SUPPLEMENTARY MATERIAL TO

(E)-4-(((2-amino-5-chlorophenyl)imino)methyl)-5-(hydroxymethyl)-2-methylpyridin-3-ol and its Cu(II) complex: Synthesis, DFT calculations and AIM analysis

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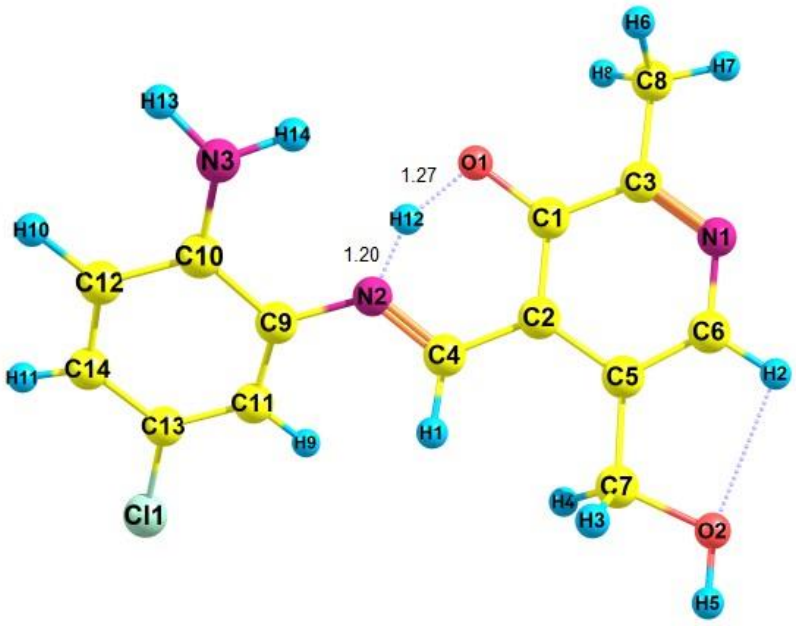

Figure S1. The B3LYP optimized geometry of the TSEnol-Keto of the *meta* isomer.

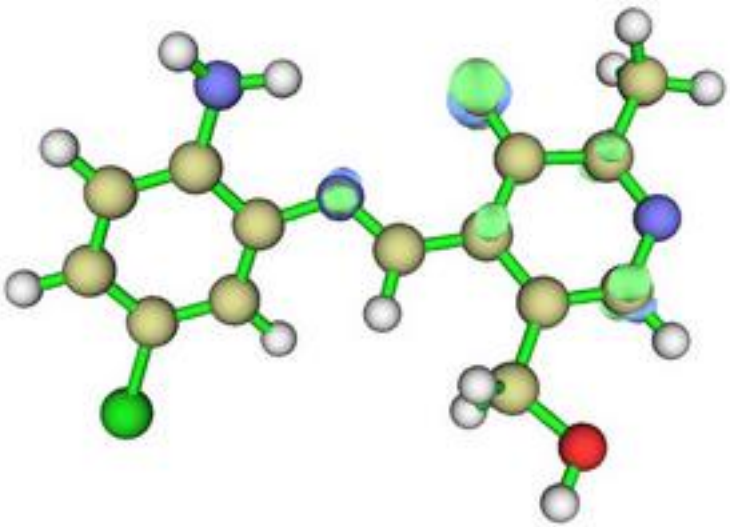

Figure S2. Optimized geometry and the isosurface Fukui map of the $\mathbf{L}^{-}$.

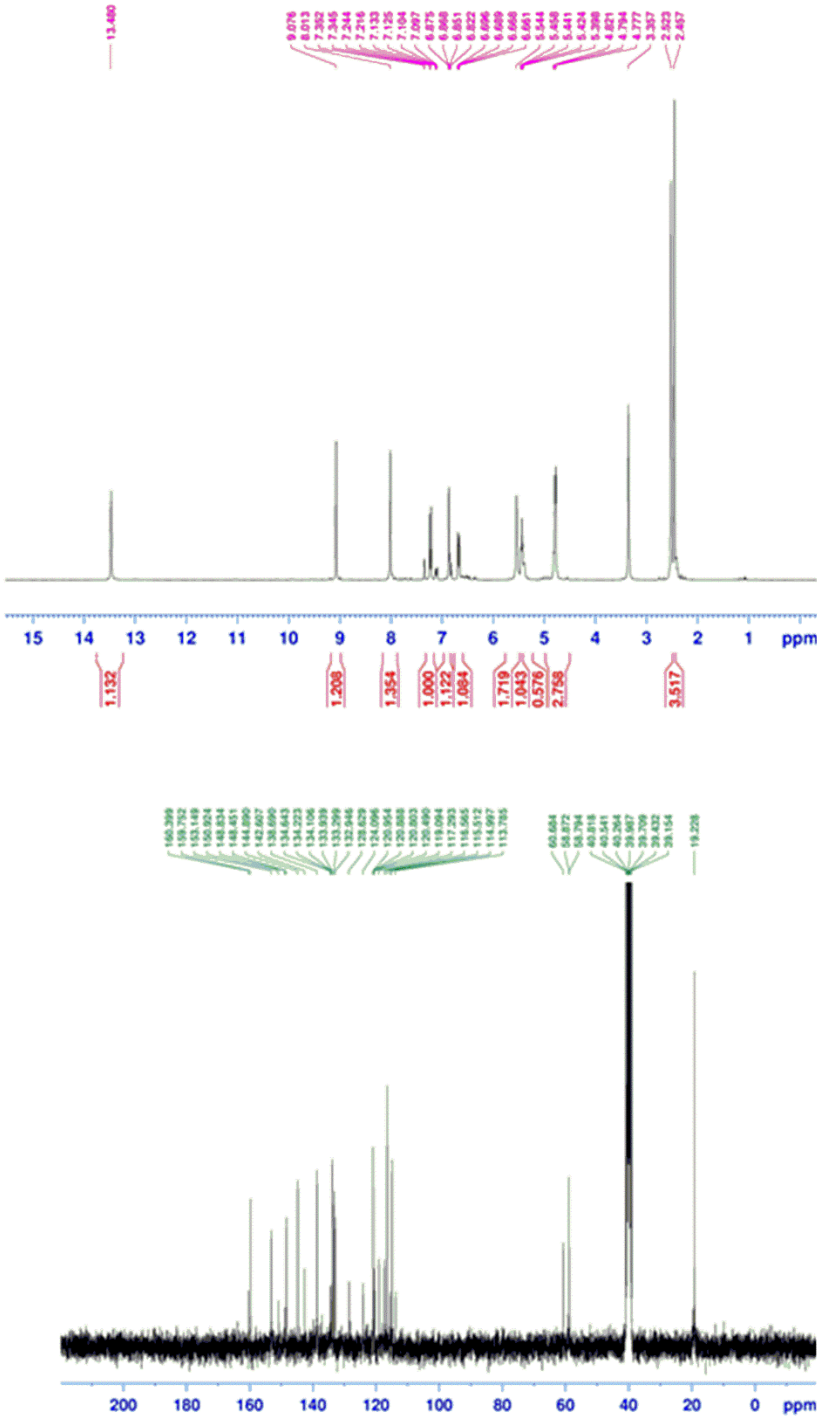

Figure S3. The ^{1}H- and ^{13}C-NMR spectra of the **HL** Schiff base.

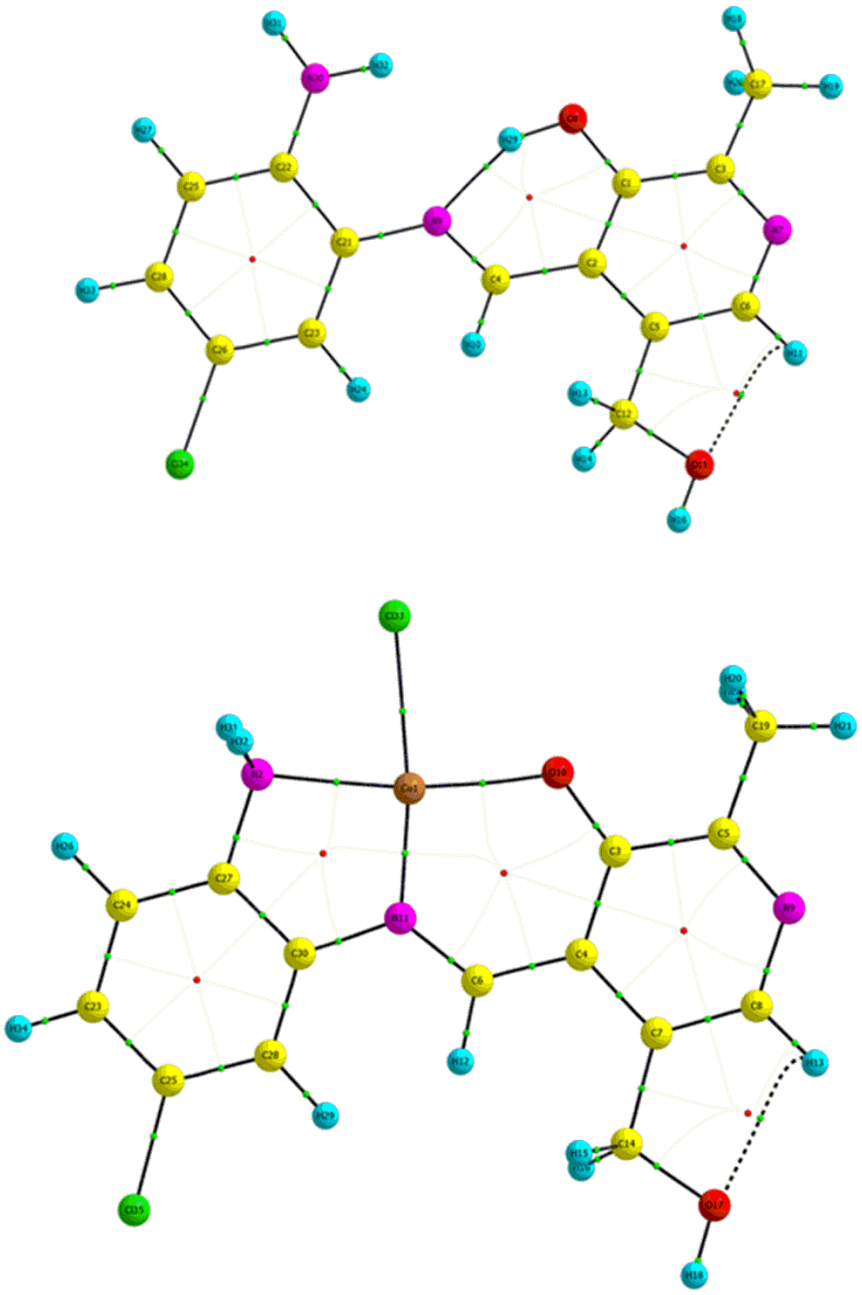

Figure S4. The QTAIM molecular graphs of the **HL** Schiff base and [Cu(**L**)Cl] complex.

Table S1. The elemental analysis of the investigated compounds.

Species	Calculated (%)				Experimental (%)				Chemical formula
	C	H	N	Metal	C	H	N	Metal	
HL	57.64	4.84	14.40	-	57.34	4.76	15.01	-	$C_{14}H_{14}ClN_3O_2$
[Cu(**L**)Cl]	43.15	3.36	10.78	16.31	43.52	3.48	10.46	17.02	$C_{14}H_{13}Cl_2CuN_3O_2$

Table S2. Relative electronic energies (E+ZPE) for the investigated species of the **HL** Schiff base (in term of $kJ.mol^{-1}$).

Species	E+ZPE		ΔG (Methanol solution)
	Methanol solution	Gas phase	
Enol tautomer of the *meta* isomer	0	0	0
Keto tautomer of the *meta* isomer	27.38	29.15	24.59
Enol tautomer of the *para* isomer	24.23	26.34	20.94
Keto tautomer of the *para* isomer	30.89	33.67	28.63
TSEnol-Keto	164.90	159.11	123.91

Table S3. Important experimental and the DFT-computed IR vibrational frequencies (cm^{-1}) of the **HL** Schiff base (Enol tautomer of the *meta* isomer) and [Cu(**L**)Cl] complex.

Experimental frequencies		Calculated frequencies				Vibrational assignment
		HL		[Cu(**L**)Cl]		
HL	[Cu(**L**)Cl]	Frequency	Intensity ($km.mol^{-1}$)	Frequency	Intensity ($km.mol^{-1}$)	
-	547 (m)	-	-	532	41	υ_{asym}(Cu-N, Cu-O)
-	640 (w)	-	-	618	5	υ_{sym}(Cu-N, Cu-O)
765 (m)	767 (m)	759	16	744	9	Breathing of the aromatic rings
846 (w)	851 (w)	834	24	836	14	δ_{op}(aromatic hydrogens)
809 (m)	-	802	79	-	-	δ_{op}(H12)
912 (w)	915 (w)	886	51	892	23	υ(C13-Cl1)
1032 (vs)	1027 (s)	1039	73	1037	95	υ(C1-O1)
1208 (m)	1188 (m)	1173	126	1160	94	υ(C9-N2)
1298 (m)	1262 (m)	1284	105	1249	228	υ(C9-N2)+ υ(Ar-C)
1380 (vs)	1416 (vs)	1370	112	1421	137	υ(C1-O1)
1471 (m)		1456	68	1482	186	υ(C9-N2)
1521 (m)	1507 (m)	1535	16	1496	127	υ_{asym}(C=C) of the benzene ring
		1557	32	1540	24	υ_{sym}(C=C) of the benzene ring
		1570	98	1563	108	υ(C=N, C=C) of the right pyridine rings + υ(C4-N2)
1617 (vs)	1605 (vs)	1584	125	1567	58	υ(C=N, C=C) of the pyridine rings
		1592	221	1581	279	υ(C4=N2)
2746 (m)	2741 (s)	2852	40	2852	65	υ_{sym}(C-H) of -CH_2- groups
2840 (s)	2838 (s)	2876	30	2876	36	υ_{asym}(C-H) of -CH_2- groups
2919 (s)	2918 (s)	2914	20	2930	14	υ_{sym}(C-H) of the methyl groups
3110 (vs, br)	3096 (vs, br)	2954	36	3032	15	υ(C4-H1)
		3015	11	3034	14	υ_{asym}(C-H) of the methyl groups
		3087-3056	3	3289-3073	4	υ_{asym}(C-H) of the aromatic hydrogens
3463 (m, br)	3362 (s)	3126	471	-	-	υ(O1-H12)
		3443	28	3353	45	υ_{sym}(H-N-H) of the -NH_2 amine group
	3444 (s)	3547	39	3417	48	υ_{asym}(H-N-H) of the -NH_2 amine group
		3260	59	3703	55	υ(O2-H5)

Table S4. Important topological parameters of the investigated species (energies in term of kJ.mol^{-1}).

Bond	ρ(r)	$\nabla^2\rho$	V_b	G_b	H_b	$-G_b/V_b$
HL Schiff base						
C1-O1	0.299251	-0.38595	-2027.82	887.36	-1140.45	0.44
O1-H12	0.331725	-2.29726	-1873.5	183.54	-1689.97	0.10
N2…H12	0.049647	0.1126	-120.763	97.30	-23.48	0.81
C4-N2	0.365541	-0.84807	-2401.46	922.68	-1478.80	0.38
C9-N2	0.292365	-0.82668	-1365.14	411.53	-953.62	0.30
C10-N3	0.305063	-0.89704	-1471.92	441.84	-1030.08	0.30
C7-O2	0.254508	-0.48479	-1429.14	555.62	-873.54	0.39
O2-H5	0.366696	-2.55259	-2048.69	187.41	-1861.28	0.09
O2…H2	0.015167	0.075335	-31.9744	40.69	8.72	1.27
C13-Cl1	0.189252	-0.26191	-504.796	166.52	-338.26	0.33
[Cu(**L**)Cl] complex						
C1-O1	0.344981	-0.17071	-2851.17	1369.62	-1481.55	0.48
C4-N2	0.348704	-0.70745	-2619.77	1077.93	-1541.85	0.41
C9-N2	0.294602	-0.93463	-1471.63	429.38	-1042.28	0.29
C10-N3	0.276305	-0.83136	-1209.91	332.37	-877.52	0.27
C7-O2	0.258655	-0.54536	-1562.55	602.46	-960.07	0.39
O2-H5	0.350059	-1.811	-1535.56	173.99	-1361.55	0.11
C13-Cl1	0.187947	-0.24896	-487.747	162.25	-325.51	0.33
Cu-O1	0.075907	0.521302	-315.888	328.86	12.98	1.04
Cu-N2	0.166307	0.872714	-1020.69	796.48	-224.21	0.78
Cu-N3	0.07758	0.441895	-304.898	297.34	-7.58	0.98
Cu-Cl2	0.063669	0.272222	-201.315	189.91	-11.41	0.94
O2…H2	0.015259	0.071397	-31.9744	39.39	7.43	1.23