Synthesis and characterization of some water soluble Zn(II) complexes with (*E*)-*N*-(pyridin-2-ylmethylene)arylamine that regulate tumour cell death by interacting with DNA†

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ELECTRONIC SUPPLEMENTARY INFORMATION

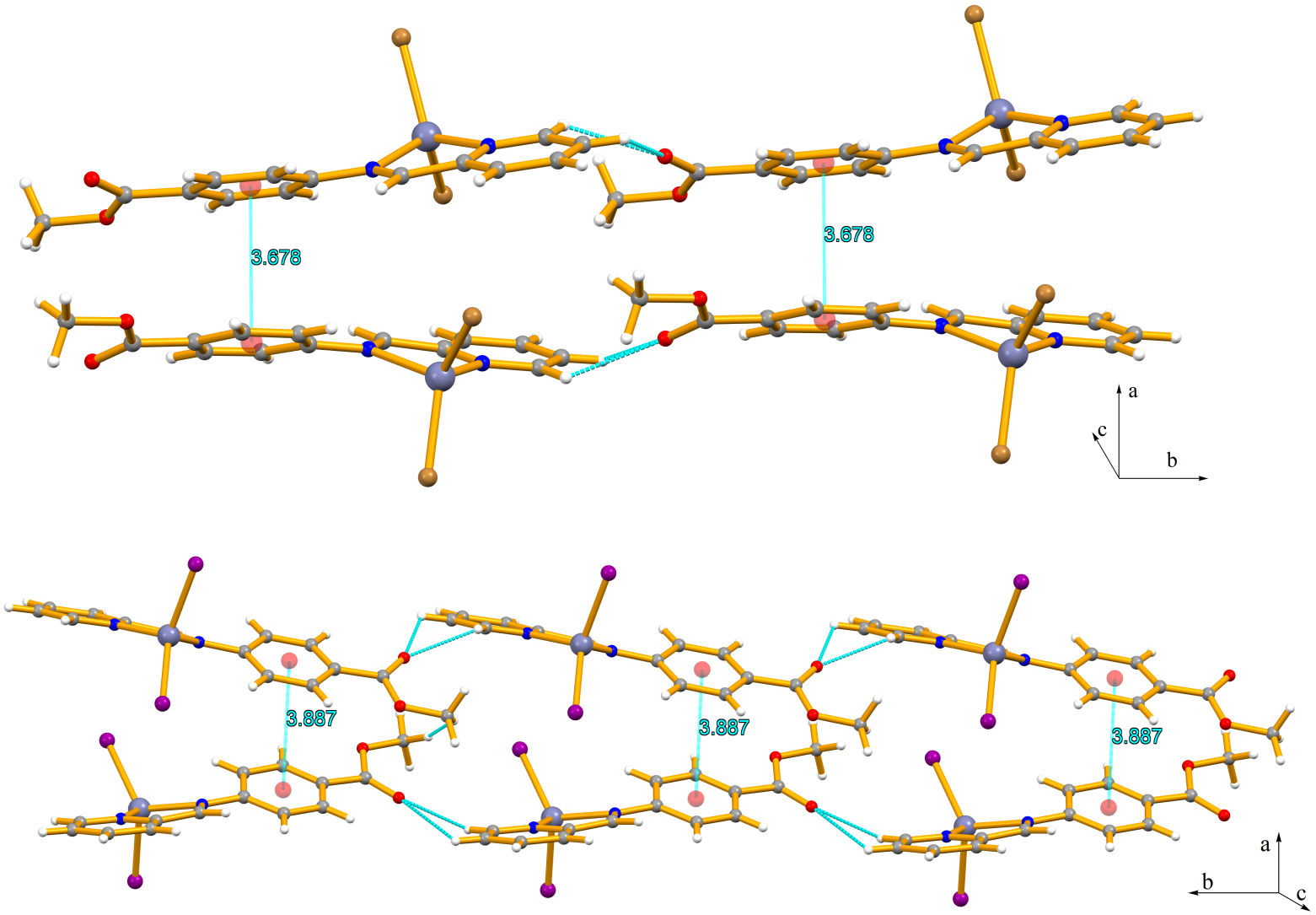

Fig. S1 Fragments of the crystal packing of **6** (top) and **7** (bottom) showing the 1D chains, running along the crystallographic *b* axis, which result from C–H···O interactions (represented as dashed light blue lines); the strongest *interchain* contacts involving the phenyl rings are also shown (*centroids* are represented as pink balls, and *centroid*···*centroid* distances as light blue lines).

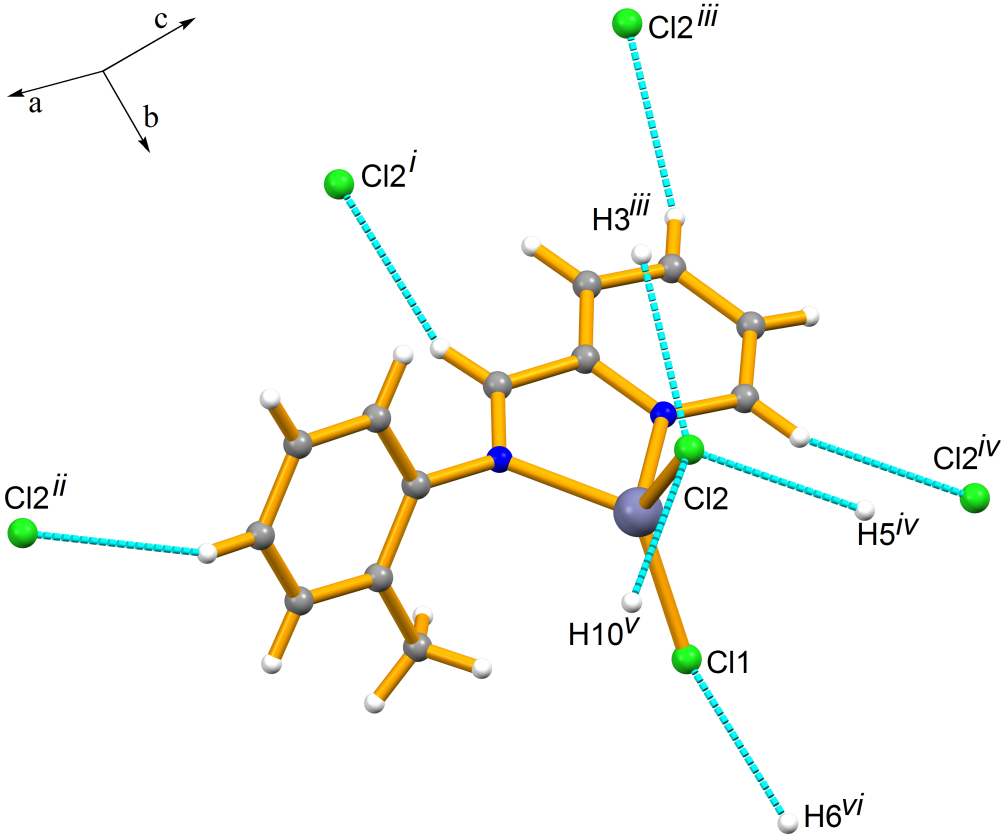

Fig. S2 The C–H···Cl contacts in the structure of **3**. Symmetry codes to generate equivalent atoms: *i*) x, –1 + y, z; *ii*) 1–x, –1/2 + y, ½ –z; *iii*) –x, 1–y, –z; *iv*) –x, 2–y, –z.

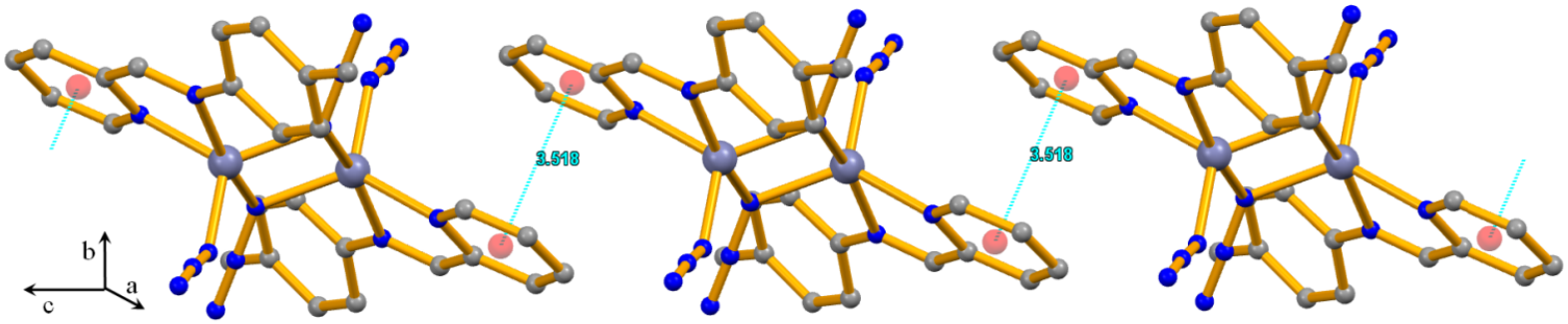

Fig. S3 Fragment of the crystal packing of **9** showing the π···π stacking interactions involving the pyridyl rings of adjacent molecules (*centroids* are represented as pink balls), which lead to 1D chains along the crystallographic *c* axis.

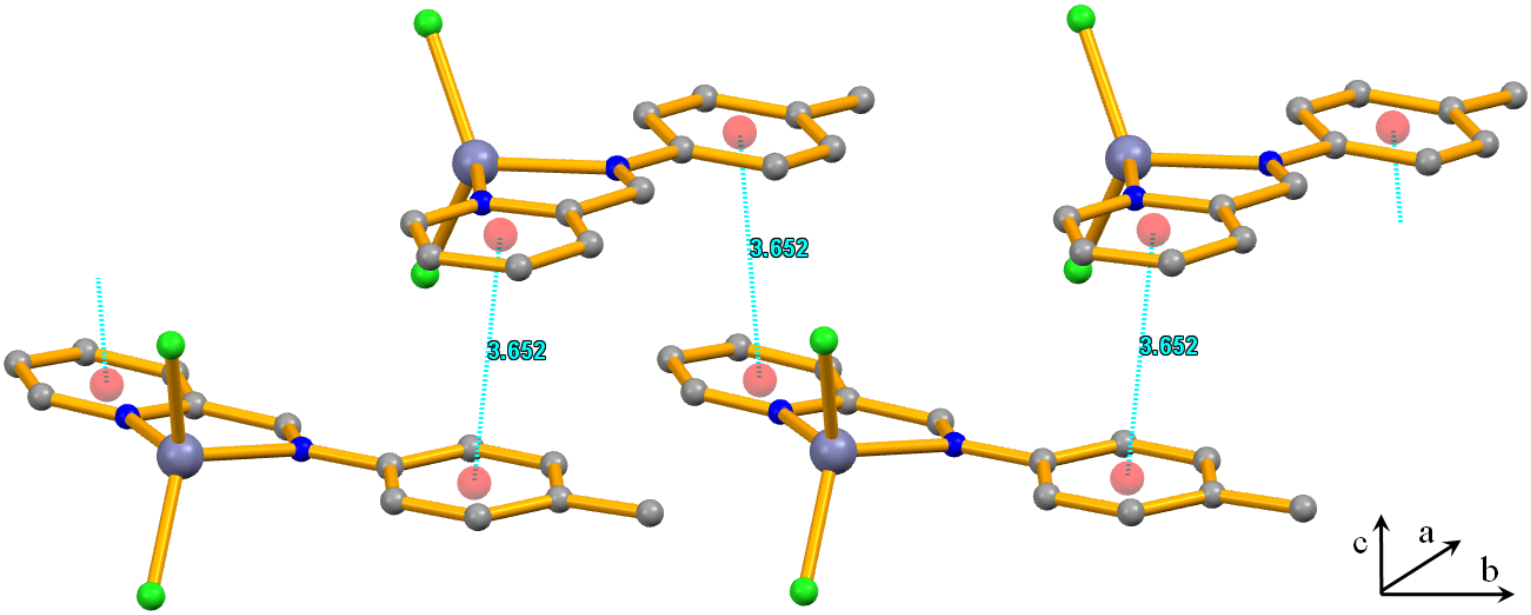

Fig. S4 Fragment of the crystal packing of **4** showing the π···π stacking interactions involving the pyridyl and phenyl rings of adjacent molecules (*centroids* are represented as pink balls), which lead to zig-zag chains along the crystallographic *b* axis.

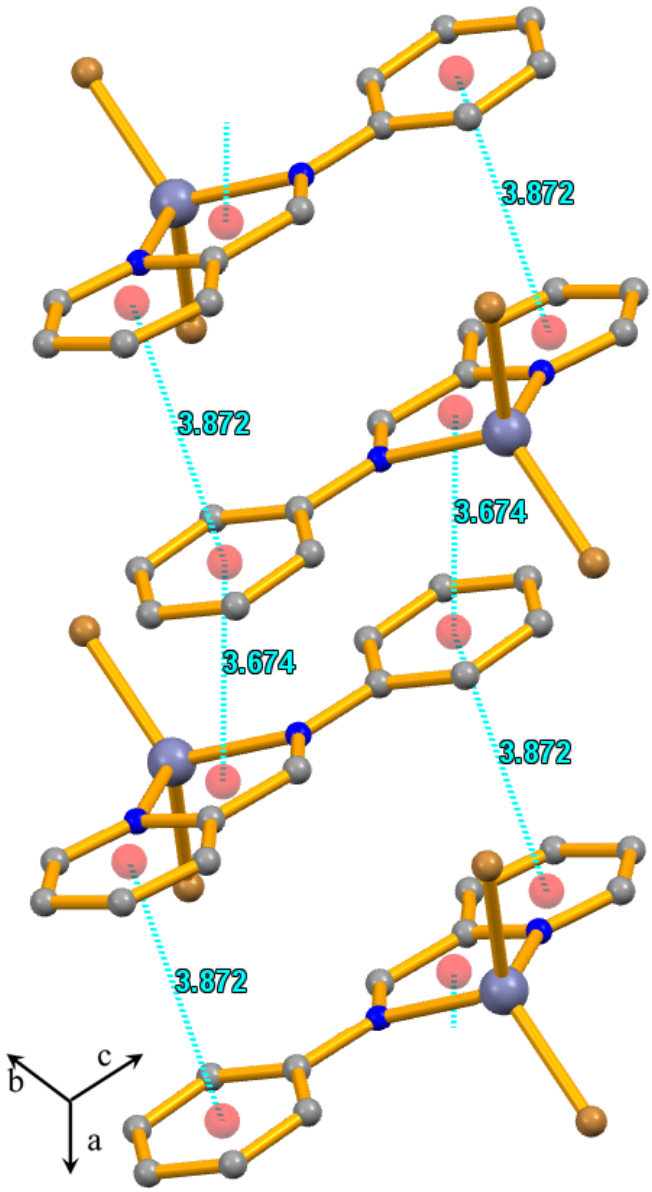

Fig. S5 Fragment of the crystal packing of **2** showing the π···π stacking interactions involving the metallacycle and the phenyl ring of an adjacent molecule (*centroids* are represented as pink balls) thus leading to centrosymmetric pairing of the molecules. These pairs are involved in further π(phenyl)···π(pyridyl) interactions on each side and the combined interactions form stacks of molecules along the crystallographic *a* axis.

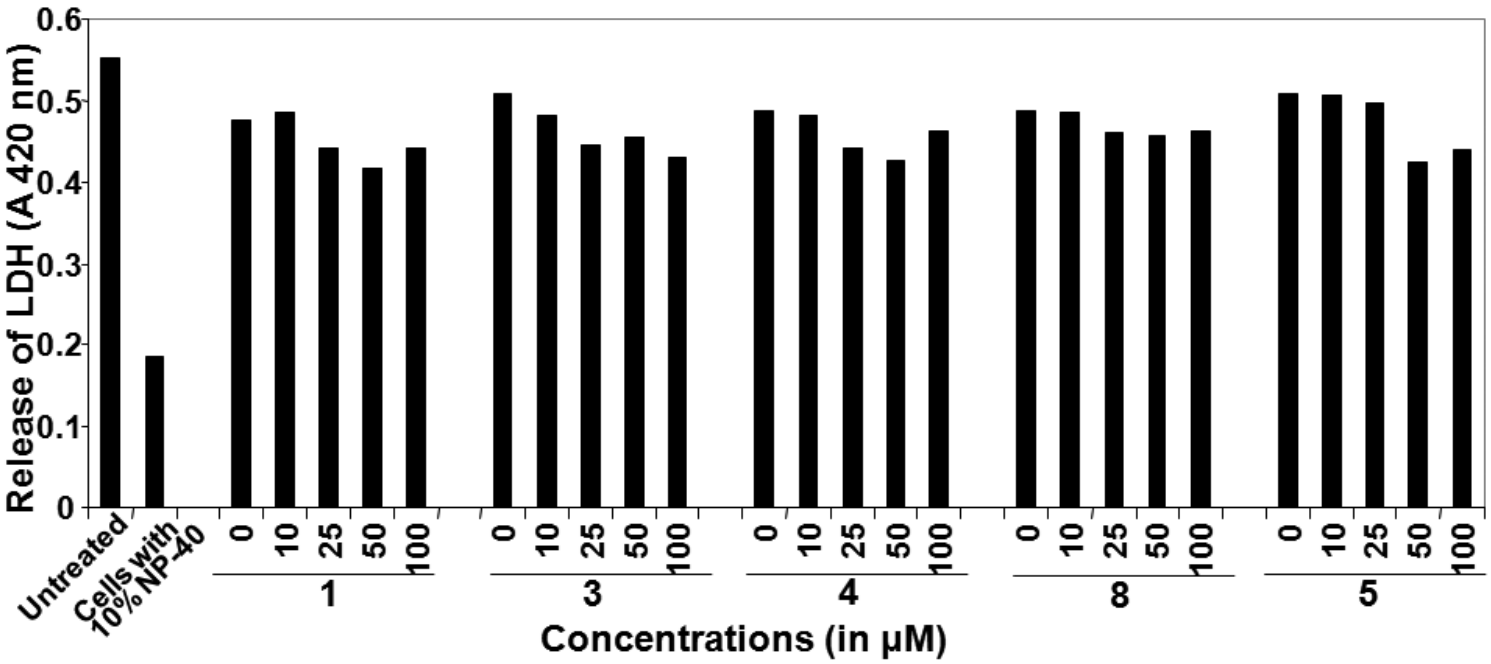

Fig. S6 Effect of zinc compounds (**1**, **3**-**5** and **8)** on cytolysis. HeLa cells (50,000/well of 24-well plate), cultured overnight were treated with different concentrations of zinc compounds for 72 h. Culture supernatants were collected and used to measure LDH activity. For total cellular LDH activity, untreated cells were incubated with 10% NP-40 for 30 min and the supernatant was used and considered as total cellular LDH activity.

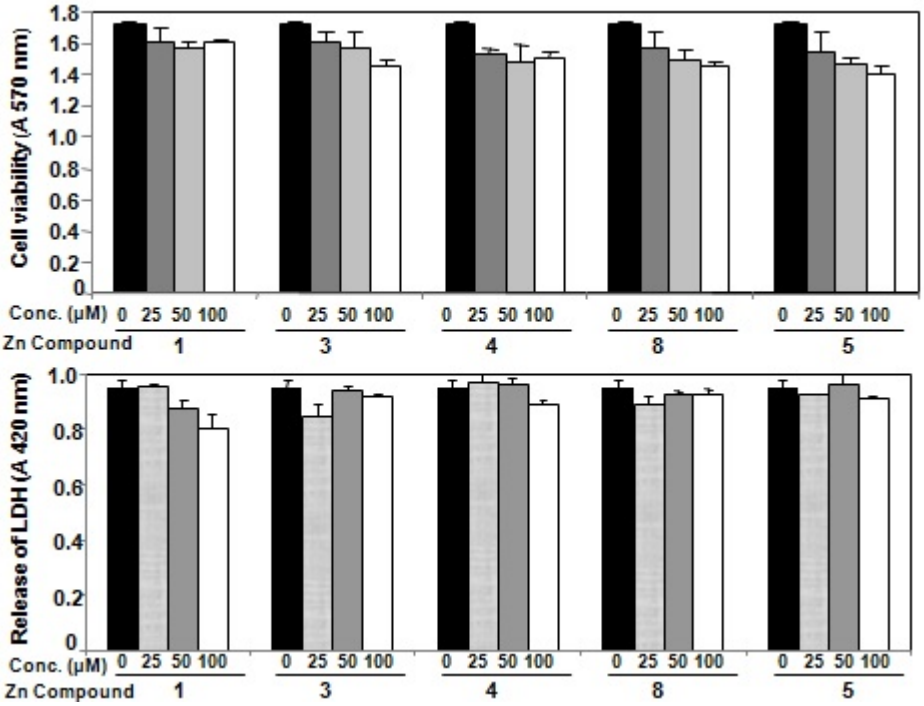

Fig. S7 PBMC isolated from fresh blood as described in the methodology section. PBMC were treated with zinc compounds for 72 h and MTT assayed (Fig. 5) and LDH measured from culture supernatant (Fig. S6).