

Supplementary Information

Synthesis and characterization of Co(II) and Fe(II) peptide conjugates as hydrolytic cleaving agents and their preferential enantiomeric disposition for CT-DNA: Structural investigation of L-enantiomers by DFT and molecular docking studies.

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Complex L-1 Bond	Bond length	Complex L-2 Bond	Bond length
O(9)–Co(25)	1.77012	O(9)–Fe(25)	1.747
N(10)–Co(25)	1.97694	N(10)–Fe(25)	2.001
Co(25)–O(26)	1.86435	Fe(25)–O(26)	1.857
Co(25)–N(35)	1.86435	Fe(25)–N(35)	1.796
Co(25)–O(50)	2.0724	Fe(25)–O(50)	2.097
Co(25)–O(51)	2.02395	Fe(25)–O(51)	2.127

Table. S1 Selected bond lengths for complexes L-1 and L-2.

Complex L-1 Bond	Bond angle	Complex L-2 Bond	Bond angle
N(10)–Co(25)–O(50)	92.5050	N(10)–Fe(25)–O(50)	89.6601
O(50)–Co(25)–O(26)	80.6012	O(50)–Fe(25)–O(26)	82.8500
O(26)–Co(25)–N(35)	87.2324	O(26)–Fe(25)–N(35)	87.0918
N(35)–Co(25)–N(10)	100.1184	N(35)–Fe(25)–N(10)	100.4485
N(10)–Co(25)–O(51)	91.27995	N(10)–Fe(25)–O(51)	90.1809
O(51)–Co(25)–N(35)	58.872	O(51)–Fe(25)–N(25)	91.7278
O(51)–Co(25)–O(26)	90.8479	O(51)–Fe(25)–O(26)	88.9407
O(51)–Co(25)–O(50)	78.7635	O(51)–Fe(25)–O(50)	75.0981
O(51)–Co(25)–O(9)	169.0894	O(51)–Fe(25)–O(9)	165.2265
O(50)–Co(25)–N(35)	164.869	O(50)–Fe(25)–N(35)	163.5028
O(26)–Co(25)–N(10)	172.246	O(26)–Fe(25)–N(10)	172.4323
O(9)–Co(25)–O(50)	90.616	O(9)–Fe(25)–O(50)	90.6419
O(9)–Co(25)–O(26)	89.859	O(9)–Fe(25)–O(26)	93.1555
O(9)–Co(25)–N(35)	98.362	O(9)–Fe(25)–N(35)	102.9781

Table. S2 Selected bond angles for complexes L-1 and L-2.

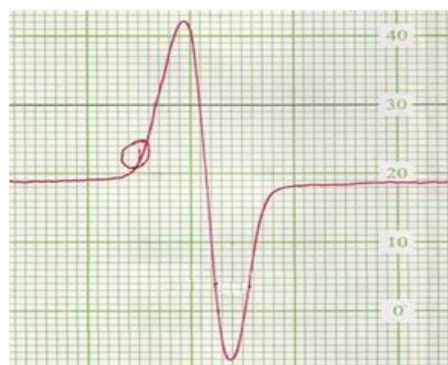


Fig. S1 EPR spectra of **L-1** at 300 K in DMSO solution.

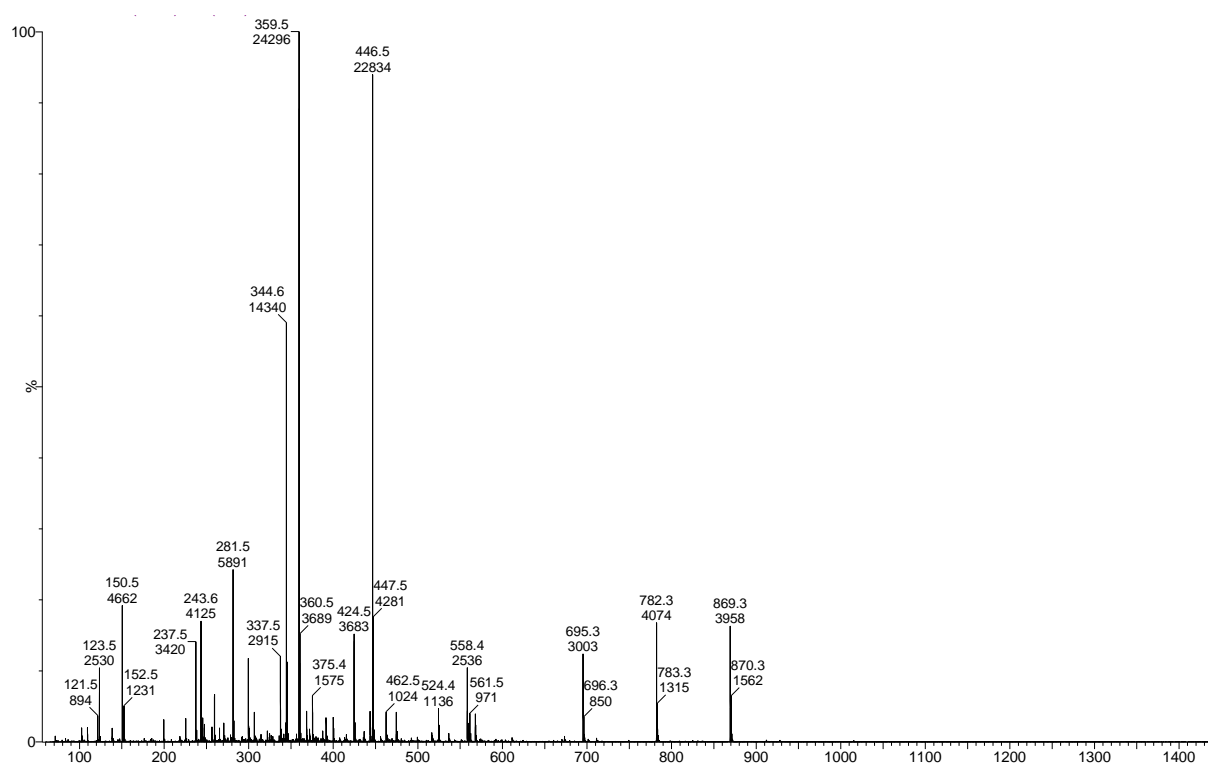


Fig. S2(i) ESI-Mass spectra of complex **L-1**.

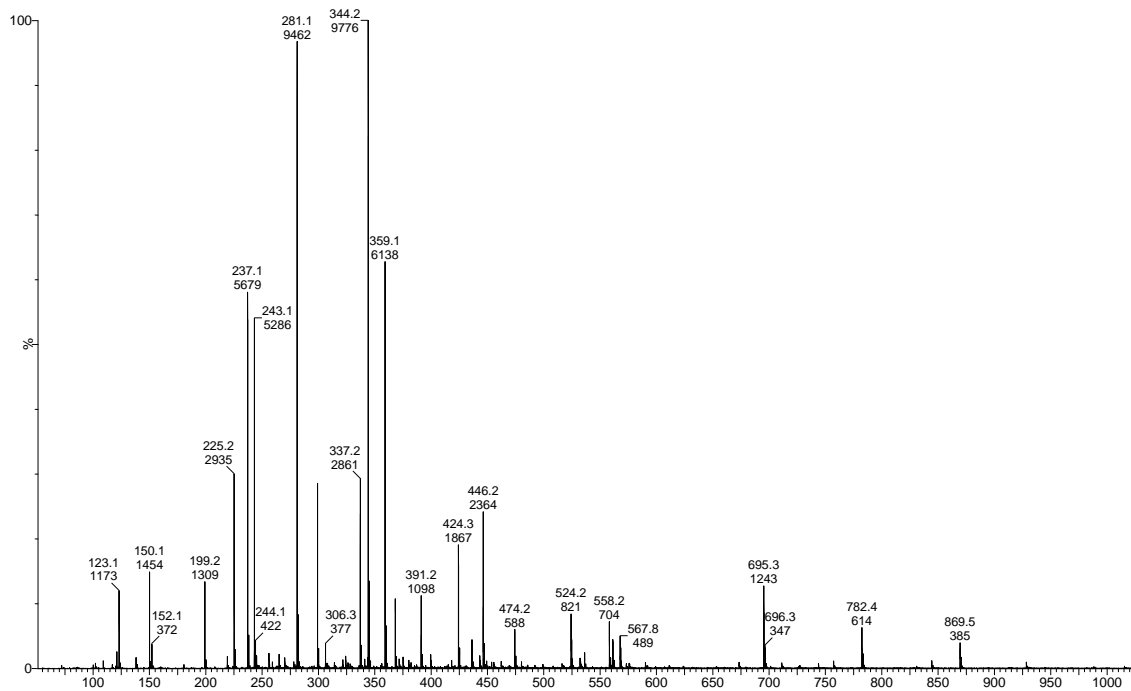


Fig. S2(ii) ESI-Mass spectra of complex D-1.

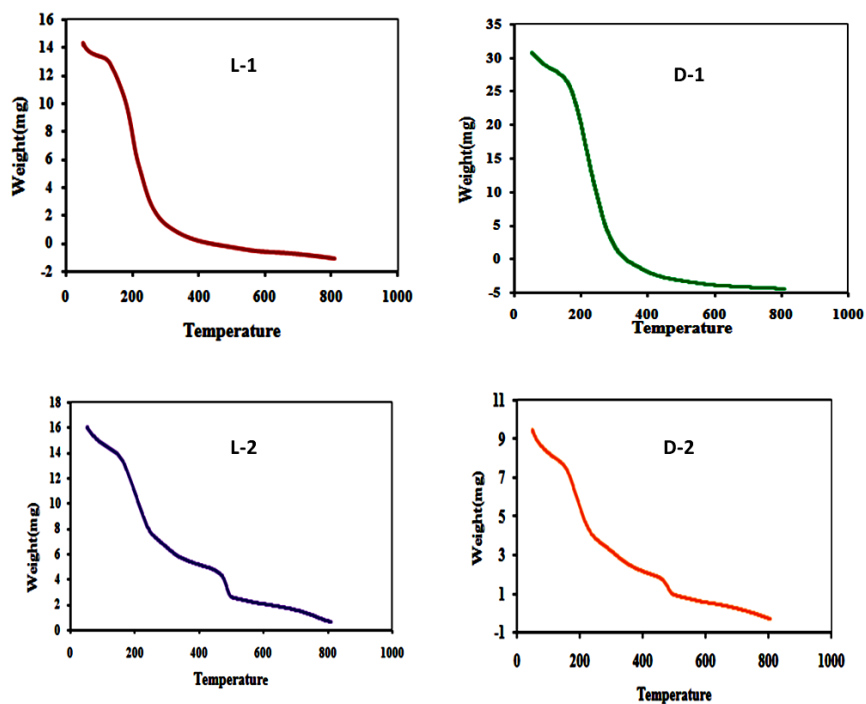


Fig. S3 TGA profile for complexes L/D-1 and 2.

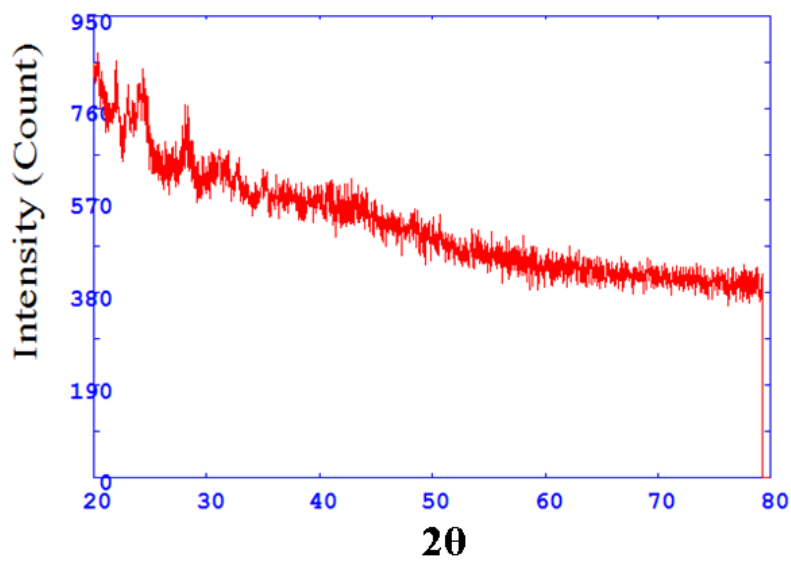


Fig. S4 X-ray diffraction pattern of complex **L-1**.

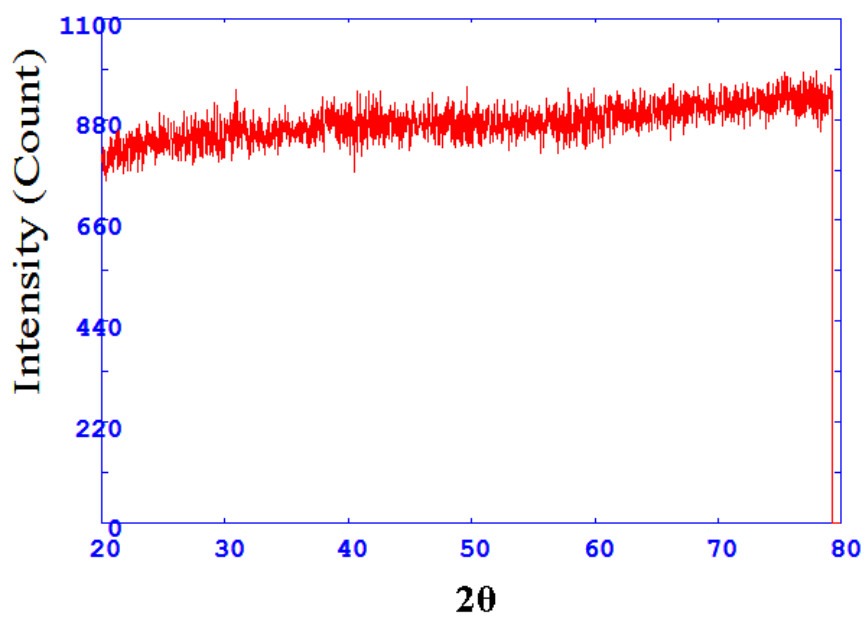


Fig. S5 X-ray diffraction pattern of complex **L-2**.

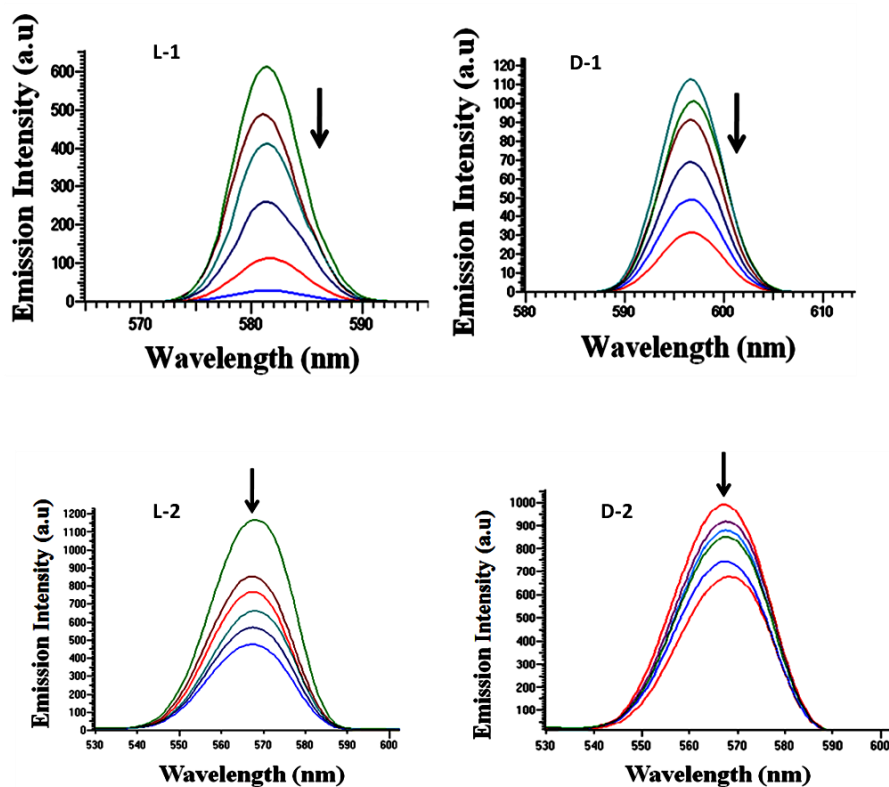


Fig. S6 Fluorescence emission spectra of the EB–CT–DNA system in the absence and presence of complexes **L/D-1** and **2** at 25°C. [Complex], [EB], [DNA]= 10^{-5} M.

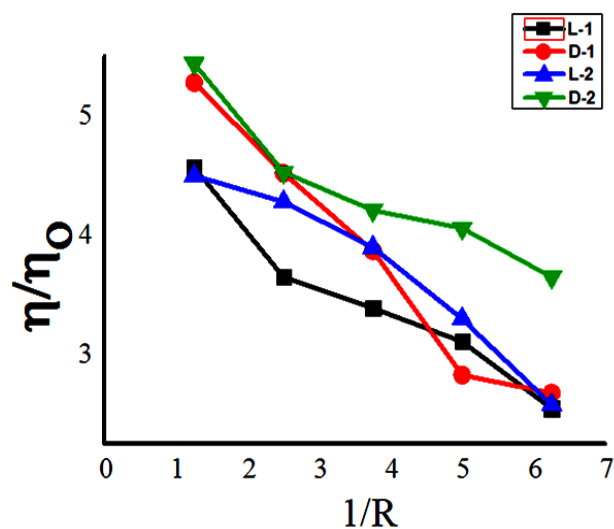
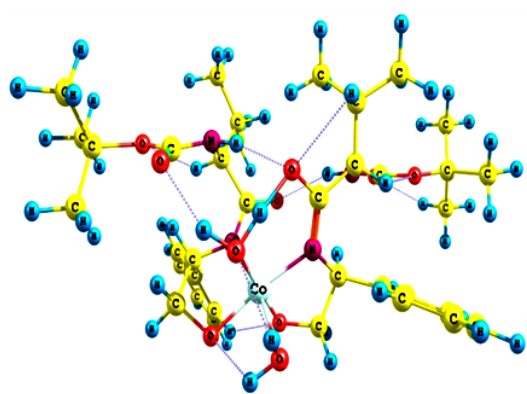
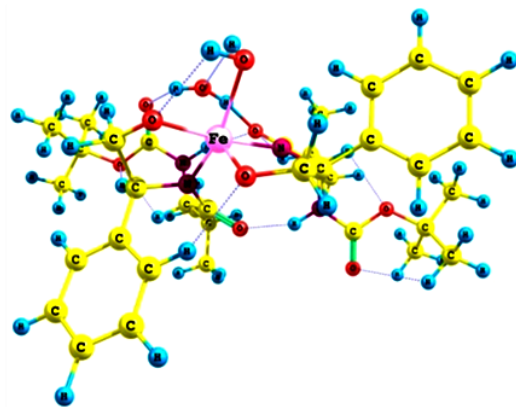


Fig. S7 Effect of increasing amounts of complexes **L/D-1** and **2** on the relative viscosity (η/η_0) of DNA in Tris–HCl buffer (pH 7.2).

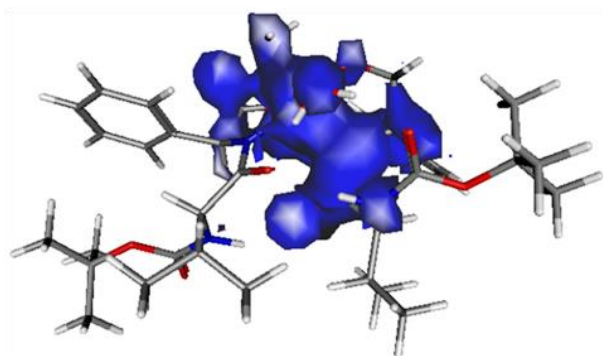


L-1

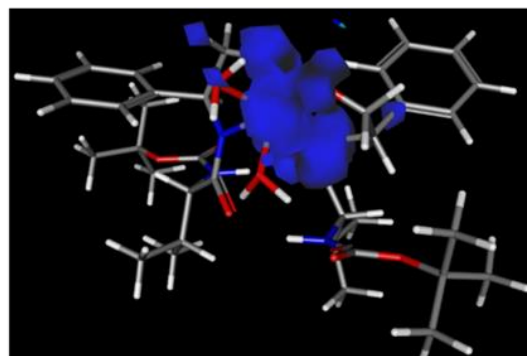


L-2

Fig. S8 DFT optimized structure of complexes **L-1** and **L-2**.



L-1



L-2

Fig. S9 3-D isodensity surface of Fukai MO nucleophilic susceptibility of **L-1** and **L-2**.