

## Supporting Information

### **Developing Novel Zinc(II) and Copper(II) Schiff Base Complexes: Combined Experimental and Theoretical Investigation on Their DNA/Protein Binding Study and Anticancer Activity**

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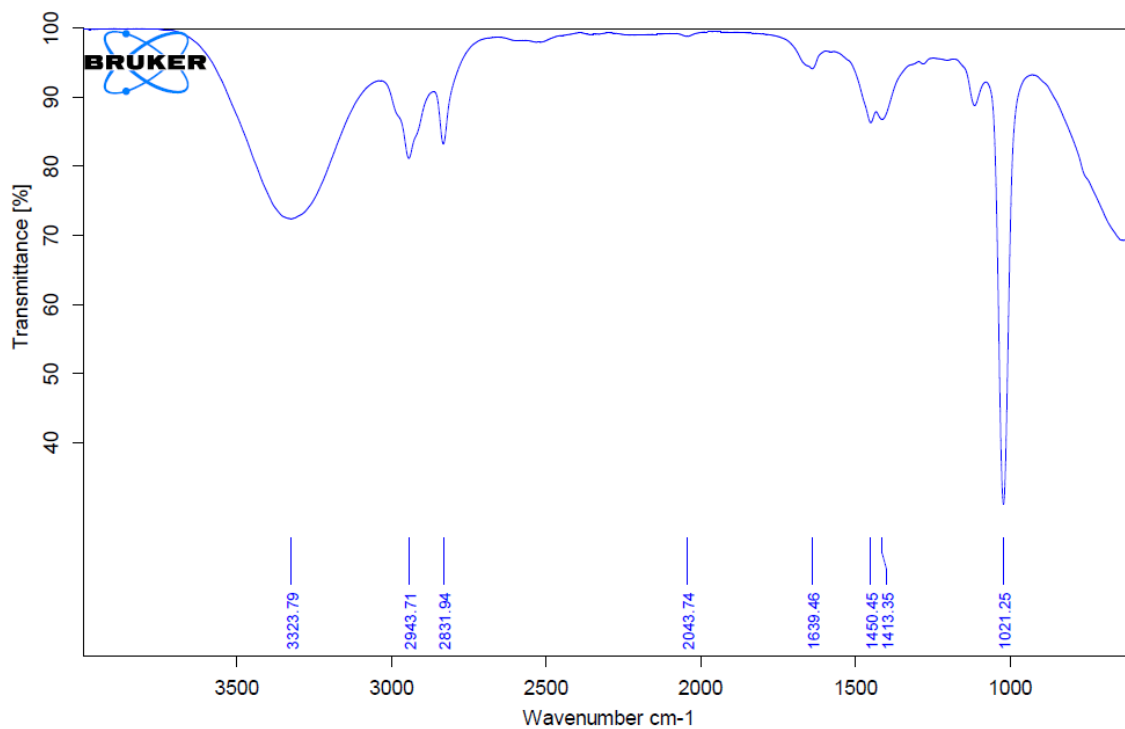


Fig. S1 FT-IR spectrum of ligand (HL).

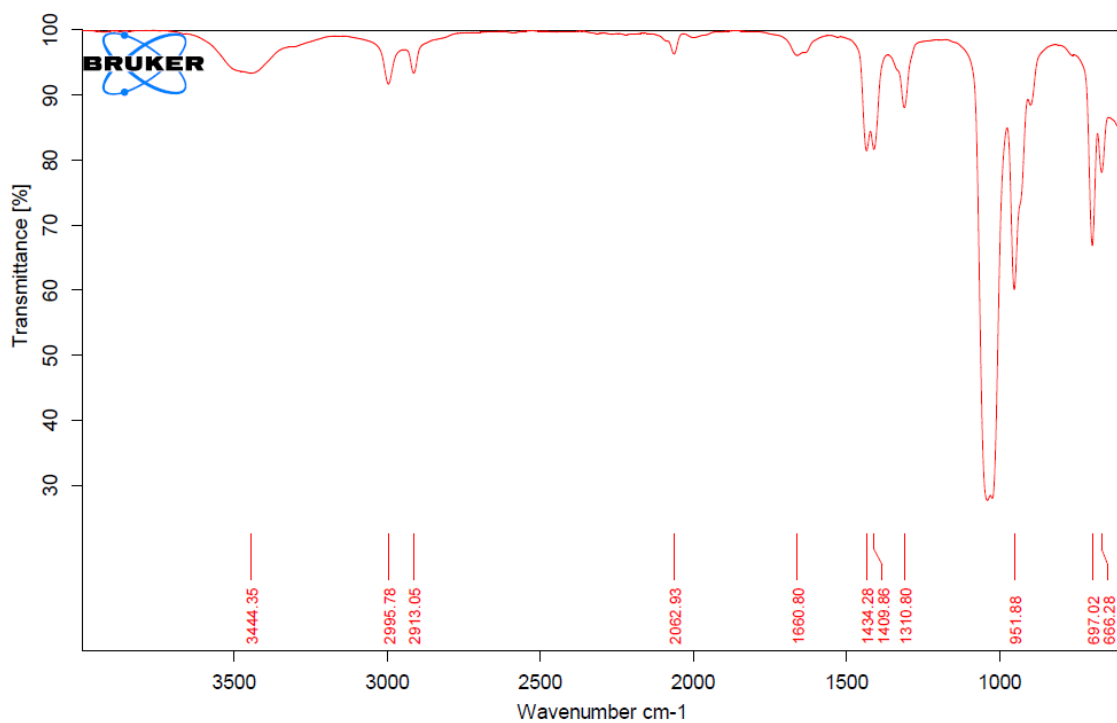
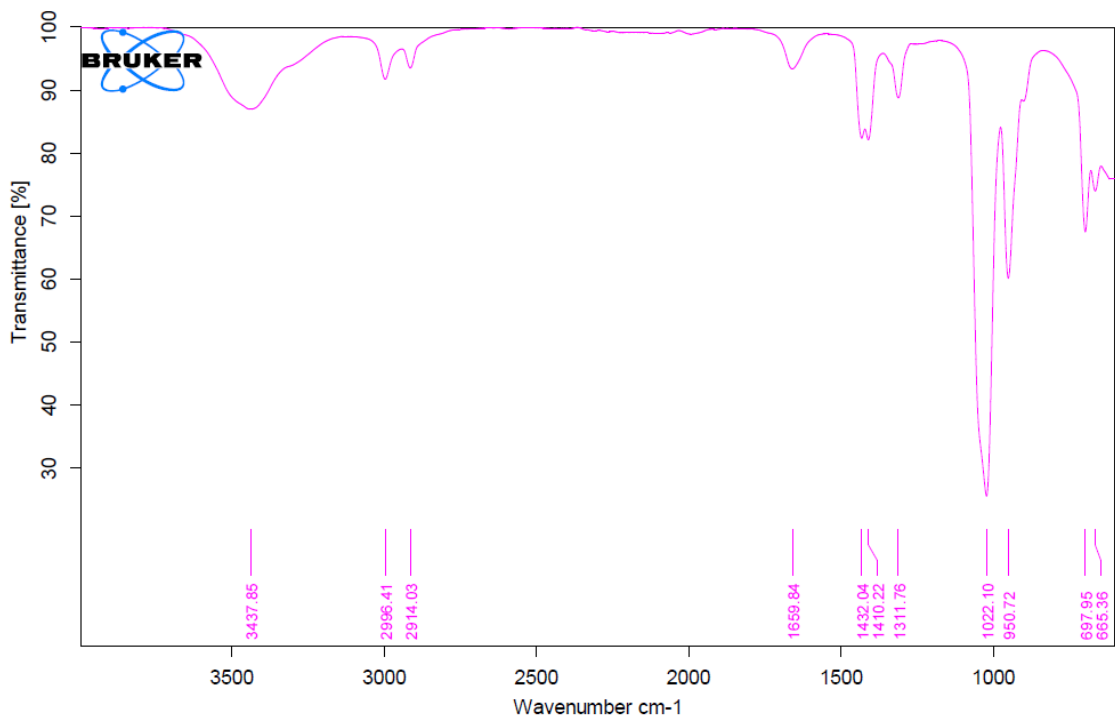
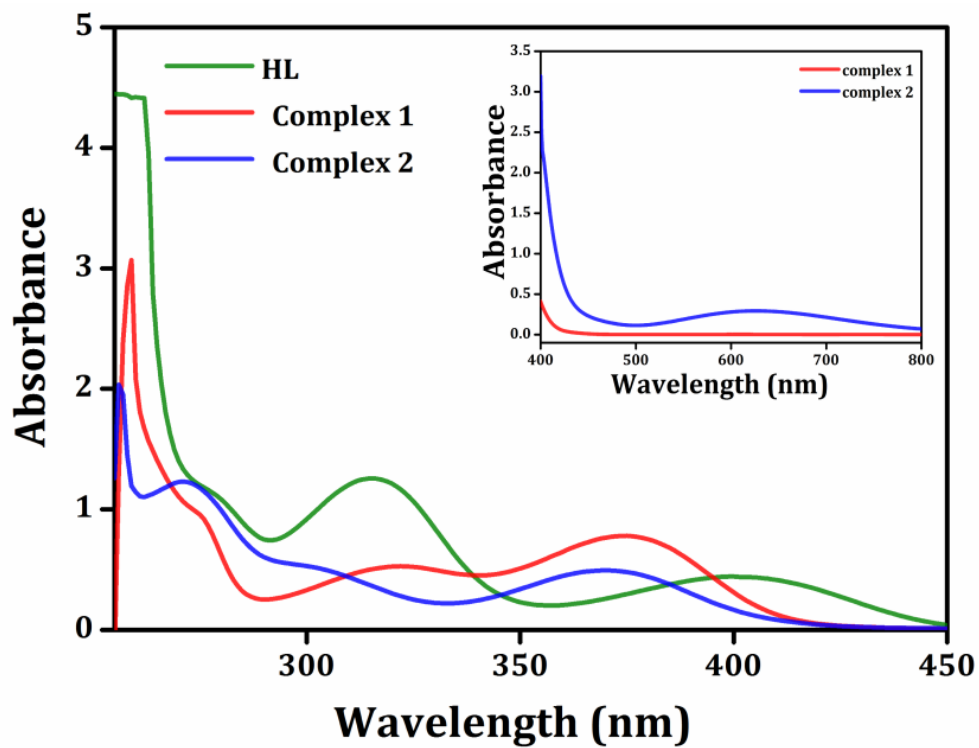


Fig. S2 FT-IR spectrum of Complex 1.



**Fig. S3** FT-IR spectrum of Complex 2.



**Fig. S4** UV-Vis spectra of ligand and complexes.

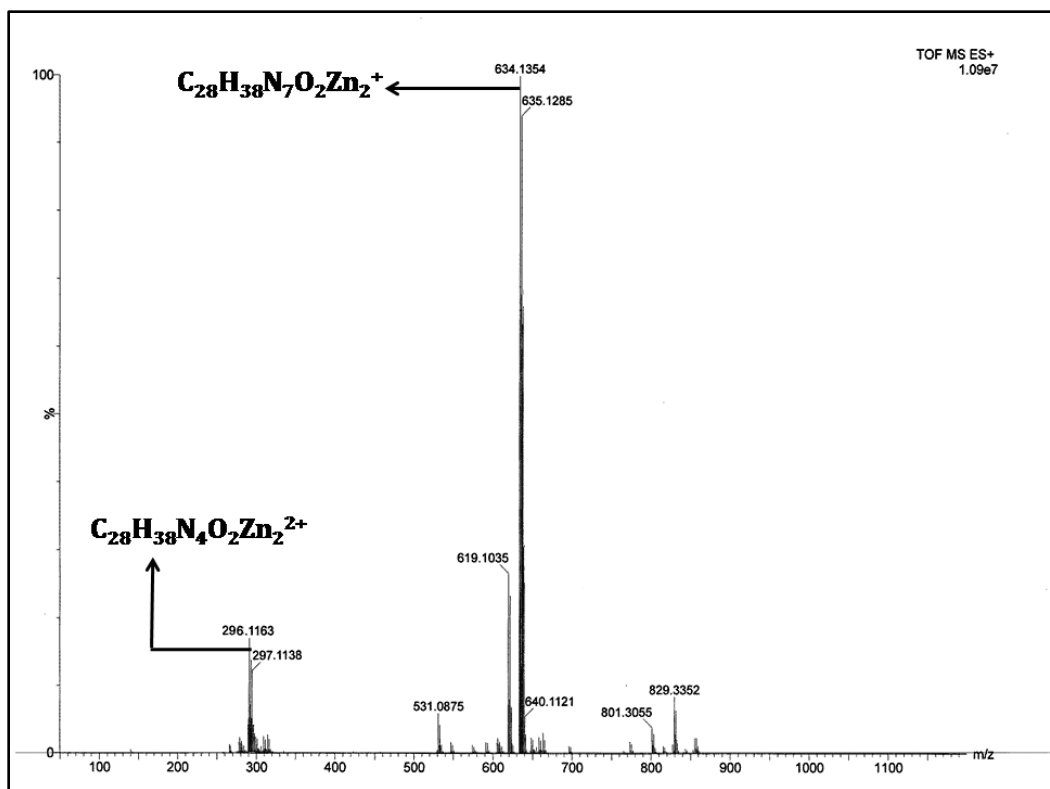


Fig. S5 ESI Mass Spectral analysis of complex 1.

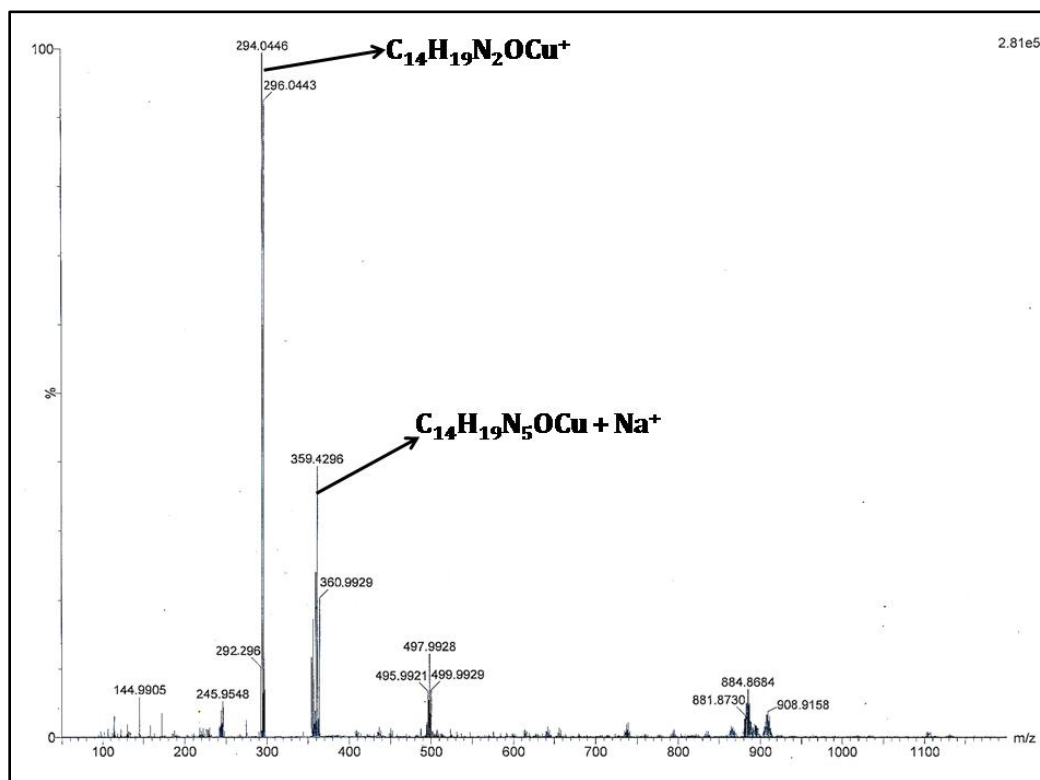


Fig. S6 ESI Mass Spectral analysis of complex 2.

**Table S1** Selected bond lengths and bond angles of Complex 1.

Complex 1					
Bond length (Å)		Bond angle (°)			
Zn1-O1	1.9800(12)	O1-Zn1-N1	89.83(5)	O1-Zn1-O1a	77.54(4)
Zn1-N1	2.1376(14)	O1-Zn1-N3	120.57(7)	N3-Zn1-N6	119.56(8)
Zn1-N3	2.0293(19)	O1-Zn1-N6	119.86(6)	O1a-Zn1-N1	167.28(5)
Zn1-N6	2.0291(16)	N1-Zn1-N3	91.05(7)	O1a-Zn1-N3	96.66(8)
Zn1-O1a	2.1736(11)	N1-Zn1-N6	90.54(6)	O1a-Zn1-N6	94.42(5)

**Table S2** Selected bond lengths and bond angles of Complex 2.

Complex 2					
Bond length (Å)		Bond angle (°)			
Cu1-O1	1.897(4)	O1-Cu1-N2	93.77(18)	N1-Cu1-N10	88.30(18)
Cu1-N1	2.075(5)	O1-Cu1-N1	178.63(18)	N2-Cu1-N10	78.59(17)
Cu1-N2	1.936(5)	O1-Cu1-N3	90.42(19)	N3-Cu1-N10	111.8(2)
Cu1-N3	1.970(6)	N1-Cu1-N2	84.87(19)	O1-Cu1-N10	91.28(16)
Cu1-N10	2.839(5)	N1-Cu1-N3	90.9(2)	N2-Cu1-N3	168.8(2)

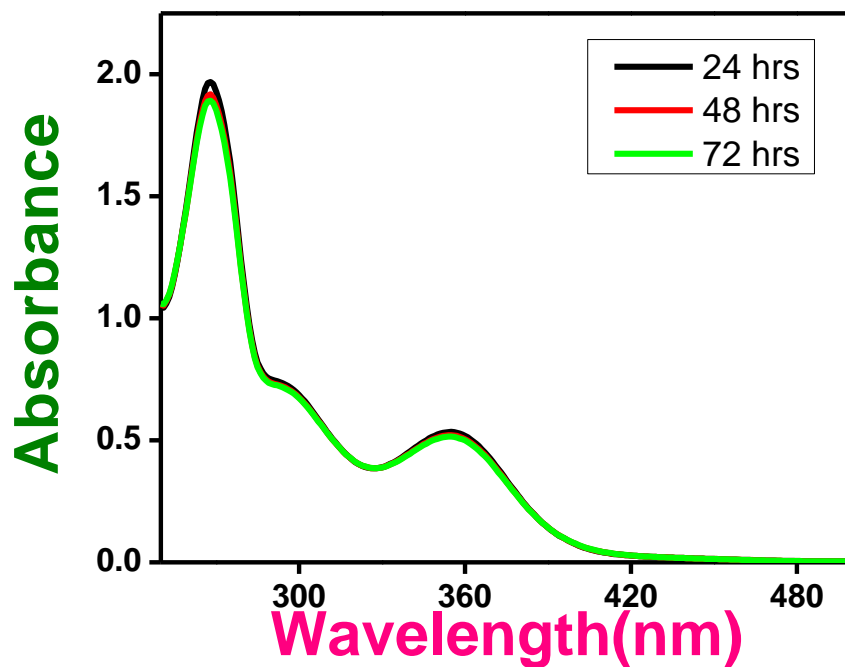


Fig. S7 Time dependent absorbance graph for complex 1 in CP buffer at pH 7.4.

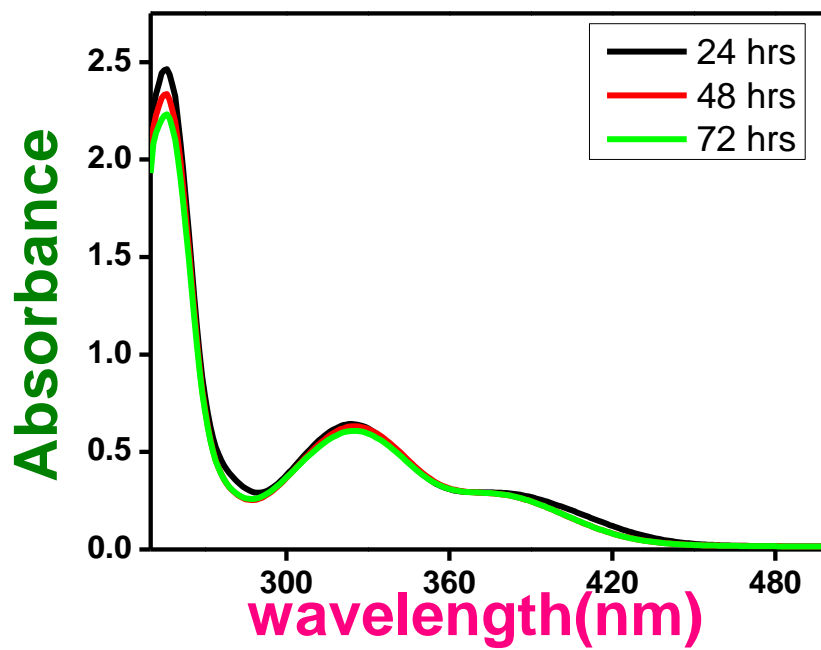


Fig. S8 Time dependent absorbance graph for complex 2 in CP buffer at pH 7.4.

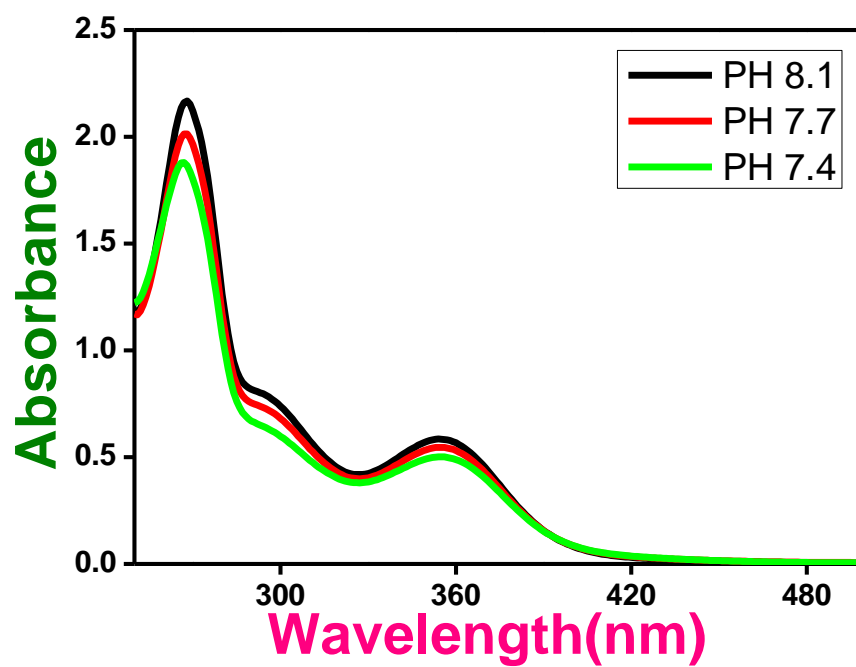


Fig. S9 pH dependent absorbance graph for complex 1.

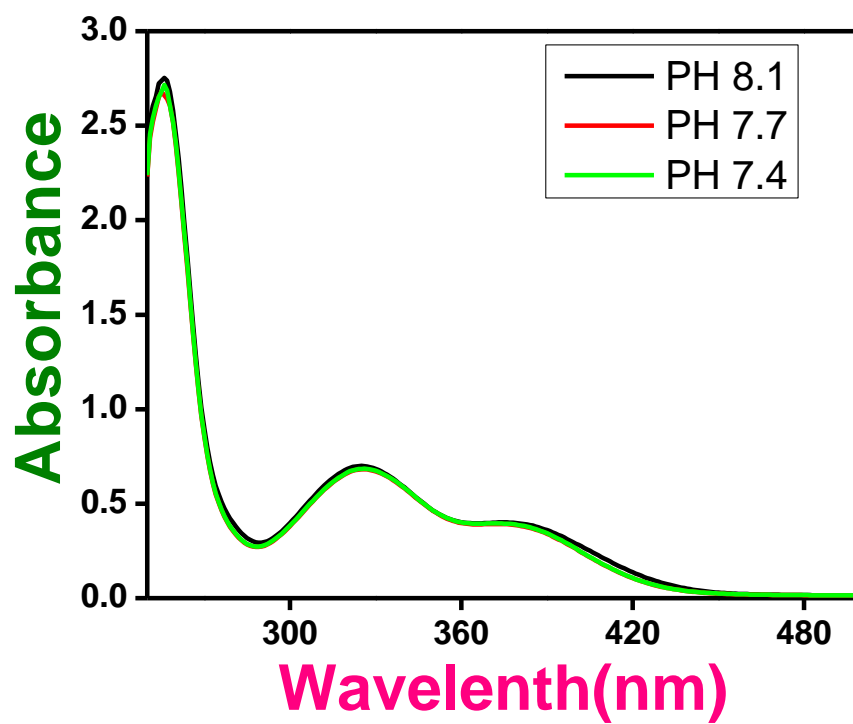
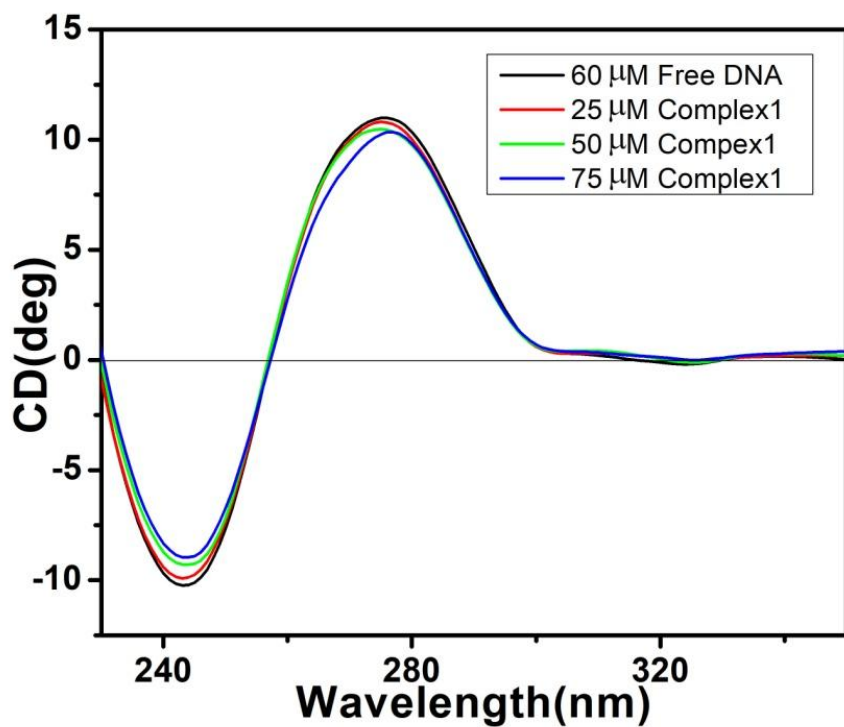
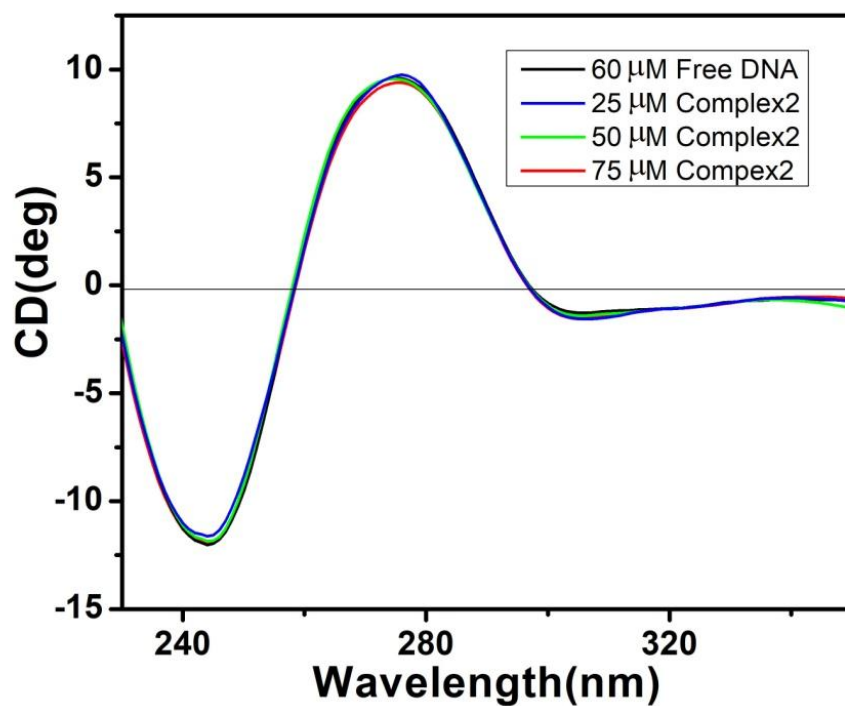


Fig. S10 pH dependent absorbance graph for complex 2.

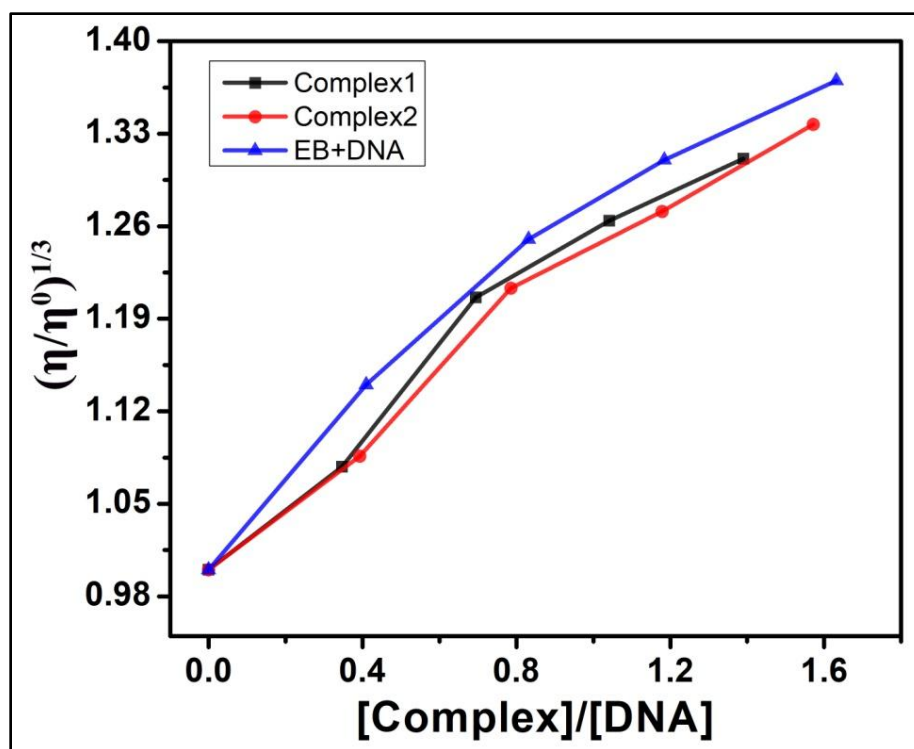




**Fig. S11** CD spectral changes in CT DNA (60 $\mu$ M) upon addition of complex 1 (D/P=10.0) in 10mM CP buffer (blue line indicates the CD of CT-DNA).



**Fig. S12** CD spectral changes in CT DNA (60 $\mu$ M) upon addition of complex 2 (D/P=10.0) in 10mM CP buffer (blue line indicates the CD of CT-DNA).



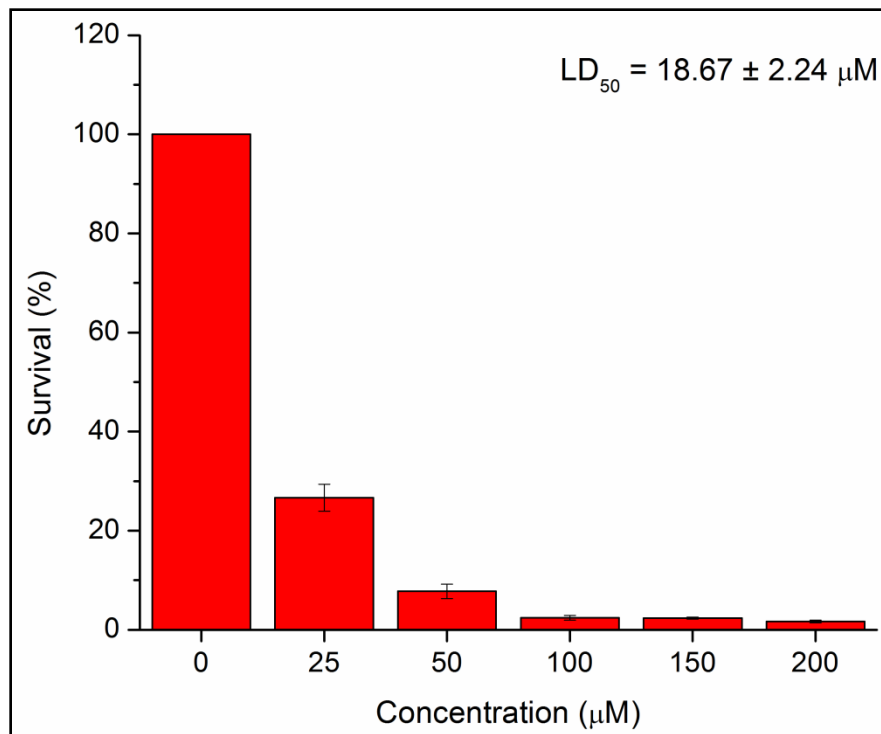
**Fig. S13** Viscosity measurement of DNA-EtBr and DNA-Complex 1 / 2 conjugate.

**Table S3** DNA - metal complexes patch dock score.

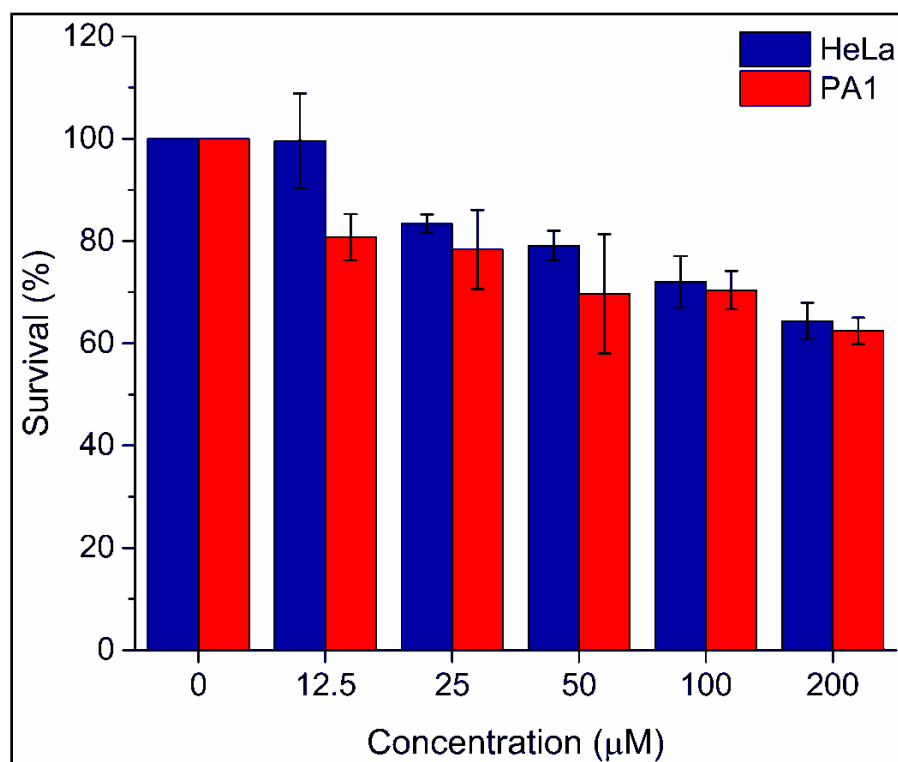
Complex	Patch Dock score	ACE (Kcal/mole)
Complex 1	3474	-498.00
Complex 2	4920	-516.71

**Table S4** HSA - metal complexes patch dock score.

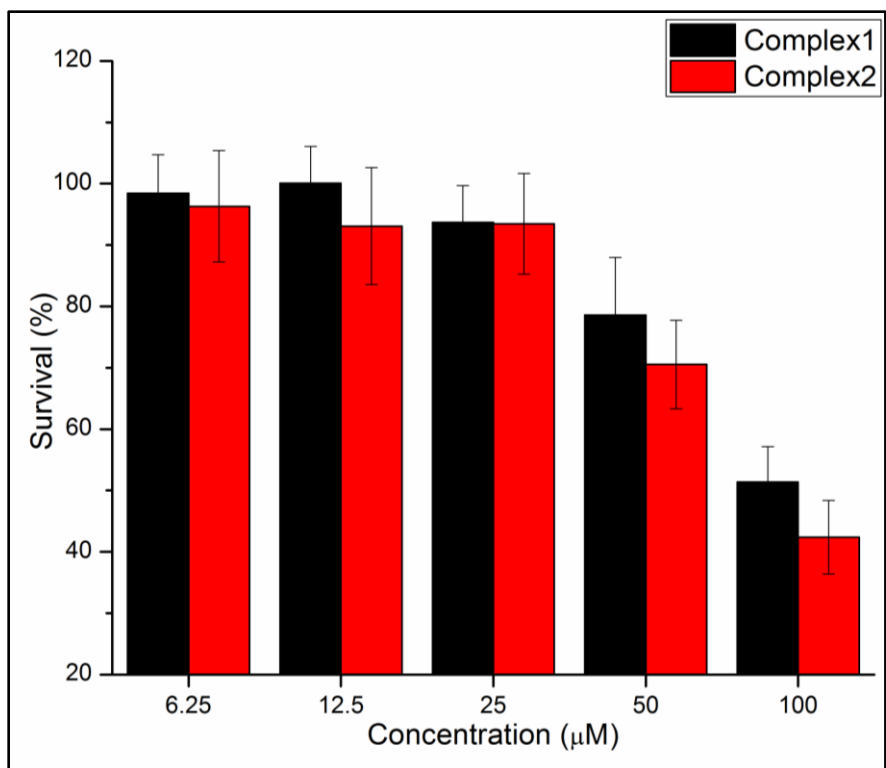
Complex	Patch Dock score	ACE (Kcal/mole)
Complex 1	7398	-61.88
Complex 2	5860	-41.17



**Fig. S14** MTT assay using cis-platin as Positive control on HeLa cell line (LD<sub>50</sub> = 18.67 ± 2.24 µM).



**Fig. S15** Cell viability of HeLa and PA1 cell line upon treatment with the Schiff base ligand (24 hrs).



**Fig. S16** Effect of complex 1 & 2 on Normal cell line (hEG) in a dose dependant manner.