Antiproliferative activity of Fe(II), Co(II), Ni(II), Cu(II), and Zn(II) complexes of dithiocarbamate: Synthesis, structural characterization, and thermal studies

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1. FTIR Spectra:

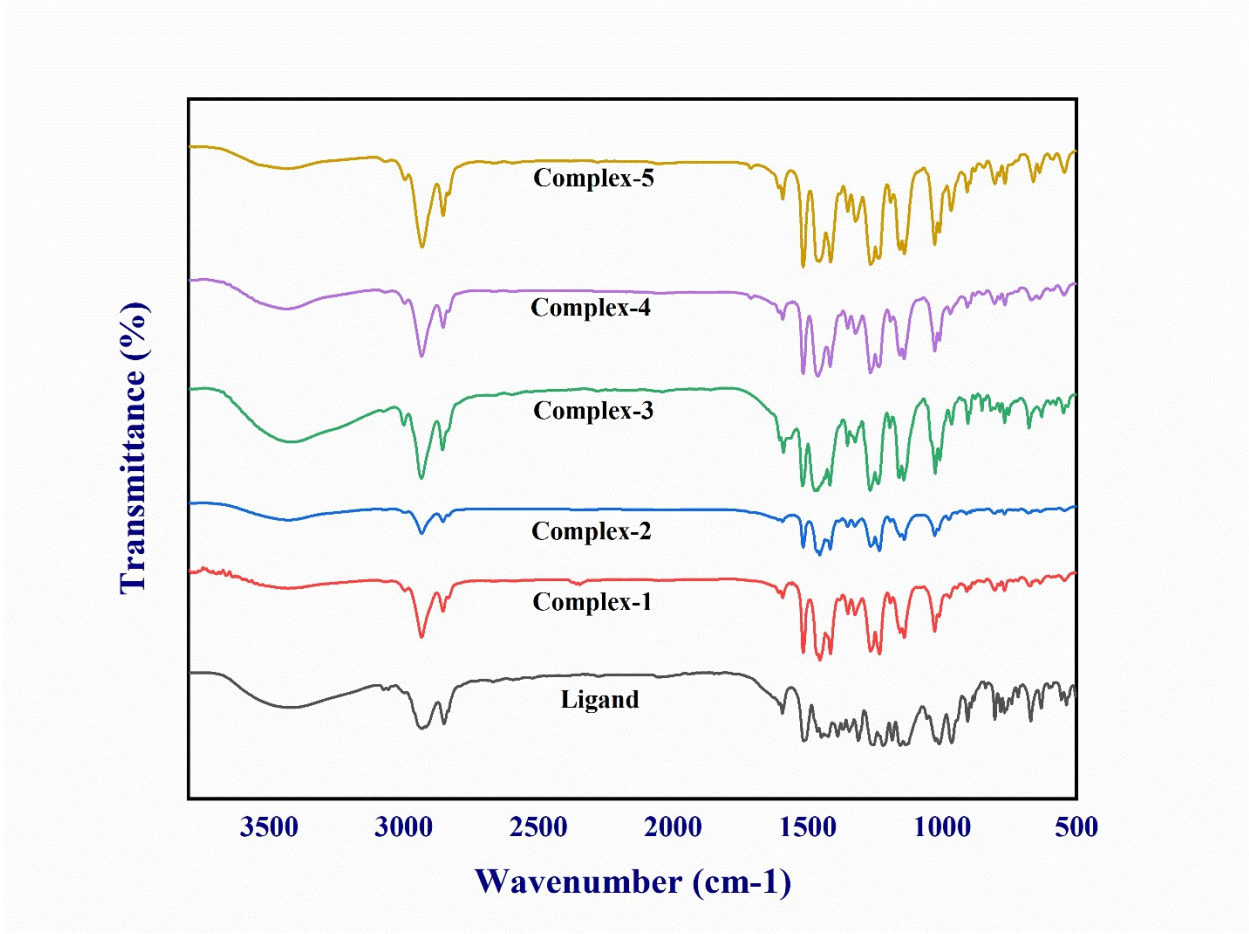

Fig. S1: FTIR spectra of ligand and complexes **1-5**.

2. NMR Spectra:

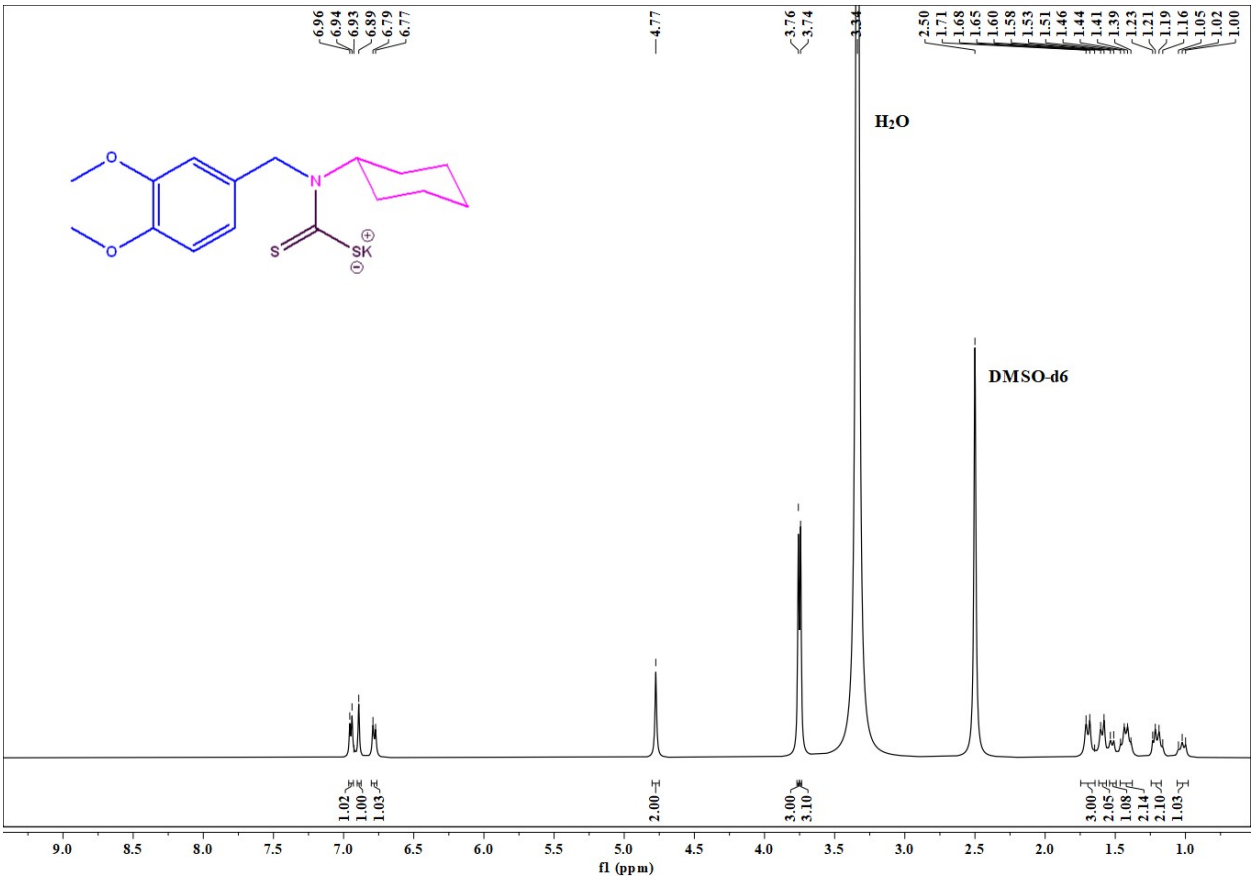

Fig. S2: ^{1}H NMR spectrum of ligand.

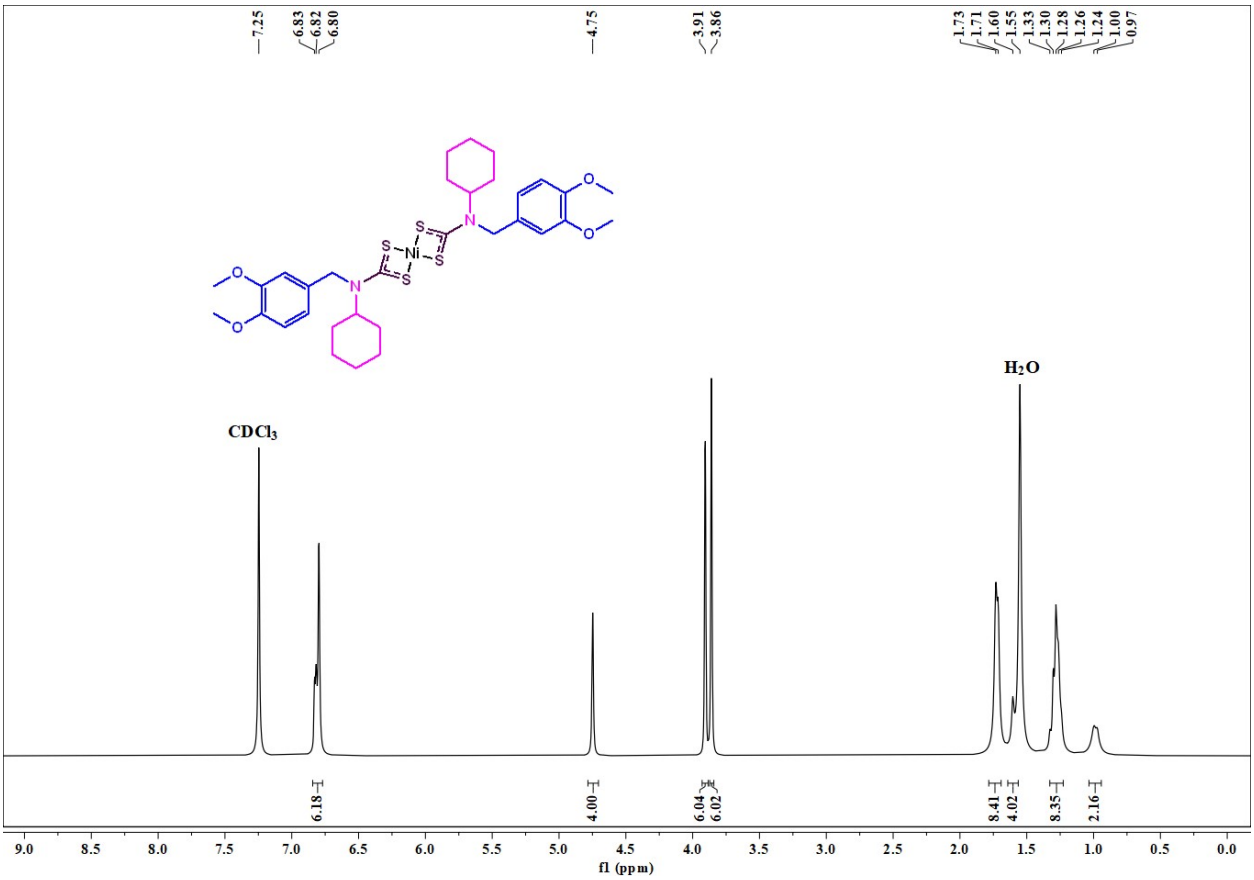

Fig. S3: ^{1}H NMR spectrum of complex **3**.

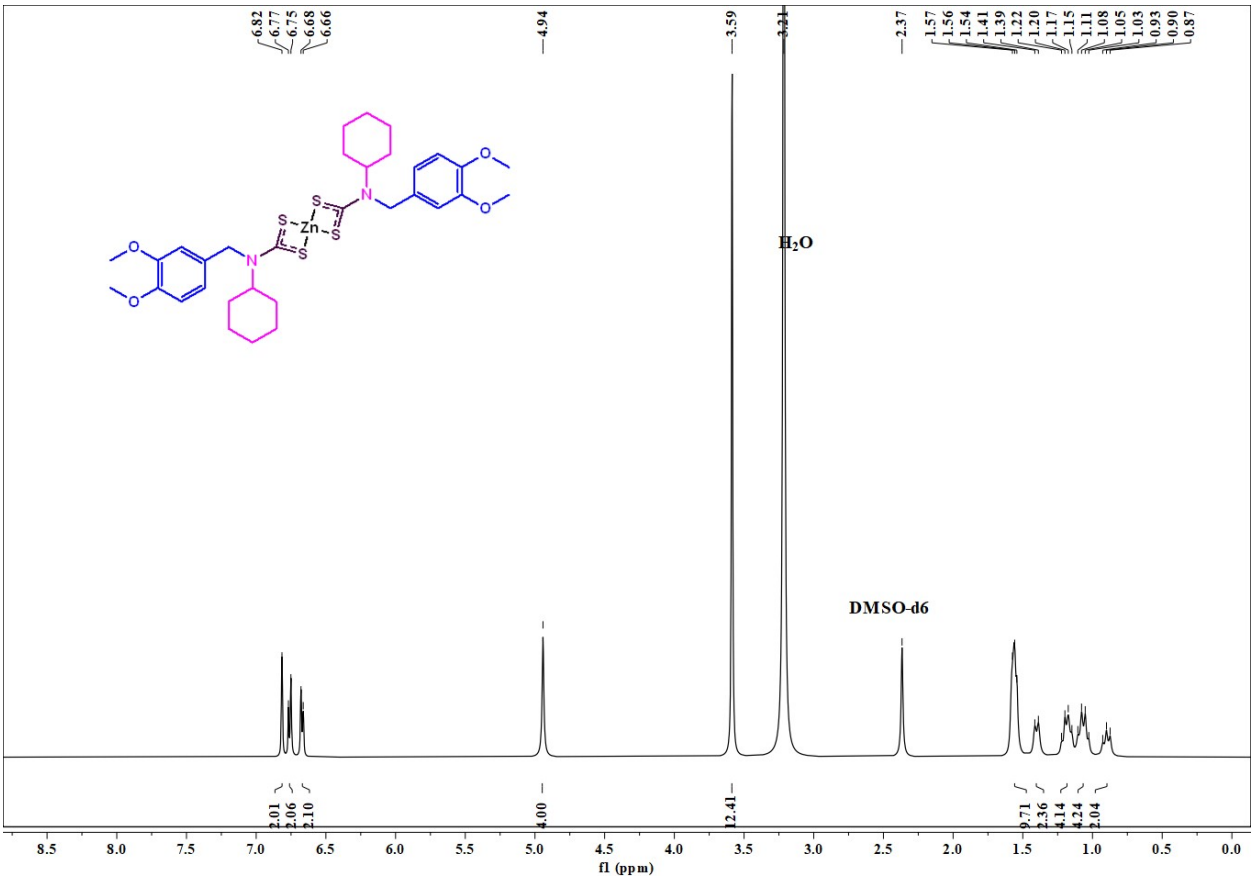

Fig. S4: ^{1}H NMR spectrum of complex **5**.

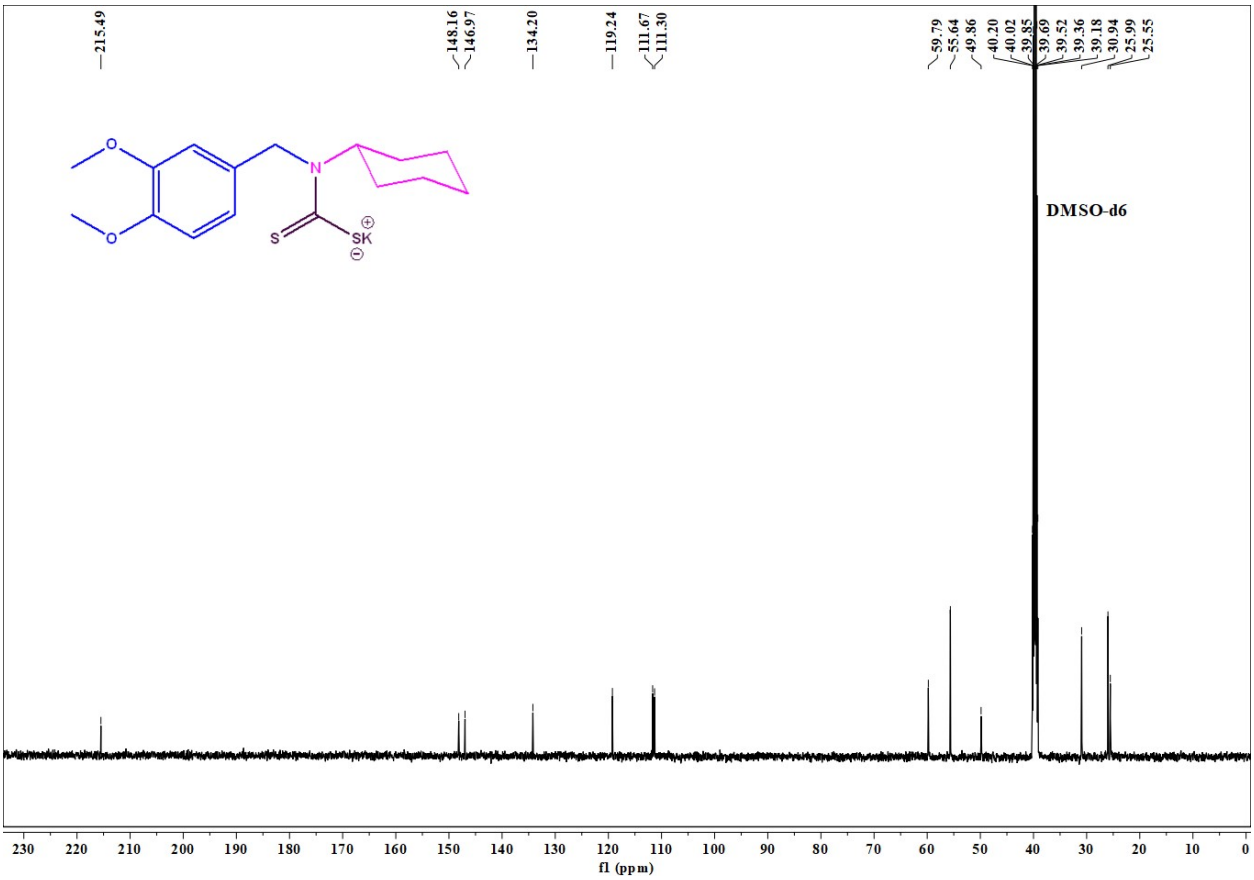

Fig. S5: ^{13}C NMR spectrum of ligand.

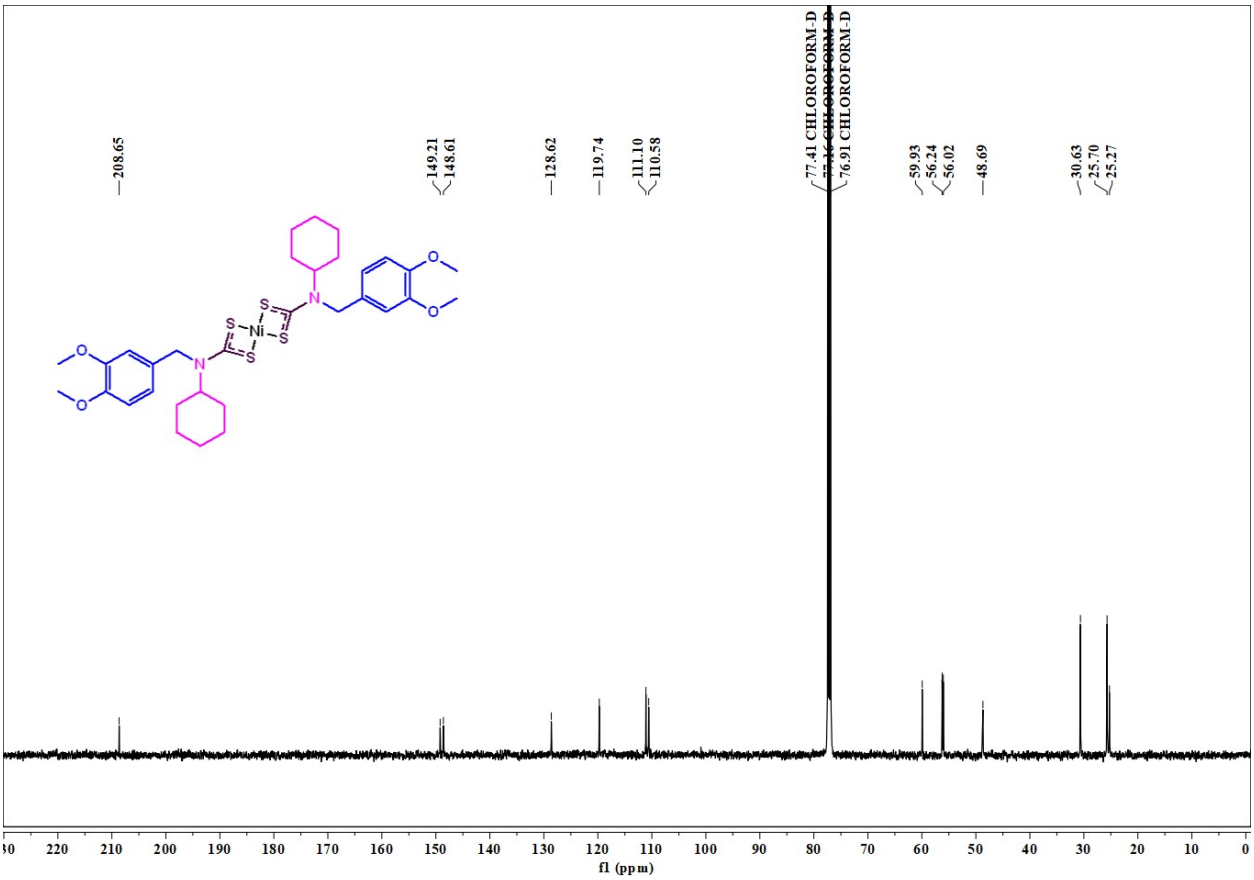

Fig. S6: ^{13}C NMR spectrum of complex **3**.

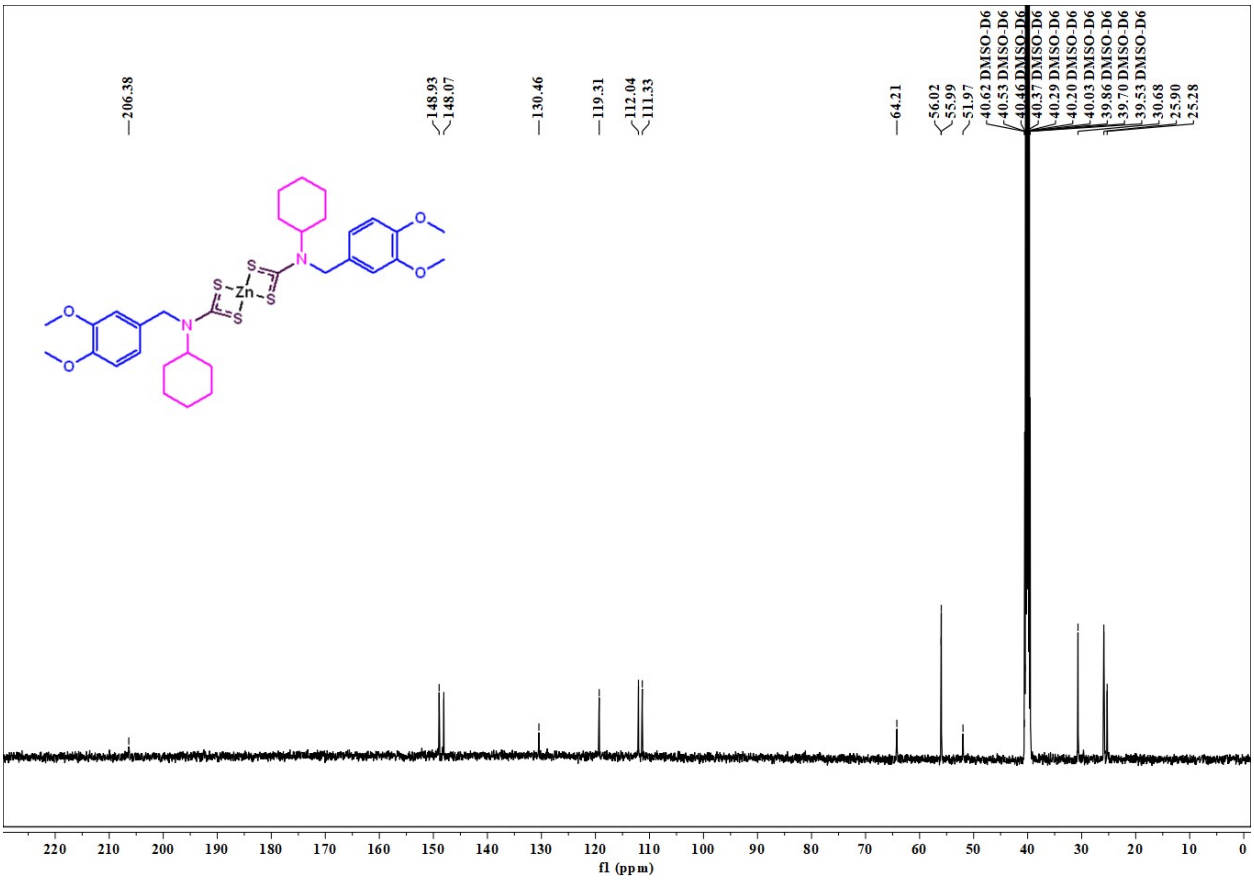

Fig. S7: ^{13}C NMR spectrum of complex **5**.

3. HRMS Spectra:

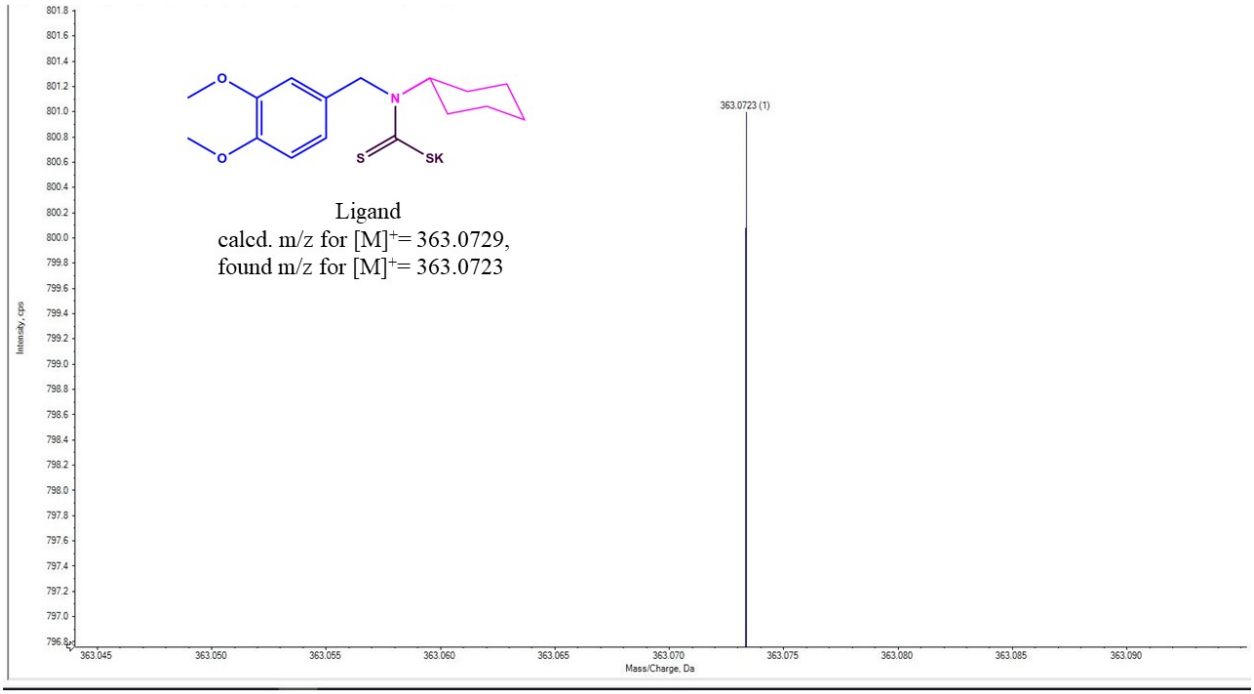

Fig. S8: HRMS spectrum of ligand.

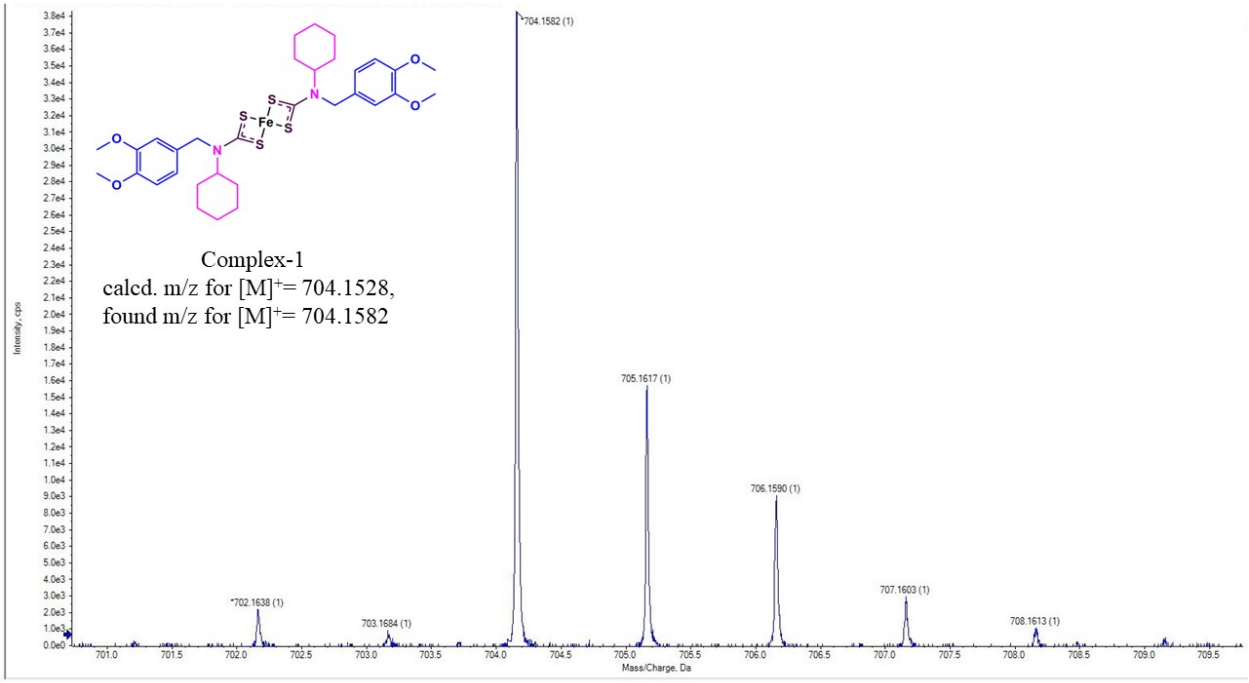

Fig. S9: HRMS spectrum of complex **1**.

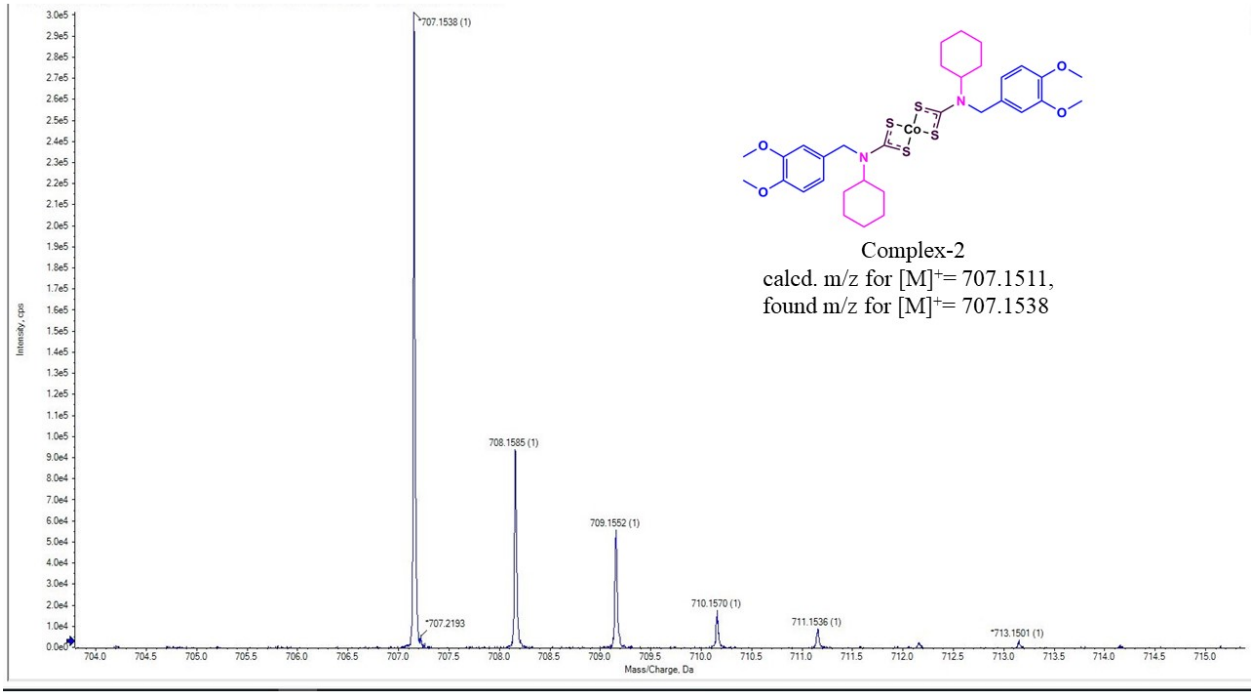

Fig. S10: HRMS spectrum of complex **2**.

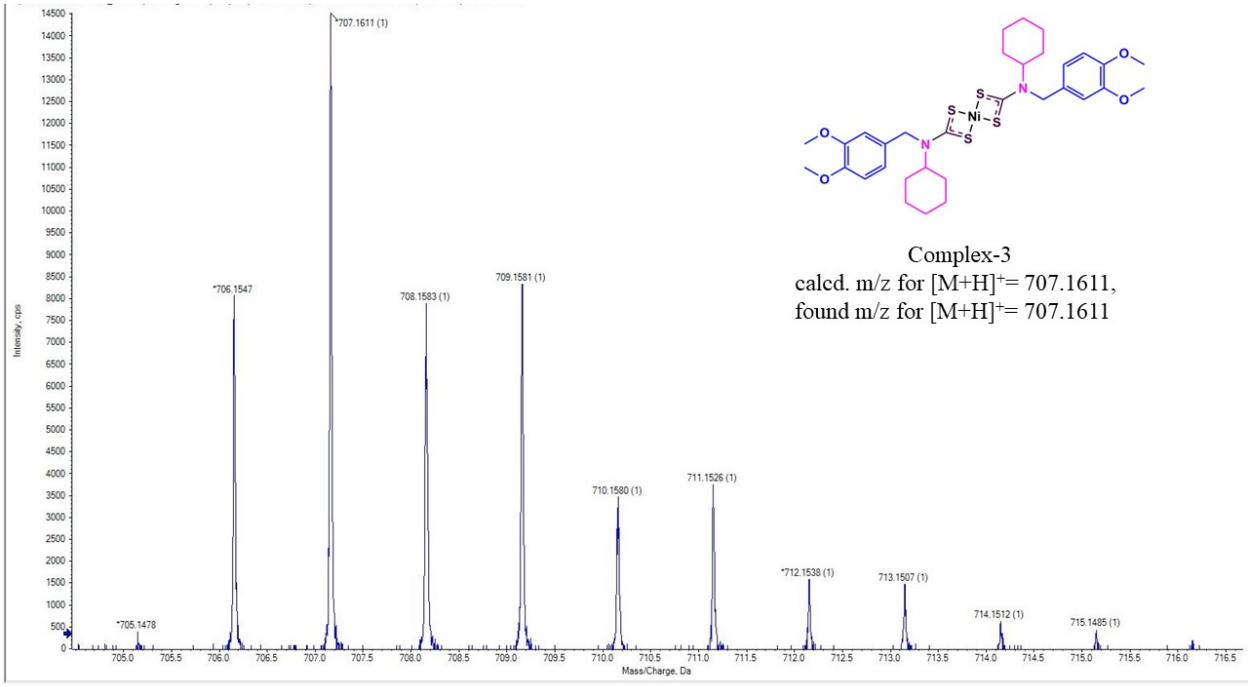

Fig. S11: HRMS spectrum of complex **3**.

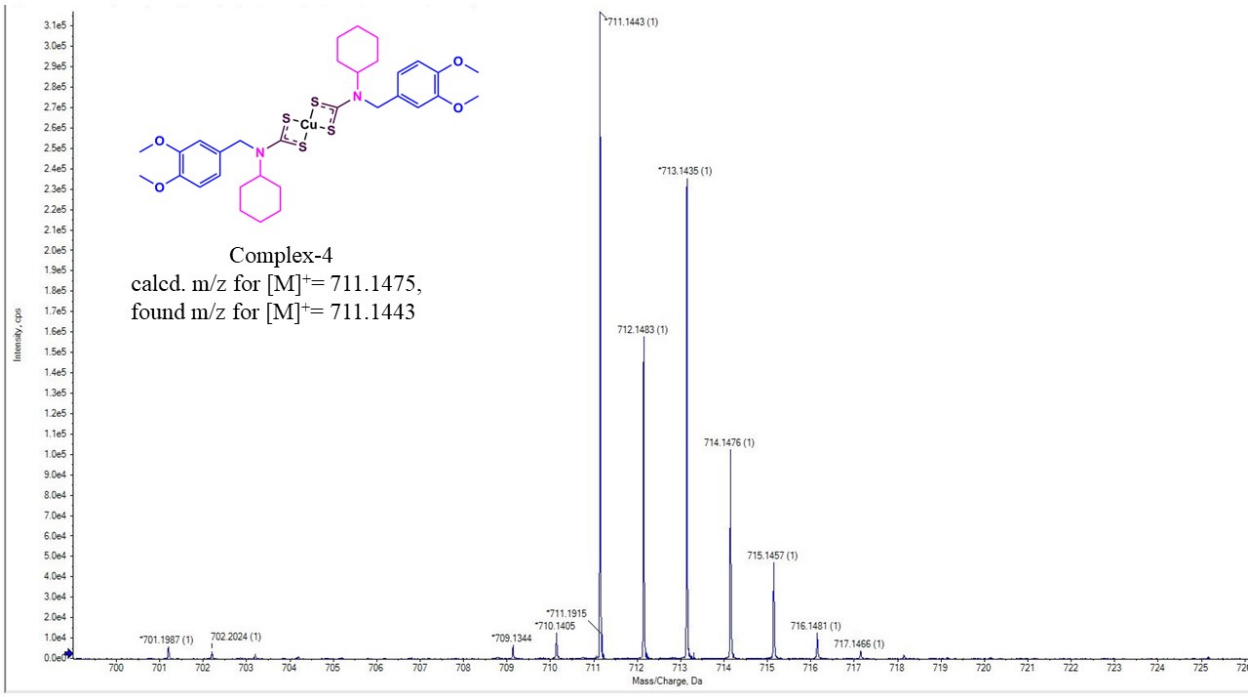

Fig. S12: HRMS spectrum of complex **4**.

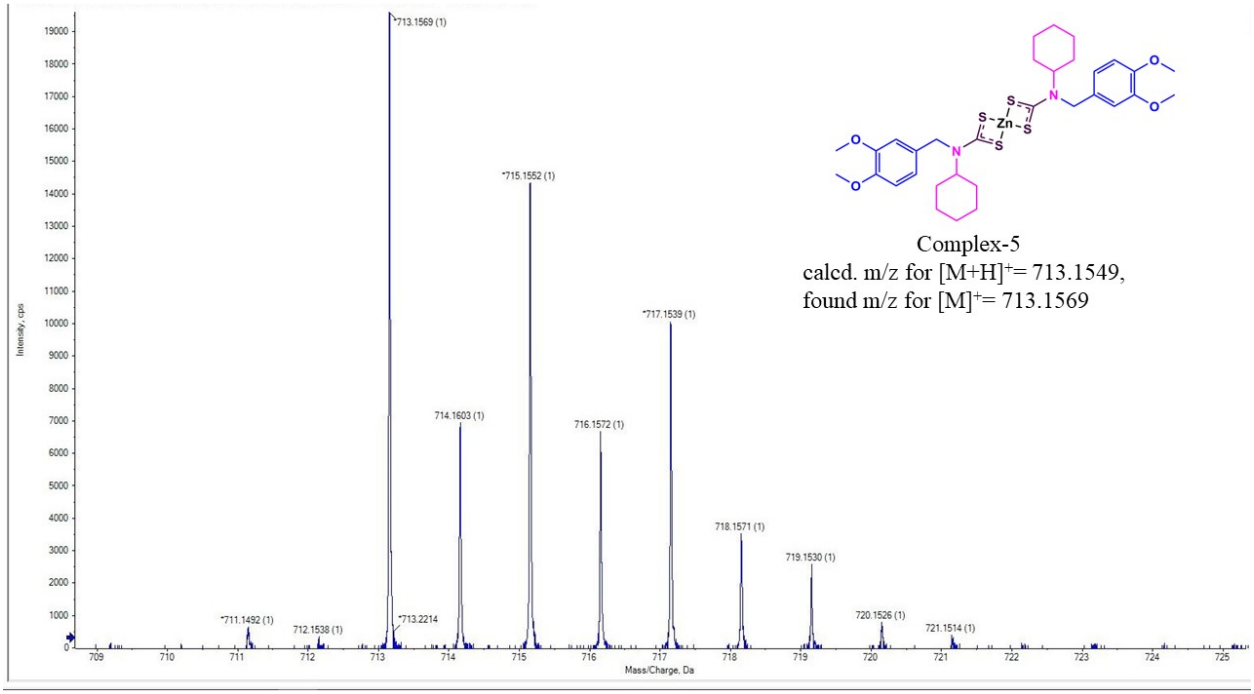

Fig. S13: HRMS spectrum of complex **5**.

4. X-ray crystallography

X-Ray diffraction measurements of complexes **4** and **5** were performed using Oxford Gemini and Bruker three-circle diffractometer equipped with a CrysAlisPro/CrysAlis CCD software using a graphite mono-chromated Mo Kα (λ= 0.71073 Å) radiation source at 296 K. The details of the temperature and monochromator of diffractometers are mentioned in the crystallographic data tables. Multi-scan absorption correction was applied to the X-ray data collection for all the compounds. The structures were solved by direct methods (SHELXS-08) and refined against all data by full matrix least-square on F2 using anisotropic displacement parameters for all non-hydrogen atoms. All hydrogen atoms were included in the refinement at geometrically ideal position and refined with a riding model[1]. The MERCURY package and ORTEP-3 for Windows program were used for generating structures[2,3]. Single crystals of complex **5** was kept at 100.00 K during data collection. The material was recrystallized from methanol by slow evaporation.

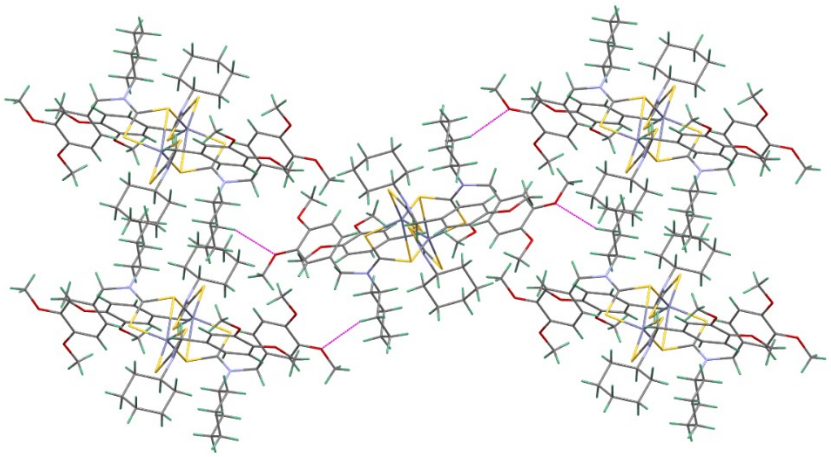

Fig. S14: Showing the intermolecular C-H···O hydrogen bonding interactions leading to wave like structures.

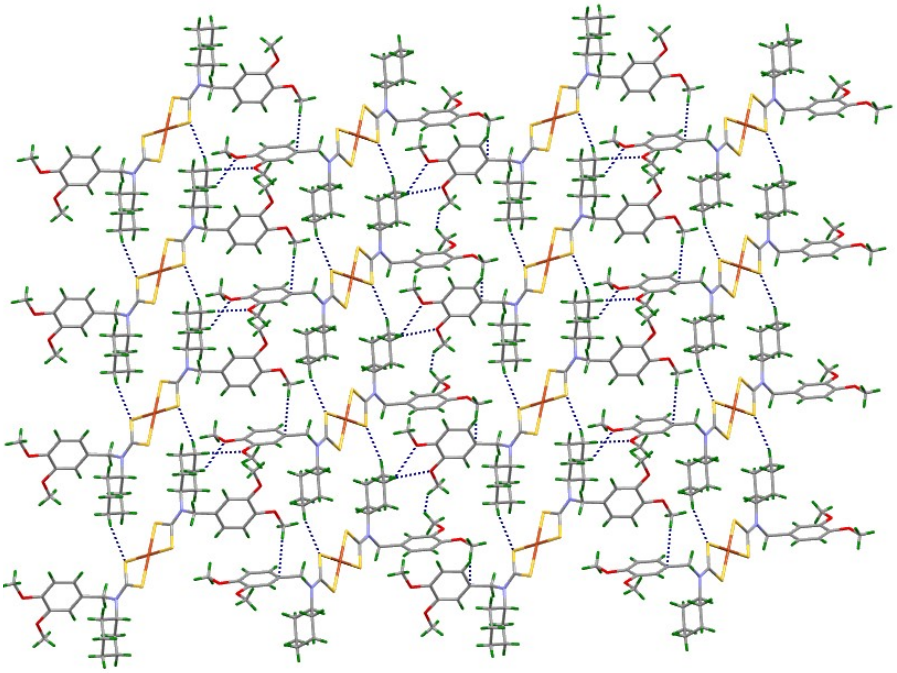

Fig. S15: Showing the intermolecular C-H···S hydrogen bonding interactions leading to ladder-like structures.

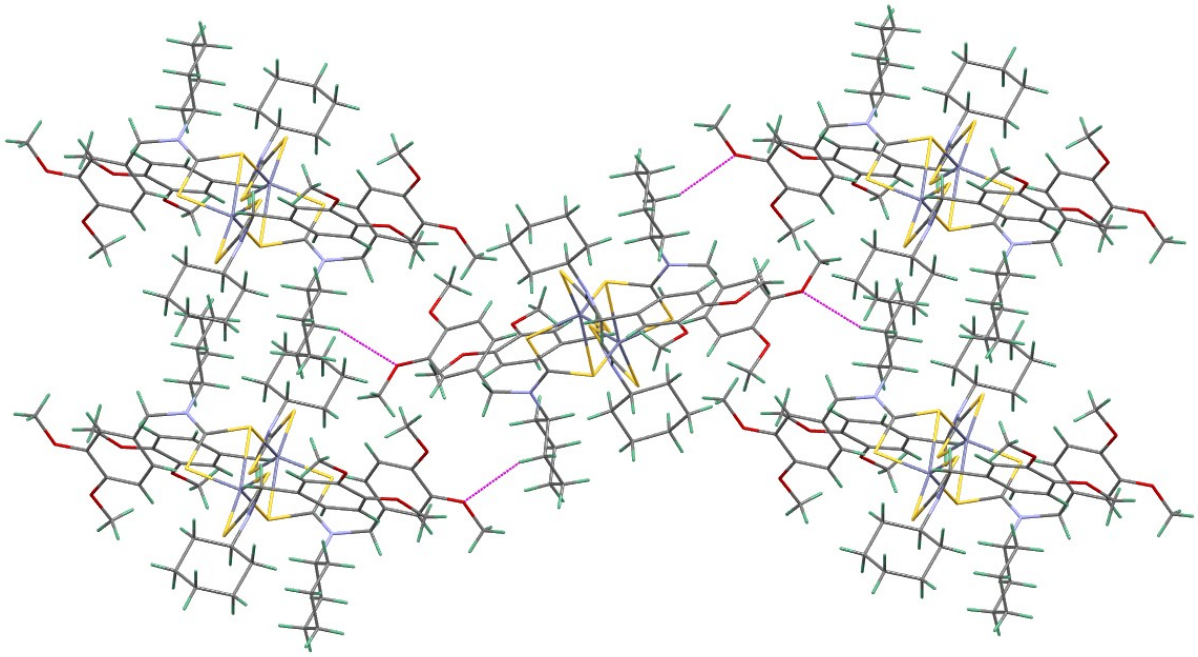

Fig. S16: Showing the intermolecular C-H···O hydrogen bonding interactions leading to a 2D supramolecular architecture.

Table S1. Hydrogen bond parameters for complex **4**.

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
C(9)-H(9)...S(1)	0.98	2.54	3.0345(16)	111.0
C(2)-H(2B)...S(2)	0.97	2.49	3.0276(18)	114.6

Symmetry transformations used to generate equivalent atoms: #1 -x,-y,-z+1

Table S2. Hydrogen bond parameters for complex **5**.

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
C(27)-H(27)...S(3)	0.98	2.50	3.041(3)	114.6
C(9)-H(9)...S(2)	0.98	2.52	3.006(2)	110.6
C(2)-H(2B)...S(1)	0.97	2.52	3.009(3)	111.0

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+1

5. Biological application

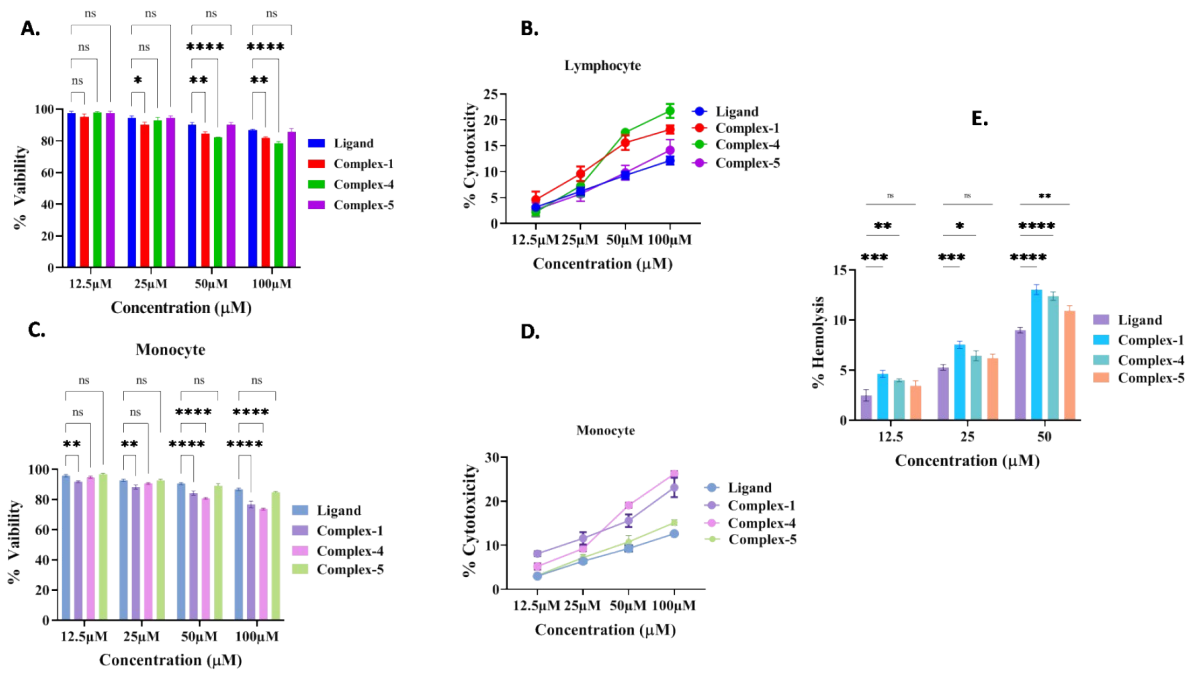

Fig. S17: Biocompatibility and hemocompatibility study of complexes **1**, **4** & **5**. Biocompatibility analysis in human monocytes and lymphocytes in the presence of indicated formulations as judged by viability (A & C) and cytotoxicity (B & D) of the lymphocytes and monocytes. Percent hemolysis of RBC following treatment for 4 hours in the presence of varying concentrations of the indicated formulations (E).

6. References:

[1] G.M. Sheldrick, ActaCrystallogr. Section A, 2008, 64, 112-122.

[2] C.F. Macrae, I.J. Bruno, J.A. Chisholm, P.R. Edgington, P. McCabe, E. Pidcock, L. Rodriguez-Monge, R. Taylor, J.Van de Streek, P.A., Wood, Appl. Cryst., 2008, 41, 466-470.

[3] L.J. Farrugia, J. Appl. Cryst., 2012, 45, 849-854.