Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Experimental and Theoretical Evaluation on the Antioxidant Activity of a Copper (II) Complex Based on Lidocaine and Ibuprofen Amide-Phenanthroline Agents

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LIST OF SUPPORTING INFORMATION

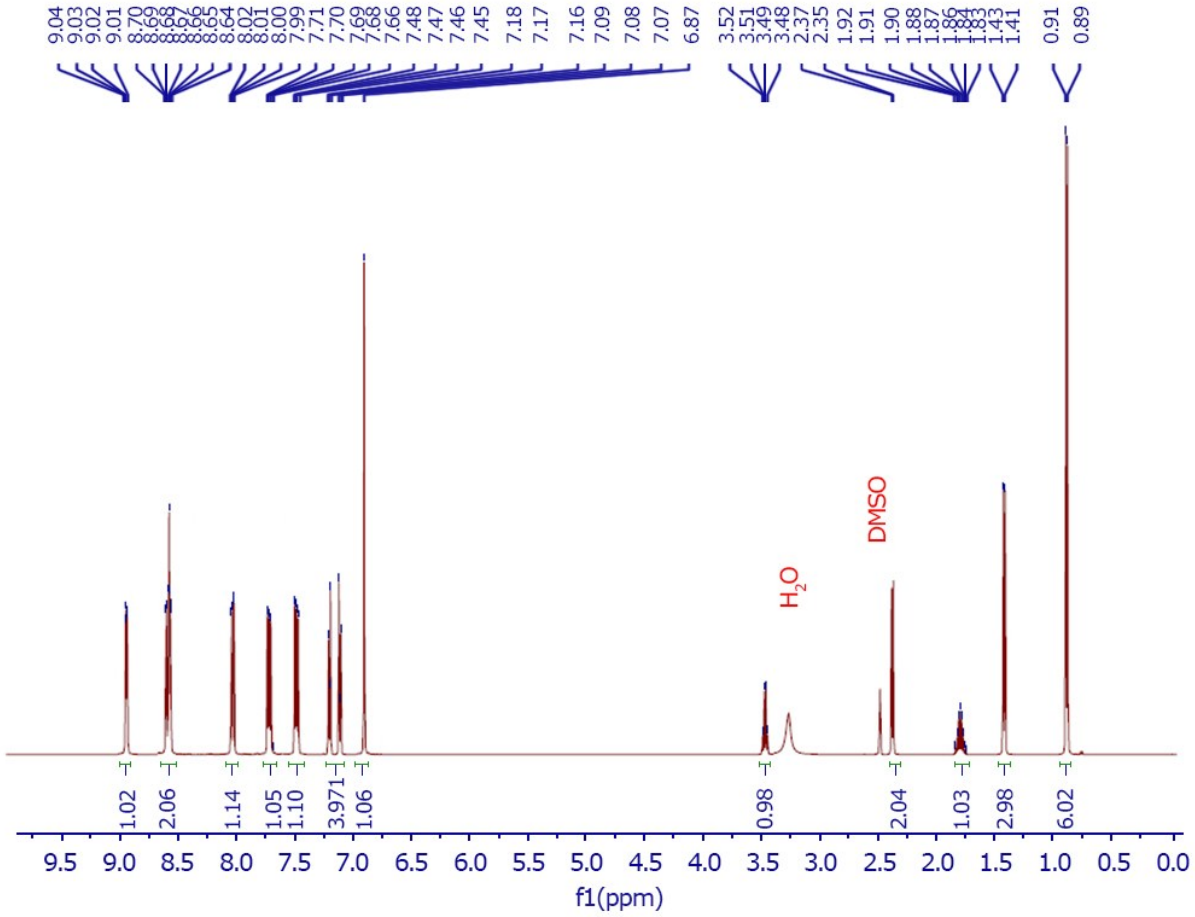


Figure S1. ^{1}H NMR spectrum of ligand ibuprofen amide-phenanthroline (Ibu-phen) (DMSO-d_6).

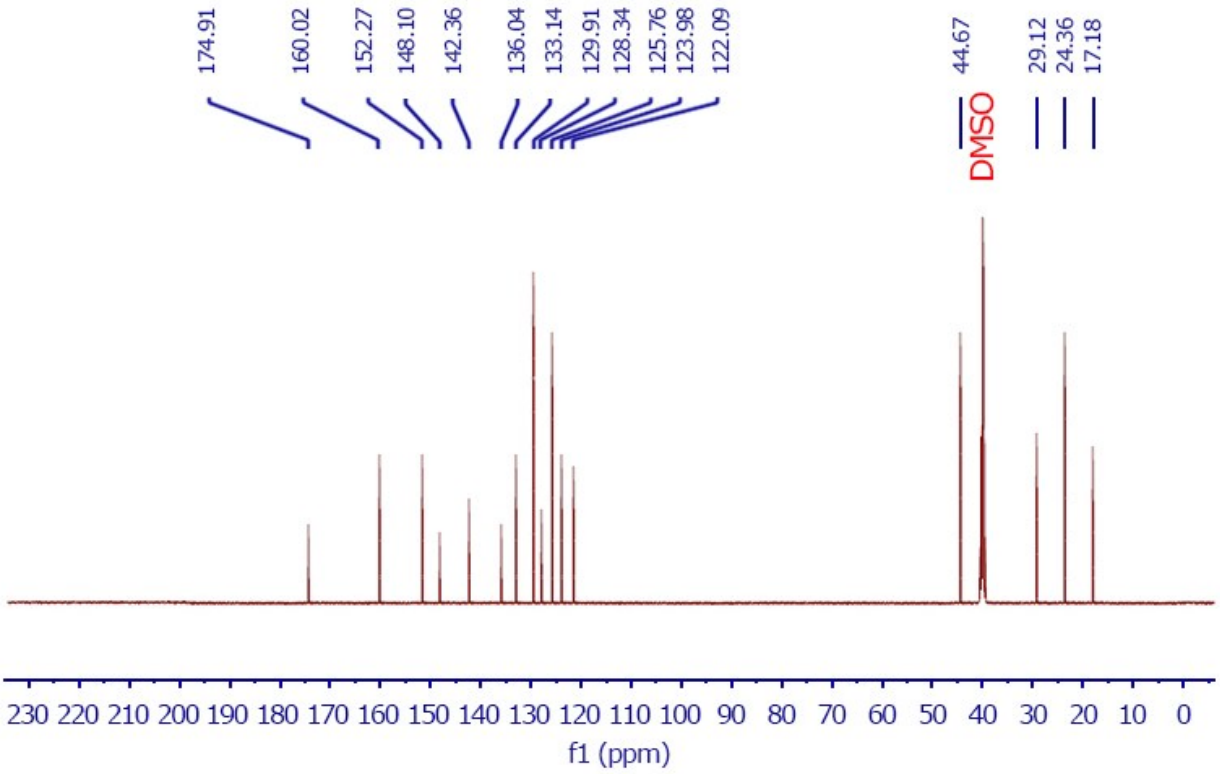


Figure S2. ^{13}C NMR spectrum of ligand ibuprofen amide-phenanthroline (Ibu-phen) (DMSO-d_6).

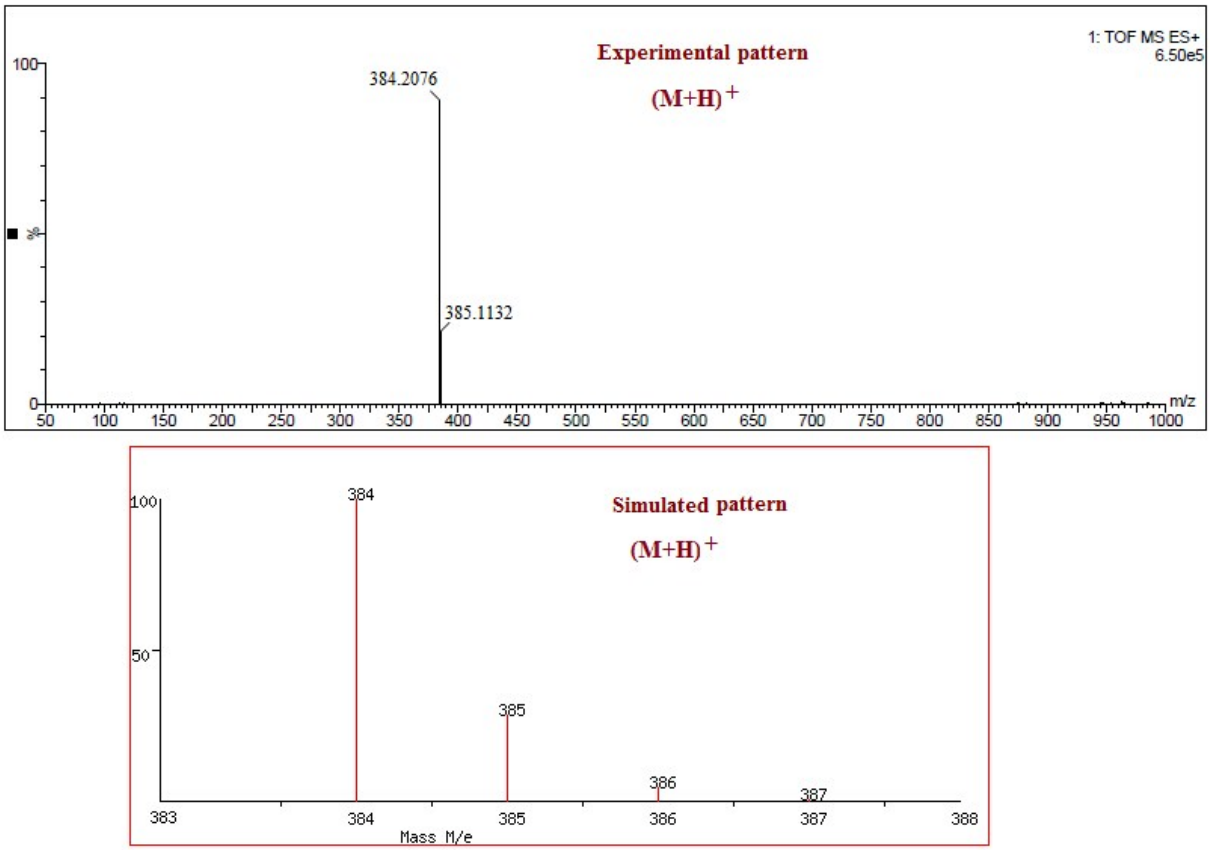


Figure S3. TOF MS spectrum of ligand ibuprofen amide-phenanthroline (Ibu-phen).

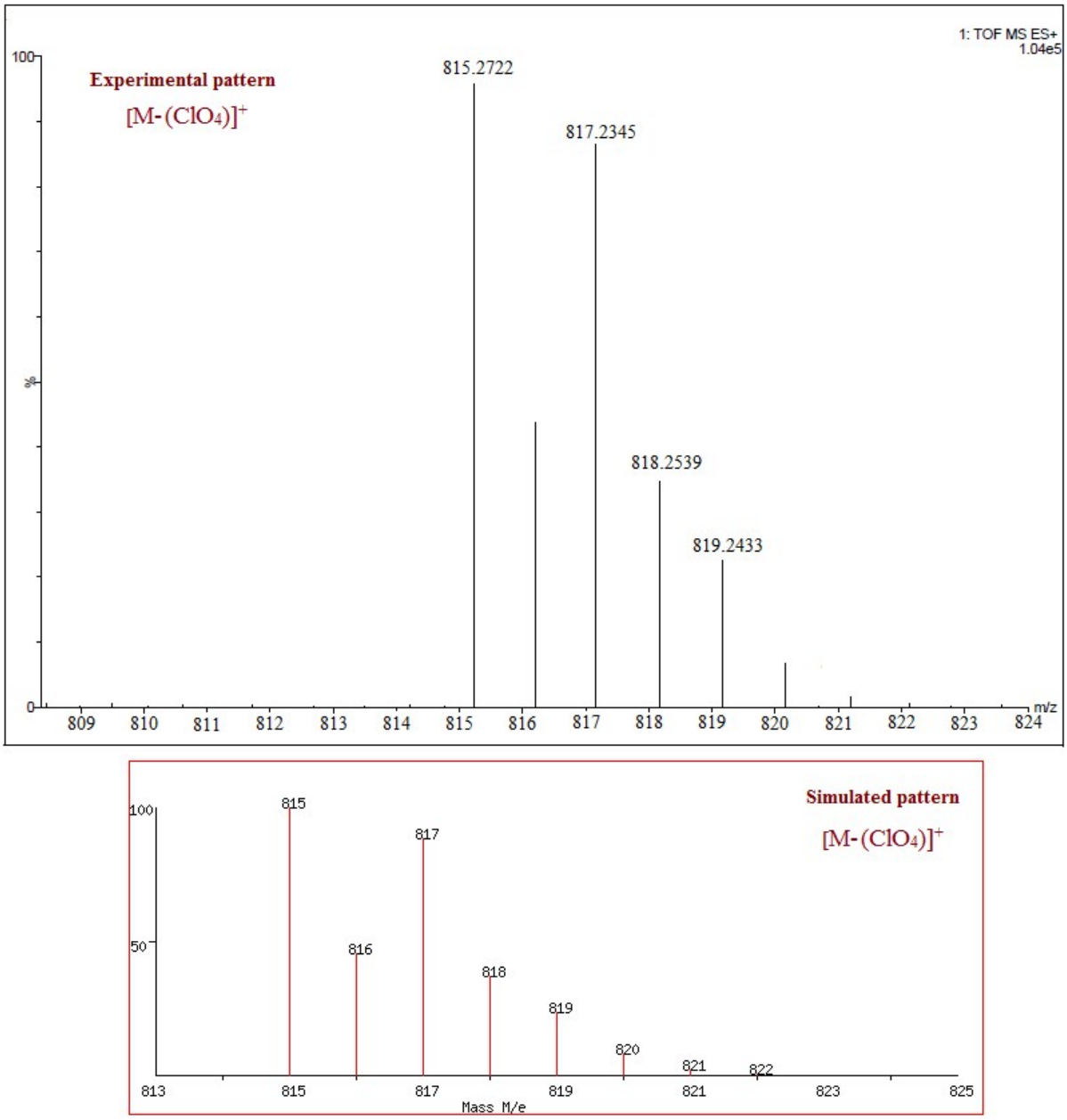


Figure S4. TOF MS spectrum of copper (II) complex.

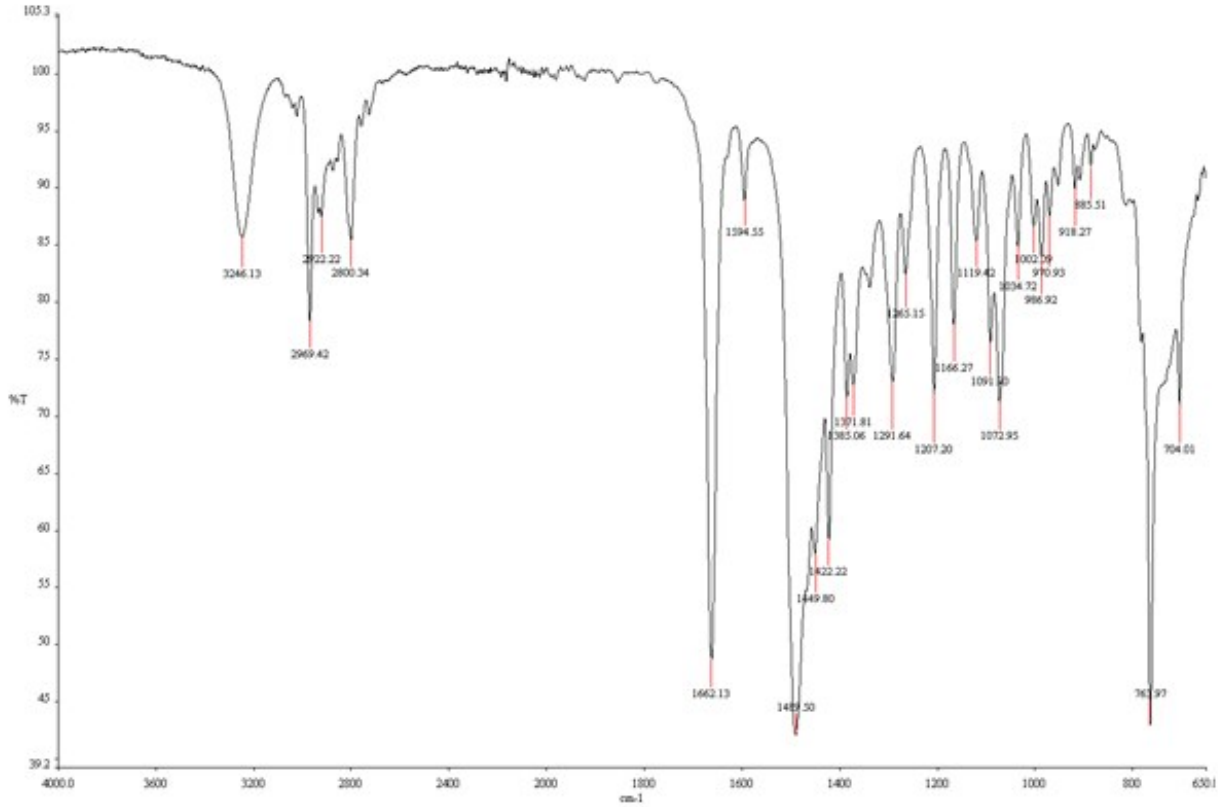


Figure S5. FT-IR of ligand LC

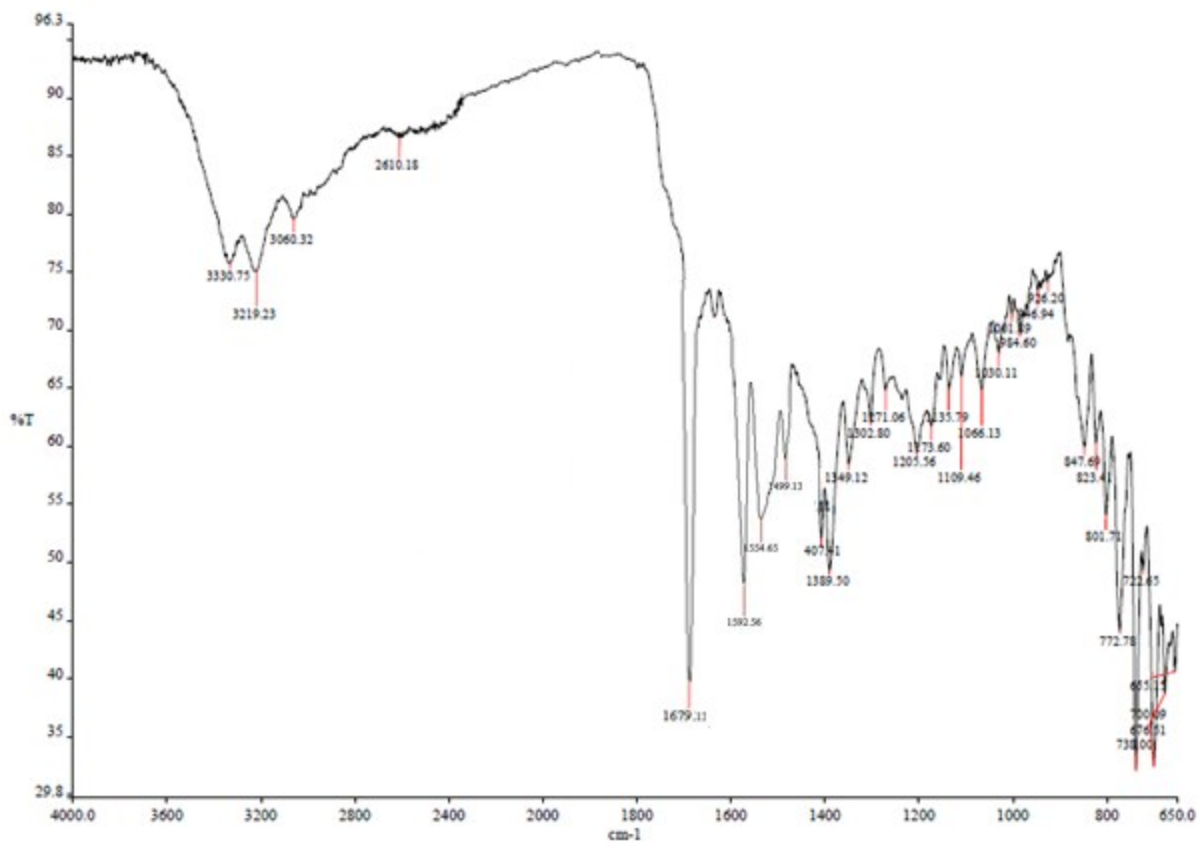


Figure S6. FT-IR of ligand Ibu-phen

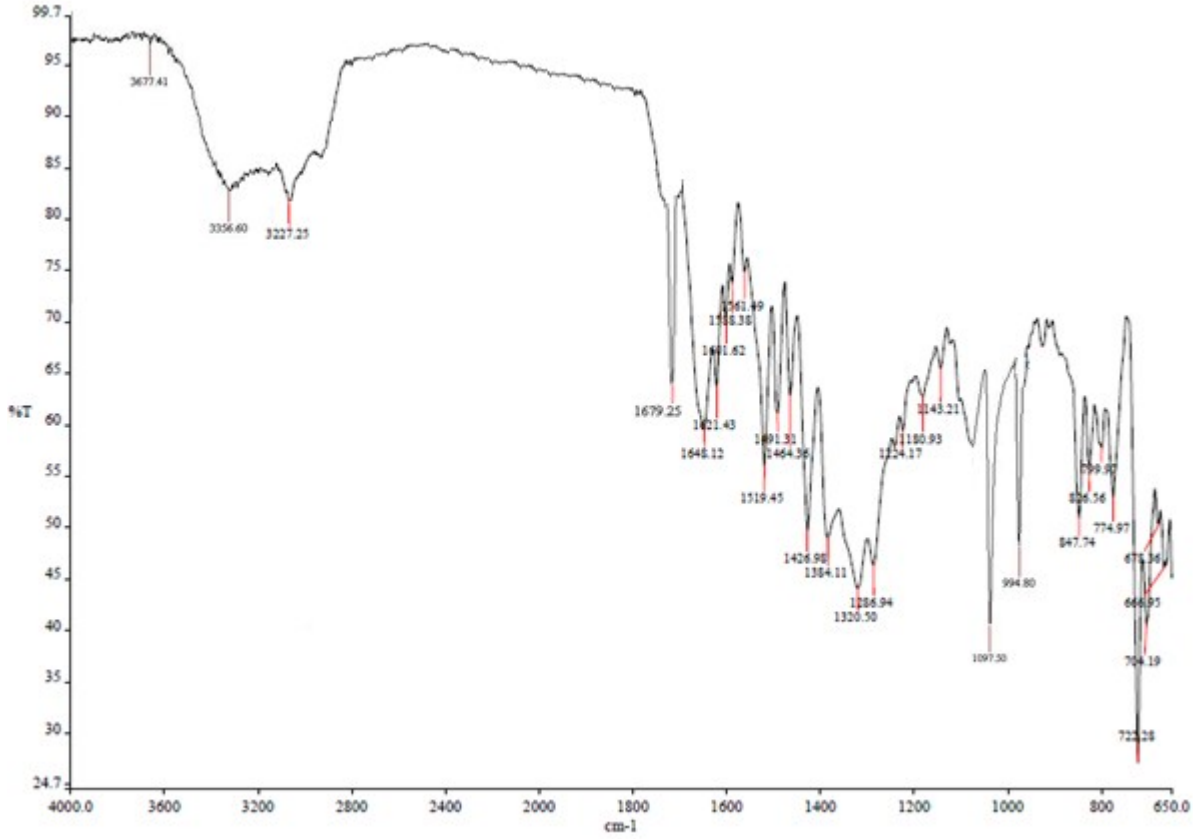


Figure S7. FT-IR of copper (II) complex

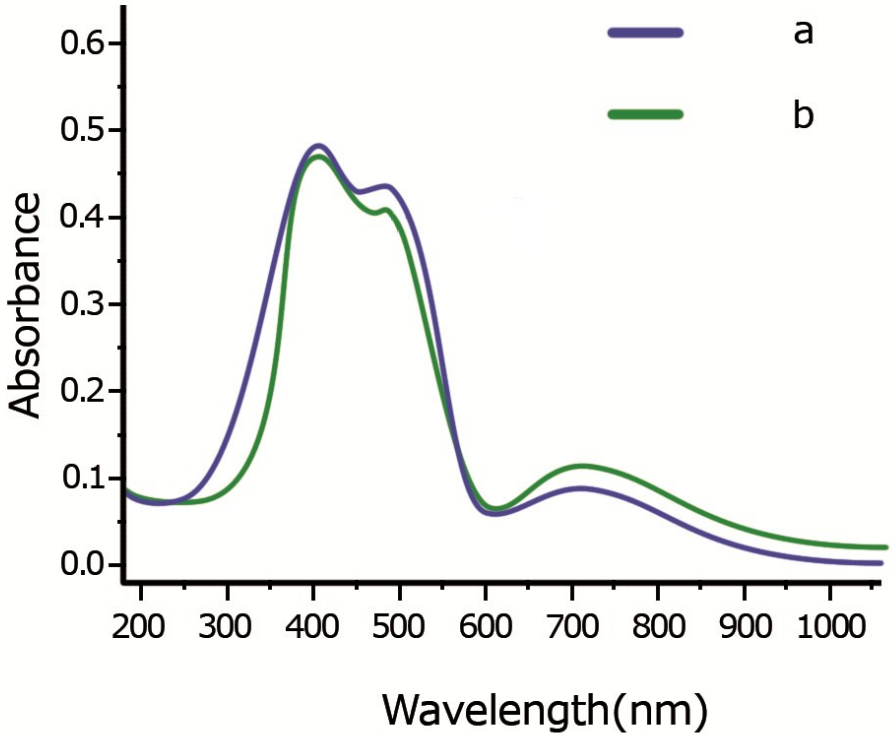


Figure S8. UV-Vis spectra of copper (II) complex in DMSO solution (**a**) and solid state (**b**).

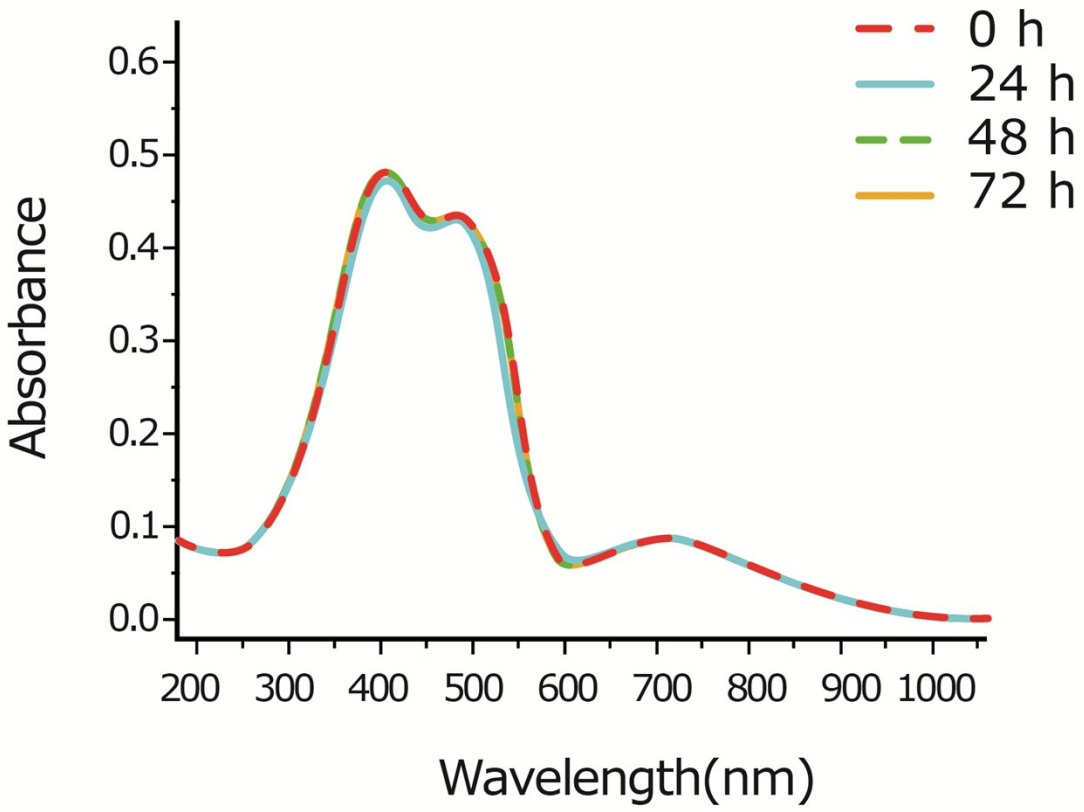
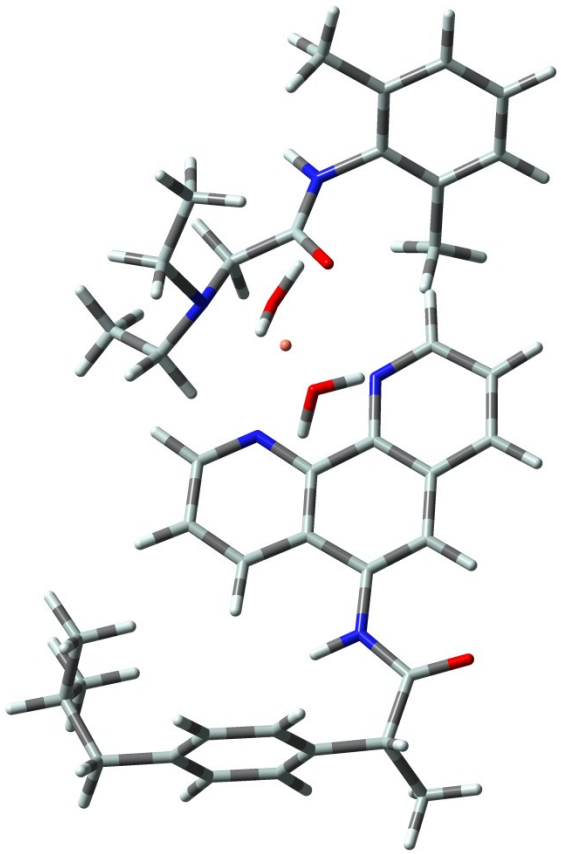


Figure S9. UV/Vis spectra of copper (II) complex in DMSO solution at room temperature during 72h.

Table S1. Cartesian coordinates and molecular enthalpies of copper (II) complex structures for different multiplicities from 2 to 8 optimized at M05-2X/LanL2DZ level of theory.

Cartesian coordinates				**Multiplicity = 2**
2 2				
O	4.43015200	-2.94646300	-3.64407200	
C	6.64647300	3.10689200	1.57653000	
C	7.86517100	2.46505800	0.86090100	
C	7.51176400	1.33448300	-0.08049600	
C	6.87722700	-0.79984000	-1.85974900	
C	6.47210500	-1.90782800	-2.81847100	
C	5.66834400	3.74750200	0.58021700	
C	5.91997500	2.10198800	2.48337300	
C	7.46834900	0.00190700	0.36850700	
C	7.24648300	1.57906900	-1.44103500	
C	7.15412100	-1.05002400	-0.50383500	
C	6.93161800	0.53056100	-2.31483700	
C	7.15002100	-3.26846400	-2.55136000	
C	4.95723900	-2.13043200	-2.86436200	
H	7.05055600	3.90288700	2.21139200	
H	8.55725300	2.09767700	1.62508100	
H	8.38838100	3.24892200	0.30449000	
H	6.74066200	-1.60385400	-3.83549000	
H	5.22502800	2.98840200	-0.07571600	
H	6.17216700	4.48048000	-0.05620200	
H	4.86237500	4.26569600	1.11099100	
H	5.11779600	2.59728100	3.04115900	
H	5.48458900	1.28651900	1.89306400	
H	6.60435200	1.65540600	3.21028500	
H	7.70854000	-0.21624400	1.40323700	
H	7.31316300	2.59229900	-1.82131000	
H	7.15497300	-2.06613900	-0.12832000	
H	6.74910800	0.74300800	-3.36316100	
H	8.23396300	-3.14572000	-2.54535900	
H	6.84340900	-3.69397200	-1.59291200	
H	6.87589300	-3.97468100	-3.33504100	
N	4.21175500	-1.36298400	-1.97195000	
H	4.77876200	-0.75554800	-1.39564400	
C	3.07414000	0.55222200	-0.14471800	
C	2.28357200	-0.38758800	-0.85766200	
C	2.46744000	1.45233200	0.71926600	
C	0.88708400	-0.35560200	-0.62801000	
C	2.82667000	-1.34763300	-1.81625800	
C	1.07111500	1.40550800	0.89635000	
H	3.05299100	2.18679000	1.25318900	
C	0.01713000	-1.22187200	-1.37216500	
C	1.97624500	-2.17172900	-2.52399100	
H	0.58648900	2.10649400	1.55622100	



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C	-1.71890900	-2.77169800	-2.83584800
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H	-3.23299900	-1.71907100	-1.65193800
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H	4.14925200	0.60872000	-0.26584000
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C	-7.71819300	0.97326700	-0.11445300
C	-5.00025900	-3.25659700	0.68002600
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H	-4.00064600	-2.96306300	0.33649000
H	-8.33843000	-2.95981000	-2.59207700
Cu	-1.75995900	0.19445300	0.33526400
O	-1.54409600	-1.70684100	1.75248600
H	-0.78523000	-2.01669300	2.27972800
H	-1.98738100	-2.44890700	1.30046600
O	-1.96814800	1.81395200	-1.22621000
H	-2.73226600	1.78382100	-1.82972000
H	-1.20351700	2.26070700	-1.63110900
Energy calculation at M05-2X/LanL2DZ			**HF=-2286.8279716**

Cartesian coordinates			**Multiplicity = 6**
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O	4.67464200	-1.71597400	-0.84696000
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C	5.91250400	-0.01679900	-2.05938700
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C	9.90420100	-0.82852500	3.15665100
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C	9.29628100	0.86905900	-0.58610800
C	7.50219300	-1.33093000	-0.52356500
C	8.09326100	0.96981200	-1.24310600
C	6.13261600	-0.85152700	-3.36648700
C	4.66602800	-0.57871800	-1.36811100
H	11.87351200	-0.09003000	2.70157000
H	11.28216100	-1.49248800	0.84684600
H	11.70441100	0.16515600	0.32780900
H	5.75626100	1.02742600	-2.34056900
H	9.44730500	1.70291200	2.11161100
H	11.14360600	2.15300600	1.80897000
H	10.57854700	1.86632100	3.45363600
H	9.98142600	-0.55265500	4.21093900
H	8.86117000	-0.68510200	2.85599200
H	10.15106800	-1.89110600	3.07654400
H	8.97009100	-2.33453000	0.66208800
H	10.00443400	1.68771400	-0.59660700
H	6.78673300	-2.14142600	-0.51369800
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H	7.01216700	-0.49862200	-3.90719400
H	6.25888200	-1.90596300	-3.11724500
H	5.25975400	-0.74694900	-4.01377900
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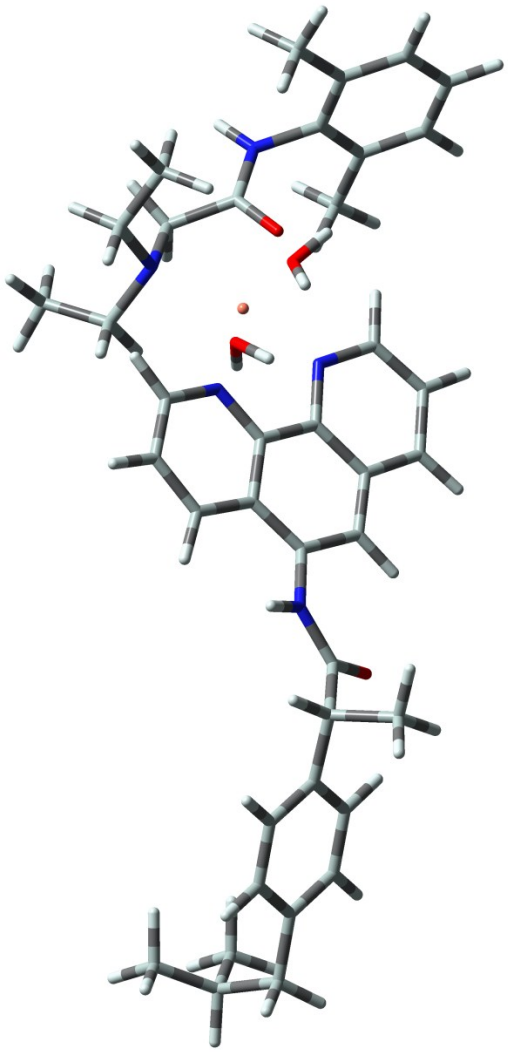

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H	-4.21171500	2.87189700	3.65566900
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H	-4.99924600	2.33236600	-1.59615200
H	-6.33492900	2.42594500	-0.42107500
H	-5.82513800	3.86683100	-1.28622600
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H	-6.77747500	-4.96242300	0.22437800
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H	-6.28617500	-2.64208800	2.73302400
H	-5.50699500	-4.04747400	2.00812600
H	-4.82584600	-2.43055000	1.76395300
H	-8.18072700	-4.68959400	-1.80359800
Cu	-2.85279100	0.75663300	-0.37446600
O	-2.76931600	-0.76220300	2.29347900
H	-2.48061500	-1.27746600	3.06645400
H	-2.30369300	-1.02485900	1.47145300
O	-3.42497700	0.88731900	-2.49929200
H	-4.05110700	0.16707300	-2.69915700
H	-2.79870600	1.06639500	-3.22118400
Energy calculation at M05-2X/LanL2DZ			HF=-2286.6231164

Cartesian coordinates			**Multiplicity = 8**
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O	5.29078900	-0.40028400	-0.69638500
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C	8.92806900	-0.99806000	0.03395300
C	7.47862500	0.63545800	-1.77232200
C	6.19767000	1.28447400	-2.21356300
C	8.61028100	-0.34024300	3.05085500
C	7.17471600	-2.24926500	2.20608000
C	7.97657300	-1.53716600	-0.90318400
C	9.22660500	0.40364500	-0.07314500
C	7.79671900	-0.76730200	-2.15036500
C	8.40216100	1.21988400	-0.87075700
C	5.99295800	1.13585100	-3.74151800
C	5.06455700	0.59136800	-1.43321100
H	9.11234700	-2.42931900	3.12777700
H	9.53035100	-2.88200700	0.82796700
H	10.49626900	-1.48933200	1.38199100
H	6.21096300	2.34581600	-1.94063900
H	8.04577900	0.36711000	2.43493000
H	9.62569000	0.04228800	3.18899600
H	8.13336800	-0.36864300	4.03358900
H	6.65408900	-2.32135100	3.16396200
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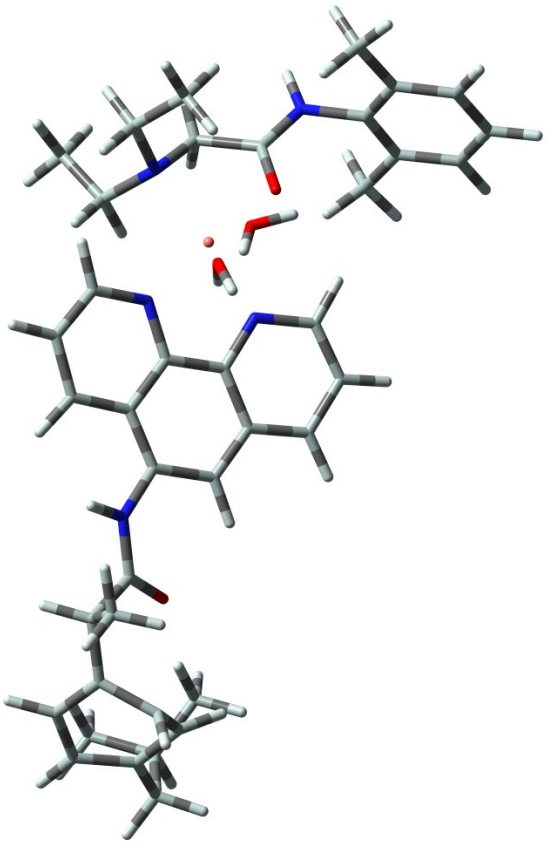

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H	8.43267900	2.29714700	-0.74484000
H	6.83222800	1.57847800	-4.28092500
H	5.91796900	0.08123800	-4.01486600
H	5.08310600	1.63976800	-4.07396600
N	3.82367200	1.15474200	-1.61488900
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C	1.49563900	1.62406900	-1.17639100
C	0.39685900	3.76502700	-1.63953000
C	0.19071600	1.09680400	-0.87886000
C	2.58264300	0.71782200	-1.13656300
C	-0.82099800	3.19307700	-1.35822800
H	0.44072900	4.80041400	-1.94667500
C	0.00654500	-0.27441200	-0.53240900
C	2.39326300	-0.70780900	-0.75808900
H	-1.73947200	3.75049600	-1.47049100
C	1.12074300	-1.19410300	-0.49016200
H	3.25732400	-1.35093600	-0.70437100
C	0.83949300	-2.56290900	-0.17820600
C	-1.52950600	-2.03629400	-0.02897300
C	-0.51146900	-2.96251800	0.02484400
H	1.64466800	-3.28305100	-0.13430600
H	-2.57177700	-2.29473000	0.09521100
H	-0.74968500	-4.00020200	0.21247000
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N	-1.27081100	-0.66794300	-0.25917800
N	-0.94301300	1.87176200	-0.92936300
O	-4.12593400	-0.33918000	-0.07148700
N	-3.79324800	2.27415500	0.56914400
N	-6.02518000	-0.60231200	1.17114200
C	-4.69992400	1.45380400	1.42487900
C	-2.85396100	3.07658100	1.44316900
C	-4.58520000	3.17668300	-0.33532100
C	-6.26224100	-1.96300700	0.72282600
C	-4.96377000	0.10770300	0.78393500
C	-7.07309300	-2.17211900	-0.40369000
C	-5.66827300	-3.01141200	1.44528700
C	-3.54146400	4.05956300	2.39954200
C	-5.52050800	2.42428500	-1.28017600
C	-7.30168400	-3.49666300	-0.80593000
C	-5.91589800	-4.32262600	1.01271300
C	-7.67109300	-1.01024500	-1.16142300
C	-4.80019600	-2.73330600	2.65069600
C	-6.72889200	-4.56397500	-0.10258200

H	-4.17382500	1.23148300	2.35690300	
H	-5.63338200	1.98166700	1.64680600	
H	-2.26418000	2.34993300	2.00396900	
H	-2.17731500	3.61707300	0.78122100	
H	-5.16684500	3.87275600	0.27950700	
H	-3.86883400	3.76621700	-0.91099000	
H	-6.66586500	-0.19856400	1.84556800	
H	-4.03955300	4.87824700	1.87762900	
H	-4.26968300	3.56586800	3.04841000	
H	-2.78313400	4.50378700	3.04833400	
H	-4.96673600	1.72903500	-1.91153300	
H	-6.29778500	1.87845600	-0.73698100	
H	-6.03015200	3.14372300	-1.92503600	
H	-7.93174600	-3.69005200	-1.66536000	
H	-5.48054700	-5.15273000	1.55557600	
H	-8.28921800	-0.37981200	-0.51564300	
H	-6.88811500	-0.37830800	-1.59281000	
H	-8.30082600	-1.36810000	-1.97618200	
H	-5.37885600	-2.27860900	3.46102900	
H	-4.37316300	-3.66152200	3.03232100	
H	-3.97996400	-2.05051300	2.40870100	
H	-6.91957100	-5.58118900	-0.41983400	
Cu	-2.57920600	0.84463000	-0.46060400	
O	-2.24405000	-0.00060600	2.46841600	
H	-1.87476800	-0.27862900	3.32430900	
H	-1.73835200	-0.35465600	1.70628100	
O	-3.16158700	0.40643300	-2.53840000	
H	-3.66338900	-0.42904400	-2.56360500	
H	-2.58292100	0.53382000	-3.30928200	
Energy calculation at M05-2X/LanL2DZ				HF=-2286.4879208

Table S2. Natural population charges of heavy atoms in the copper (II) complex calculated at the M05-2X/6-311++g(2df,2p) level of theory.

Atom	No	Natural charge	Spin Density	Atom	No	Natural charge	Spin Density
O	1	-0.6326	0.0001	C	46	-0.1016	-0.0044
C	2	-0.2374	0.0000	C	47	0.0846	-0.0056
C	3	-0.4144	0.0000	C	48	-0.2267	0.0065
C	4	-0.0314	0.0000	N	53	-0.5900	0.0626
C	5	-0.0906	-0.0001	N	54	-0.6018	0.0479
C	6	-0.3318	0.0000	O	55	-0.7547	0.0500
C	7	-0.5910	0.0000	N	56	-0.6248	0.0516
C	8	-0.5898	0.0000	N	57	-0.5870	-0.0018
C	9	-0.2025	0.0000	C	58	-0.2762	0.0049
C	10	-0.2014	0.0000	C	59	-0.1695	0.0001
C	11	-0.2202	0.0000	C	60	-0.1749	0.0031
C	12	-0.2061	0.0000	C	61	0.1003	0.0021
C	13	-0.5767	0.0000	C	62	0.7631	0.0011
C	14	0.7535	0.0000	C	63	-0.0210	-0.0006
N	32	-0.6613	0.0002	C	64	-0.0293	-0.0004
C	34	-0.0842	-0.0033	C	65	-0.6212	0.0012
C	35	-0.1364	0.0026	C	66	-0.6187	-0.0005
C	36	-0.1993	0.0039	C	67	-0.1958	0.0004
C	37	0.3058	-0.0040	C	68	-0.2054	-0.0002
C	38	0.1991	0.0003	C	69	-0.6123	0.0001
C	39	0.0924	-0.0005	C	70	-0.6071	0.0000
C	41	0.2692	-0.0001	C	71	-0.1614	0.0000

C	42	-0.1792	0.0003	Cu	94	1.1682	0.7791
C	44	-0.1186	0.0030	O	95	-0.9495	0.0003
				O	98	-0.9486	0.0000

Table S3. Natural bond orbital (NBO) analysis of the copper (II) complex calculated at the M05-2X/6-311++g(2df,2p) level of theory

Donor NBO (i)	Acceptor NBO (j)	E(2), kJ/mol
LP(1) N53	LP*(5) Cu94	120.20
LP(1) N53	LP*(6) Cu94	49.60
LP(1) N53	LP*(8) Cu94	52.70
LP(1) N54	LP*(5) Cu94	40.30
LP(1) N54	LP*(6) Cu94	98.90
LP(1) N54	LP*(7) Cu94	37.10
LP(1) O55	LP*(6) Cu94	94.2
LP(1) O55	LP*(7) Cu94	50.00
LP(1) O55	LP*(8) Cu94	32.30
LP(1) O55	LP*(9) Cu94	395.8
LP(2) O55	LP*(6) Cu94	166.00
LP(2) O55	LP*(7) Cu94	82.40
LP(2) O55	LP*(8) Cu94	26.20
LP(2) O55	LP*(9) Cu94	223.70
LP(3) O55	LP*(9) Cu94	47.00
σ(1) N56–C59	LP*(9) Cu94	237.1
LP(1) N56	LP*(5) Cu94	73.8
LP(1) N56	LP*(6) Cu94	57.6
LP(1) N56	LP*(8) Cu94	35.9
σ(1) O95–H96	LP*(9) Cu94	28.7
σ(1) O95–H97	LP*(9) Cu94	26.9
LP(2) O95	LP*(9) Cu94	81.3
σ(1) O98–H99	LP*(6) Cu94	37.1
LP(2) O98	LP*(6) Cu94	124.1
LP(2) O98	LP*(9) Cu94	844.9