Supporting material

Synthesis, Cytotoxicities, Structural Properties and Comparison of Dihalogenosubstituted-thiosemicarbazone ligands and Mixed-Ligand Ni(II) Complexes

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Supplementary Materials

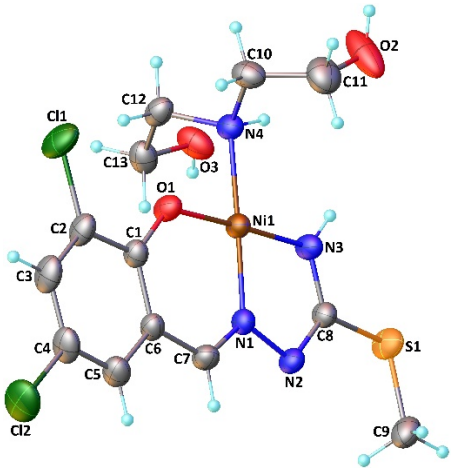

Fig. S1 Molecular structure of **Complex I** with the atom numbering. Thermal ellipsoids are shown at the 30% probability level

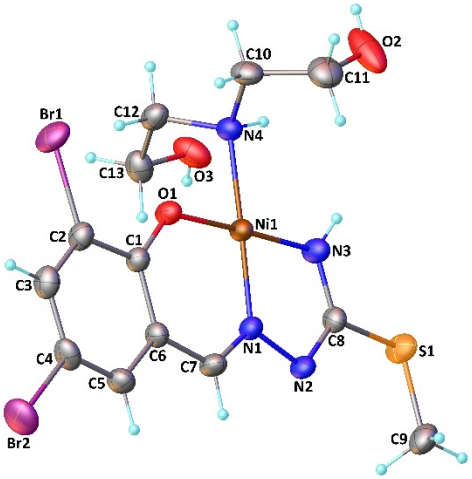

Fig. S2 Molecular structure of **Complex II** with the atom numbering. Thermal ellipsoids are shown at the 30% probability level

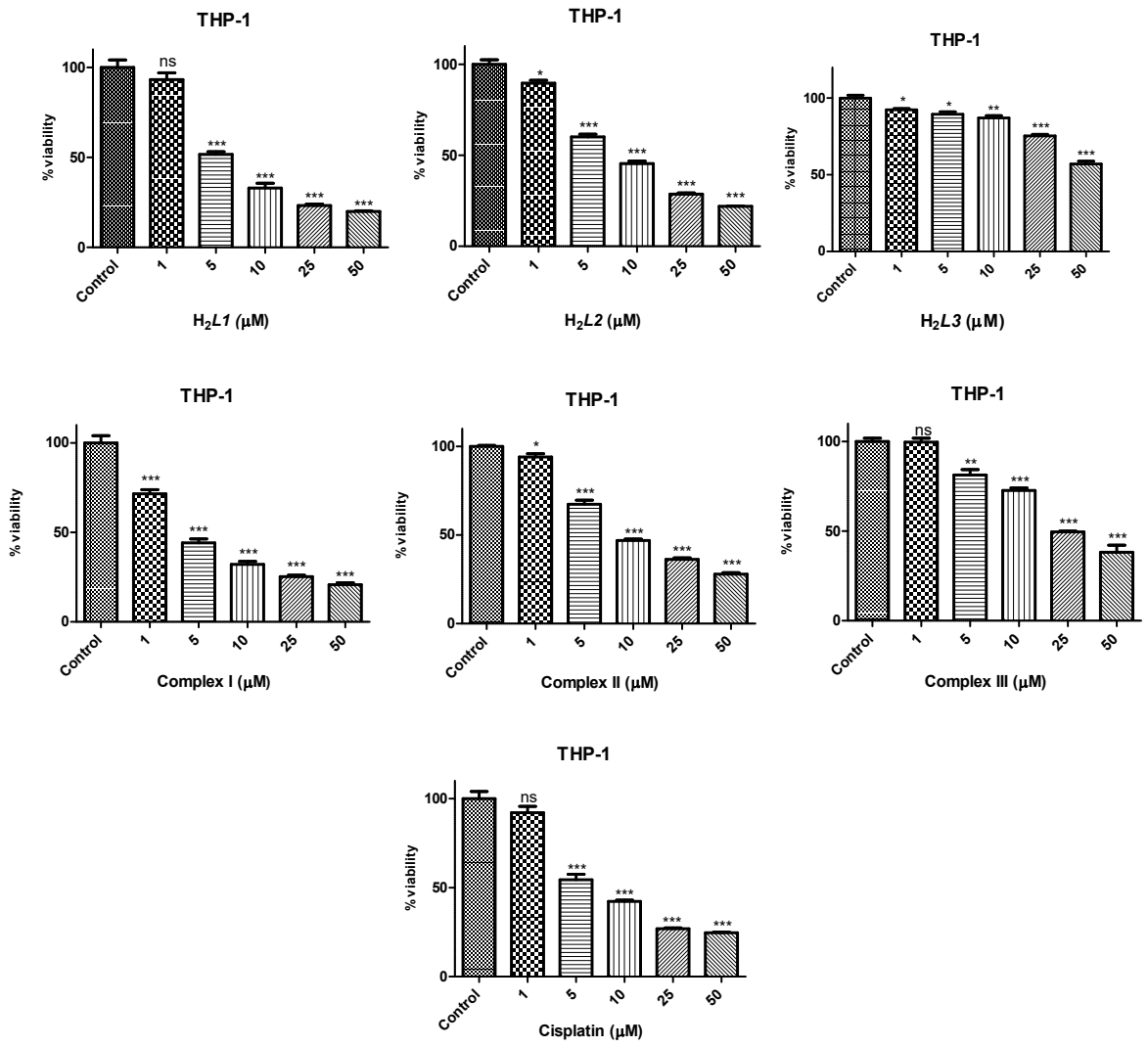

Fig. S3 The graphs showing the cell viability obtained by MTT assay in THP-1 human acute monocytic leukemia cell line treated with different concentrations **H_2*L1***, **H_2*L2***, **H_2*L3*, Complex I, Complex II, Complex III** and **Cisplatin**. ***p < 0.001, **p < 0.01, *p < 0.05, significant differences between control and each treatment group. The results represent the means of at least 3 independent experiments

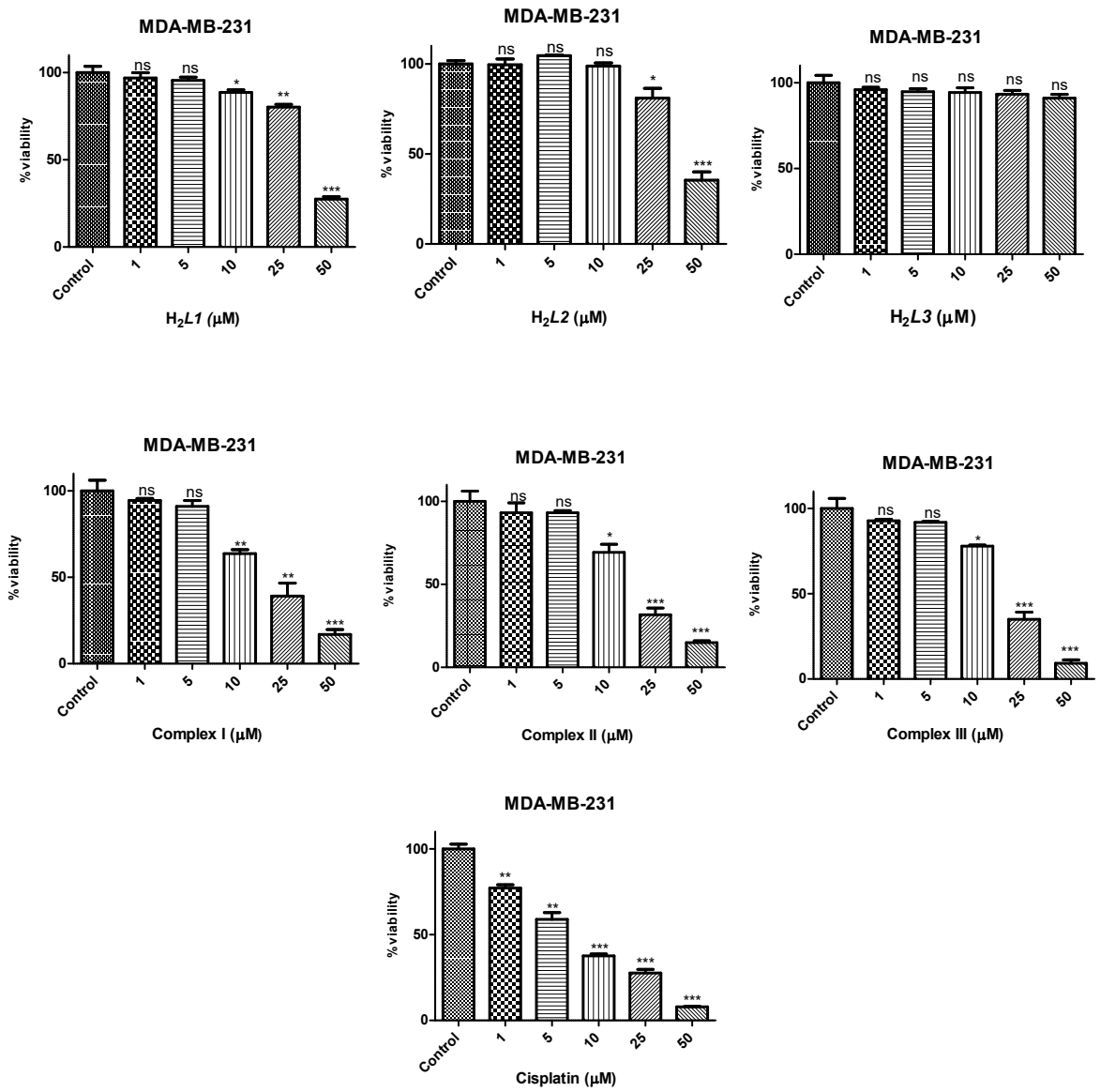

Fig. S4 The graphs showing the cell viability obtained by MTT assay in MDA-MB-231 human breast cancer cell line treated with different concentrations **H_2L1**, **H_2L2**, **H_2L3, Complex I, Complex II, Complex III** and **Cisplatin**. ***p < 0.001, **p < 0.01, *p < 0.05, significant differences between control and each treatment group, ns:not significant. The results represent the means of at least 3 independent experiments

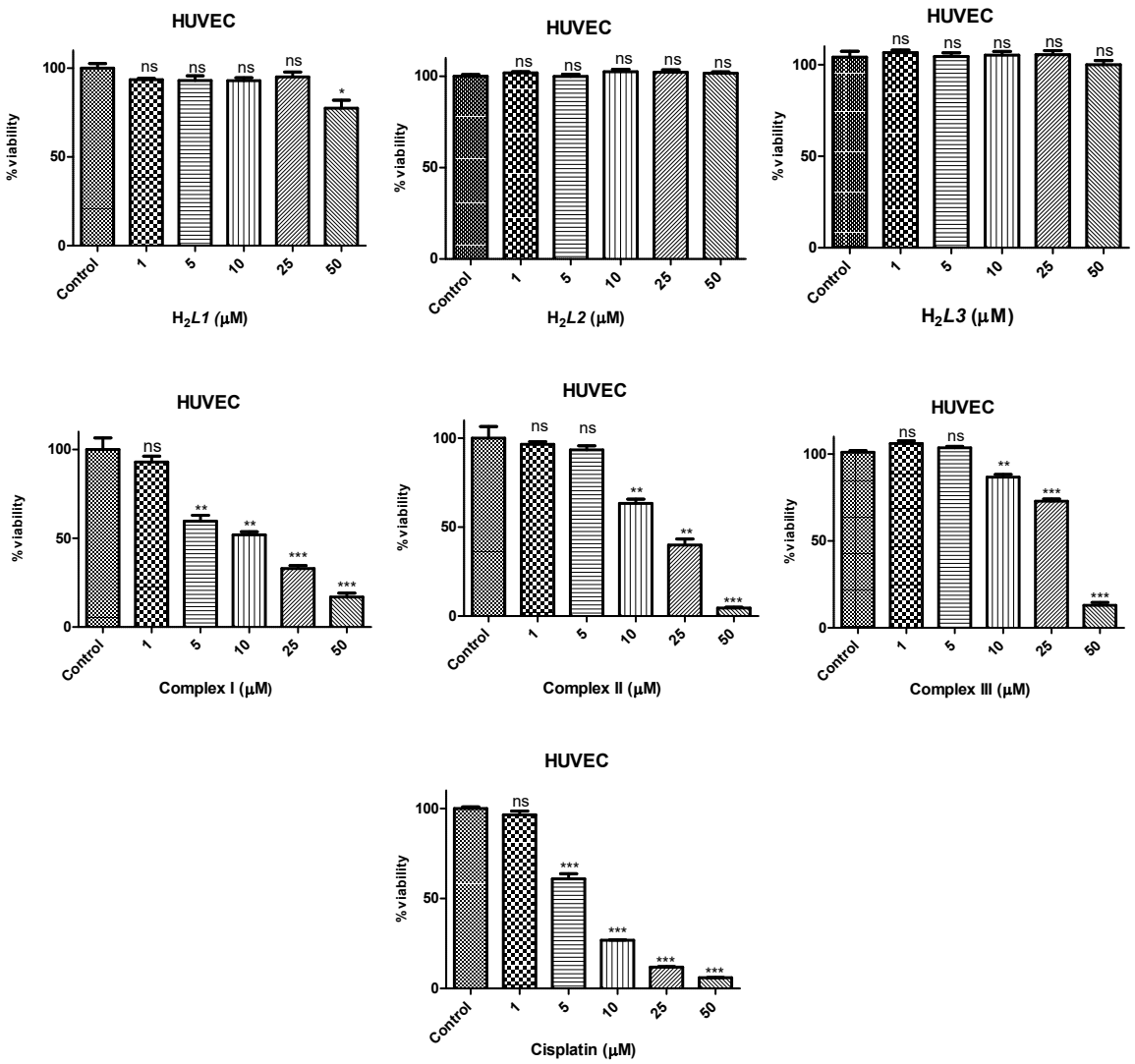

Fig. S5 The graphs showing the cell viability obtained by MTT assay in Human umbilical vein endothelial cells (HUVEC) cell line treated with different concentrations **H_2L1**, **H_2L2**, **H_2L3, Complex I, Complex II, Complex III** and **Cisplatin**.***p < 0.001, **p < 0.01, *p < 0.05, significant differences between control and each treatment group. The results represent the means of at least 3 independent experiments

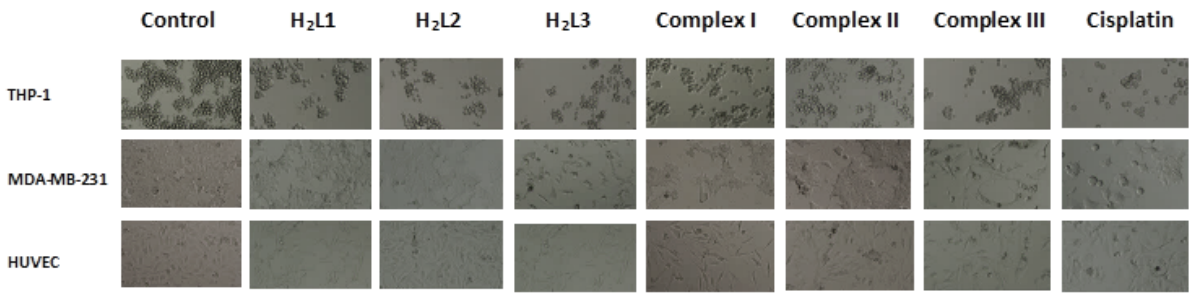

Fig. S6 Representative microscopic images (20X) of all cell lines treated with **H_2L1, H_2L2, H_2L3, Complex I, Complex II, Complex III,** and **Cisplatin** at their IC_{50} concentrations for 72 hours.

Stability Tests of the Active Compounds

Stabilities of the Substances in PBS

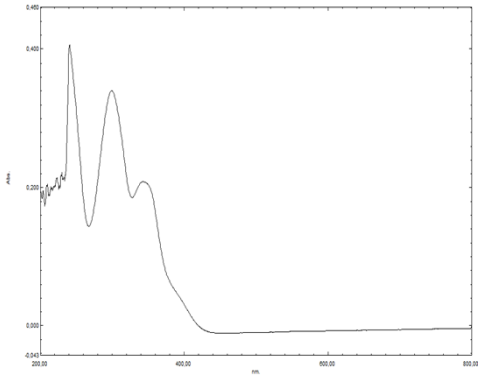

Fig. S7 UV-Vis Spectrum of the **H_2*L1*** in PBS. (%2 DMF, 40 µM)

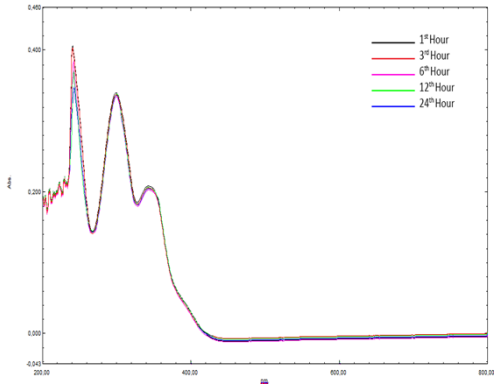

Fig. S8 Time-dependent stability of the **H_2L1** in PBS. (%2 DMF, 40 µM)

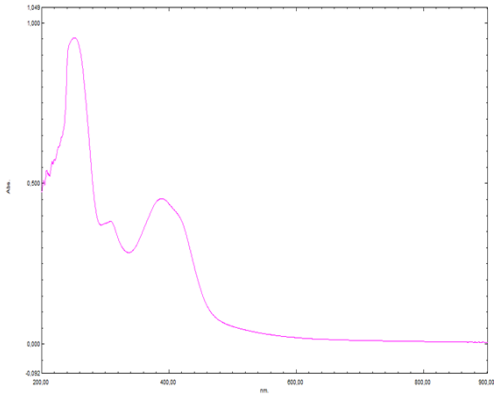

Fig. S9 UV-Vis Spectrum of the **Complex I** in PBS. (%2 DMF, 40 µM)

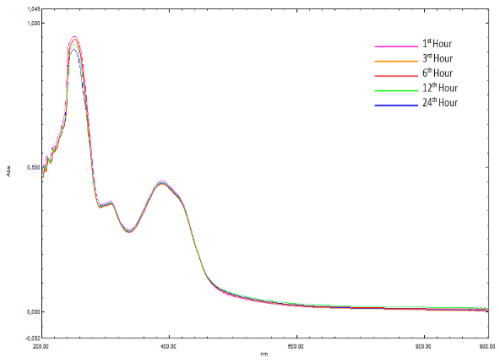

Fig. S10 Time-dependent stability of the Complex I in PBS. (%2 DMF, 40 µM)

Stabilities of the Substances in DMSO

The stabilities of biologically active substances in DMSO was measured in a time-dependent manner (0, 1, 3, 6, 12 and 24 h).

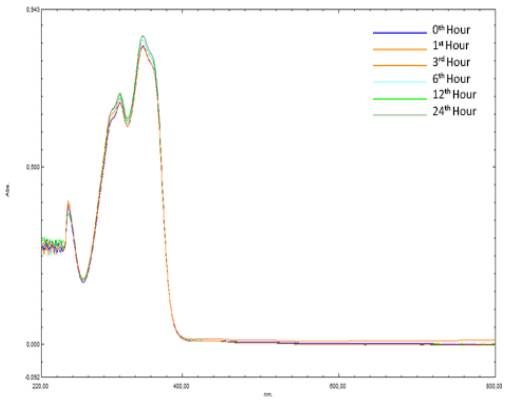

Fig. S11 Time-dependent stability of the **H_2*L1*** in DMSO.

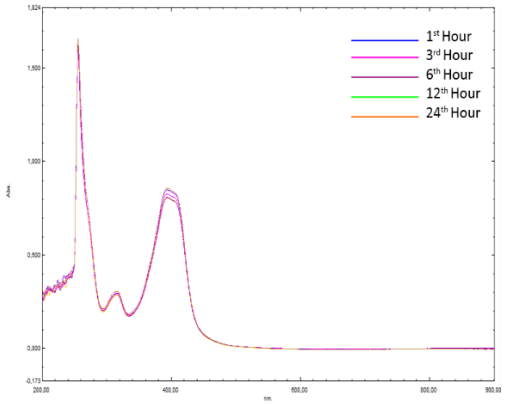

Fig. S12 Time-dependent stability of the **Complex I** in DMSO.

Stability of Substances Against pH Changes

The stability of the compounds against pH changes was examined in DMSO. (pH= 7.0, 7.2, 7.4, 7.6, 7.8)

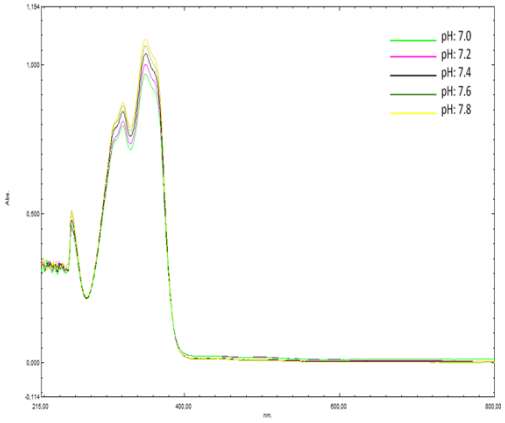

Fig. S13 pH stability of the **H_2L1** in DMSO.

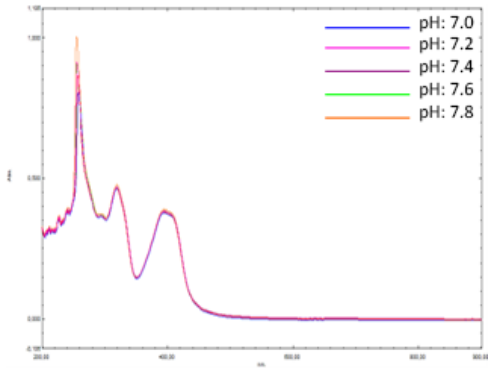

Fig. S14 pH stability of the **Complex I** in DMSO.