Supplementary material

Enhancement of the cytotoxicity of quinazolinone Schiff base derivatives by copper coordination

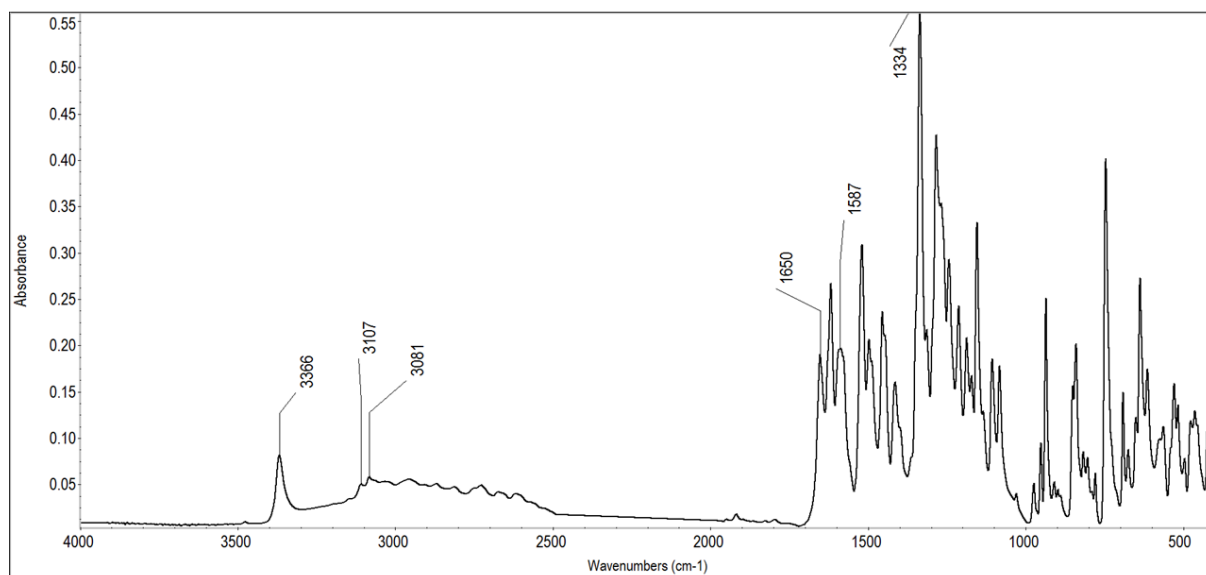Ilona Gurgul[1], Jana Hricovíniová[2], Olga Mazuryk[1], Zuzana Hricovíniová[3,*] and Małgorzata Brindell[1,*]

Figure S1. The FT-IR spectrum of the free ligand **L1**.
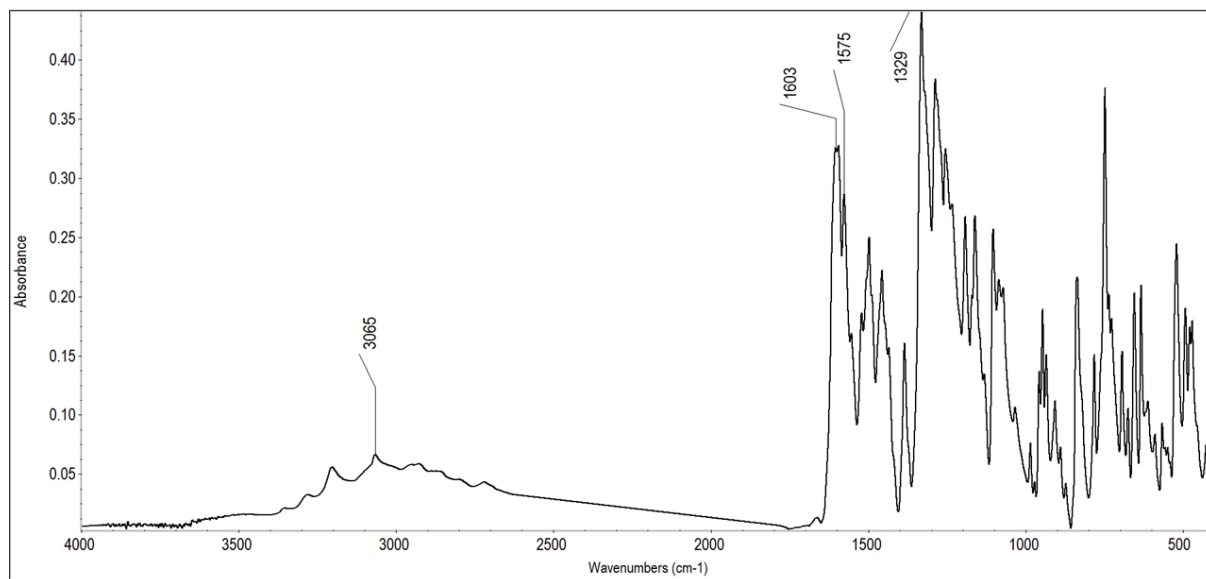

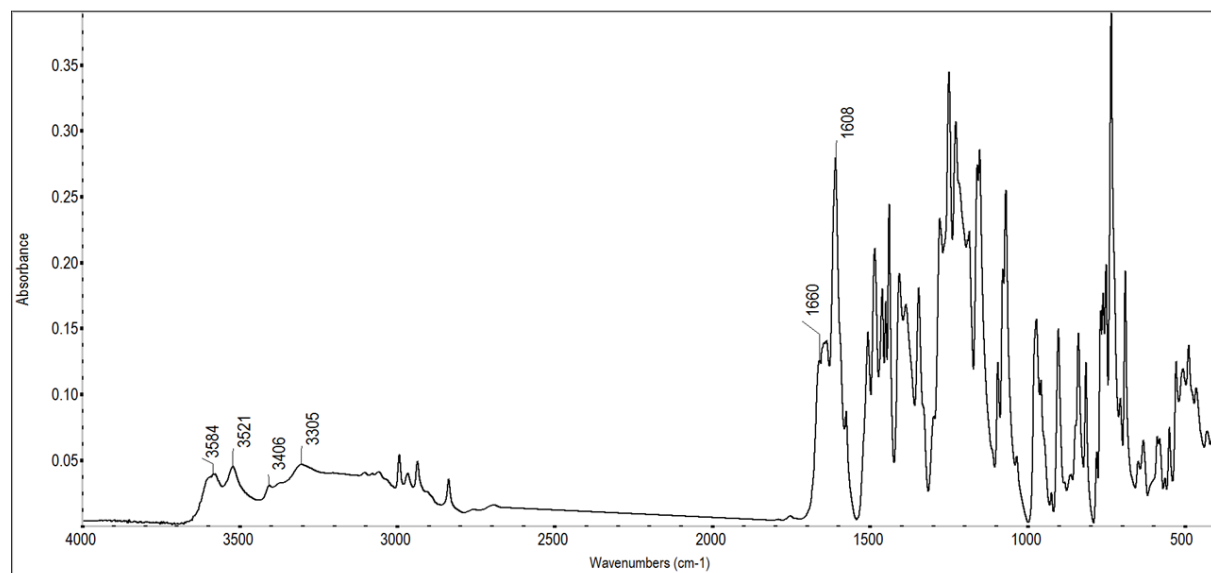**Figure S2**. The FT-IR spectrum of the **Cu-L1** complex.

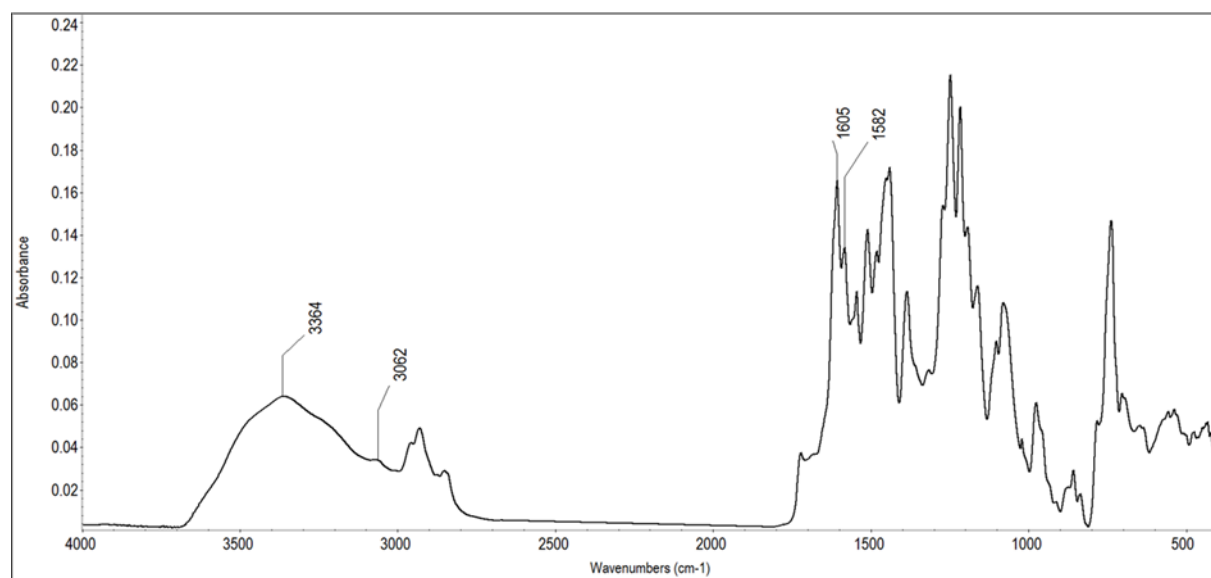**Figure S3**. The FT-IR spectrum of the free ligand **L2**.

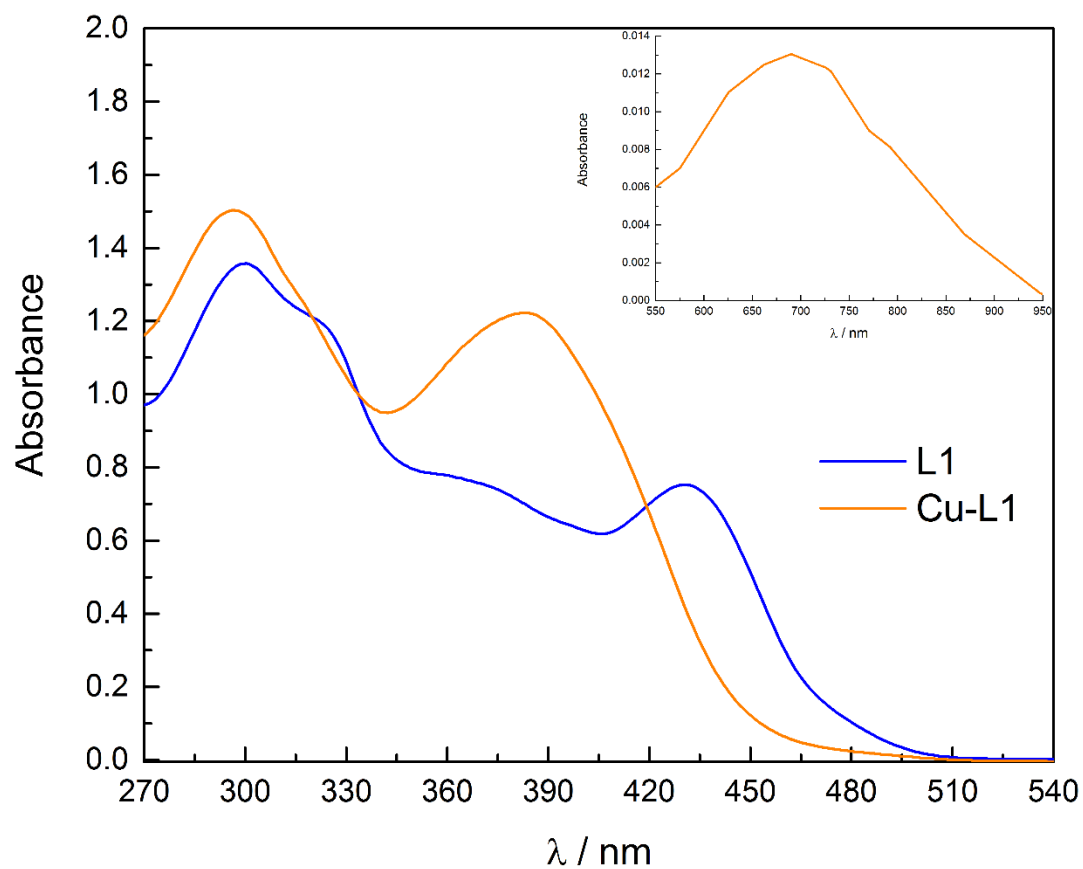**Figure S4**. The FT-IR spectrum of the **Cu-L2** complex.

Figure S5. The electronic absorption spectra of the free ligand **L1** (blue line) and the **Cu-L1** complex (orange line) measured in DMSO at 0.1 mM concentration. The inset shows absorption band of **Cu-L1** complex obtained at higher concentration (1 mM) in order to register the d-d transitions.

Figure S6. The electronic absorption spectra of the ligand **L2** (blue line) and the **Cu-L2** complex (orange line) measured in DMSO at 0.1 mM concentration. The inset shows absorption band of **Cu-L2** complex obtained at higher concentration (1 mM) in order to register the d-d transitions.
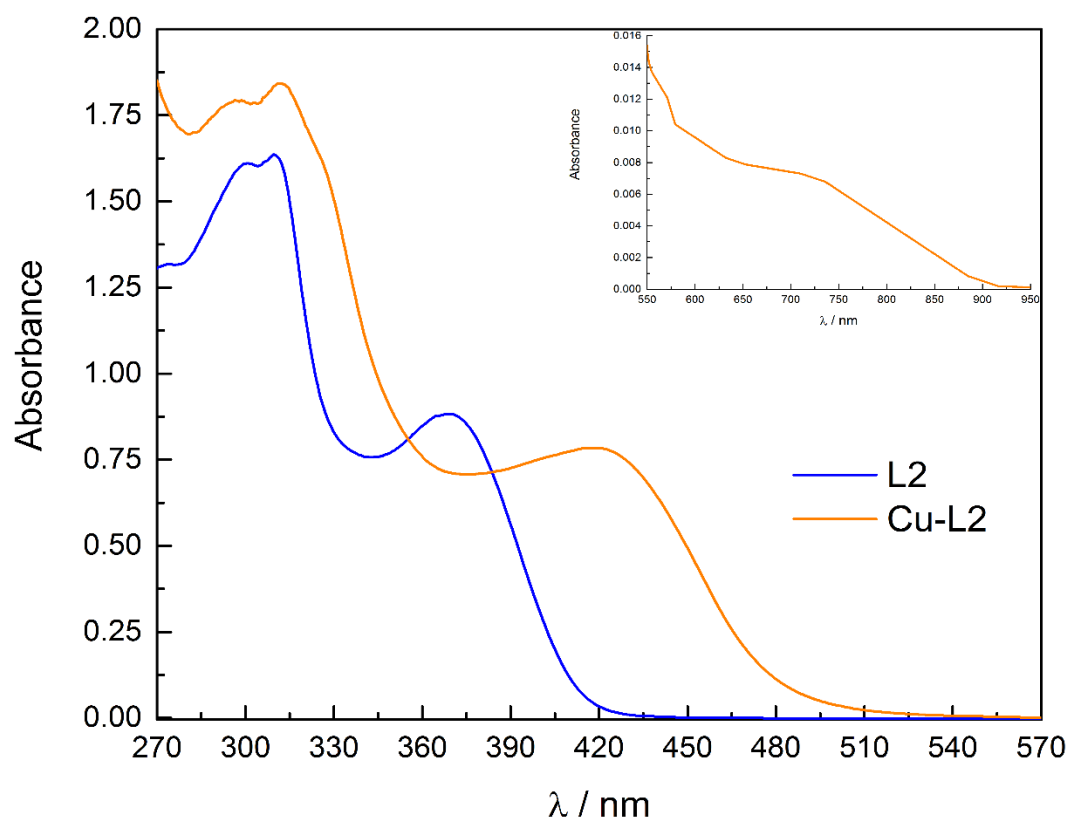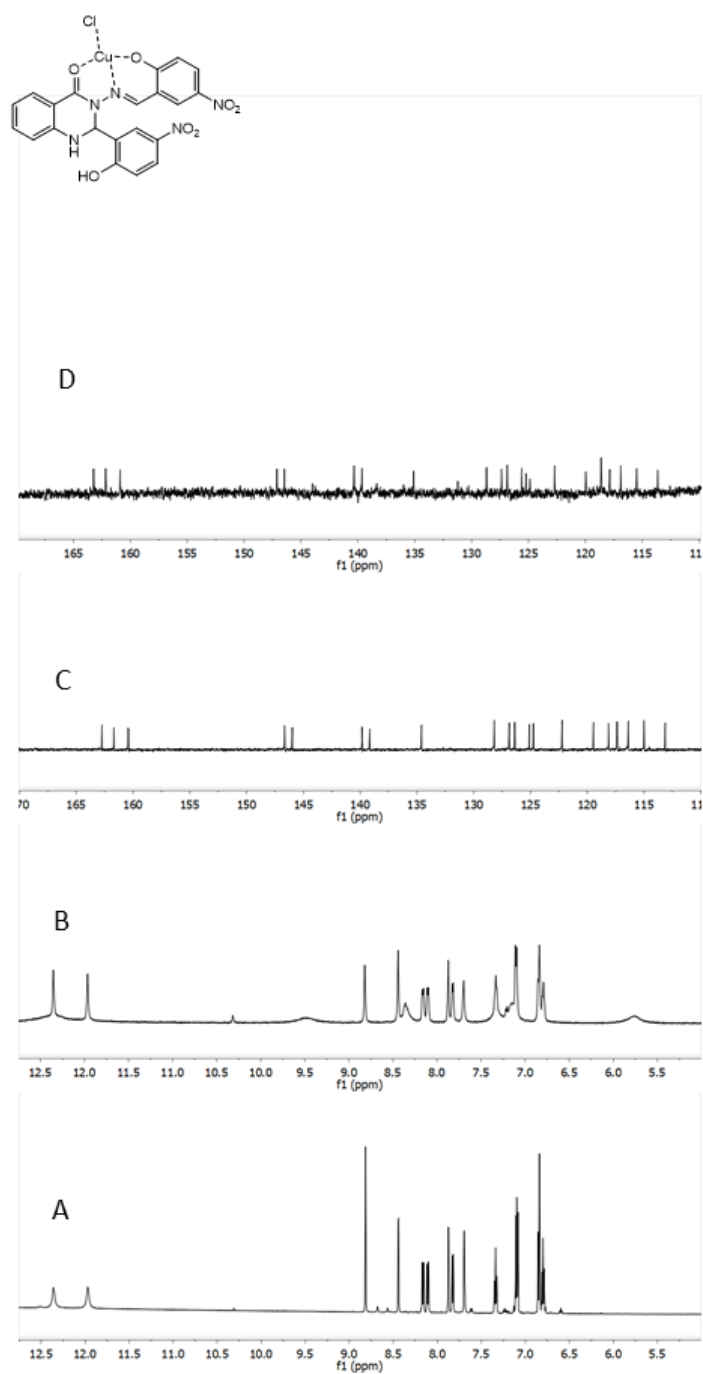
Figure S7. ¹H NMR and ¹³C spectra of the ligand **L1** (A and C, respectively) and its copper complex (with 30 % excess of the ligand **L1**) **Cu-L1** (B and D).

Figure S8. ¹H NMR and ¹³C spectra of the ligand **L2** (A and C, respectively) and its copper complex (with 30 % excess of the ligand **L2**) **Cu-L2** (B and D).
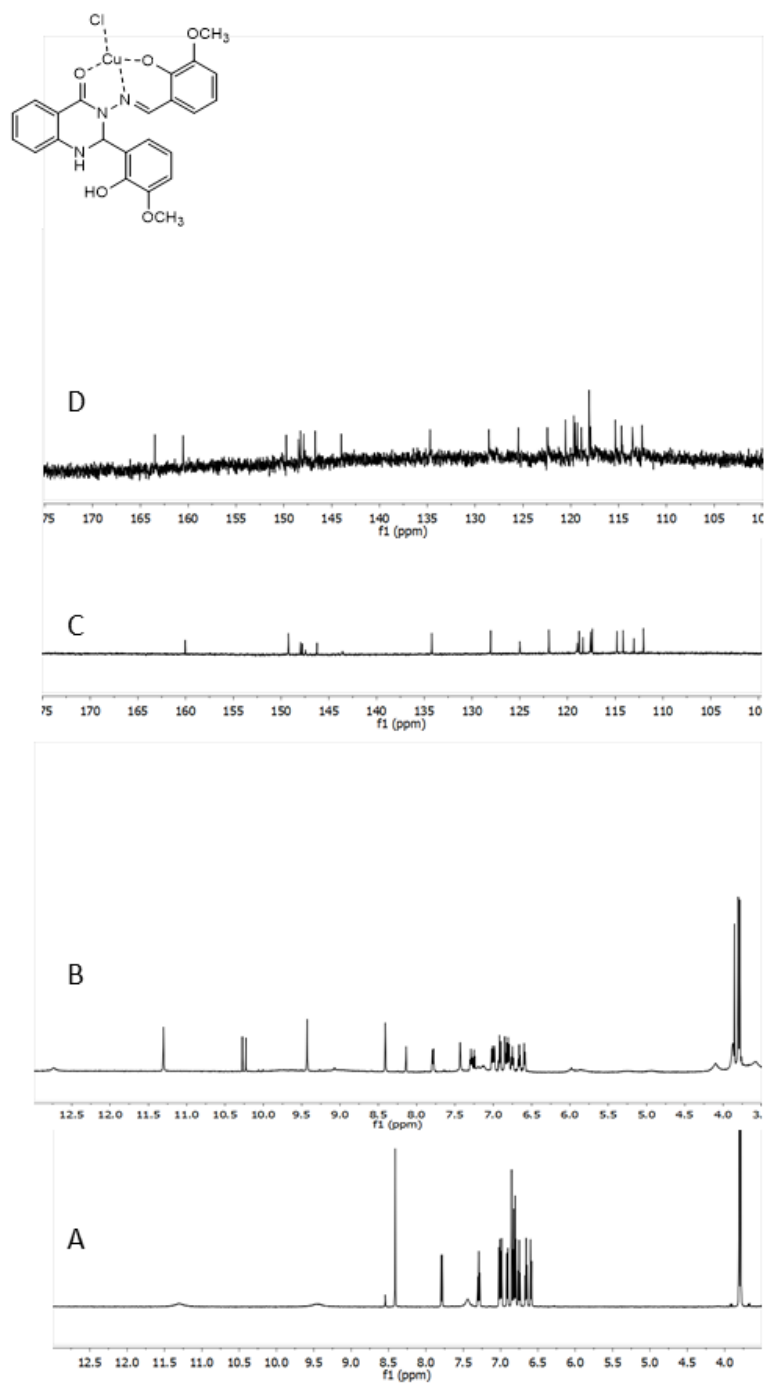
Table S1. The selected theoretical bond lengths (in Å) data of the studied **Cu-L1** and **Cu-L2** complexes obtained from gas-phase DFT calculations using APFD/LanL2DZ approach.

Atom 1	Atom 2	Length / Å	
		Cu-L1	**Cu-L2**
Cu	Cl	2.23	2.24
Cu	O4	1.98	1.96
Cu	O2″	1.90	1.89
Cu	N4	1.99	1.98
Cu	O	2.22	2.27
O4	C4	1.27	1.28
N3	C4	1.38	1.38
N3	N4	1.39	1.40
C9	N4	1.31	1.31
C9	C1″	1.43	1.43
C2″	C1″	1.45	1.44
C2″	O2″	1.31	1.32

Table S2. The selected theoretical bond angles (in degrees) data of the studied **Cu-L1** and **Cu-L2** complexes obtained from gas-phase DFT calculations using APFD/LanL2DZ approach.

Atom 1	Atom 2	Atom 3	Angle / deg	
			Cu-L1	**Cu-L2**
Cl	Cu	N4	172.3	174.7
Cl	Cu	O4	91.9	94.0
Cl	Cu	O2″	96.1	93.3
Cl	Cu	O	85.5	88.2
N4	Cu	O2″	91.5	91.2
N4	Cu	O4	80.9	81.5
O2″	Cu	O4	166.3	172.7
O2″	Cu	O	109.0	87.1
O4	Cu	O	82.7	94.1
Cu	O2″	C2″	129.4	129.7
Cu	O4	C4	113.0	113.4
O4	C4	N3	119.2	119.3
C9	N4	N3	121.6	121.2
C4	N3	C2	123.5	122.5
O2″	C2″	C1′	124.3	124.2

Table S3. The selected theoretical dihedral angles (in degrees) data of the studied **Cu-L1** and **Cu-L2** complexes obtained from gas-phase DFT calculations in the using APFD/LanL2DZ approach.

Atom 1	Atom 2	Atom 3	Atom 4	Angle / deg	
				Cu-L1	Cu-L2
C4	O4	Cu	O2″	70.5	14.0
C4	N3	N4	C9	178.4	179.4
O4	Cu	O2″	C2″	-63.4	27.1
O4	Cu	N4	N3	-11.0	-8.2
O2″	Cu	N4	N3	-179.5	170.1
O	Cu	N4	N3	71.4	83.6
O	Cu	O2″	C2″	84.3	111.5
O	Cu	N4	C9	-99.2	-89.9
Cl	Cu	N4	N3	6.9	-20.1
Cl	Cu	O2″	C2″	171.6	-159.7
Cu	O2″	C2″	C1″	3.8	-16.6
C1″	C9	N4	N3	-178.1	-178.9
C9	N4	N3	C4	178.4	179.4
C9	N4	N3	C2	8.7	16.0
N3	C2	C1′	C6′	10.1	6.5