Supporting Information

Syntheses, crystal structures, DNA binding, DNA cleavage and DFT study of Co(III) complexes involving azo appended Schiff base ligands

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CONTENTS:

Table S1. Mulliken charge distribution of complexes **1-3**.

1	**2**	**3**
1 Co 0.378817	1 Co 0.376428	1 Co 0.377869
2 O -0.566254	2 O -0.527782	2 O -0.531500
3 C 0.335974	3 O -0.491498	3 O -0.494055
4 C 0.304393	4 O -0.464516	4 O -0.474108
5 C -0.037245	5 O -0.528412	5 O -0.520834
7 C 0.220323	6 O -0.488221	6 O -0.493821
8 C -0.053657	7 O -0.497273	7 O -0.365940
10 C 0.033091	8 N -0.372988	8 N -0.382122
11 O -0.507009	9 N -0.189060	9 N -0.241730
12 C 0.315756	11 N -0.265872	10 N -0.266769
16 N -0.265253	12 N -0.266240	11 N -0.270949
17 N -0.271584	13 N -0.381019	12 N -0.381666
18 C 0.218687	14 N -0.188158	13 N -0.212701
19 C 0.004794	16 N -0.265617	14 N -0.262439
21 C -0.047335	17 N -0.260969	15 N -0.266635
23 C 0.131988	18 C 0.375014	16 C 0.369490
24 C -0.050298	19 C 0.313555	17 C 0.306367
26 C 0.024902	20 C -0.030026	18 C -0.025213
28 C 0.031700	22 C 0.232163	20 C 0.225898
32 C 0.221663	23 C -0.033868	21 C -0.038791
34 N -0.380935	25 C 0.068799	23 C 0.071109
35 C 0.242943	26 C 0.326801	24 C 0.321167
38 C -0.014239	30 C 0.266382	28 C 0.264419
39 C 0.042693	32 C 0.217029	30 C 0.212248
43 C 0.058692	35 C 0.291213	33 C 0.318249
47 C 0.228025	38 C 0.222370	36 C 0.232495
50 N 0.088697	41 C 0.296269	39 C 0.300408
53 O -0.566563	44 C 0.223039	42 C 0.218852
54 C 0.336067	45 C 0.013192	43 C 0.014222
55 C 0.304116	47 C 0.029559	45 C 0.021282
56 C -0.037117	49 C 0.045755	47 C 0.047834
58 C 0.220417	51 C 0.018269	49 C 0.010656
59 C -0.053180	53 C 0.033287	51 C 0.035121
61 C 0.032730	55 C 0.369330	53 C 0.367677
62 O -0.506911	56 C 0.317870	54 C 0.313643
63 C 0.315872	57 C -0.022060	55 C -0.017844
67 N -0.265256	59 C 0.225524	57 C 0.219548

68 N -0.271604 69 C 0.219015 70 C 0.004590 72 C -0.047038 74 C 0.131715 75 C -0.050127 77 C 0.024583 79 C 0.031698 83 C 0.221886 85 N -0.380785 86 C 0.242708 89 C -0.014061 90 C 0.042589 94 C 0.058715 98 C 0.228075 101 N 0.088538 Sum of Mulliken charges with hydrogens summed into heavy atoms = 1.00000	60 C -0.030941 62 C 0.056760 63 C 0.331253 67 C 0.257261 69 C 0.218435 72 C 0.293984 75 C 0.209981 78 C 0.314293 81 C 0.222630 82 C 0.020272 84 C 0.018357 86 C 0.050703 88 C 0.013778 90 C 0.034965 Sum of Mulliken charges with hydrogens summed into heavy atoms = 1.00000	58 C -0.035758 60 C 0.055204 61 C 0.326826 65 C 0.256260 67 C 0.229803 70 C 0.281852 73 C 0.280771 76 C 0.253624 77 C 0.224187 78 C 0.015593 80 C 0.018965 82 C 0.047166 84 C 0.011666 86 C 0.032402 Sum of Mulliken charges with hydrogens summed into heavy atoms = 1.00000

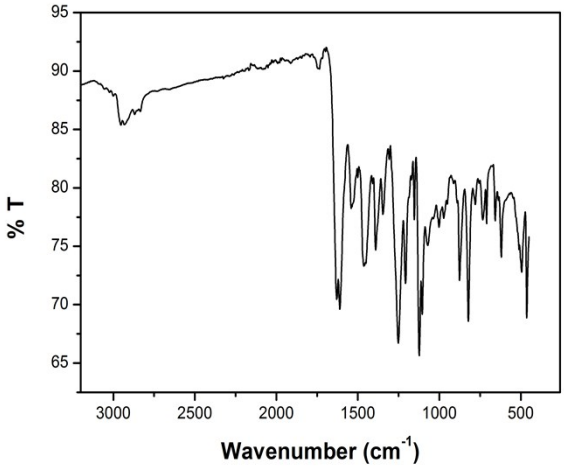

Fig. S1. FTIR spectrum of ligand **HL[1]**.

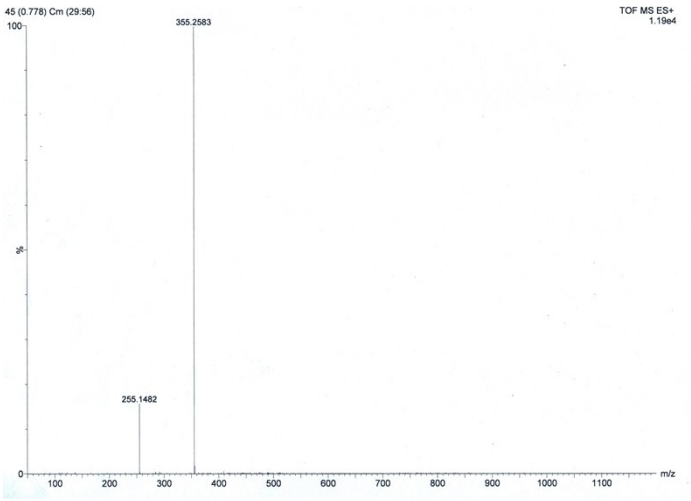

Fig. S2. ESI-MS spectrum of ligand **HL[1]**.

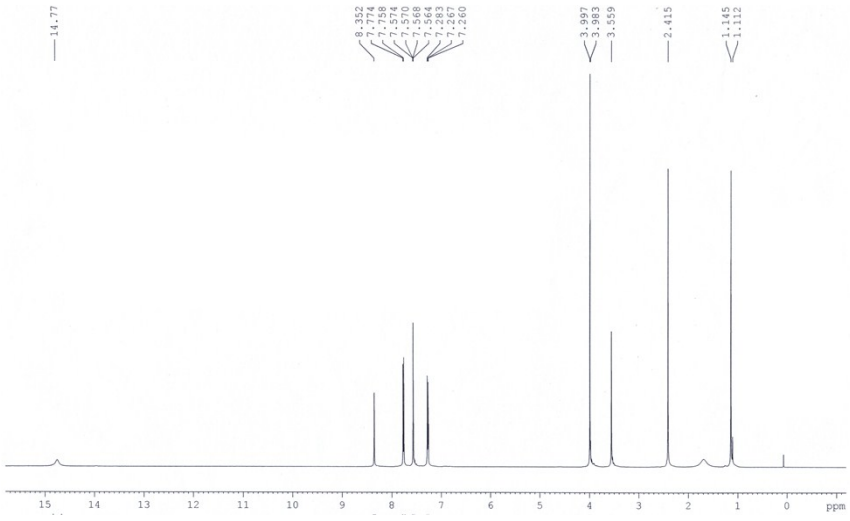

Fig. S3. [1]HNMR Spectrum of ligand **HL[1]**.

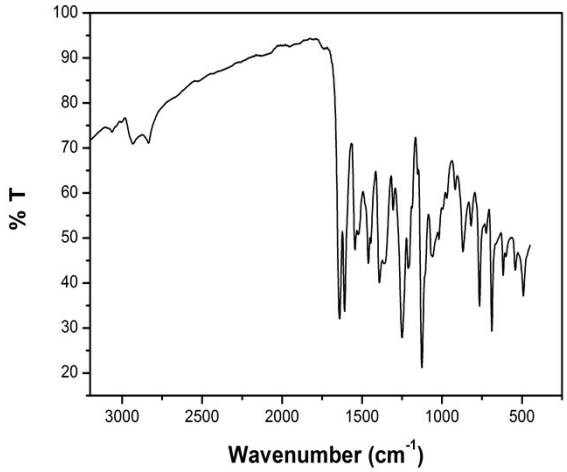

Fig. S4. FTIR spectrum of ligand **HL²**.

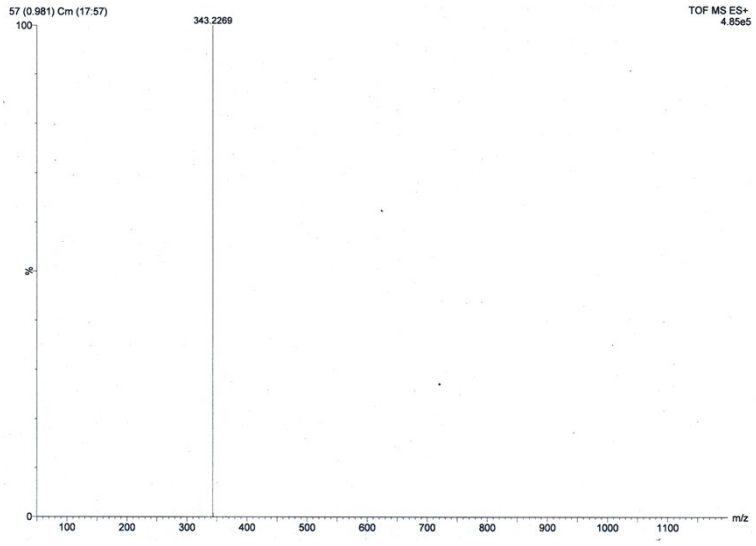

Fig. S5. ESI-MS spectrum of ligand **HL²**.

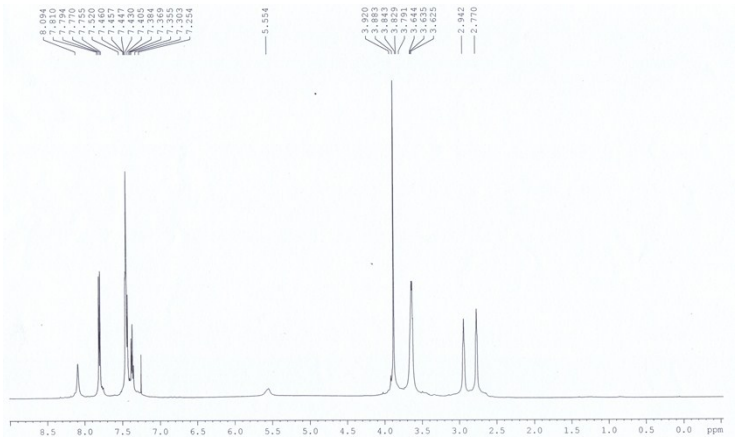

Fig. S6. [1]HNMR Spectrum of ligand **HL²**.

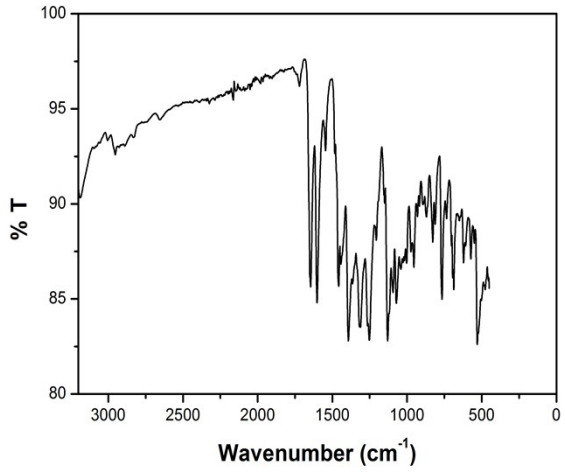

Fig. S7. FTIR spectrum of complex **1.**

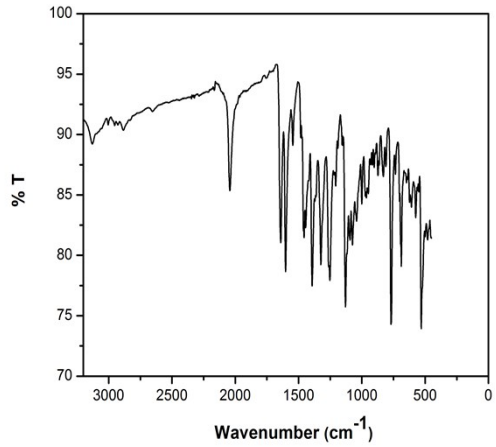

Fig. S8. FTIR spectrum of complex **2**.

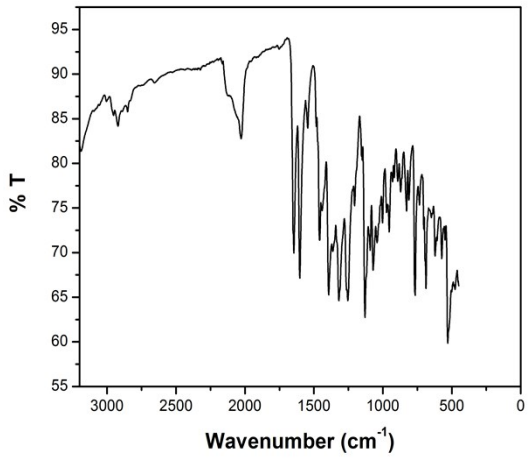

Fig. S9. FTIR spectrum of complex **3**.

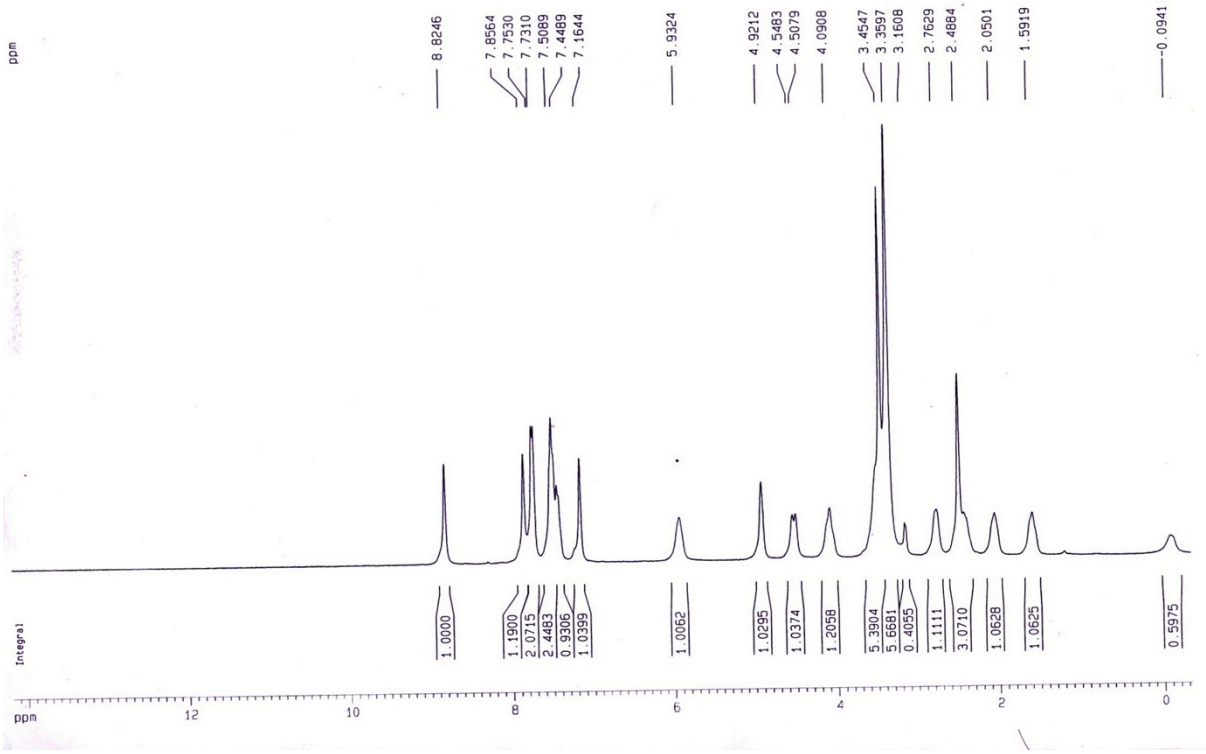

Fig. S10. [1]HNMR Spectrum of complex **3**.

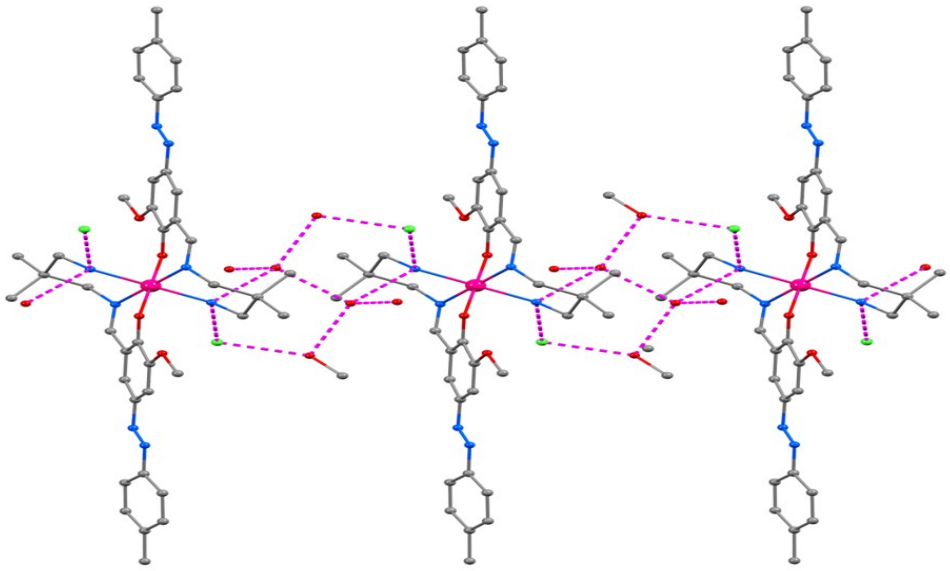

Fig. S11. 1D supramolecular architecture of complex **1** propagating along the *b* axis showing H-bonding interactions. Hydrogen atoms of least interest are omitted for clarity.

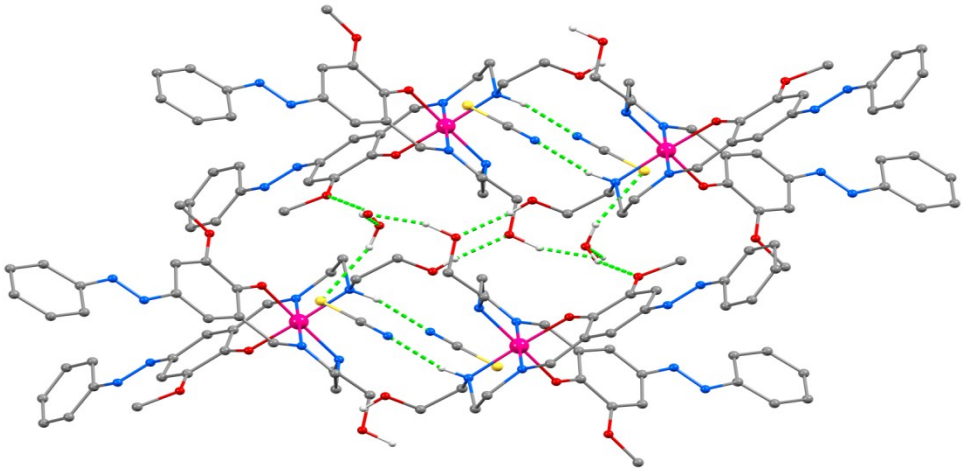

Fig. S12. 1D supramolecular architecture of complex **2** propagating along the *a* axis showing H-bonding interaction. Hydrogen atoms of least interest are omitted for clarity

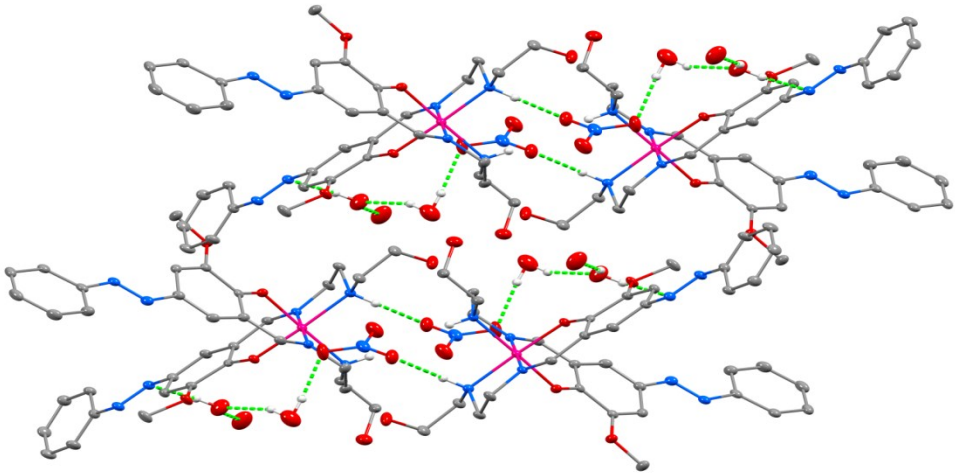

Fig. S13. 1D supramolecular architecture of complex **3** propagating along the *b* axis showing H-bonding interaction. Hydrogen atoms of least interest are omitted for clarity.

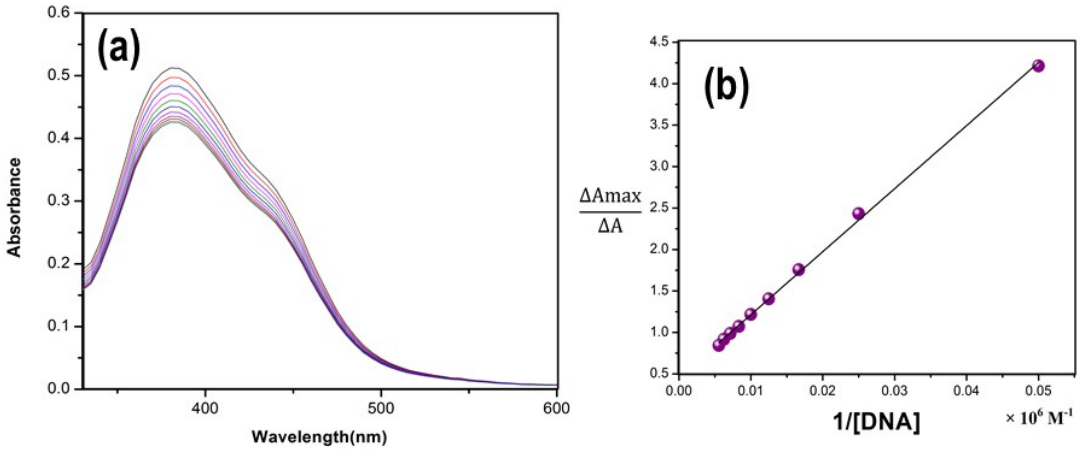

Fig. S14. (a) UV-vis spectra of 2×10^{-5} (M) complex **2** with incremental addition of CT-DNA (0-15 eq.); (b) Benesi Hildebrand equation for**.**

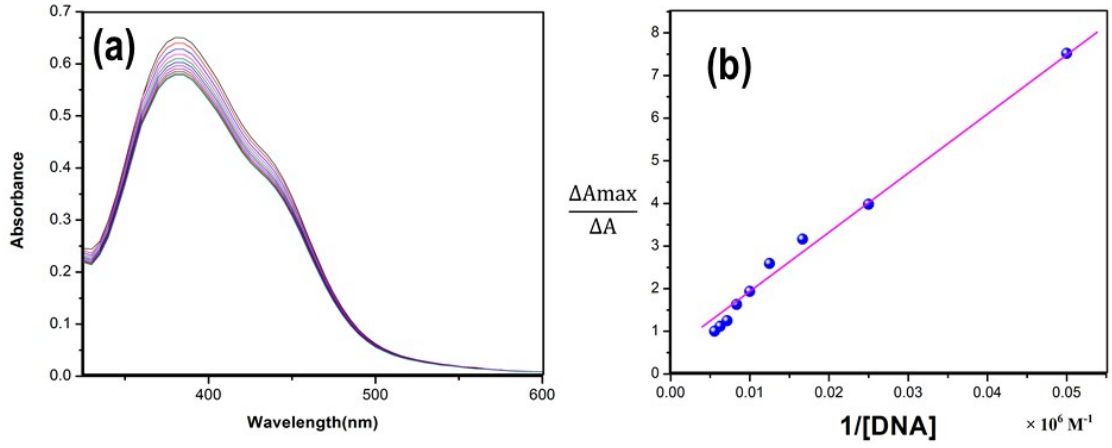

Fig. S15. (a) UV-vis spectra of 2×10^{-5} (M) complex **3** with incremental addition of CT-DNA (0-15 eq.); (b) Benesi Hildebrand equation for**.**

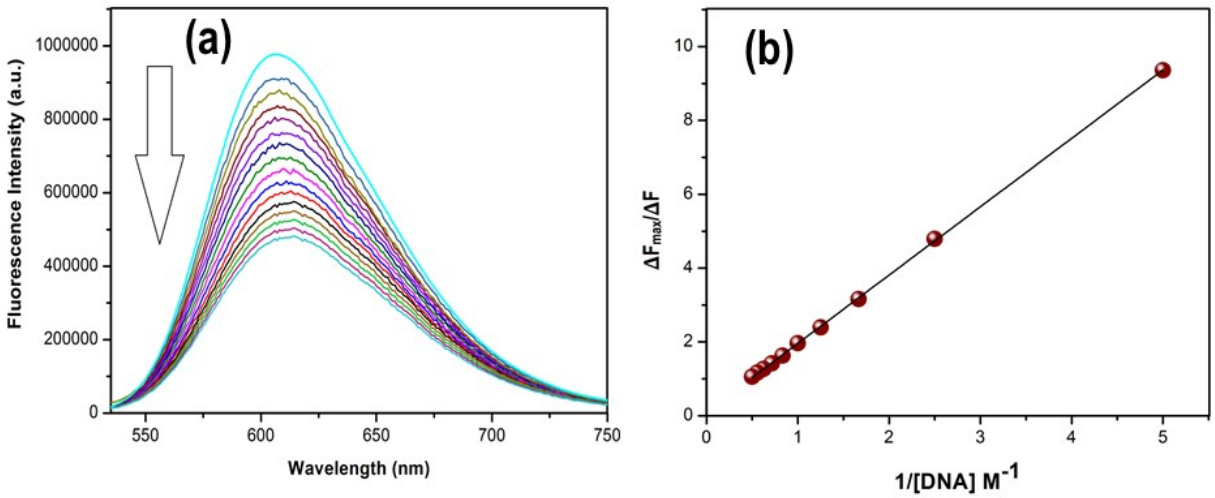

Fig. S16. Fluorescence spectra of a) 20 μM EB bound DNA with incremental addition of complex **2** (0-180 μM). b) Stern-Volmer plot for the quenching of fluorescence of Ethidium bromide (EB)-DNA complex caused by complex **2**.

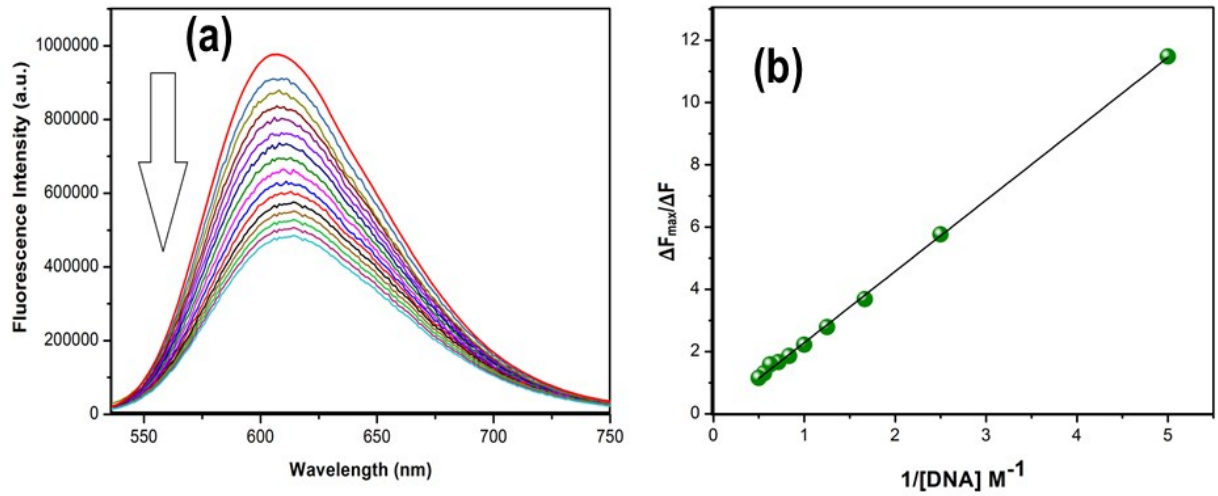

Fig. S17. Fluorescence spectra of a) 20 μM EB bound DNA with incremental addition of complex **3** (0-180 μM). b) Stern-Volmer plot for the quenching of fluorescence of Ethidium bromide (EB)-DNA complex caused by complex **3**.

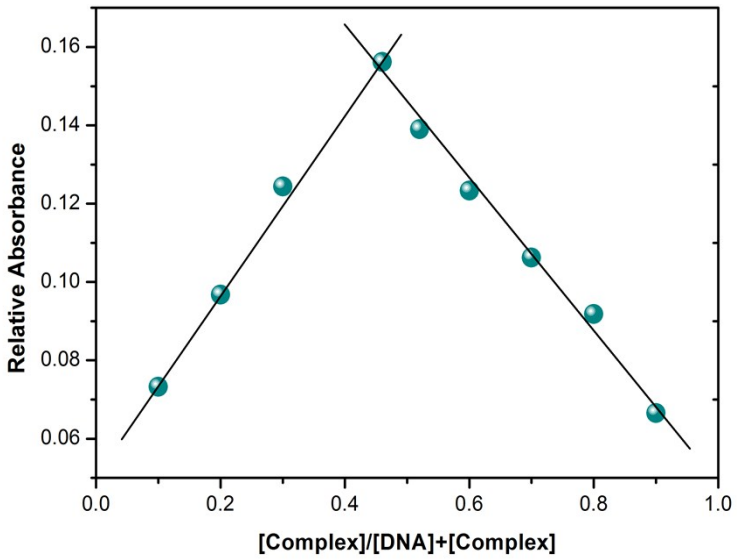

Fig. S18. Job's plot of complex **1**.

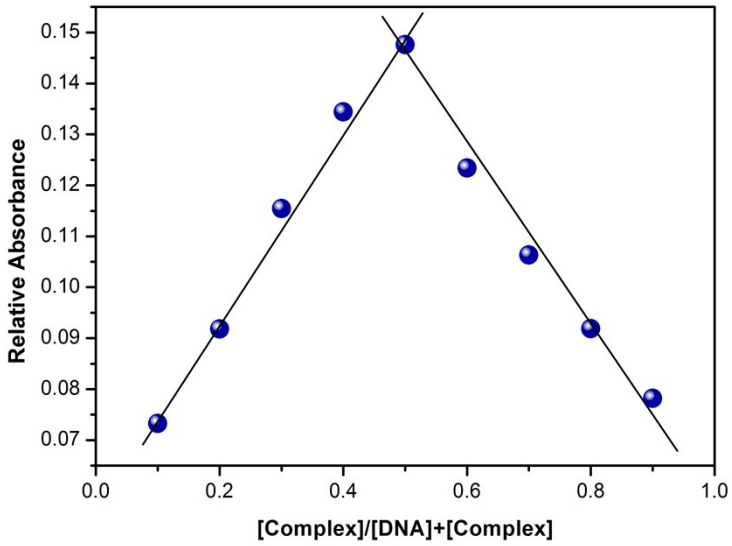

Fig. S19. Job's plot of complex **2**.

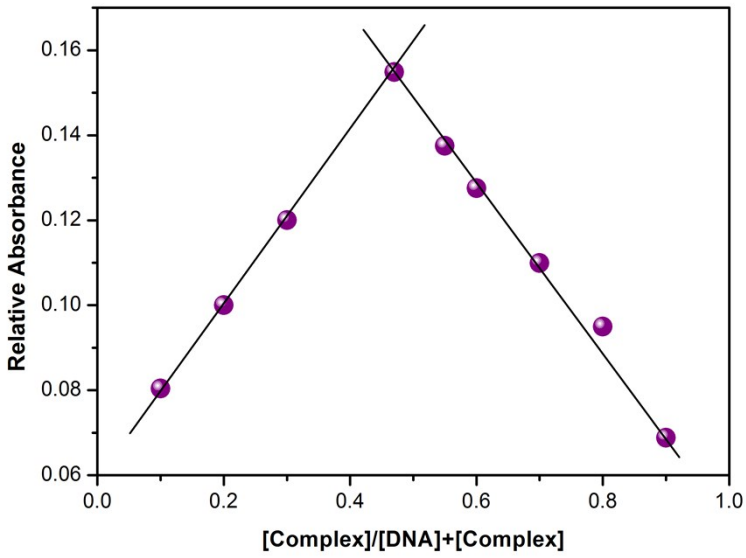

Fig. S20. Job's plot of complex **3**.

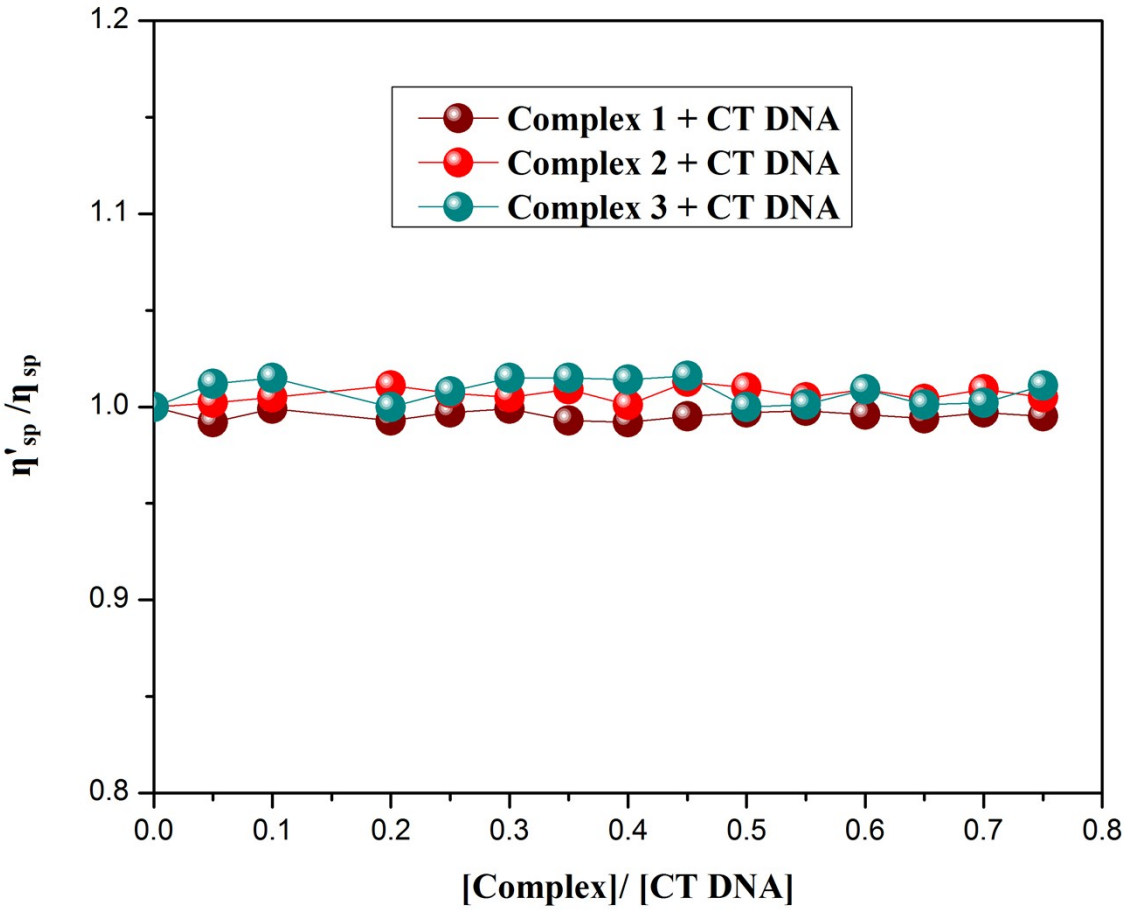

Fig. S21. Relative specific viscosity measurements of complex **1-3** in presence of CT DNA.

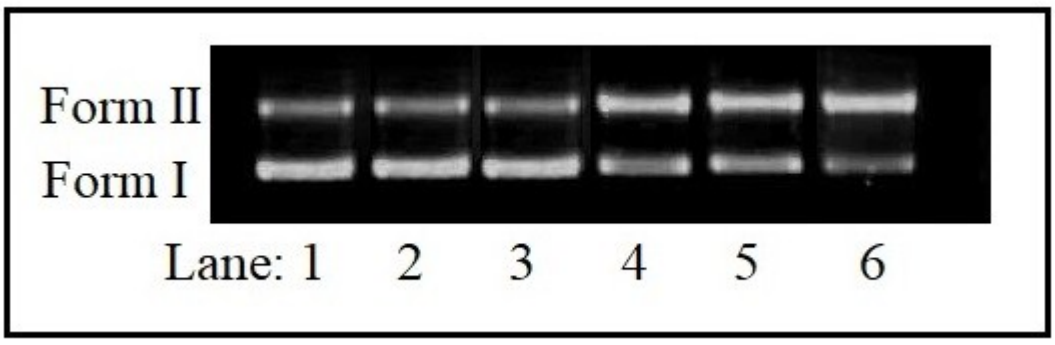

Fig. S22. Gel electrophoresis diagram showing DNA cleavage activity of the complex **2**. pUC19 plasmid DNA was incubated with increasing concentration of **2** for 1.5 h at 37 °C in 10 mM Tris-HCl, pH 7.2. Lane 1: pUC19 plasmid DNA + buffer, Lane 2: pUC19 plasmid

DNA + buffer + N,N-dimethylformamide (DMF), Lane 3: pUC19 plasmid DNA + buffer + 200μM H_2O_2, Lane 4-6: pUC19 plasmid DNA + buffer + 200μM H_2O_2 + complex **2** with concentrations 25, 50, 75 μM, respectively.

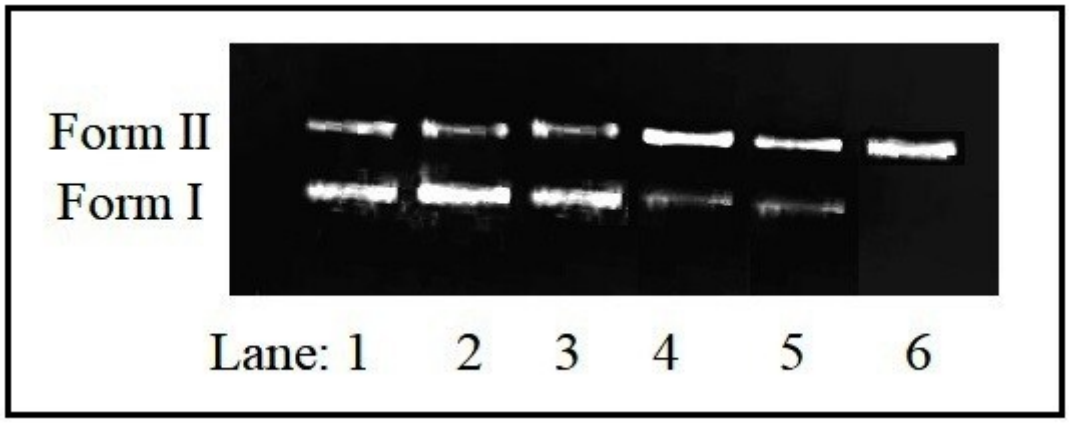

Fig. S23. Gel electrophoresis diagram showing DNA cleavage activity of the complex **3**. pUC19 plasmid DNA was incubated with increasing concentration of **3** for 1.5 h at 37 °C in 10 mM Tris-HCl, pH 7.2. Lane 1: pUC19 plasmid DNA + buffer, Lane 2: pUC19 plasmid DNA + buffer + N,N-dimethylformamide (DMF), Lane 3: pUC19 plasmid DNA + buffer + 200μM H_2O_2, Lane 4-6: pUC19 plasmid DNA + buffer + 200μM H_2O_2 + complex **3** with concentrations 25, 50, 75 μM, respectively.