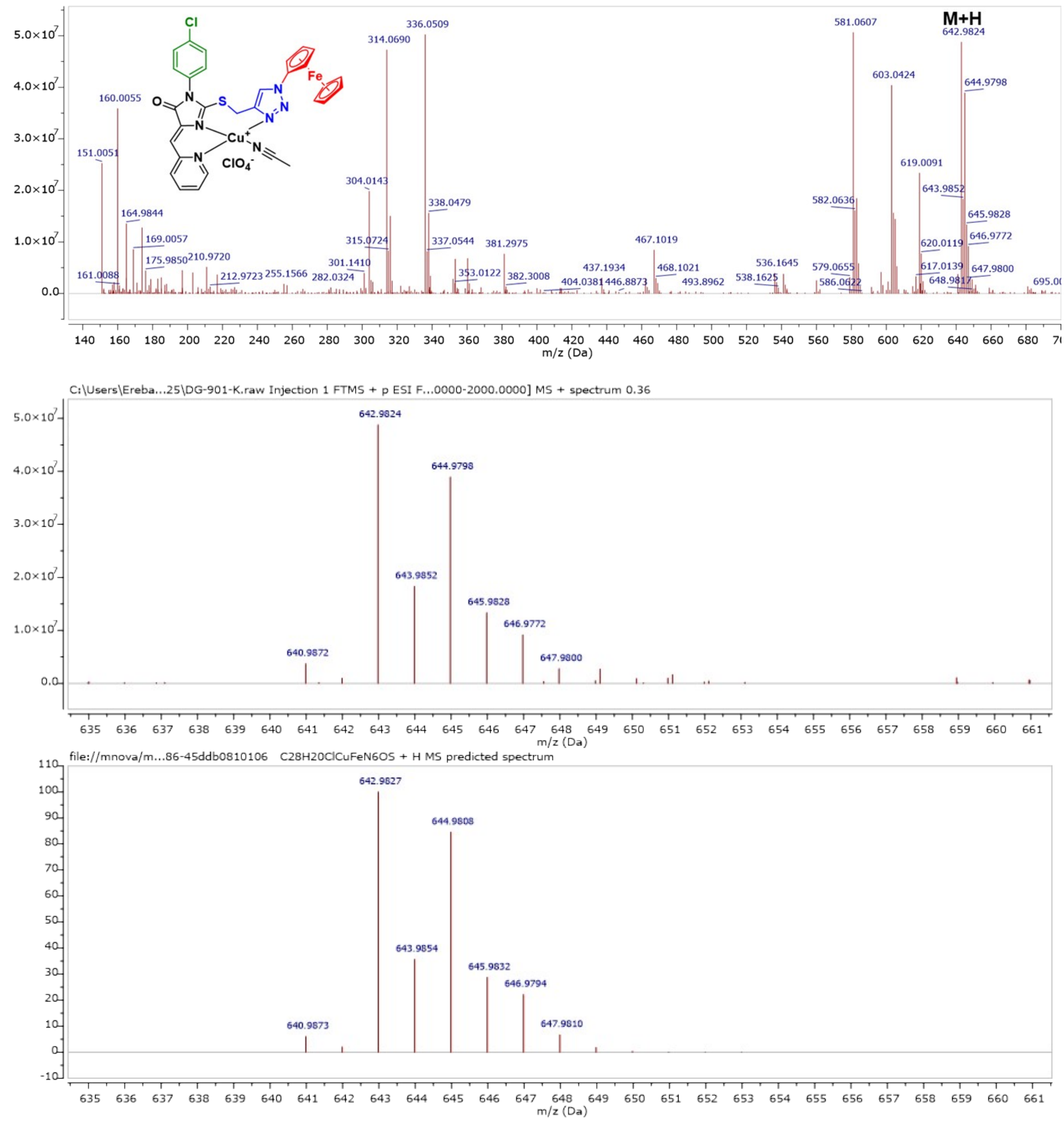


Fig. S59. Full (top), experimental [M+H] (middle) and predicted [M+H] (bottom) HRMS Spectra of compound **14c**.

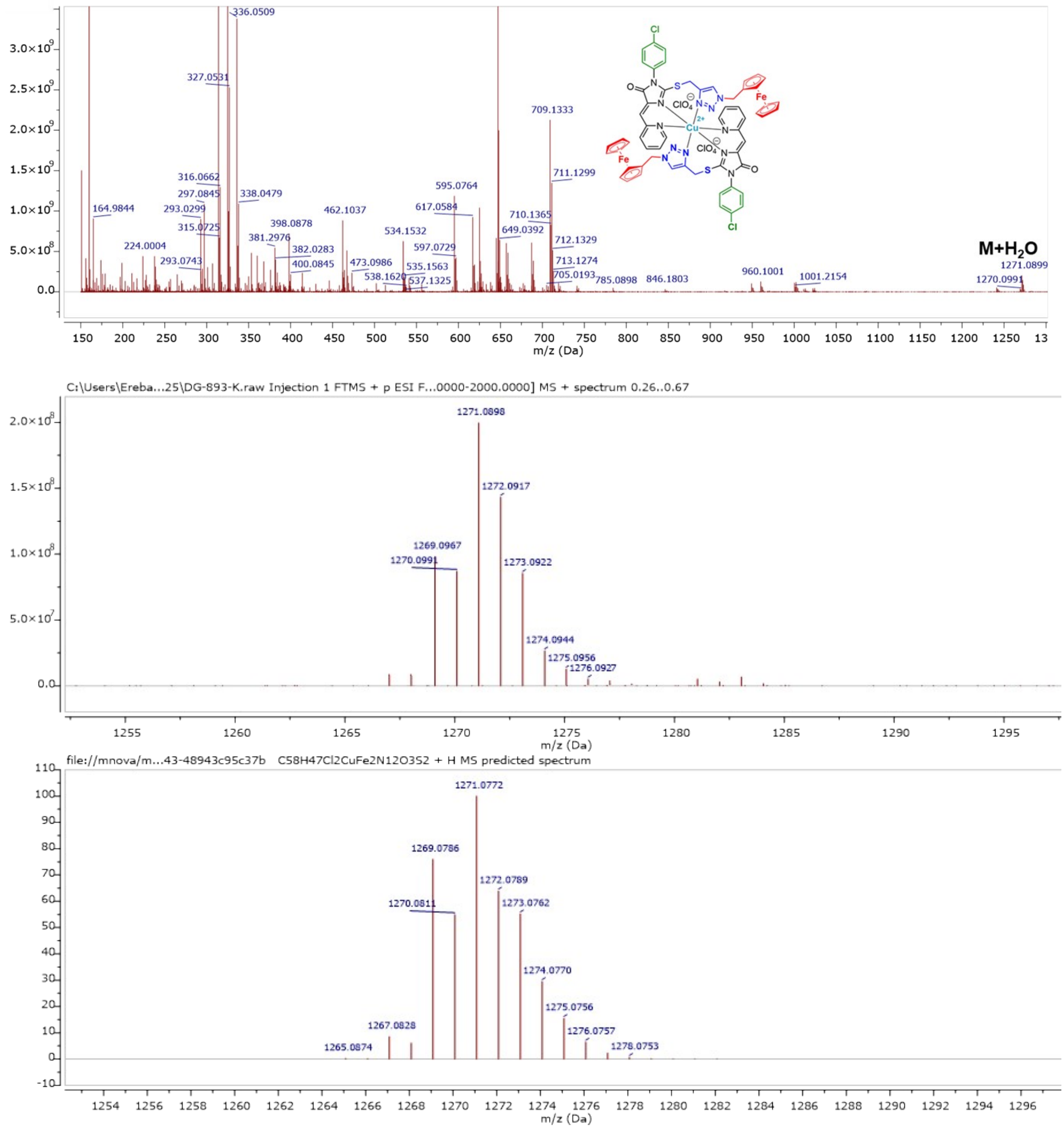


Fig. S60. Full (top), experimental [M+H$_2$O] (middle) and predicted [M+H$_2$O] (bottom) HRMS Spectra of compound **15c**.

Single crystal X-Ray diffraction studies

Numerous attempts to obtain single crystals of compounds **15c** suitable for X-ray diffraction analysis have always resulted in small crystals prone to twinning. We conducted several diffractometric experiments with different data sets and varying quantities and quality of reflections, the best of which is presented below. The data we obtained completely satisfy us and resolve beyond a doubt the question of the structure of the copper complex.

For single crystal of **15c** 40506 reflection with θ max =53.416° were measured on a STOE StadiVari Pilatus 100 K diffractometer, Cu-Kα radiation (1.54186 Å), from a GeniX3D Cu HF generator with a microfocus X-ray tube and Xenocs FOX3DHF multilayer thin-film ellipsoidal monochromator (France). Data collection and processing of the recorded diffraction peaks were performed using the X-Area 1.67 software package (STOE & Cie GmbH, Darmstadt, Germany, 2013). The intensities of the reflections on the frames obtained from the 2D detector were scaled using the LANA program (incorporated in the X-Area package), upon which diffraction data processing minimizes the intensity differences of symmetrically equivalent reflections (multiscan method). **15c** at 295 K, monoclinic; space group P 21/n; cell parameters: a = 11.6539(4), b=18.4849(6), c=30.3200(10)Å, α=90, β=91.854(3), γ=90 °, V=6528.2(4) Å ^{3}, Z = 4 Crystal structure solution and refinement were performed using SHELX-97 package. Atomic positions were located using dual method and refined using a combination of Fourier synthesis and least-square refinement in isotropic and **anisotropic** approximations. The positions of hydrogen atoms at heteroatoms (N, O) were determined from the Fourier syntheses and refined freely. The positions of the hydrogen atoms at the carbon atoms were calculated and refined in the isotropic approximation using a riding model. Refinement was made against 7429 reflections. 876 parameters were refined using 1012 restraints. The final R = 0.1269 against 7429 observed reflections, GOF= 0.877, wR2 = 0. 1448 for all reflections. The structure has been deposited at the Cambridge Crystallographic Data Center with the reference CCDC number 2503895.

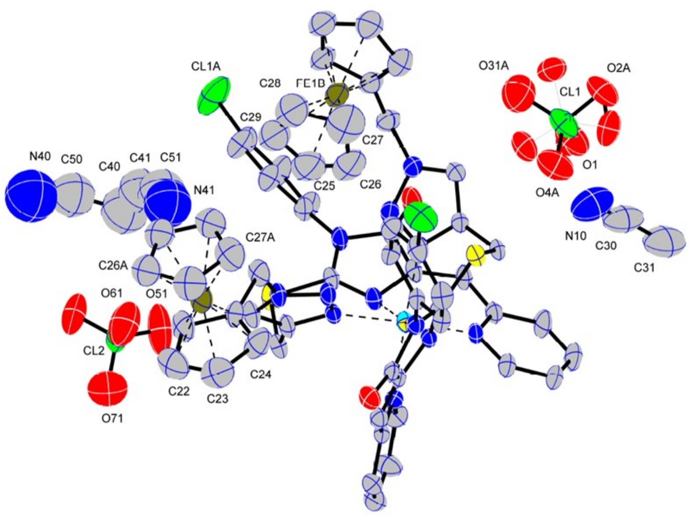


Figure S61. Molecular structure of **15c** (H-atoms are omitted, for clarity) shows the disorder in the structure of the perchlorate anion (CL1) and the solvate molecules of acetonitrile, the disorder of one of which (N41, N40), like perchlorate (CL1), is modeled by the separation of atoms. The occupancy of the positions is 0.5. Disordering of the oxygen atoms of the perchlorate anion (CL2) and the carbon atoms of the pentadiene cycles (C25 C26 C27) expressed in elongated vibration ellipsoids is also visible.

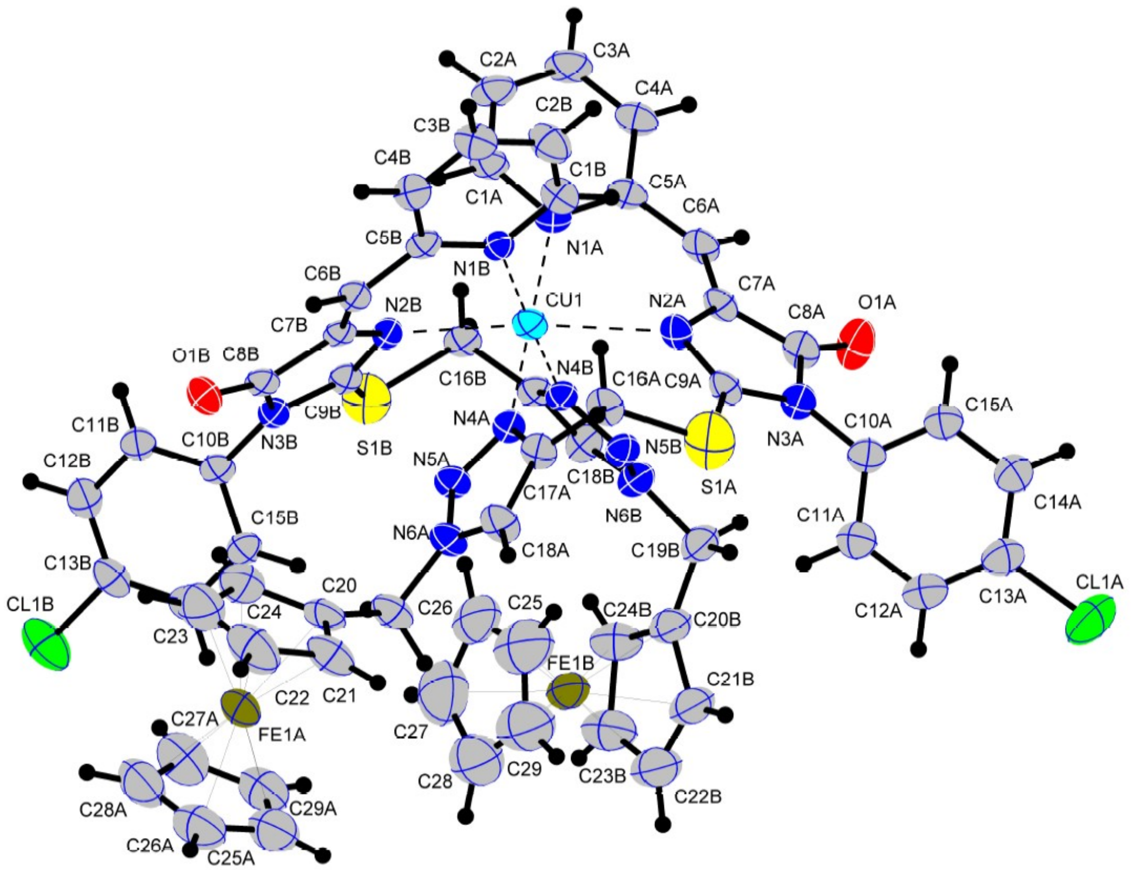


Figure S62. Molecular structure of **15c** with thermal ellipsoids. Perchlorate anions and solvent molecules are omitted for clarity.

X-Ray diffraction tables

Table S1. Crystal data and structure refinement for dg902k2n2.

Identification code	dg902k2n2	
Empirical formula	C62 H52 Cl4 Cu Fe2 N14 O10 S2	
Formula weight	1534.33	
Temperature	295(2) K	
Wavelength	1.54186 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 11.6539(4) Å	α= 90°.
	b = 18.4849(6) Å	β= 91.854(3)°.
	c = 30.3200(10) Å	γ = 90°.
Volume	6528.2(4) Å^3	
Z	4	
Density (calculated)	1.561 Mg/m^3	
Absorption coefficient	6.583 mm^{-1}	
F(000)	3132	

Crystal size	0.14 x 0.11 x 0.08 mm^3
Theta range for data collection	4.680 to 53.416°.
Index ranges	-12<=h<=12, -19<=k<=9, -31<=l<=31
Reflections collected	40506
Independent reflections	7429 [R(int) = 0.1358]
Completeness to theta = 53.416°	96.4 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7429 / 1012 / 876
Goodness-of-fit on F^2	0.877
Final R indices [I>2sigma(I)]	R1 = 0.0561, wR2 = 0.1229
R indices (all data)	R1 = 0.1269, wR2 = 0.1448
Largest diff. peak and hole	0.520 and -0.355 e.$Å^{-3}$

Table S2. Bond lengths [Å] and angles [°] for dg902k2n2.

Cu(1)-N(4A)	2.019(5)
Cu(1)-N(4B)	2.048(5)
Cu(1)-N(1A)	2.050(5)
Cu(1)-N(1B)	2.068(5)
Cu(1)-N(2B)	2.365(5)
Cu(1)-N(2A)	2.410(6)
Fe(1A)-C(23)	1.979(11)
Fe(1A)-C(27A)	1.997(11)
Fe(1A)-C(24)	2.013(9)
Fe(1A)-C(20)	2.013(7)
Fe(1A)-C(21)	2.017(9)
Fe(1A)-C(28A)	2.026(10)
Fe(1A)-C(22)	2.028(11)
Fe(1A)-C(26A)	2.050(10)
Fe(1A)-C(25A)	2.055(10)
Fe(1A)-C(29A)	2.059(10)
Cl(1A)-C(13A)	1.725(9)
S(1A)-C(9A)	1.710(7)
S(1A)-C(16A)	1.797(7)
O(1A)-C(8A)	1.192(8)
N(1A)-C(1A)	1.344(8)
N(1A)-C(5A)	1.351(8)
N(2A)-C(9A)	1.326(8)

N(2A)-C(7A)	1.406(8)
N(3A)-C(8A)	1.376(8)
N(3A)-C(9A)	1.376(8)
N(3A)-C(10A)	1.436(9)
N(4A)-N(5A)	1.341(7)
N(4A)-C(17A)	1.356(8)
N(5A)-N(6A)	1.330(7)
N(6A)-C(18A)	1.337(8)
N(6A)-C(19A)	1.485(8)
C(1A)-C(2A)	1.347(9)
C(1A)-H(1A)	0.9300
C(2A)-C(3A)	1.362(10)
C(2A)-H(2A)	0.9300
C(3A)-C(4A)	1.379(10)
C(3A)-H(3A)	0.9300
C(4A)-C(5A)	1.391(9)
C(4A)-H(4A)	0.9300
C(5A)-C(6A)	1.449(9)
C(6A)-C(7A)	1.336(8)
C(6A)-H(6A)	0.9300
C(7A)-C(8A)	1.480(10)
C(10A)-C(15A)	1.353(10)
C(10A)-C(11A)	1.366(10)
C(11A)-C(12A)	1.380(10)
C(11A)-H(11A)	0.9300
C(12A)-C(13A)	1.362(11)
C(12A)-H(12A)	0.9300
C(13A)-C(14A)	1.353(10)
C(14A)-C(15A)	1.402(10)
C(14A)-H(14A)	0.9300
C(15A)-H(15A)	0.9300
C(16A)-C(17A)	1.475(9)
C(16A)-H(16A)	0.9700
C(16A)-H(16B)	0.9700
C(17A)-C(18A)	1.358(9)
C(18A)-H(18A)	0.9300
C(19A)-C(20)	1.479(10)
C(19A)-H(19A)	0.9700

C(19A)-H(19B)	0.9700
C(25A)-C(29A)	1.384(12)
C(25A)-C(26A)	1.387(13)
C(25A)-H(25A)	0.9300
C(26A)-C(28A)	1.384(13)
C(26A)-H(26A)	0.9300
C(28A)-C(27A)	1.418(13)
C(28A)-H(28A)	0.9300
C(27A)-C(29A)	1.391(13)
C(27A)-H(27A)	0.9300
C(29A)-H(29A)	0.9300
Fe(1B)-C(21B)	1.986(9)
Fe(1B)-C(24B)	1.994(9)
Fe(1B)-C(27)	2.005(13)
Fe(1B)-C(20B)	2.017(9)
Fe(1B)-C(25)	2.025(13)
Fe(1B)-C(23B)	2.025(10)
Fe(1B)-C(22B)	2.028(10)
Fe(1B)-C(26)	2.032(11)
Fe(1B)-C(29)	2.035(12)
Fe(1B)-C(28)	2.036(12)
S(1B)-C(9B)	1.730(7)
S(1B)-C(16B)	1.811(7)
Cl(1B)-C(13B)	1.731(8)
O(1B)-C(8B)	1.193(7)
N(1B)-C(1B)	1.346(8)
N(1B)-C(5B)	1.360(8)
N(2B)-C(9B)	1.307(7)
N(2B)-C(7B)	1.405(8)
N(3B)-C(9B)	1.370(8)
N(3B)-C(8B)	1.407(8)
N(3B)-C(10B)	1.445(8)
N(4B)-N(5B)	1.314(7)
N(4B)-C(17B)	1.363(8)
N(5B)-N(6B)	1.340(7)
N(6B)-C(18B)	1.333(8)
N(6B)-C(19B)	1.462(8)
C(1B)-C(2B)	1.367(9)

C(1B)-H(1B)	0.9300
C(2B)-C(3B)	1.366(10)
C(2B)-H(2B)	0.9300
C(3B)-C(4B)	1.373(9)
C(3B)-H(3B)	0.9300
C(4B)-C(5B)	1.392(9)
C(4B)-H(4B)	0.9300
C(5B)-C(6B)	1.453(9)
C(6B)-C(7B)	1.334(8)
C(6B)-H(6B)	0.9300
C(7B)-C(8B)	1.490(9)
C(10B)-C(11B)	1.370(9)
C(10B)-C(15B)	1.379(9)
C(11B)-C(12B)	1.385(9)
C(11B)-H(11B)	0.9300
C(12B)-C(13B)	1.380(10)
C(12B)-H(12B)	0.9300
C(13B)-C(14B)	1.359(10)
C(14B)-C(15B)	1.398(9)
C(14B)-H(14B)	0.9300
C(15B)-H(15B)	0.9300
C(16B)-C(17B)	1.473(9)
C(16B)-H(16C)	0.9700
C(16B)-H(16D)	0.9700
C(17B)-C(18B)	1.356(9)
C(18B)-H(18B)	0.9300
C(19B)-C(20B)	1.477(10)
C(19B)-H(19A)	0.9700
C(19B)-H(19B)	0.9700
C(20B)-C(24B)	1.409(11)
C(20B)-C(21B)	1.430(11)
C(21B)-C(22B)	1.361(12)
C(21B)-H(21B)	0.9300
C(22B)-C(23B)	1.389(12)
C(22B)-H(22B)	0.9300
C(23B)-C(24B)	1.434(12)
C(23B)-H(23B)	0.9300
C(24B)-H(24B)	0.9300

N(10)-C(30)	1.090(18)
C(30)-C(31)	1.401(18)
C(31)-H(31A)	0.9600
C(31)-H(31B)	0.9600
C(31)-H(31C)	0.9600
C(25)-C(26)	1.279(16)
C(25)-C(29)	1.281(16)
C(25)-H(25)	0.9300
C(26)-C(27)	1.521(17)
C(26)-H(26)	0.9300
C(27)-C(28)	1.478(16)
C(27)-H(27)	0.9300
C(28)-C(29)	1.347(15)
C(28)-H(28)	0.9300
C(29)-H(29)	0.9300
Cl(1)-O(4)	1.395(15)
Cl(1)-O(2)	1.408(13)
Cl(1)-O(31)	1.412(14)
Cl(1)-O(1)	1.418(11)
Cl(2)-O(51)	1.327(7)
Cl(2)-O(71)	1.356(10)
Cl(2)-O(81)	1.373(7)
Cl(2)-O(61)	1.412(8)
C(20)-C(21)	1.391(10)
C(20)-C(24)	1.430(11)
C(21)-C(22)	1.404(12)
C(21)-H(21)	0.9300
C(22)-C(23)	1.354(13)
C(22)-H(22)	0.9300
C(23)-C(24)	1.417(13)
C(23)-H(23)	0.9300
C(24)-H(24)	0.9300
O(4A)-Cl(3)	1.378(14)
Cl(3)-O(2A)	1.392(14)
Cl(3)-O(31A)	1.421(15)
Cl(3)-O(3)	1.424(12)
C(40)-C(50)	1.4795
C(40)-H(40A)	0.9600

C(40)-H(40B)	0.9600
C(40)-H(40C)	0.9600
C(50)-N(40)	1.1226
C(41)-C(51)	1.4749
C(41)-H(41A)	0.9600
C(41)-H(41B)	0.9600
C(41)-H(41C)	0.9600
C(51)-N(41)	1.2282

N(4A)-Cu(1)-N(4B)	91.5(2)
N(4A)-Cu(1)-N(1A)	177.3(2)
N(4B)-Cu(1)-N(1A)	90.9(2)
N(4A)-Cu(1)-N(1B)	91.8(2)
N(4B)-Cu(1)-N(1B)	176.7(2)
N(1A)-Cu(1)-N(1B)	85.9(2)
N(4A)-Cu(1)-N(2B)	85.8(2)
N(4B)-Cu(1)-N(2B)	90.7(2)
N(1A)-Cu(1)-N(2B)	95.5(2)
N(1B)-Cu(1)-N(2B)	89.3(2)
N(4A)-Cu(1)-N(2A)	89.3(2)
N(4B)-Cu(1)-N(2A)	85.4(2)
N(1A)-Cu(1)-N(2A)	89.5(2)
N(1B)-Cu(1)-N(2A)	94.9(2)
N(2B)-Cu(1)-N(2A)	173.68(19)
C(23)-Fe(1A)-C(27A)	124.2(5)
C(23)-Fe(1A)-C(24)	41.6(4)
C(27A)-Fe(1A)-C(24)	108.0(5)
C(23)-Fe(1A)-C(20)	68.3(4)
C(27A)-Fe(1A)-C(20)	125.1(4)
C(24)-Fe(1A)-C(20)	41.6(3)
C(23)-Fe(1A)-C(21)	67.7(5)
C(27A)-Fe(1A)-C(21)	160.5(4)
C(24)-Fe(1A)-C(21)	69.5(4)
C(20)-Fe(1A)-C(21)	40.4(3)
C(23)-Fe(1A)-C(28A)	109.0(5)
C(27A)-Fe(1A)-C(28A)	41.3(4)
C(24)-Fe(1A)-C(28A)	125.0(5)
C(20)-Fe(1A)-C(28A)	162.8(4)

C(21)-Fe(1A)-C(28A)	155.8(4)
C(23)-Fe(1A)-C(22)	39.5(4)
C(27A)-Fe(1A)-C(22)	158.1(5)
C(24)-Fe(1A)-C(22)	69.1(5)
C(20)-Fe(1A)-C(22)	68.0(4)
C(21)-Fe(1A)-C(22)	40.6(3)
C(28A)-Fe(1A)-C(22)	121.5(4)
C(23)-Fe(1A)-C(26A)	124.6(5)
C(27A)-Fe(1A)-C(26A)	67.5(5)
C(24)-Fe(1A)-C(26A)	161.3(5)
C(20)-Fe(1A)-C(26A)	155.9(4)
C(21)-Fe(1A)-C(26A)	120.9(4)
C(28A)-Fe(1A)-C(26A)	39.7(4)
C(22)-Fe(1A)-C(26A)	107.8(5)
C(23)-Fe(1A)-C(25A)	159.7(5)
C(27A)-Fe(1A)-C(25A)	66.8(5)
C(24)-Fe(1A)-C(25A)	157.3(4)
C(20)-Fe(1A)-C(25A)	121.7(4)
C(21)-Fe(1A)-C(25A)	107.5(4)
C(28A)-Fe(1A)-C(25A)	66.8(5)
C(22)-Fe(1A)-C(25A)	124.1(5)
C(26A)-Fe(1A)-C(25A)	39.5(4)
C(23)-Fe(1A)-C(29A)	159.7(5)
C(27A)-Fe(1A)-C(29A)	40.1(4)
C(24)-Fe(1A)-C(29A)	122.5(4)
C(20)-Fe(1A)-C(29A)	108.5(4)
C(21)-Fe(1A)-C(29A)	123.8(4)
C(28A)-Fe(1A)-C(29A)	67.8(4)
C(22)-Fe(1A)-C(29A)	159.7(5)
C(26A)-Fe(1A)-C(29A)	66.7(4)
C(25A)-Fe(1A)-C(29A)	39.3(3)
C(9A)-S(1A)-C(16A)	101.7(3)
C(1A)-N(1A)-C(5A)	115.7(6)
C(1A)-N(1A)-Cu(1)	117.9(5)
C(5A)-N(1A)-Cu(1)	126.4(5)
C(9A)-N(2A)-C(7A)	105.2(6)
C(9A)-N(2A)-Cu(1)	135.4(5)
C(7A)-N(2A)-Cu(1)	106.2(4)

C(8A)-N(3A)-C(9A)	109.1(6)
C(8A)-N(3A)-C(10A)	121.5(6)
C(9A)-N(3A)-C(10A)	129.3(6)
N(5A)-N(4A)-C(17A)	109.2(6)
N(5A)-N(4A)-Cu(1)	118.2(4)
C(17A)-N(4A)-Cu(1)	132.5(5)
N(6A)-N(5A)-N(4A)	105.3(5)
N(5A)-N(6A)-C(18A)	112.5(6)
N(5A)-N(6A)-C(19A)	118.7(6)
C(18A)-N(6A)-C(19A)	128.8(6)
N(1A)-C(1A)-C(2A)	125.2(7)
N(1A)-C(1A)-H(1A)	117.4
C(2A)-C(1A)-H(1A)	117.4
C(1A)-C(2A)-C(3A)	119.4(8)
C(1A)-C(2A)-H(2A)	120.3
C(3A)-C(2A)-H(2A)	120.3
C(2A)-C(3A)-C(4A)	117.8(8)
C(2A)-C(3A)-H(3A)	121.1
C(4A)-C(3A)-H(3A)	121.1
C(3A)-C(4A)-C(5A)	120.0(8)
C(3A)-C(4A)-H(4A)	120.0
C(5A)-C(4A)-H(4A)	120.0
N(1A)-C(5A)-C(4A)	121.8(7)
N(1A)-C(5A)-C(6A)	120.9(7)
C(4A)-C(5A)-C(6A)	117.3(7)
C(7A)-C(6A)-C(5A)	131.2(7)
C(7A)-C(6A)-H(6A)	114.4
C(5A)-C(6A)-H(6A)	114.4
C(6A)-C(7A)-N(2A)	129.7(7)
C(6A)-C(7A)-C(8A)	121.1(7)
N(2A)-C(7A)-C(8A)	109.1(6)
O(1A)-C(8A)-N(3A)	127.1(8)
O(1A)-C(8A)-C(7A)	129.6(8)
N(3A)-C(8A)-C(7A)	103.3(7)
N(2A)-C(9A)-N(3A)	113.3(6)
N(2A)-C(9A)-S(1A)	128.3(6)
N(3A)-C(9A)-S(1A)	118.4(6)
C(15A)-C(10A)-C(11A)	120.2(8)

C(15A)-C(10A)-N(3A)	117.8(7)
C(11A)-C(10A)-N(3A)	121.6(7)
C(10A)-C(11A)-C(12A)	120.3(8)
C(10A)-C(11A)-H(11A)	119.9
C(12A)-C(11A)-H(11A)	119.9
C(13A)-C(12A)-C(11A)	119.2(8)
C(13A)-C(12A)-H(12A)	120.4
C(11A)-C(12A)-H(12A)	120.4
C(14A)-C(13A)-C(12A)	121.2(9)
C(14A)-C(13A)-Cl(1A)	118.0(7)
C(12A)-C(13A)-Cl(1A)	120.8(7)
C(13A)-C(14A)-C(15A)	119.1(8)
C(13A)-C(14A)-H(14A)	120.5
C(15A)-C(14A)-H(14A)	120.5
C(10A)-C(15A)-C(14A)	119.9(8)
C(10A)-C(15A)-H(15A)	120.1
C(14A)-C(15A)-H(15A)	120.1
C(17A)-C(16A)-S(1A)	113.4(5)
C(17A)-C(16A)-H(16A)	108.9
S(1A)-C(16A)-H(16A)	108.9
C(17A)-C(16A)-H(16B)	108.9
S(1A)-C(16A)-H(16B)	108.9
H(16A)-C(16A)-H(16B)	107.7
N(4A)-C(17A)-C(18A)	108.0(7)
N(4A)-C(17A)-C(16A)	123.7(6)
C(18A)-C(17A)-C(16A)	128.2(7)
N(6A)-C(18A)-C(17A)	105.0(7)
N(6A)-C(18A)-H(18A)	127.5
C(17A)-C(18A)-H(18A)	127.5
C(20)-C(19A)-N(6A)	112.7(6)
C(20)-C(19A)-H(19A)	109.1
N(6A)-C(19A)-H(19A)	109.1
C(20)-C(19A)-H(19B)	109.1
N(6A)-C(19A)-H(19B)	109.1
H(19A)-C(19A)-H(19B)	107.8
C(29A)-C(25A)-C(26A)	109.2(12)
C(29A)-C(25A)-Fe(1A)	70.5(6)
C(26A)-C(25A)-Fe(1A)	70.1(6)

C(29A)-C(25A)-H(25A)	125.4
C(26A)-C(25A)-H(25A)	125.4
Fe(1A)-C(25A)-H(25A)	125.6
C(28A)-C(26A)-C(25A)	108.4(12)
C(28A)-C(26A)-Fe(1A)	69.2(6)
C(25A)-C(26A)-Fe(1A)	70.5(6)
C(28A)-C(26A)-H(26A)	125.8
C(25A)-C(26A)-H(26A)	125.8
Fe(1A)-C(26A)-H(26A)	126.1
C(26A)-C(28A)-C(27A)	106.8(12)
C(26A)-C(28A)-Fe(1A)	71.1(6)
C(27A)-C(28A)-Fe(1A)	68.3(6)
C(26A)-C(28A)-H(28A)	126.6
C(27A)-C(28A)-H(28A)	126.6
Fe(1A)-C(28A)-H(28A)	125.6
C(29A)-C(27A)-C(28A)	108.4(12)
C(29A)-C(27A)-Fe(1A)	72.4(6)
C(28A)-C(27A)-Fe(1A)	70.5(6)
C(29A)-C(27A)-H(27A)	125.8
C(28A)-C(27A)-H(27A)	125.8
Fe(1A)-C(27A)-H(27A)	123.0
C(25A)-C(29A)-C(27A)	107.1(11)
C(25A)-C(29A)-Fe(1A)	70.2(6)
C(27A)-C(29A)-Fe(1A)	67.6(6)
C(25A)-C(29A)-H(29A)	126.4
C(27A)-C(29A)-H(29A)	126.4
Fe(1A)-C(29A)-H(29A)	127.3
C(21B)-Fe(1B)-C(24B)	69.1(4)
C(21B)-Fe(1B)-C(27)	172.1(5)
C(24B)-Fe(1B)-C(27)	113.7(6)
C(21B)-Fe(1B)-C(20B)	41.9(3)
C(24B)-Fe(1B)-C(20B)	41.1(3)
C(27)-Fe(1B)-C(20B)	144.8(5)
C(21B)-Fe(1B)-C(25)	114.2(6)
C(24B)-Fe(1B)-C(25)	136.0(5)
C(27)-Fe(1B)-C(25)	69.4(7)
C(20B)-Fe(1B)-C(25)	110.2(5)
C(21B)-Fe(1B)-C(23B)	67.6(4)

C(24B)-Fe(1B)-C(23B)	41.8(3)
C(27)-Fe(1B)-C(23B)	109.1(6)
C(20B)-Fe(1B)-C(23B)	69.4(4)
C(25)-Fe(1B)-C(23B)	177.0(6)
C(21B)-Fe(1B)-C(22B)	39.6(3)
C(24B)-Fe(1B)-C(22B)	69.1(4)
C(27)-Fe(1B)-C(22B)	133.4(6)
C(20B)-Fe(1B)-C(22B)	69.1(4)
C(25)-Fe(1B)-C(22B)	142.8(6)
C(23B)-Fe(1B)-C(22B)	40.1(3)
C(21B)-Fe(1B)-C(26)	142.5(5)
C(24B)-Fe(1B)-C(26)	113.2(5)
C(27)-Fe(1B)-C(26)	44.3(5)
C(20B)-Fe(1B)-C(26)	113.9(4)
C(25)-Fe(1B)-C(26)	36.8(4)
C(23B)-Fe(1B)-C(26)	140.5(6)
C(22B)-Fe(1B)-C(26)	177.0(5)
C(21B)-Fe(1B)-C(29)	108.5(5)
C(24B)-Fe(1B)-C(29)	171.6(5)
C(27)-Fe(1B)-C(29)	69.8(6)
C(20B)-Fe(1B)-C(29)	131.9(5)
C(25)-Fe(1B)-C(29)	36.8(4)
C(23B)-Fe(1B)-C(29)	145.6(5)
C(22B)-Fe(1B)-C(29)	114.6(5)
C(26)-Fe(1B)-C(29)	63.4(5)
C(21B)-Fe(1B)-C(28)	131.3(5)
C(24B)-Fe(1B)-C(28)	148.7(5)
C(27)-Fe(1B)-C(28)	42.9(5)
C(20B)-Fe(1B)-C(28)	169.9(5)
C(25)-Fe(1B)-C(28)	64.1(6)
C(23B)-Fe(1B)-C(28)	116.8(5)
C(22B)-Fe(1B)-C(28)	110.0(5)
C(26)-Fe(1B)-C(28)	67.0(5)
C(29)-Fe(1B)-C(28)	38.7(4)
C(9B)-S(1B)-C(16B)	101.1(3)
C(1B)-N(1B)-C(5B)	118.6(6)
C(1B)-N(1B)-Cu(1)	115.6(5)
C(5B)-N(1B)-Cu(1)	125.7(5)

C(9B)-N(2B)-C(7B)	105.6(6)
C(9B)-N(2B)-Cu(1)	133.8(4)
C(7B)-N(2B)-Cu(1)	108.5(4)
C(9B)-N(3B)-C(8B)	108.6(6)
C(9B)-N(3B)-C(10B)	126.9(6)
C(8B)-N(3B)-C(10B)	124.5(6)
N(5B)-N(4B)-C(17B)	110.0(6)
N(5B)-N(4B)-Cu(1)	119.9(5)
C(17B)-N(4B)-Cu(1)	129.7(5)
N(4B)-N(5B)-N(6B)	106.1(5)
C(18B)-N(6B)-N(5B)	110.8(6)
C(18B)-N(6B)-C(19B)	129.7(7)
N(5B)-N(6B)-C(19B)	119.5(6)
N(1B)-C(1B)-C(2B)	122.6(8)
N(1B)-C(1B)-H(1B)	118.7
C(2B)-C(1B)-H(1B)	118.7
C(3B)-C(2B)-C(1B)	119.8(8)
C(3B)-C(2B)-H(2B)	120.1
C(1B)-C(2B)-H(2B)	120.1
C(2B)-C(3B)-C(4B)	118.3(8)
C(2B)-C(3B)-H(3B)	120.9
C(4B)-C(3B)-H(3B)	120.9
C(3B)-C(4B)-C(5B)	120.9(7)
C(3B)-C(4B)-H(4B)	119.5
C(5B)-C(4B)-H(4B)	119.5
N(1B)-C(5B)-C(4B)	119.8(7)
N(1B)-C(5B)-C(6B)	121.4(7)
C(4B)-C(5B)-C(6B)	118.9(7)
C(7B)-C(6B)-C(5B)	130.8(7)
C(7B)-C(6B)-H(6B)	114.6
C(5B)-C(6B)-H(6B)	114.6
C(6B)-C(7B)-N(2B)	129.9(7)
C(6B)-C(7B)-C(8B)	120.7(7)
N(2B)-C(7B)-C(8B)	109.4(6)
O(1B)-C(8B)-N(3B)	126.9(7)
O(1B)-C(8B)-C(7B)	131.1(7)
N(3B)-C(8B)-C(7B)	101.9(6)
N(2B)-C(9B)-N(3B)	114.3(6)

N(2B)-C(9B)-S(1B)	129.1(5)
N(3B)-C(9B)-S(1B)	116.6(5)
C(11B)-C(10B)-C(15B)	120.7(7)
C(11B)-C(10B)-N(3B)	120.1(7)
C(15B)-C(10B)-N(3B)	119.1(7)
C(10B)-C(11B)-C(12B)	119.7(7)
C(10B)-C(11B)-H(11B)	120.2
C(12B)-C(11B)-H(11B)	120.2
C(13B)-C(12B)-C(11B)	119.4(8)
C(13B)-C(12B)-H(12B)	120.3
C(11B)-C(12B)-H(12B)	120.3
C(14B)-C(13B)-C(12B)	121.5(8)
C(14B)-C(13B)-Cl(1B)	119.1(7)
C(12B)-C(13B)-Cl(1B)	119.4(7)
C(13B)-C(14B)-C(15B)	119.2(8)
C(13B)-C(14B)-H(14B)	120.4
C(15B)-C(14B)-H(14B)	120.4
C(10B)-C(15B)-C(14B)	119.6(7)
C(10B)-C(15B)-H(15B)	120.2
C(14B)-C(15B)-H(15B)	120.2
C(17B)-C(16B)-S(1B)	110.9(5)
C(17B)-C(16B)-H(16C)	109.5
S(1B)-C(16B)-H(16C)	109.5
C(17B)-C(16B)-H(16D)	109.5
S(1B)-C(16B)-H(16D)	109.5
H(16C)-C(16B)-H(16D)	108.0
C(18B)-C(17B)-N(4B)	106.5(7)
C(18B)-C(17B)-C(16B)	130.1(7)
N(4B)-C(17B)-C(16B)	123.2(6)
N(6B)-C(18B)-C(17B)	106.4(7)
N(6B)-C(18B)-H(18B)	126.8
C(17B)-C(18B)-H(18B)	126.8
N(6B)-C(19B)-C(20B)	116.9(7)
N(6B)-C(19B)-H(19A)	108.1
C(20B)-C(19B)-H(19A)	108.1
N(6B)-C(19B)-H(19B)	108.1
C(20B)-C(19B)-H(19B)	108.1
H(19A)-C(19B)-H(19B)	107.3

C(24B)-C(20B)-C(21B)	105.3(8)
C(24B)-C(20B)-C(19B)	127.3(8)
C(21B)-C(20B)-C(19B)	127.3(9)
C(24B)-C(20B)-Fe(1B)	68.6(5)
C(21B)-C(20B)-Fe(1B)	67.9(5)
C(19B)-C(20B)-Fe(1B)	129.0(6)
C(22B)-C(21B)-C(20B)	110.4(10)
C(22B)-C(21B)-Fe(1B)	71.8(6)
C(20B)-C(21B)-Fe(1B)	70.2(5)
C(22B)-C(21B)-H(21B)	124.8
C(20B)-C(21B)-H(21B)	124.8
Fe(1B)-C(21B)-H(21B)	124.8
C(21B)-C(22B)-C(23B)	108.4(10)
C(21B)-C(22B)-Fe(1B)	68.5(6)
C(23B)-C(22B)-Fe(1B)	69.9(6)
C(21B)-C(22B)-H(22B)	125.8
C(23B)-C(22B)-H(22B)	125.8
Fe(1B)-C(22B)-H(22B)	127.4
C(22B)-C(23B)-C(24B)	107.8(10)
C(22B)-C(23B)-Fe(1B)	70.1(6)
C(24B)-C(23B)-Fe(1B)	67.9(6)
C(22B)-C(23B)-H(23B)	126.1
C(24B)-C(23B)-H(23B)	126.1
Fe(1B)-C(23B)-H(23B)	127.5
C(20B)-C(24B)-C(23B)	108.0(9)
C(20B)-C(24B)-Fe(1B)	70.3(5)
C(23B)-C(24B)-Fe(1B)	70.3(6)
C(20B)-C(24B)-H(24B)	126.0
C(23B)-C(24B)-H(24B)	126.0
Fe(1B)-C(24B)-H(24B)	125.0
N(10)-C(30)-C(31)	174.2(19)
C(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(26)-C(25)-C(29)	113.1(19)

C(26)-C(25)-Fe(1B)	71.9(9)
C(29)-C(25)-Fe(1B)	72.0(9)
C(26)-C(25)-H(25)	123.4
C(29)-C(25)-H(25)	123.4
Fe(1B)-C(25)-H(25)	124.1
C(25)-C(26)-C(27)	109.7(15)
C(25)-C(26)-Fe(1B)	71.3(8)
C(27)-C(26)-Fe(1B)	66.9(7)
C(25)-C(26)-H(26)	125.1
C(27)-C(26)-H(26)	125.1
Fe(1B)-C(26)-H(26)	128.2
C(28)-C(27)-C(26)	96.9(13)
C(28)-C(27)-Fe(1B)	69.7(7)
C(26)-C(27)-Fe(1B)	68.8(7)
C(28)-C(27)-H(27)	131.5
C(26)-C(27)-H(27)	131.5
Fe(1B)-C(27)-H(27)	122.3
C(29)-C(28)-C(27)	109.7(14)
C(29)-C(28)-Fe(1B)	70.6(8)
C(27)-C(28)-Fe(1B)	67.5(7)
C(29)-C(28)-H(28)	125.1
C(27)-C(28)-H(28)	125.1
Fe(1B)-C(28)-H(28)	128.4
C(25)-C(29)-C(28)	110.0(17)
C(25)-C(29)-Fe(1B)	71.2(9)
C(28)-C(29)-Fe(1B)	70.7(8)
C(25)-C(29)-H(29)	125.0
C(28)-C(29)-H(29)	125.0
Fe(1B)-C(29)-H(29)	124.7
O(4)-Cl(1)-O(2)	109.6(12)
O(4)-Cl(1)-O(31)	107.8(11)
O(2)-Cl(1)-O(31)	107.2(10)
O(4)-Cl(1)-O(1)	112.1(14)
O(2)-Cl(1)-O(1)	108.4(14)
O(31)-Cl(1)-O(1)	111.7(15)
O(51)-Cl(2)-O(71)	105.7(7)
O(51)-Cl(2)-O(81)	116.7(6)
O(71)-Cl(2)-O(81)	105.2(6)

O(51)-Cl(2)-O(61)	109.3(5)
O(71)-Cl(2)-O(61)	108.7(7)
O(81)-Cl(2)-O(61)	110.9(5)
C(21)-C(20)-C(24)	109.1(8)
C(21)-C(20)-C(19A)	124.1(8)
C(24)-C(20)-C(19A)	126.6(8)
C(21)-C(20)-Fe(1A)	70.0(5)
C(24)-C(20)-Fe(1A)	69.2(5)
C(19A)-C(20)-Fe(1A)	123.2(5)
C(20)-C(21)-C(22)	107.9(10)
C(20)-C(21)-Fe(1A)	69.7(5)
C(22)-C(21)-Fe(1A)	70.1(6)
C(20)-C(21)-H(21)	126.0
C(22)-C(21)-H(21)	126.0
Fe(1A)-C(21)-H(21)	125.8
C(23)-C(22)-C(21)	107.5(11)
C(23)-C(22)-Fe(1A)	68.3(7)
C(21)-C(22)-Fe(1A)	69.3(6)
C(23)-C(22)-H(22)	126.2
C(21)-C(22)-H(22)	126.2
Fe(1A)-C(22)-H(22)	127.7
C(22)-C(23)-C(24)	111.6(12)
C(22)-C(23)-Fe(1A)	72.2(7)
C(24)-C(23)-Fe(1A)	70.5(6)
C(22)-C(23)-H(23)	124.2
C(24)-C(23)-H(23)	124.2
Fe(1A)-C(23)-H(23)	124.7
C(23)-C(24)-C(20)	103.8(10)
C(23)-C(24)-Fe(1A)	68.0(6)
C(20)-C(24)-Fe(1A)	69.2(5)
C(23)-C(24)-H(24)	128.1
C(20)-C(24)-H(24)	128.1
Fe(1A)-C(24)-H(24)	126.3
O(4A)-Cl(3)-O(2A)	114.6(14)
O(4A)-Cl(3)-O(31A)	108.2(16)
O(2A)-Cl(3)-O(31A)	106.8(14)
O(4A)-Cl(3)-O(3)	108.0(17)
O(2A)-Cl(3)-O(3)	112.2(17)

O(31A)-Cl(3)-O(3)	106.7(17)
C(50)-C(40)-H(40A)	109.5
C(50)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(50)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
N(40)-C(50)-C(40)	163.2
C(51)-C(41)-H(41A)	109.5
C(51)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5
C(51)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5
H(41B)-C(41)-H(41C)	109.5
N(41)-C(51)-C(41)	161.4

Symmetry transformations used to generate equivalent atoms:

Table S3. Torsion angles [°] for dg902k2n2.

C(17A)-N(4A)-N(5A)-N(6A)	0.4(7)
Cu(1)-N(4A)-N(5A)-N(6A)	-177.0(4)
N(4A)-N(5A)-N(6A)-C(18A)	-0.3(7)
N(4A)-N(5A)-N(6A)-C(19A)	-178.7(6)
C(5A)-N(1A)-C(1A)-C(2A)	1.2(10)
Cu(1)-N(1A)-C(1A)-C(2A)	179.7(6)
N(1A)-C(1A)-C(2A)-C(3A)	-2.1(11)
C(1A)-C(2A)-C(3A)-C(4A)	2.1(12)
C(2A)-C(3A)-C(4A)-C(5A)	-1.5(12)
C(1A)-N(1A)-C(5A)-C(4A)	-0.6(9)
Cu(1)-N(1A)-C(5A)-C(4A)	-178.9(5)
C(1A)-N(1A)-C(5A)-C(6A)	-179.8(6)
Cu(1)-N(1A)-C(5A)-C(6A)	1.8(9)
C(3A)-C(4A)-C(5A)-N(1A)	0.8(11)
C(3A)-C(4A)-C(5A)-C(6A)	-179.9(7)
N(1A)-C(5A)-C(6A)-C(7A)	-24.4(11)
C(4A)-C(5A)-C(6A)-C(7A)	156.3(7)
C(5A)-C(6A)-C(7A)-N(2A)	-2.7(13)

C(5A)-C(6A)-C(7A)-C(8A)	-179.2(7)
C(9A)-N(2A)-C(7A)-C(6A)	-176.7(7)
Cu(1)-N(2A)-C(7A)-C(6A)	35.5(8)
C(9A)-N(2A)-C(7A)-C(8A)	0.2(7)
Cu(1)-N(2A)-C(7A)-C(8A)	-147.7(4)
C(9A)-N(3A)-C(8A)-O(1A)	178.6(8)
C(10A)-N(3A)-C(8A)-O(1A)	1.4(12)
C(9A)-N(3A)-C(8A)-C(7A)	-1.7(7)
C(10A)-N(3A)-C(8A)-C(7A)	-179.0(6)
C(6A)-C(7A)-C(8A)-O(1A)	-2.2(12)
N(2A)-C(7A)-C(8A)-O(1A)	-179.3(8)
C(6A)-C(7A)-C(8A)-N(3A)	178.1(6)
N(2A)-C(7A)-C(8A)-N(3A)	1.0(7)
C(7A)-N(2A)-C(9A)-N(3A)	-1.3(8)
Cu(1)-N(2A)-C(9A)-N(3A)	132.0(5)
C(7A)-N(2A)-C(9A)-S(1A)	177.0(5)
Cu(1)-N(2A)-C(9A)-S(1A)	-49.7(9)
C(8A)-N(3A)-C(9A)-N(2A)	2.0(8)
C(10A)-N(3A)-C(9A)-N(2A)	179.0(7)
C(8A)-N(3A)-C(9A)-S(1A)	-176.4(5)
C(10A)-N(3A)-C(9A)-S(1A)	0.5(10)
C(16A)-S(1A)-C(9A)-N(2A)	5.0(7)
C(16A)-S(1A)-C(9A)-N(3A)	-176.7(5)
C(8A)-N(3A)-C(10A)-C(15A)	53.1(10)
C(9A)-N(3A)-C(10A)-C(15A)	-123.5(8)
C(8A)-N(3A)-C(10A)-C(11A)	-119.4(8)
C(9A)-N(3A)-C(10A)-C(11A)	64.0(11)
C(15A)-C(10A)-C(11A)-C(12A)	-1.0(13)
N(3A)-C(10A)-C(11A)-C(12A)	171.3(7)
C(10A)-C(11A)-C(12A)-C(13A)	-2.4(13)
C(11A)-C(12A)-C(13A)-C(14A)	4.2(14)
C(11A)-C(12A)-C(13A)-Cl(1A)	-175.1(7)
C(12A)-C(13A)-C(14A)-C(15A)	-2.7(14)
Cl(1A)-C(13A)-C(14A)-C(15A)	176.7(6)
C(11A)-C(10A)-C(15A)-C(14A)	2.5(12)
N(3A)-C(10A)-C(15A)-C(14A)	-170.1(7)
C(13A)-C(14A)-C(15A)-C(10A)	-0.7(13)
C(9A)-S(1A)-C(16A)-C(17A)	79.8(5)

N(5A)-N(4A)-C(17A)-C(18A)	-0.4(8)
Cu(1)-N(4A)-C(17A)-C(18A)	176.4(5)
N(5A)-N(4A)-C(17A)-C(16A)	176.8(6)
Cu(1)-N(4A)-C(17A)-C(16A)	-6.4(10)
S(1A)-C(16A)-C(17A)-N(4A)	-88.0(7)
S(1A)-C(16A)-C(17A)-C(18A)	88.6(8)
N(5A)-N(6A)-C(18A)-C(17A)	0.0(8)
C(19A)-N(6A)-C(18A)-C(17A)	178.2(7)
N(4A)-C(17A)-C(18A)-N(6A)	0.3(8)
C(16A)-C(17A)-C(18A)-N(6A)	-176.8(7)
N(5A)-N(6A)-C(19A)-C(20)	-116.4(7)
C(18A)-N(6A)-C(19A)-C(20)	65.5(10)
C(29A)-C(25A)-C(26A)-C(28A)	-0.8(12)
Fe(1A)-C(25A)-C(26A)-C(28A)	59.0(7)
C(29A)-C(25A)-C(26A)-Fe(1A)	-59.8(7)
C(25A)-C(26A)-C(28A)-C(27A)	-0.6(12)
Fe(1A)-C(26A)-C(28A)-C(27A)	59.2(7)
C(25A)-C(26A)-C(28A)-Fe(1A)	-59.8(7)
C(26A)-C(28A)-C(27A)-C(29A)	1.8(12)
Fe(1A)-C(28A)-C(27A)-C(29A)	62.8(7)
C(26A)-C(28A)-C(27A)-Fe(1A)	-61.0(7)
C(26A)-C(25A)-C(29A)-C(27A)	1.9(12)
Fe(1A)-C(25A)-C(29A)-C(27A)	-57.6(7)
C(26A)-C(25A)-C(29A)-Fe(1A)	59.6(7)
C(28A)-C(27A)-C(29A)-C(25A)	-2.3(12)
Fe(1A)-C(27A)-C(29A)-C(25A)	59.3(7)
C(28A)-C(27A)-C(29A)-Fe(1A)	-61.6(7)
C(17B)-N(4B)-N(5B)-N(6B)	1.4(7)
Cu(1)-N(4B)-N(5B)-N(6B)	-172.3(4)
N(4B)-N(5B)-N(6B)-C(18B)	0.3(7)
N(4B)-N(5B)-N(6B)-C(19B)	-178.5(6)
C(5B)-N(1B)-C(1B)-C(2B)	-0.9(10)
Cu(1)-N(1B)-C(1B)-C(2B)	-177.3(6)
N(1B)-C(1B)-C(2B)-C(3B)	1.9(12)
C(1B)-C(2B)-C(3B)-C(4B)	-1.6(12)
C(2B)-C(3B)-C(4B)-C(5B)	0.4(11)
C(1B)-N(1B)-C(5B)-C(4B)	-0.3(9)
Cu(1)-N(1B)-C(5B)-C(4B)	175.7(5)

C(1B)-N(1B)-C(5B)-C(6B)	179.5(6)
Cu(1)-N(1B)-C(5B)-C(6B)	-4.6(9)
C(3B)-C(4B)-C(5B)-N(1B)	0.5(10)
C(3B)-C(4B)-C(5B)-C(6B)	-179.2(6)
N(1B)-C(5B)-C(6B)-C(7B)	-20.1(11)
C(4B)-C(5B)-C(6B)-C(7B)	159.7(7)
C(5B)-C(6B)-C(7B)-N(2B)	0.0(12)
C(5B)-C(6B)-C(7B)-C(8B)	-178.8(6)
C(9B)-N(2B)-C(7B)-C(6B)	180.0(7)
Cu(1)-N(2B)-C(7B)-C(6B)	31.6(8)
C(9B)-N(2B)-C(7B)-C(8B)	-1.1(7)
Cu(1)-N(2B)-C(7B)-C(8B)	-149.5(4)
C(9B)-N(3B)-C(8B)-O(1B)	176.4(7)
C(10B)-N(3B)-C(8B)-O(1B)	-2.4(11)
C(9B)-N(3B)-C(8B)-C(7B)	-4.9(6)
C(10B)-N(3B)-C(8B)-C(7B)	176.4(6)
C(6B)-C(7B)-C(8B)-O(1B)	1.4(11)
N(2B)-C(7B)-C(8B)-O(1B)	-177.6(7)
C(6B)-C(7B)-C(8B)-N(3B)	-177.3(6)
N(2B)-C(7B)-C(8B)-N(3B)	3.7(6)
C(7B)-N(2B)-C(9B)-N(3B)	-2.2(7)
Cu(1)-N(2B)-C(9B)-N(3B)	134.3(5)
C(7B)-N(2B)-C(9B)-S(1B)	175.5(5)
Cu(1)-N(2B)-C(9B)-S(1B)	-48.1(9)
C(8B)-N(3B)-C(9B)-N(2B)	4.8(8)
C(10B)-N(3B)-C(9B)-N(2B)	-176.5(6)
C(8B)-N(3B)-C(9B)-S(1B)	-173.2(4)
C(10B)-N(3B)-C(9B)-S(1B)	5.6(9)
C(16B)-S(1B)-C(9B)-N(2B)	1.2(7)
C(16B)-S(1B)-C(9B)-N(3B)	178.9(5)
C(9B)-N(3B)-C(10B)-C(11B)	-113.7(8)
C(8B)-N(3B)-C(10B)-C(11B)	64.9(8)
C(9B)-N(3B)-C(10B)-C(15B)	67.8(9)
C(8B)-N(3B)-C(10B)-C(15B)	-113.7(7)
C(15B)-C(10B)-C(11B)-C(12B)	-1.3(10)
N(3B)-C(10B)-C(11B)-C(12B)	-179.9(6)
C(10B)-C(11B)-C(12B)-C(13B)	0.4(11)
C(11B)-C(12B)-C(13B)-C(14B)	0.8(12)

C(11B)-C(12B)-C(13B)-Cl(1B)	-177.6(5)
C(12B)-C(13B)-C(14B)-C(15B)	-1.0(12)
Cl(1B)-C(13B)-C(14B)-C(15B)	177.4(5)
C(11B)-C(10B)-C(15B)-C(14B)	1.1(10)
N(3B)-C(10B)-C(15B)-C(14B)	179.7(6)
C(13B)-C(14B)-C(15B)-C(10B)	0.1(11)
C(9B)-S(1B)-C(16B)-C(17B)	84.3(5)
N(5B)-N(4B)-C(17B)-C(18B)	-2.5(7)
Cu(1)-N(4B)-C(17B)-C(18B)	170.4(5)
N(5B)-N(4B)-C(17B)-C(16B)	174.7(6)
Cu(1)-N(4B)-C(17B)-C(16B)	-12.4(9)
S(1B)-C(16B)-C(17B)-C(18B)	91.6(8)
S(1B)-C(16B)-C(17B)-N(4B)	-84.8(7)
N(5B)-N(6B)-C(18B)-C(17B)	-1.8(8)
C(19B)-N(6B)-C(18B)-C(17B)	176.9(7)
N(4B)-C(17B)-C(18B)-N(6B)	2.5(8)
C(16B)-C(17B)-C(18B)-N(6B)	-174.4(6)
C(18B)-N(6B)-C(19B)-C(20B)	-62.9(11)
N(5B)-N(6B)-C(19B)-C(20B)	115.6(8)
N(6B)-C(19B)-C(20B)-C(24B)	50.4(12)
N(6B)-C(19B)-C(20B)-C(21B)	-131.6(9)
N(6B)-C(19B)-C(20B)-Fe(1B)	-41.1(12)
C(24B)-C(20B)-C(21B)-C(22B)	2.1(10)
C(19B)-C(20B)-C(21B)-C(22B)	-176.2(8)
Fe(1B)-C(20B)-C(21B)-C(22B)	60.8(7)
C(24B)-C(20B)-C(21B)-Fe(1B)	-58.7(6)
C(19B)-C(20B)-C(21B)-Fe(1B)	123.0(9)
C(20B)-C(21B)-C(22B)-C(23B)	-1.2(11)
Fe(1B)-C(21B)-C(22B)-C(23B)	58.6(7)
C(20B)-C(21B)-C(22B)-Fe(1B)	-59.8(6)
C(21B)-C(22B)-C(23B)-C(24B)	-0.2(12)
Fe(1B)-C(22B)-C(23B)-C(24B)	57.6(7)
C(21B)-C(22B)-C(23B)-Fe(1B)	-57.8(7)
C(21B)-C(20B)-C(24B)-C(23B)	-2.2(10)
C(19B)-C(20B)-C(24B)-C(23B)	176.2(8)
Fe(1B)-C(20B)-C(24B)-C(23B)	-60.5(7)
C(21B)-C(20B)-C(24B)-Fe(1B)	58.2(6)
C(19B)-C(20B)-C(24B)-Fe(1B)	-123.4(8)

C(22B)-C(23B)-C(24B)-C(20B)	1.6(11)
Fe(1B)-C(23B)-C(24B)-C(20B)	60.5(6)
C(22B)-C(23B)-C(24B)-Fe(1B)	-58.9(7)
C(29)-C(25)-C(26)-C(27)	-4.7(17)
Fe(1B)-C(25)-C(26)-C(27)	55.9(9)
C(29)-C(25)-C(26)-Fe(1B)	-60.6(11)
C(25)-C(26)-C(27)-C(28)	6.5(14)
Fe(1B)-C(26)-C(27)-C(28)	65.0(7)
C(25)-C(26)-C(27)-Fe(1B)	-58.5(10)
C(26)-C(27)-C(28)-C(29)	-6.3(13)
Fe(1B)-C(27)-C(28)-C(29)	58.0(10)
C(26)-C(27)-C(28)-Fe(1B)	-64.3(7)
C(26)-C(25)-C(29)-C(28)	0.2(17)
Fe(1B)-C(25)-C(29)-C(28)	-60.3(10)
C(26)-C(25)-C(29)-Fe(1B)	60.5(11)
C(27)-C(28)-C(29)-C(25)	4.5(16)
Fe(1B)-C(28)-C(29)-C(25)	60.6(10)
C(27)-C(28)-C(29)-Fe(1B)	-56.1(9)
N(6A)-C(19A)-C(20)-C(21)	-89.6(9)
N(6A)-C(19A)-C(20)-C(24)	95.9(9)
N(6A)-C(19A)-C(20)-Fe(1A)	-176.6(5)
C(24)-C(20)-C(21)-C(22)	-1.7(10)
C(19A)-C(20)-C(21)-C(22)	-177.1(7)
Fe(1A)-C(20)-C(21)-C(22)	-59.9(6)
C(24)-C(20)-C(21)-Fe(1A)	58.2(6)
C(19A)-C(20)-C(21)-Fe(1A)	-117.2(7)
C(20)-C(21)-C(22)-C(23)	1.9(11)
Fe(1A)-C(21)-C(22)-C(23)	-57.7(8)
C(20)-C(21)-C(22)-Fe(1A)	59.7(6)
C(21)-C(22)-C(23)-C(24)	-1.4(13)
Fe(1A)-C(22)-C(23)-C(24)	-59.7(8)
C(21)-C(22)-C(23)-Fe(1A)	58.3(7)
C(22)-C(23)-C(24)-C(20)	0.3(12)
Fe(1A)-C(23)-C(24)-C(20)	-60.4(6)
C(22)-C(23)-C(24)-Fe(1A)	60.7(8)
C(21)-C(20)-C(24)-C(23)	0.9(10)
C(19A)-C(20)-C(24)-C(23)	176.1(8)
Fe(1A)-C(20)-C(24)-C(23)	59.6(6)

C(21)-C(20)-C(24)-Fe(1A)	-58.7(6)
C(19A)-C(20)-C(24)-Fe(1A)	116.5(8)

Symmetry transformations used to generate equivalent atoms:

Table S4. Hydrogen bonds for dg902k2n2 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(1A)-H(1A)...N(2B)	0.93	2.63	3.239(9)	123.6
C(11A)-H(11A)...N(40)	0.93	2.59	3.514(9)	171.3
C(12A)-H(12A)...O(61)#1	0.93	2.48	3.379(11)	161.5
C(15A)-H(15A)...O(2)#2	0.93	2.53	3.248(15)	133.9
C(16A)-H(16A)...O(51)	0.97	2.56	3.171(11)	120.9
C(16A)-H(16B)...N(1B)	0.97	2.66	3.445(9)	137.8
C(18A)-H(18A)...O(61)	0.93	2.45	3.377(11)	175.7
C(1B)-H(1B)...N(2A)	0.93	2.58	3.196(10)	123.7
C(2B)-H(2B)...O(4A)#2	0.93	2.64	3.221(19)	120.8
C(11B)-H(11B)...O(2A)#3	0.93	2.52	3.380(19)	153.8
C(14B)-H(14B)...O(71)#4	0.93	2.62	3.482(13)	154.0
C(16B)-H(16C)...O(1)	0.97	2.62	3.44(3)	142.7
C(16B)-H(16D)...N(1A)	0.97	2.56	3.338(8)	136.9
C(18B)-H(18B)...O(1)	0.93	2.48	3.22(3)	137.4
C(18B)-H(18B)...O(3)	0.93	2.57	3.31(3)	136.7
C(18B)-H(18B)...O(31A)	0.93	2.63	3.45(2)	146.7

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z+1 #2 x-1,y,z #3 -x+3/2,y+1/2,-z+3/2

#4 x+1,y,z

Table S5. analysis of variance for reflections employed in refinement*

Resolution(A)	0.96	1.00	1.04	1.09	1.15	1.23	1.32	1.45	1.66	2.09	inf
N in group	782.	723.	747.	732.	749.	730.	734.	756.	737.	739.	
GooF	0.699	0.719	0.752	0.813	0.789	0.834	0.874	0.858	1.050	1.288	
K	1.037	1.037	1.037	1.012	1.015	0.999	1.014	1.014	1.010	1.006	
R1	0.299	0.283	0.235	0.232	0.182	0.123	0.091	0.066	0.054	0.047	

* The scale factor K remained close to 1.0 across all resolution shells, confirming proper data scaling.

The refinement is stable, and the number of reflections per refined parameter is satisfactory. The obtained geometric parameters of the copper complex are reasonable and correspond to those of similar compounds. The results are reproducible (three diffractometry experiments were performed). In other words, the structure, taking into account the complexity caused by disorder, has been well determined, and its reliability is beyond doubt. (The validity of the structure is confirmed, for example, by the expected Jahn-Teller effect. A strongly elongated octahedron along the N2a – Cu –N2b line).

Graphs of reflection data statistics

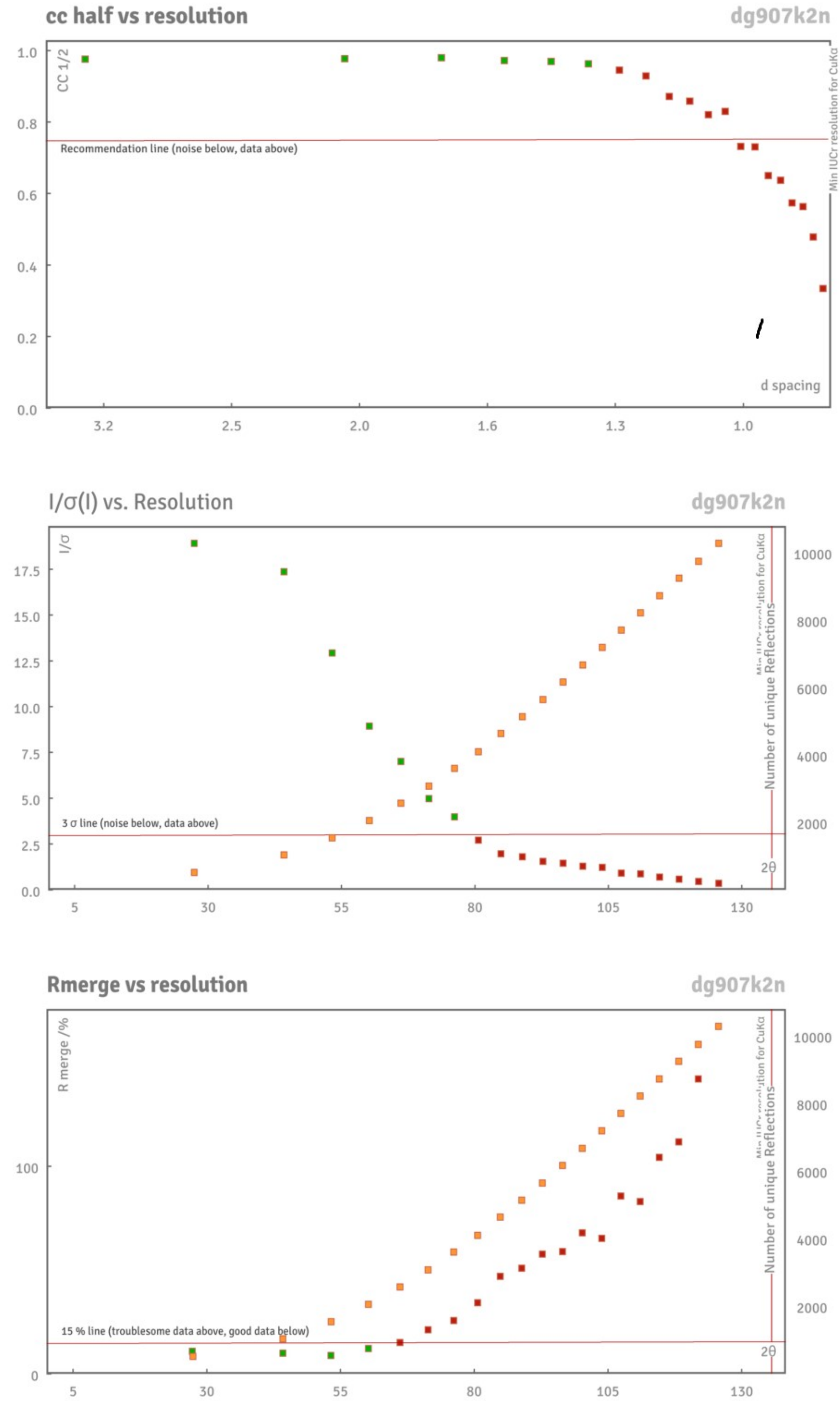


Figure S63. Graphs of reflection data statistics (kindly provided by reviewer of the manuscript).