Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

A rare dihydroxo copper(II) complex with ciprofloxacin; a combined experimental and ONIOM computational study of the interaction of the complex with DNA and BSA

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Table. S1. The DNA binding constants and parameters derived for ciprofloxacin and the Cu(II) complex.

	compound	K_{vs} M($^{-1}$)	K_q M($^{-1}s^{-1}$)	K_b M($^{-1}$)	n	Ref
DNA	Ciprofloxacin	1.09×10^4	1.09×10^{12}	3.98×10^4	1.12	1
	Cu(II) complex	1.2×10^4	1.2×10^{12}	1.17×10^4	0.88	work this

Table. S2. The BSA binding constants and parameters derived for ciprofloxacin and the Cu(II) complex.

	compound	K_{vs} M($^{-1}$)	K_q M($^{-1}s^{-1}$)	K_b M($^{-1}$)	n	Ref
BSA	Ciprofloxacin	2.33×10^4	2.33×10^{12}	2.17×10^4	0.91	2
	Cu(II) complex	6.38×10^4	6.38×10^{12}	4.08×10^4	0.97	work this

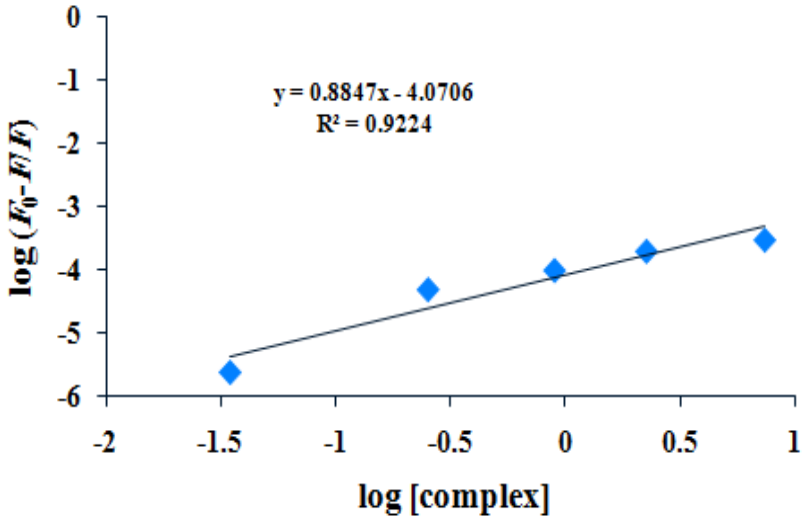

Fig. S1 Plot of log (F_0 – F)/F) *versus* log [complex].

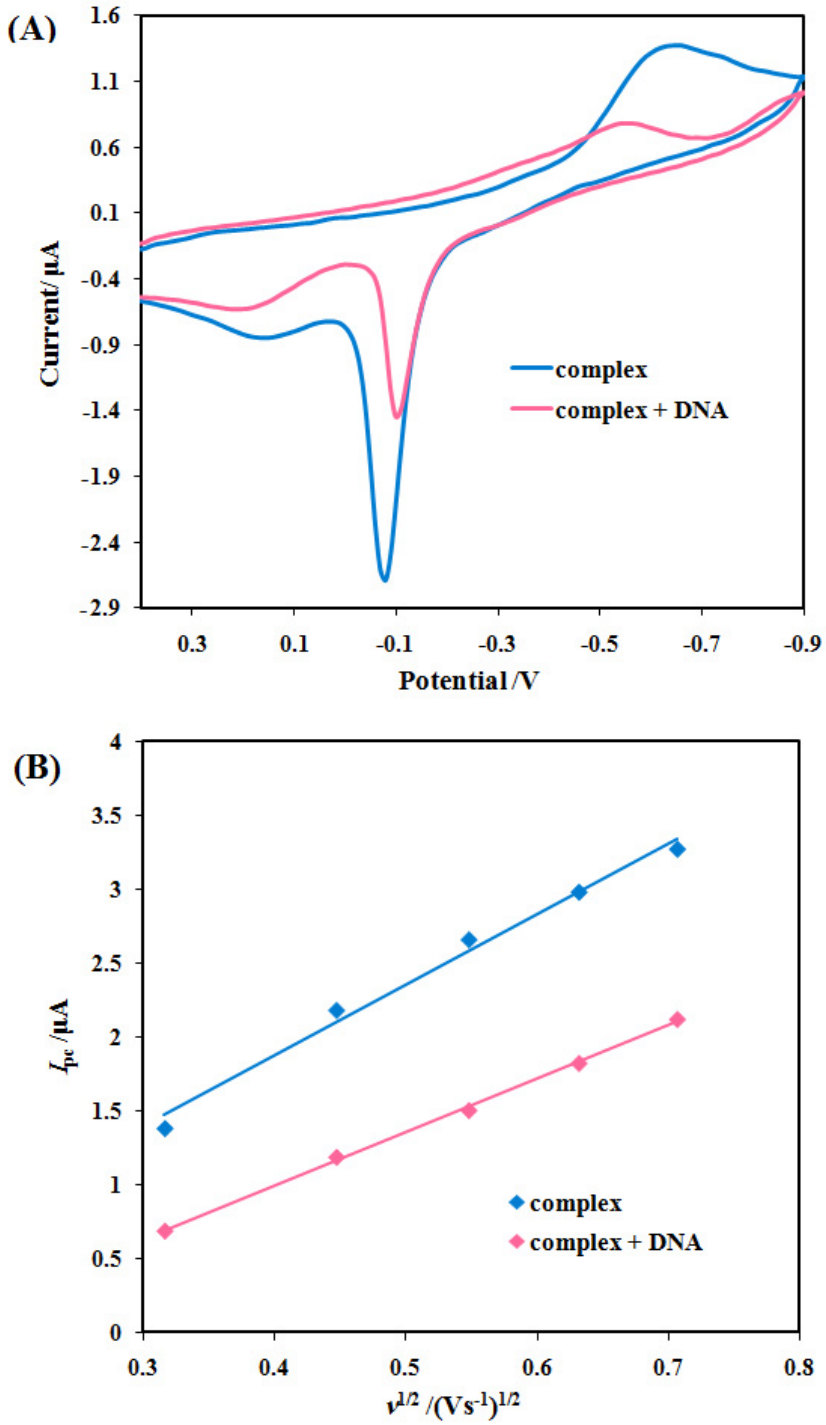

Fig. S2 (A) Cyclic voltammograms of 1.0×10^{-3} M of the *trans*-$[Cu(cip)_2(OH)_2]\cdot 2CH_3OH\cdot 6H_2O$ in the absence and presence of CT-DNA (scan rate = 0.1 V/s). (B) The plots of the cathodic peak currents of the complex in the absence and presence of CT-DNA versus the square root of the scan rates ($v^{1/2}$).

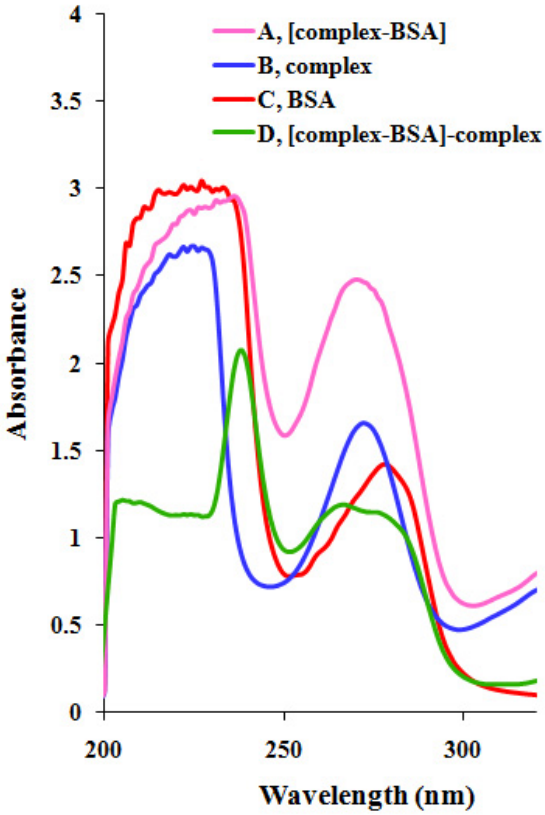

Fig. S3 Electronic absorption spectra of BSA in the presence of the Cu(II) complex. (A) (pink) The absorption spectra of BSA-complex system when the mol ratio is 1:1; (B) (blue) the absorption spectra complex only; (C) (red) the absorption spectra of BSA only; (D) (green) the difference absorption spectra between the BSA-complex and the complex at the same concentration.

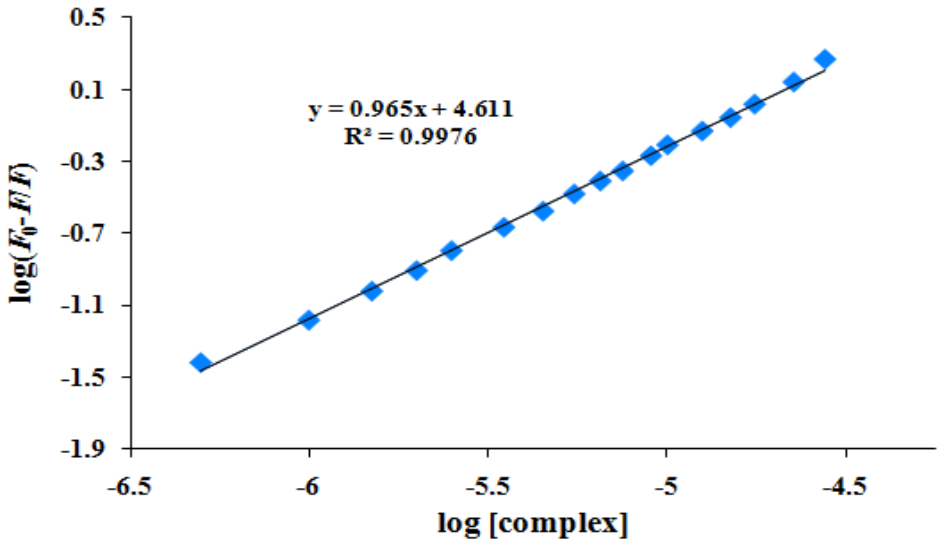

Fig. S4 Determination of the complex-BSA binding constant and the number of binding sites on BSA.

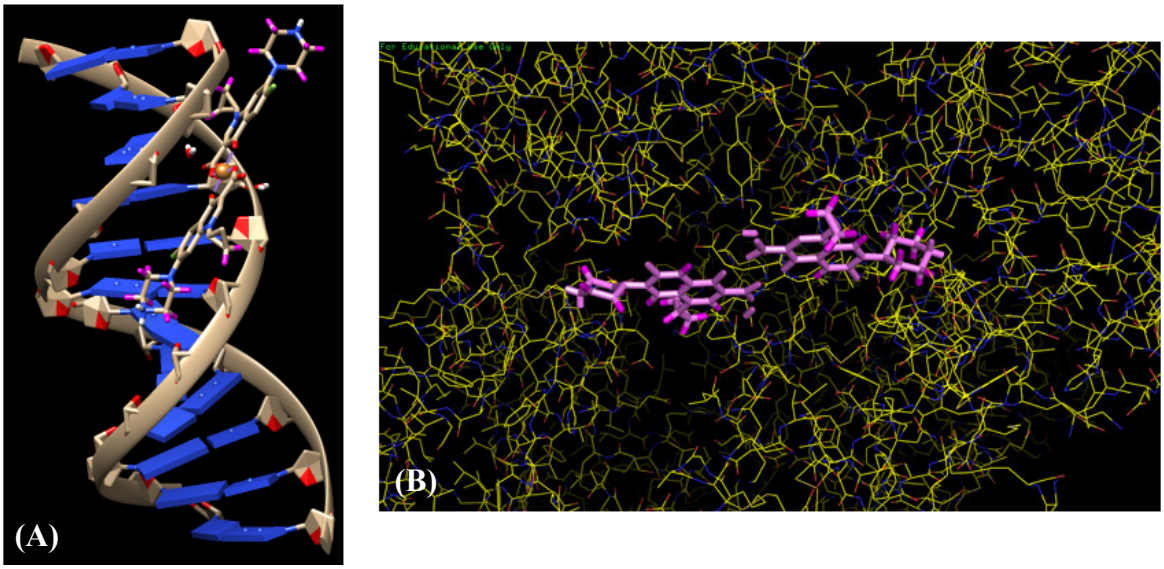

Fig. S5 Molecular docking of the complex with DNA (A) and BSA (B).

References

1 L. Fotouhi, Z. Atoofi and M. M. Heravi, *Talanta*., 2013, **103**, 194–200.

2 Y.J. Hu, Y. Ou-Yang, Y. Zhang and Y. Liu, *Protein J*., 2010, **29,** 234–241.