

Supplementary material

Exploring the antitumor potential of copper complexes based on ester derivatives of bis(pyrazol-1-yl)acetate ligands

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Table S1. XPS data analysis results: BE, FWHM values and Assignments for samples 2 , 8 , 5 and 9 .					
Sample	Signal	BE (eV)	FWHM (eV)	atomic ratios	Assignment
2	C1s	284.70	1.44	14.1	C-C aromatic + aliphatic
		286.25	1.44	2.2	C-N
		287.79	1.44	1.1	C-O-C
		289.13	1.44	1.0	COOR
	N1s	399.88	2.14	1.1	C-N
		401.77	2.14	1.0	C=N
	O1s	532.07	1.59	1.8	C=O (+ impurities)
		533.25	1.59	1.0	C-O
8	C1s	284.70	1.80	9.5	C-C aromatic + aliphatic
		285.84	1.80	3.4	C-N
		287.48	1.80	1.0	C-O-C
		288.78	1.80	1.0	COOR
	N1s	399.85	2.80	1.0	C-N
	O1s	531.01	2.69	1.2	C=O (+ impurities)
		533.11	2.69	1.0	C-O
	P2p _{3/2}	131.89	3.31	1.0	R-PPh ₃
	Cu2p _{3/2}	932.20	3.31	1.0	Cu(I) in coordination compound
5	C1s	284.70	1.45	6.8	C-C aromatic + aliphatic
		286.05	1.45	2.0	C-N
		287.41	1.45	1.0	C-O-C
		288.84	1.45	1.0	COOR
	N1s	400.92	3.20	1.0	C-N
	O1s	532.05	2.08	2.1	C=O (+ impurities)
		533.43	2.08	1.0	C-O
	Cl2p _{3/2}	199.27	2.61	0.8	Cl-Cu monomeric coord. compound
		201.31	2.61	1.0	Cu-Cl-Cu dimeric coord. compound
	Cu2p _{3/2}	932.19	2.53	1.0	Cu(I)?
		934.82	2.53	0.8	Cu(II) in coordination compound
9	C1s	284.70	1.52	14.3	C-C aromatic + aliphatic
		286.23	1.52	2.6	C-N
		287.71	1.52	1.0	C-O-C
		289.12	1.52	1.0	COOR
	N1s	400.34	2.85	1.0	C-N
	O1s	532.15	1.67	3.8	C=O (+ impurities)
		533.44	1.67	1.0	C-O
	Cl2p _{3/2}	199.11	1.86	1.0	Cl-Cu monomeric coord. compound
	Cu2p _{3/2}	932.24	2.54	1.0	Cu(I)?
		935.24	2.54	2.2	Cu(II) in coordination compound

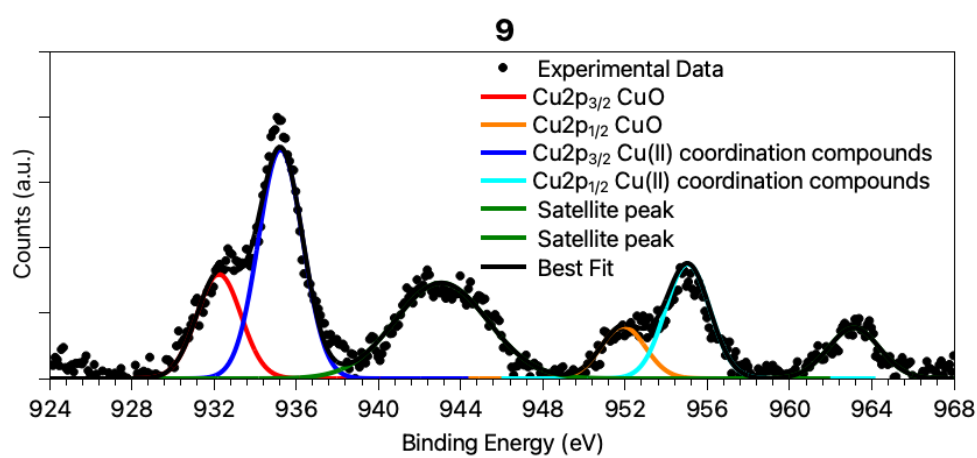
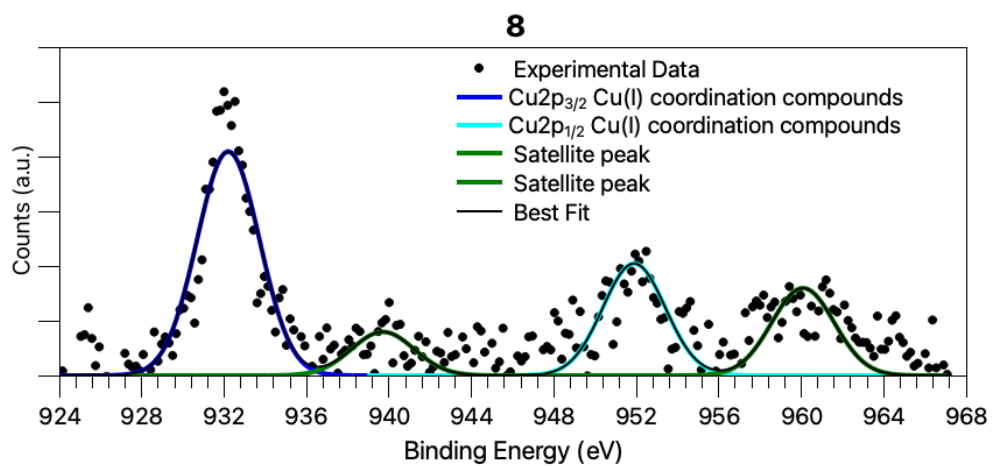


Figure S1. Cu2p spectra of complexes **8** and **9**.

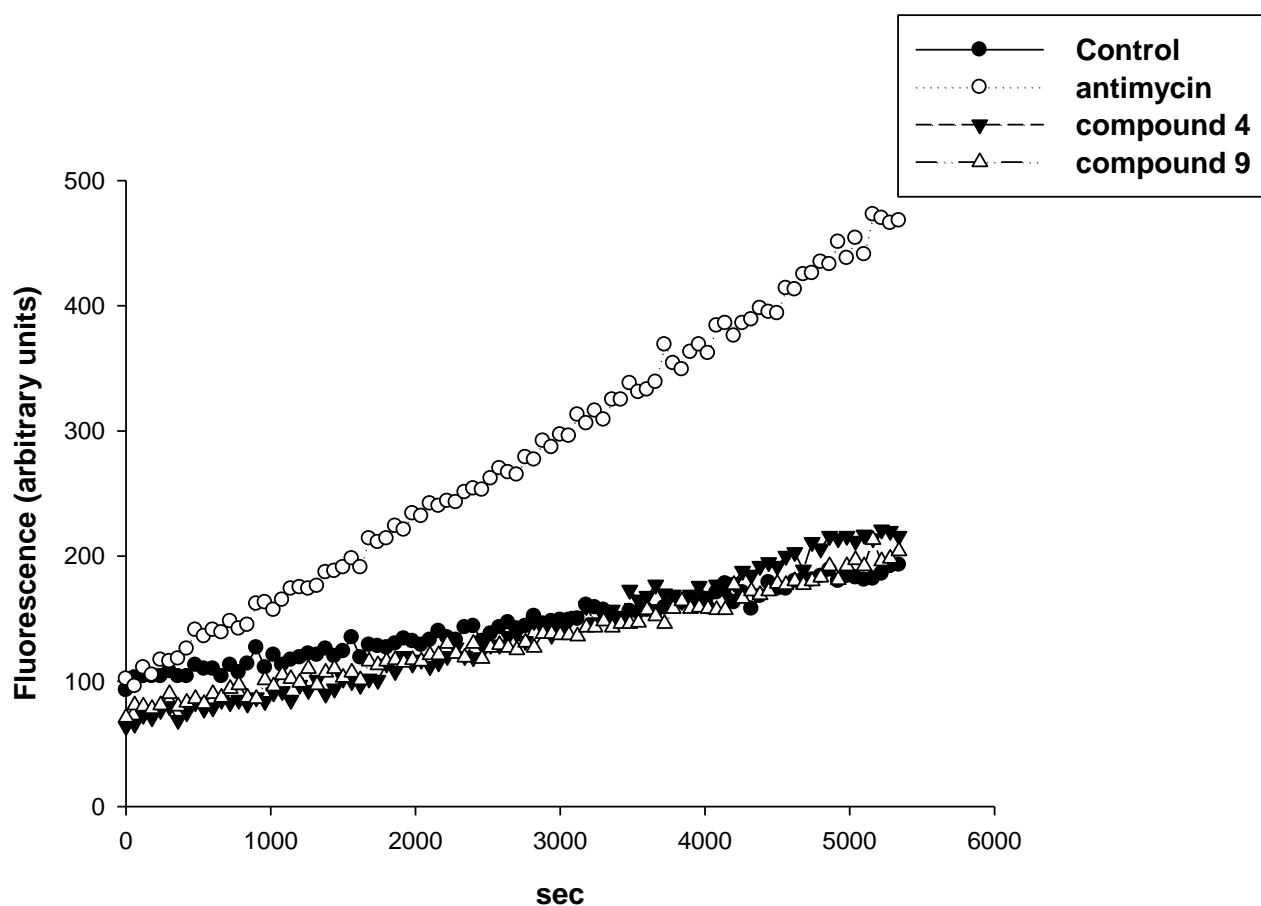


Figure S2. Cellular ROS production. Effect of tested compounds or antimycin on hydrogen peroxide formation in HCT-15 colon cancer cells. Error bars indicate S.D.

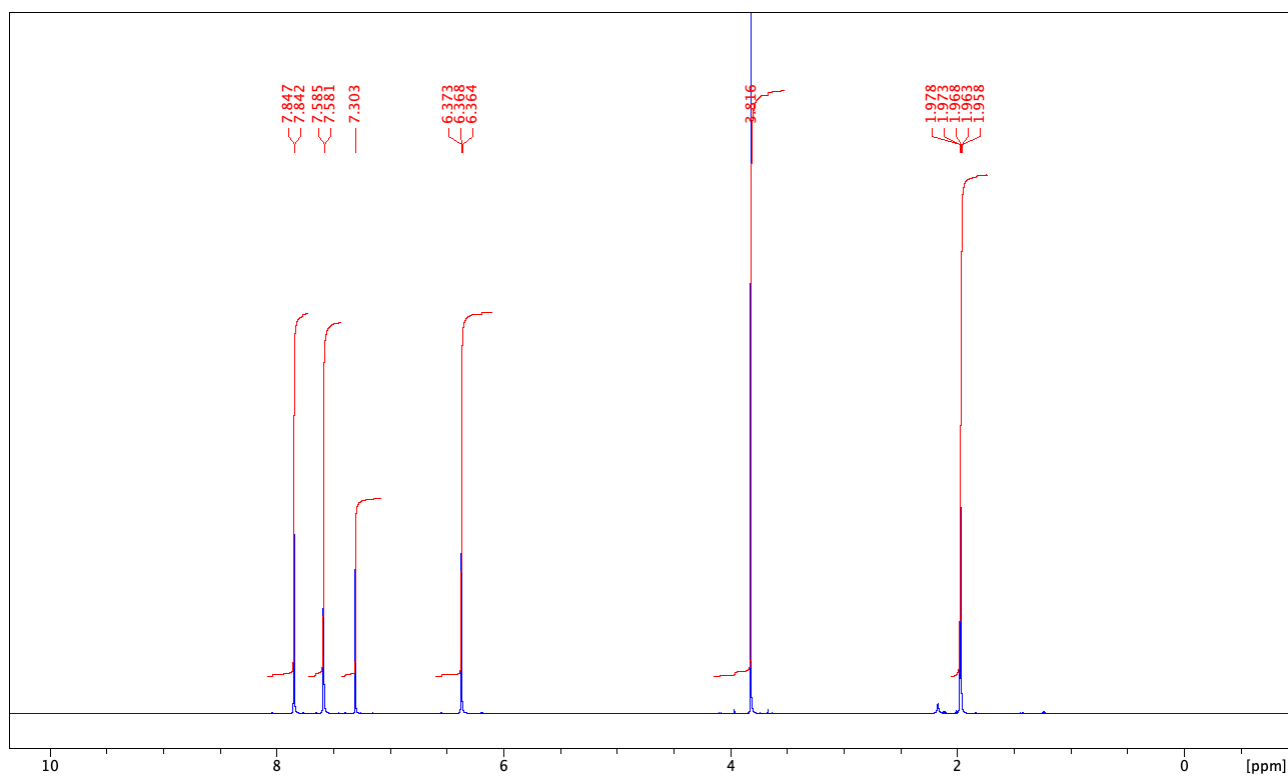


Figure S3: ¹H-NMR spectrum of [HC(pz)₂COOCH₃] (L^{OMe}, **1**) in CD₃CN.

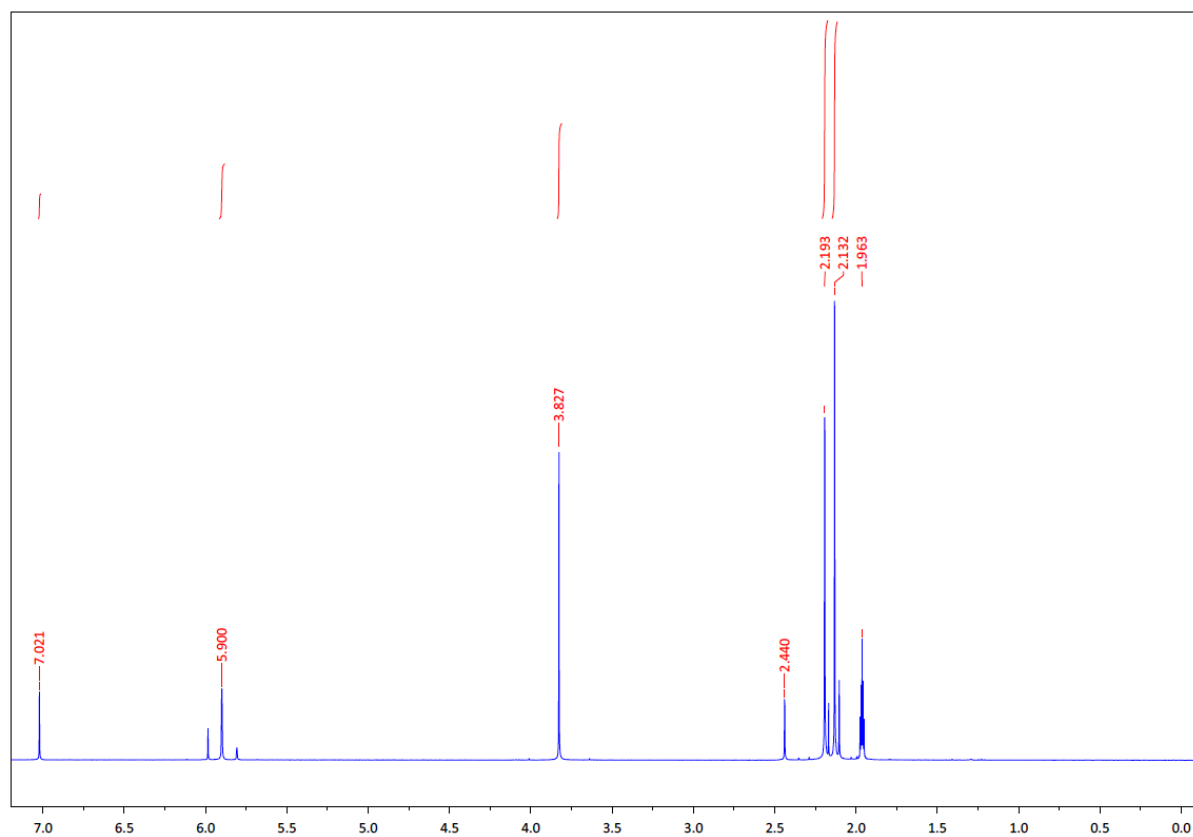


Figure S4: ¹H-NMR spectrum of [HC(pz^{Me2})₂COOCH₃] (L^{2OMe}, **2**) in CD₃CN.

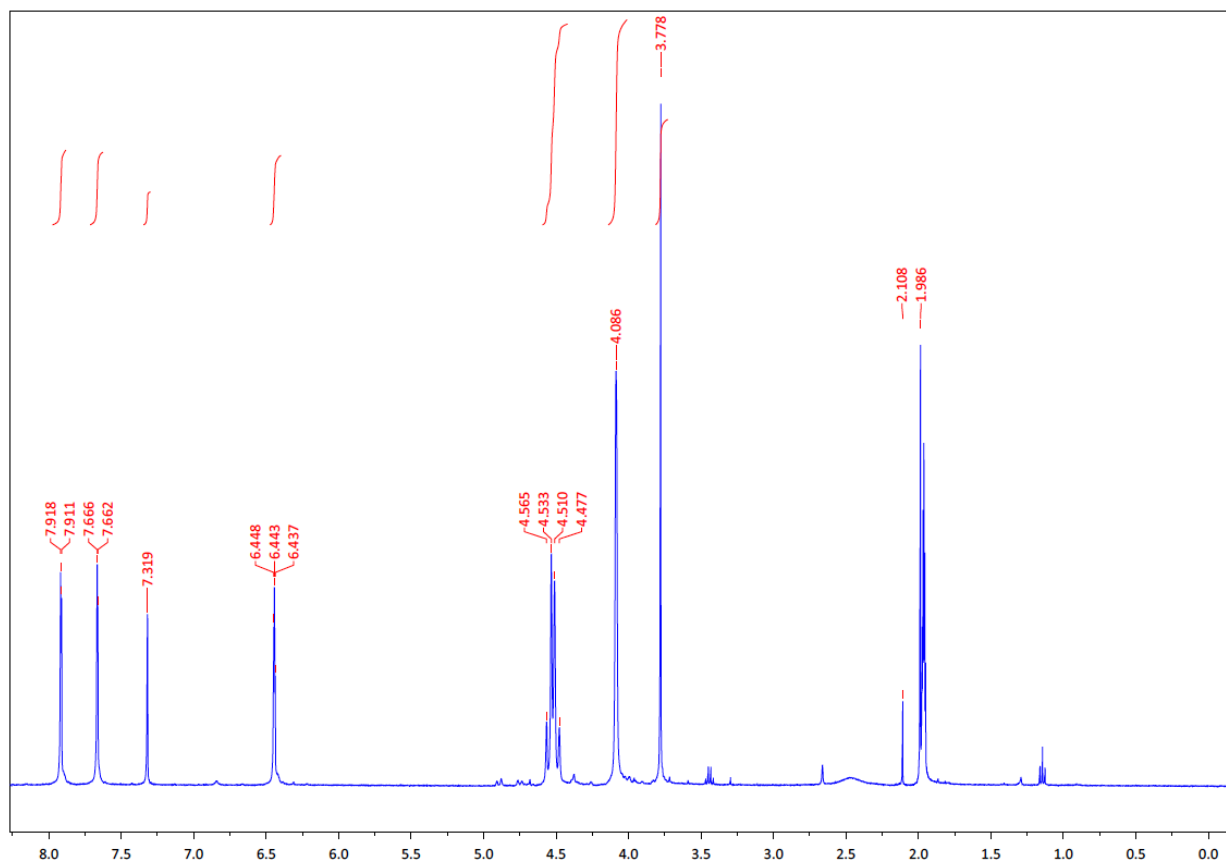


Figure S5: ^1H -NMR spectrum of $[(\text{PTA})\text{Cu}(\text{L}^{\text{OMe}})]\text{PF}_6$ (**3**) in CD_3CN .

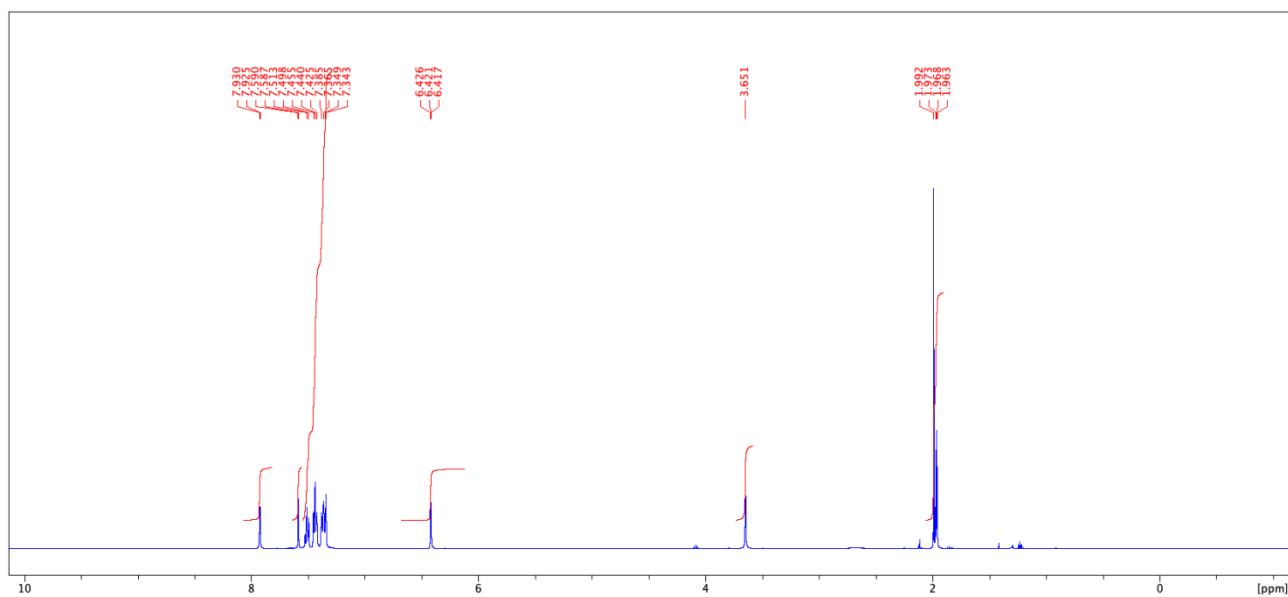


Figure S6: ^1H -NMR spectrum of $[(\text{PPh}_3)\text{Cu}(\text{L}^{\text{OMe}})]\text{PF}_6$ (**4**) in CD_3CN .

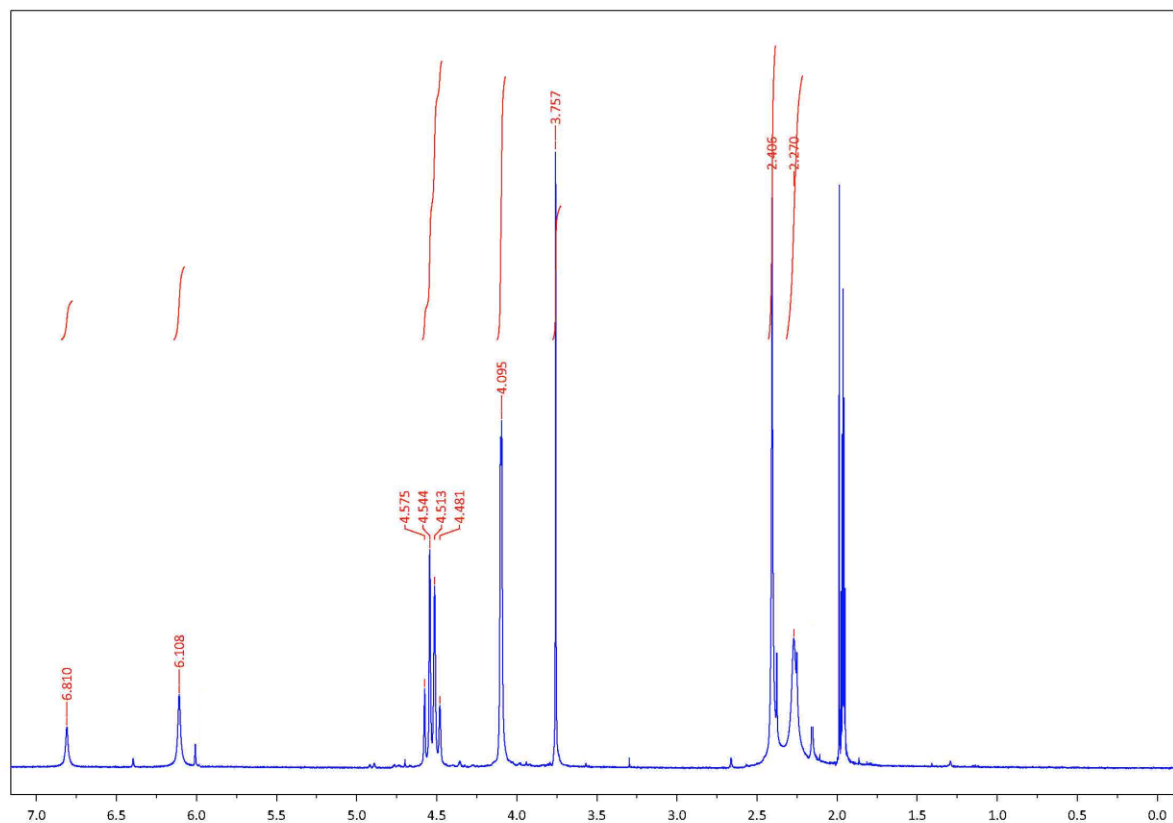


Figure S7: ^1H -NMR spectrum of $[(\text{PTA})\text{Cu}(\text{L}^{2\text{OMe}})]\text{PF}_6$ (**7**) in CD_3CN .

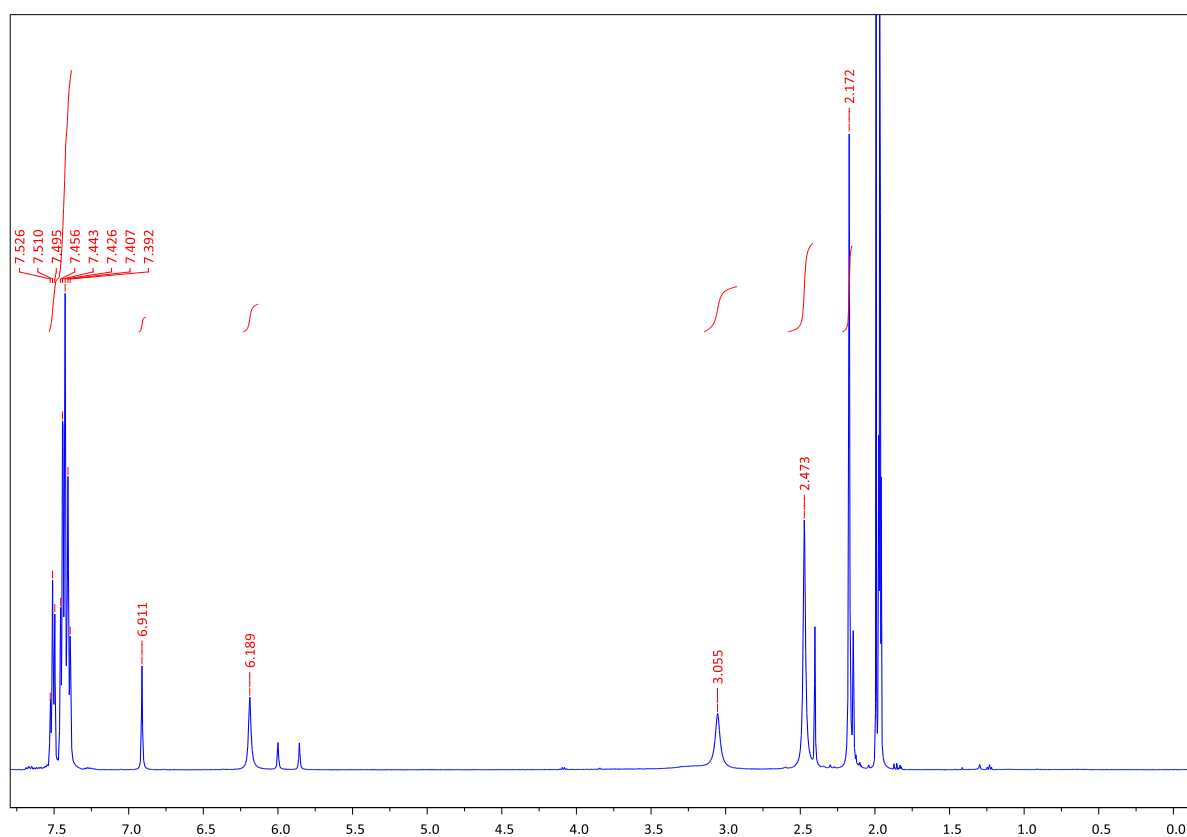


Figure S8: ^1H NMR spectrum of $[(\text{PPh}_3)\text{Cu}(\text{L}^{2\text{OMe}})]\text{PF}_6$ (**8**) in CD_3CN .