Electronic Supplementary Information (ESI) for the article "**Diethylaminophenyl-based Schiff base Cu(II) and V(IV) complexes: experimental and theoretical study and cytotoxicity assays"** by Mariana Rocha[1], M.C. Ruiz[2], G. A. Echeverría[3,+], O. E. Piro[3,+], A.L. Di Virgilio[2,+], I.E. León[2,+], Antonio Frontera[4,*] and Diego M. Gil[1,+,*]

Figure S1: IR spectra of the Schiff base H_2L and its Cu(II) and V(IV) complexes in solid state.

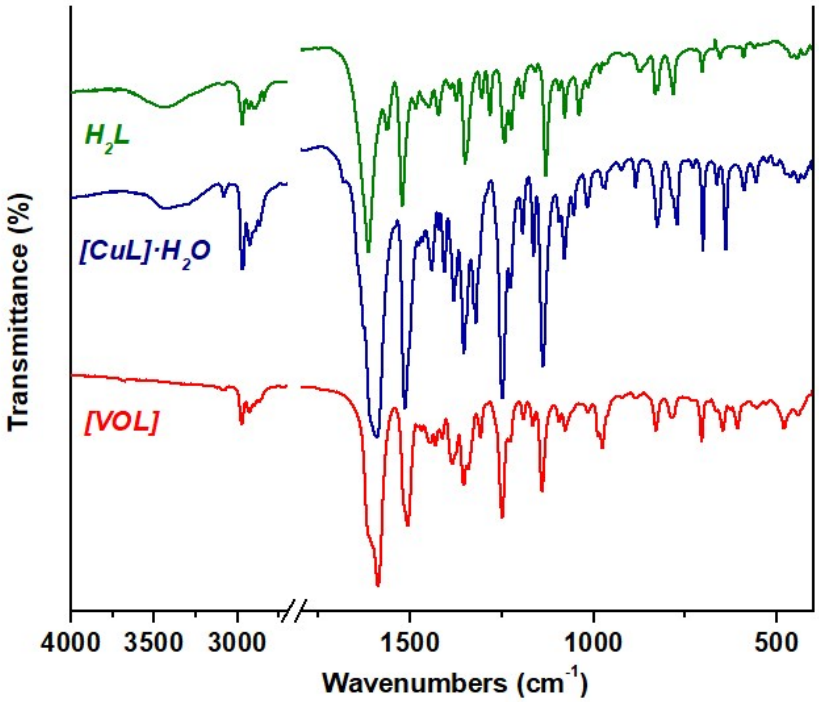

Figure S2: Electronic spectra (in solid state) of the Schiff base H_2L and its complexes.

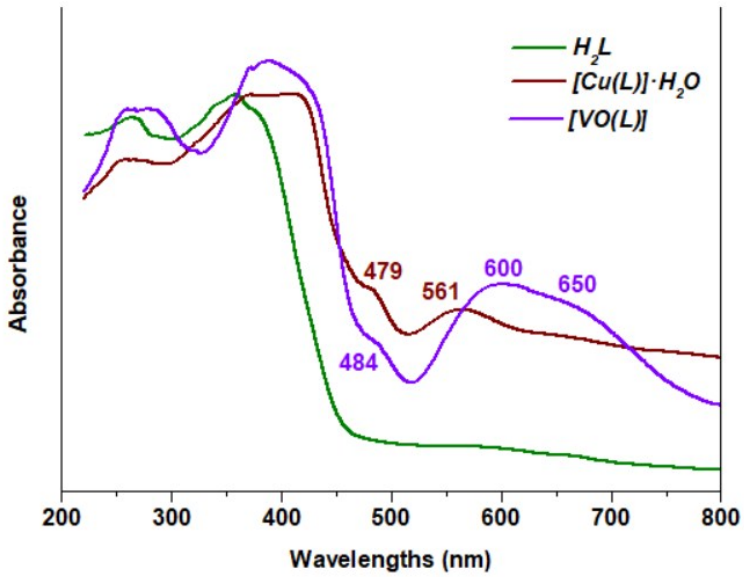

Figure S3: View of the crystal packing of compound (***1***) showing C-H···O intermolecular interactions as dashed lines.

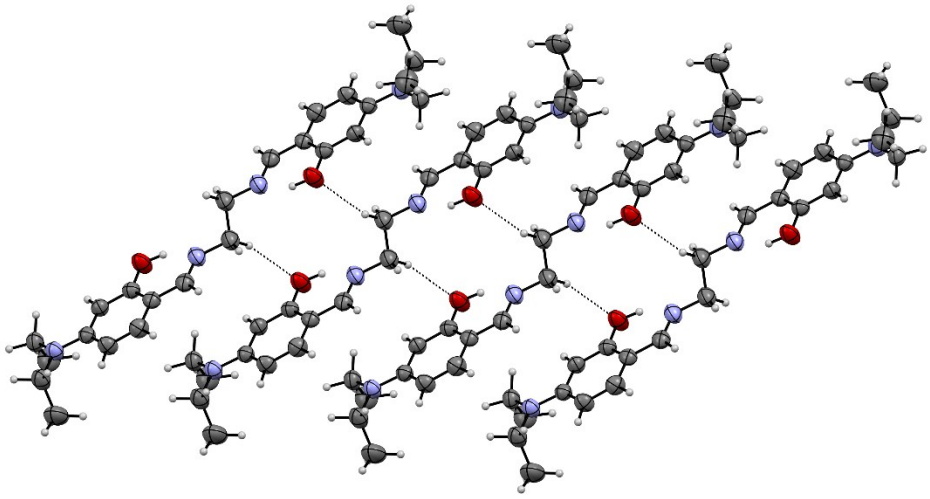

Figure S4: Self-assembled dimers present in compound (***2***) showing intramolecular Ow-H···O and intermolecular C-H···O contacts.

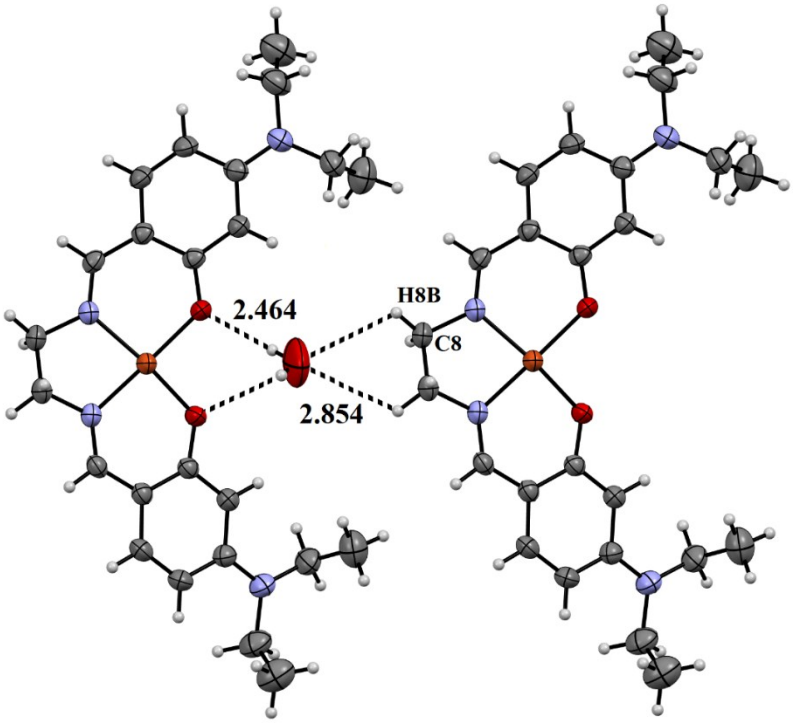

Figure S5: Self-assembled stacked dimers observed in compound (***2***).

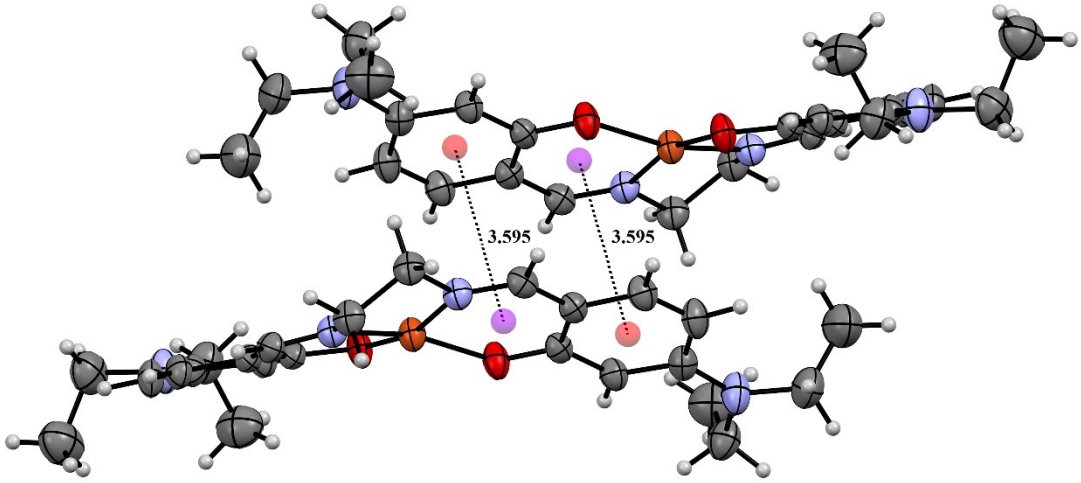

Figure S6: Hirshfeld surface of compound (***2***) mapped with *shape index* function.

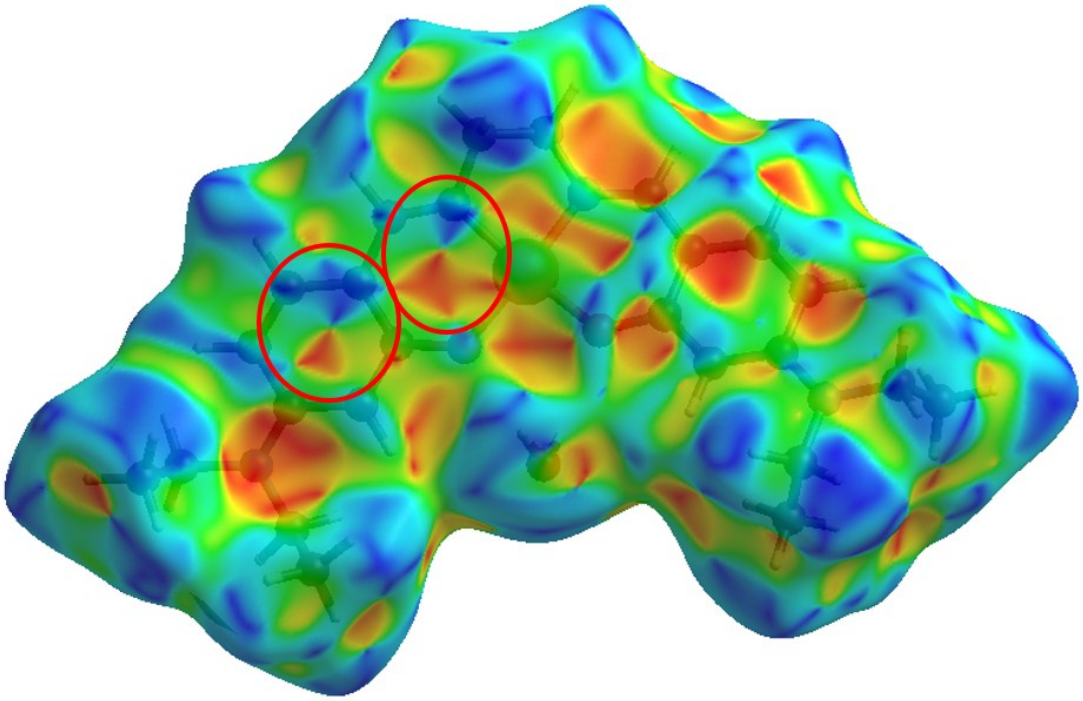

Figure S7: Effect of complexes **2** (green bars) and **3** (orange bars) on MG-63, MDA-MB-231, MCF-7 and HT-29 cell lines viability. The effect of the ligand (grey bars) and the control cells (black bars) are also shown. The results are expressed as percentage of the basal level and represent the mean ± the standard error of the mean (n = 18). *p<0.0001 differences between control and treatment.

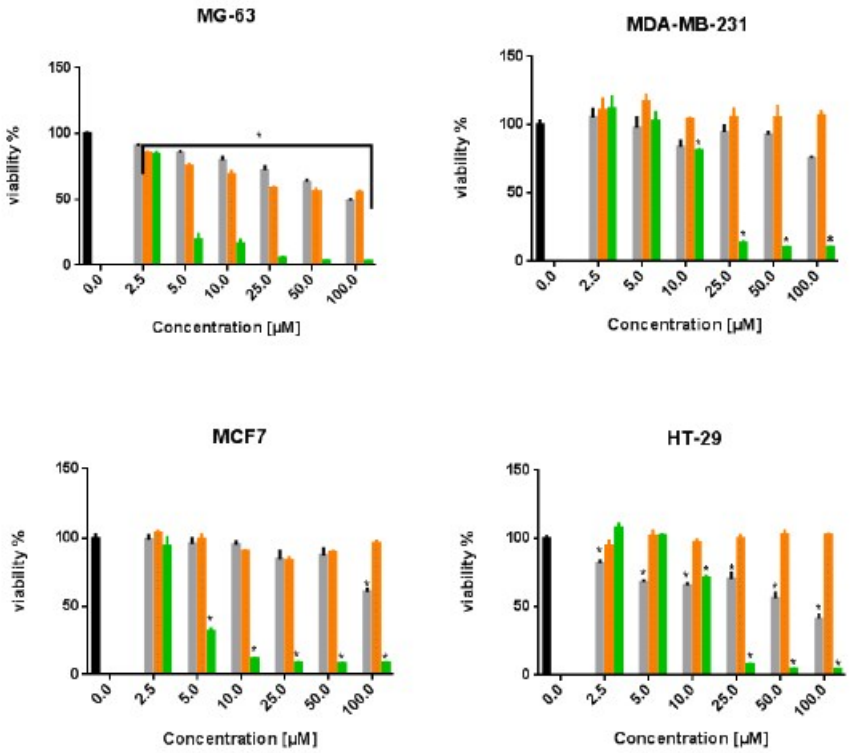

Table S1: Selected bond lengths (Å) and angles (º) in the crystal structure of the Schiff base H_2L (***1***).

Bond lengths (Å)		***Angles (º)***	
C8-N1	1.460(2)	C8-N1-C7	119.1(2)
C7-N1	1.278(3)	C1-C7-N1	122.5(2)
C1-C7	1.445(2)	C2-C1-C7	121.9(2)
C2-O	1.359(2)	O-C2-C1	120.6(2)
C4-N2	1.375(2)	C4-N2-C9	120.9(1)
C9-N2	1.460(3)	C4-N2-C10	121.6(2)
C10-N2	1.456(3)	***Dihedral angles (º)***	
C9-C11	1.510(4)	C8-N1-C7-C1	179.5(2)
C10-C12	1.500(4)	N1-C7-C1-C6	-179.7(2)
		C2-C1-C7-N1	1.8(3)
		N1-C8-C8-N1	180.0(2)