

Experimental and theoretical studies on piperidine-based heteroleptic Schiff-based Ni(II) and Cu(II) complexes investigating DNA/protein binding and antibacterial/anticancer activities

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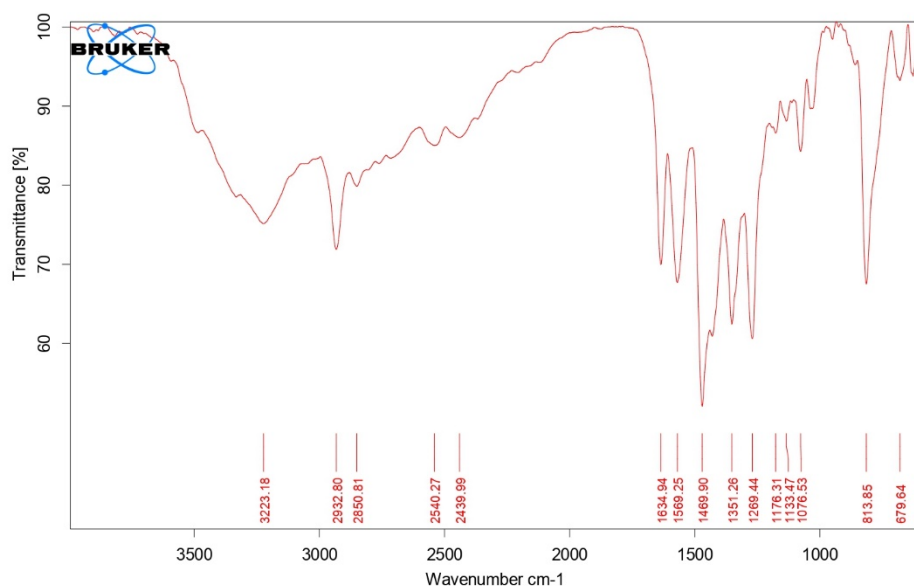


Figure S1: FTIR spectrum of ligand HL

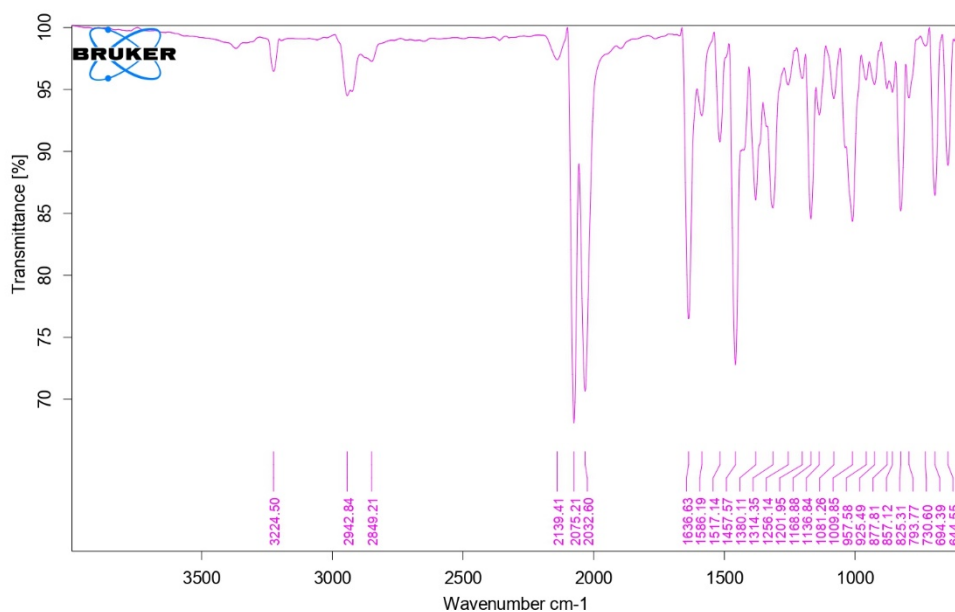


Figure S2: FTIR spectrum of complex 1

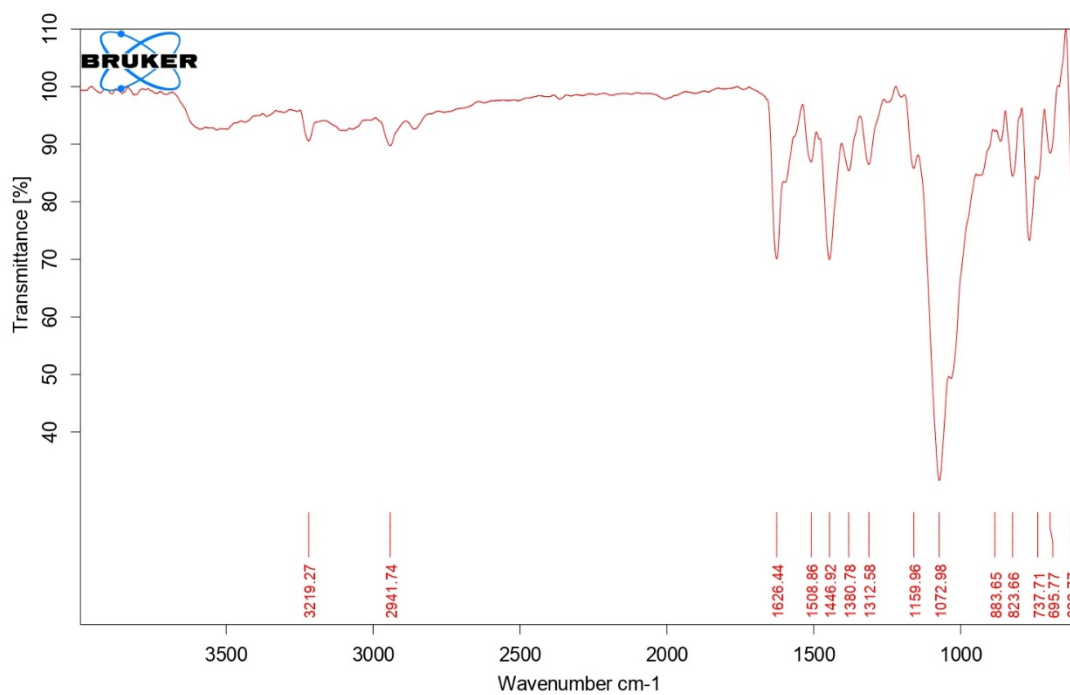


Figure S3: FTIR spectrum of complex 2

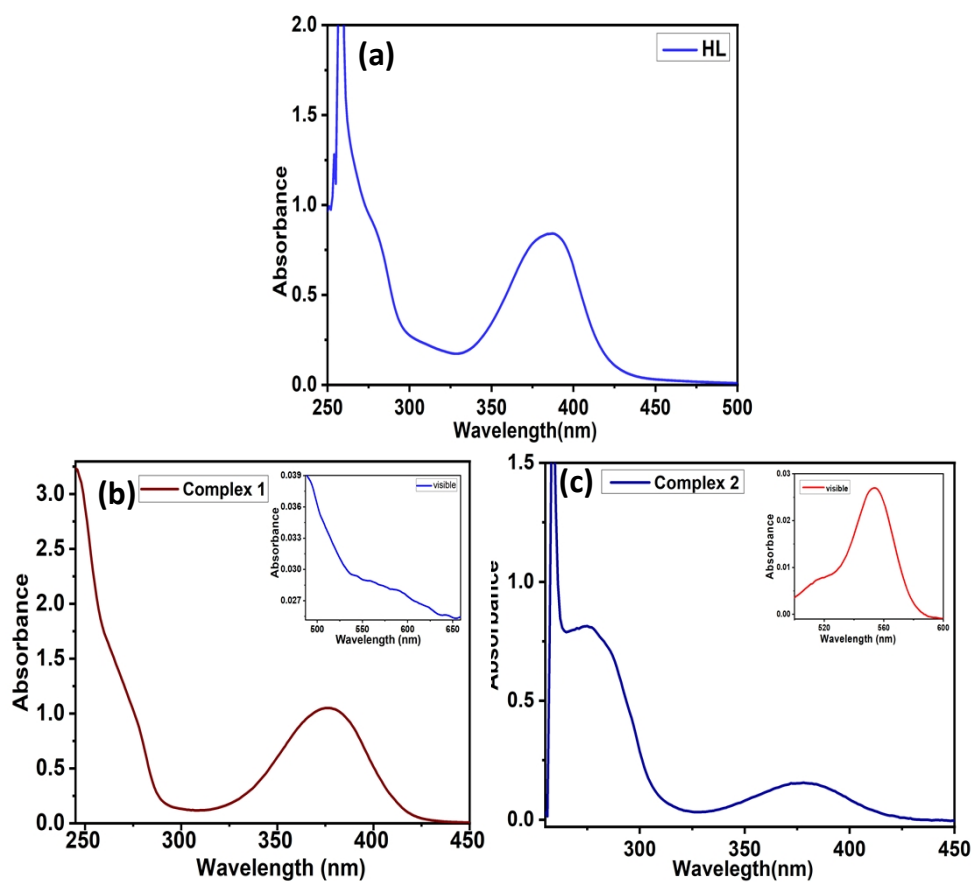


Figure S4: UV spectrum of HL, complex 1 and complex 2

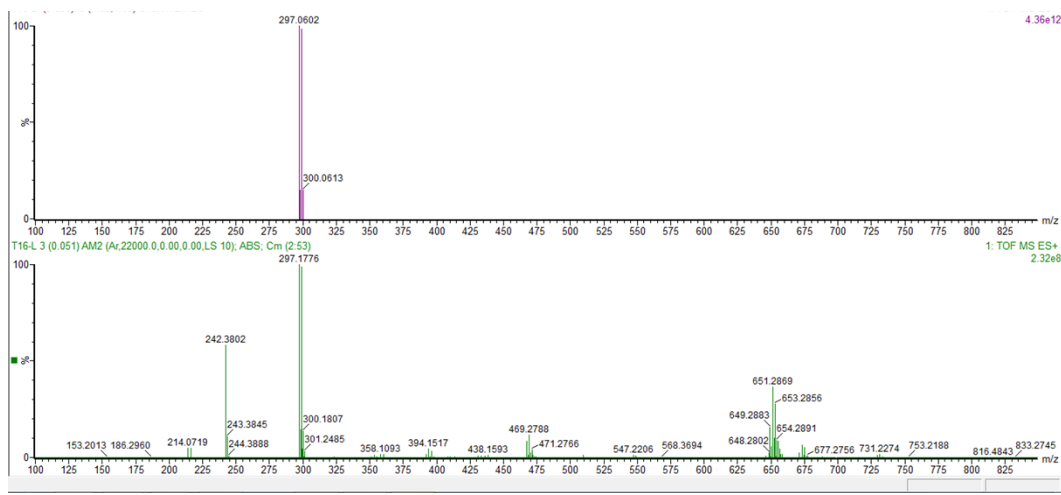


Figure S5: Mass spectrum of HL

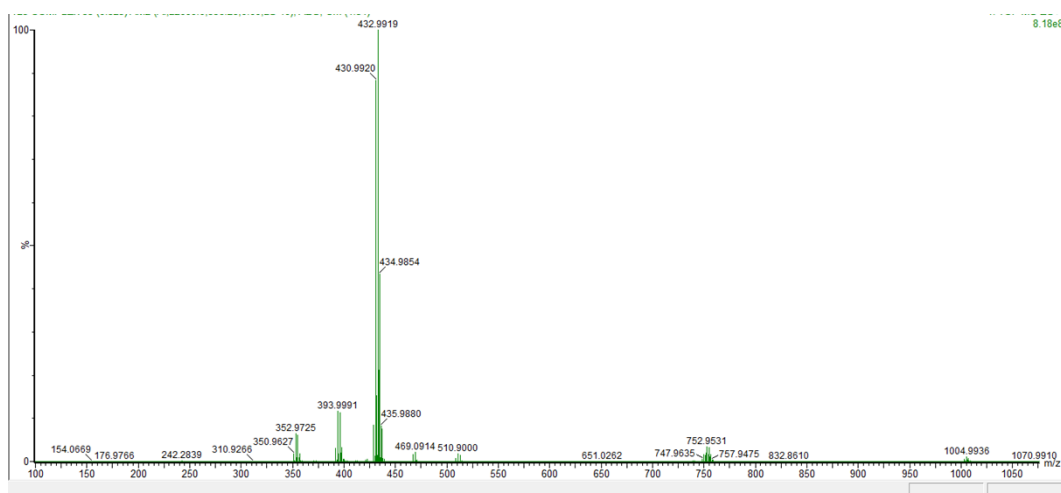


Figure S6: Mass spectrum of complex 1

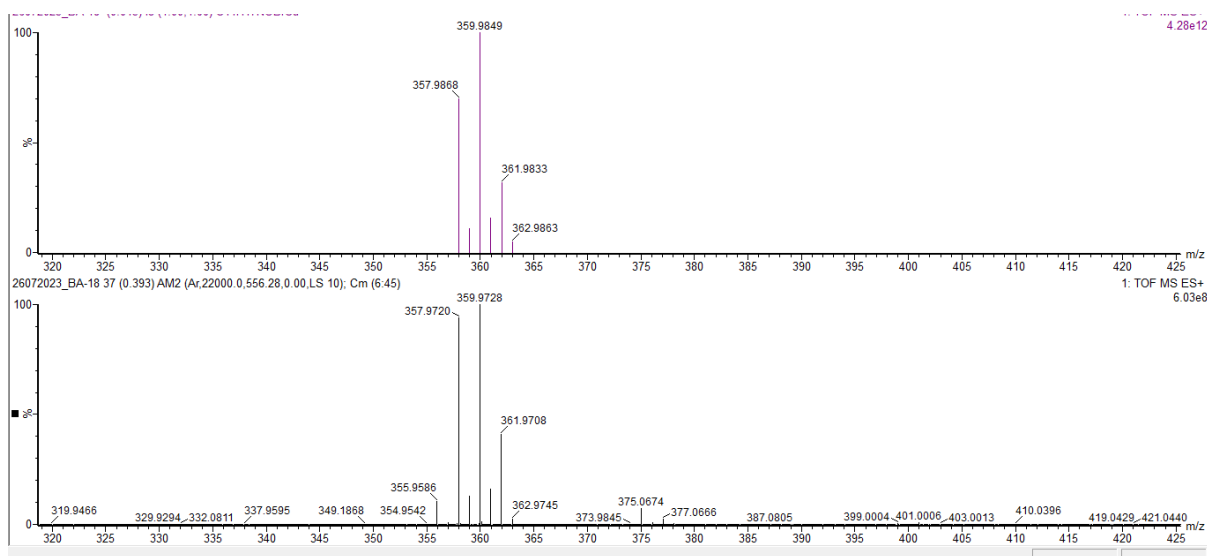


Figure S7: Mass spectrum of complex 2

Table S1: Selected bond length and bond angle table of complex **1**.

Bond length (Å)			
Ni1-O1	2.0121(15)	Ni1-N4	2.0091(18)
Ni1-O2	2.1206(17)	Ni1-N5	2.1216(18)
Ni1-N1	2.1467(17)	Ni1-N1_a	2.0941(18)
Bond angle (°)			
O1- Ni1 -O2	91.36(7)	O2- Ni1-N4	93.72(7)
O1- Ni1 -N1	93.74(7)	O2- Ni1-N5	87.03(7)
O1- Ni1-N4	90.99(7)	N1- Ni1-N4	91.18(7)
O1- Ni1 -N5	173.10(7)	N1- Ni1-N5	88.48(7)
O2- Ni1-N1	172.87(7)	N4- Ni1-N5	82.42(7)
O1- Ni1-N1_a	91.12(7)	O2- Ni1-N1_a	94.29(7)
N1_a- Ni1-N4	171.66(7)	N1_a- Ni1-N5	95.69(7)
N1- Ni1-N1_a	80.64(7)		

Table S2: Selected bond length and bond angle table of complex **2**.

Bond length (Å)			
Cu-O1	1.918(3)	Cu-N2	2.059(3)
Cu-N1	1.930(3)	Cu-N3	2.265(4)
Cu-N6	2.014(3)		
Bond angle (°)			
O1-Cu-N1	93.03(12)	N1-Cu-N3	103.28(13)
O1-Cu-N2	166.19(14)	N1-Cu-N4	177.23(12)
O1-Cu-N3	92.03(13)	N2-Cu-N3	101.78(12)
O1-Cu-N4	89.67(12)	N2-Cu-N4	93.21(12)
N1-Cu-N2	84.03(12)	N3-Cu-N4	77.22(12)

Table S3: Hydrogen bonding parameter of Complex **2**.

D-H····A	D-H(Å)	H····A(Å)	D····A(Å)	<D-H····A(°)	Symmetry
N2—H2...O2	0.9800	2.5000	3.418(6)	157.00	-1+x, y, z
Cl17—H17...O2	0.9300	2.5100	3.411(7)	163.00	x, y, z
C20 – H20 ...O4B	0.9300	2.5300	3.18(6)	127.00	x, y, z