

## Supporting Information

### **DNA/BSA binding, DNA cleavage and electrochemical properties of new multidentate copper(II) complexes**

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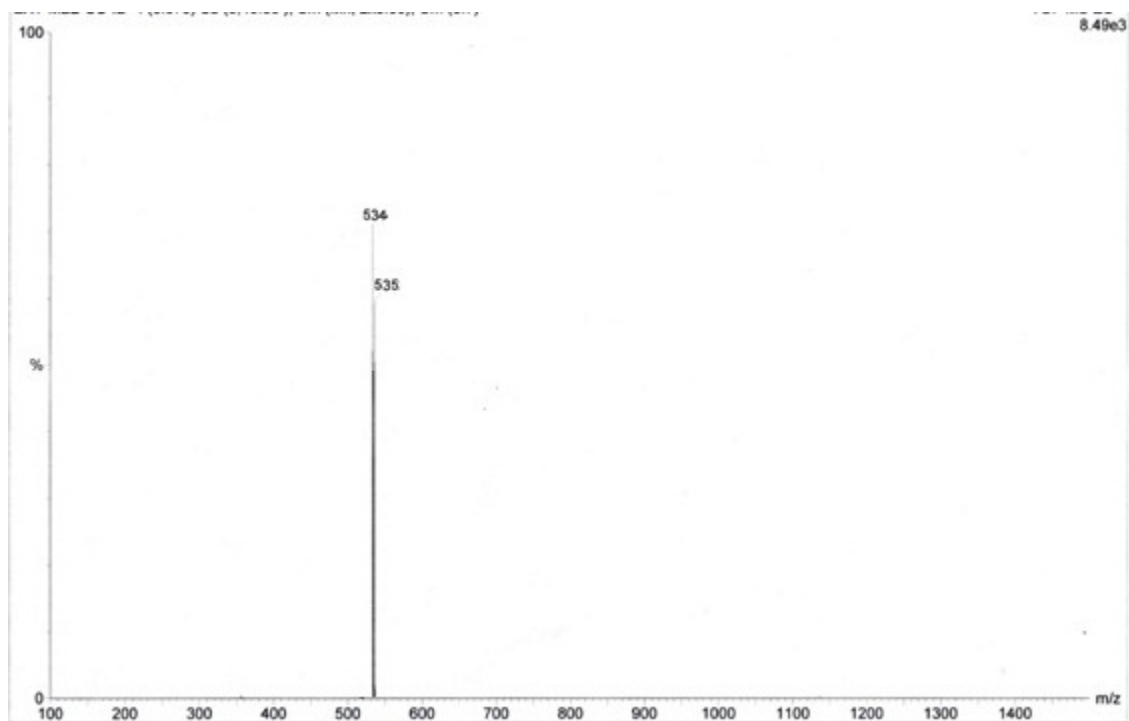
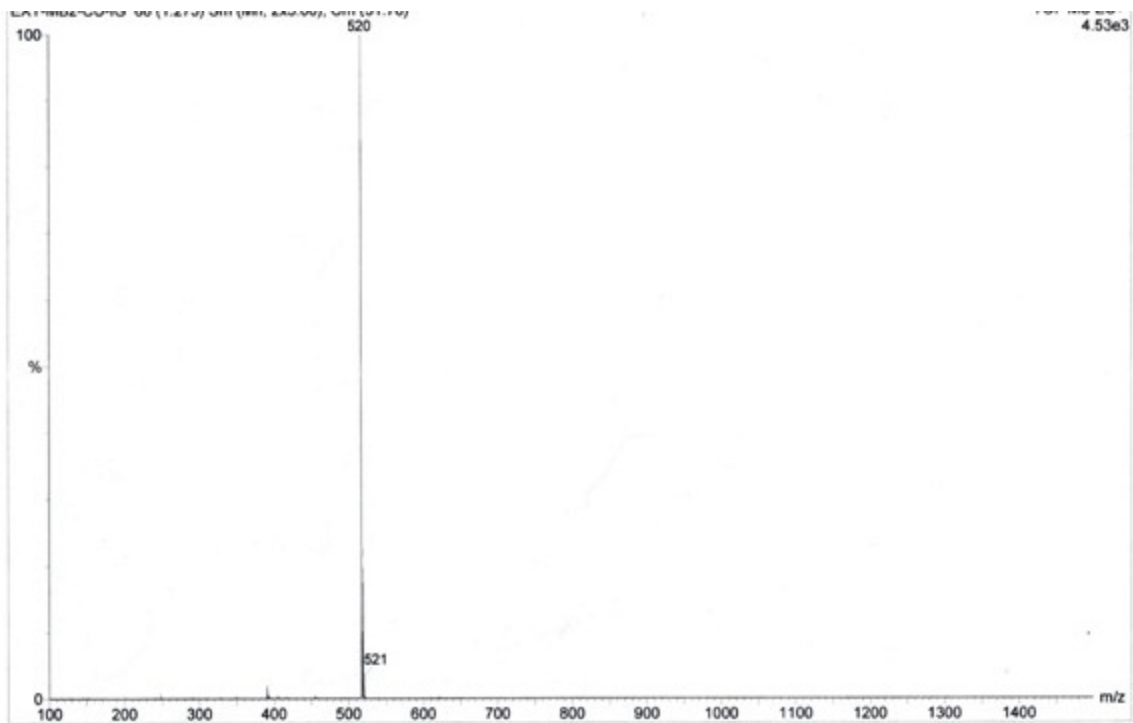


Fig. S1. ESI-MS spectrum of mono nuclear complexes (1) and (2)

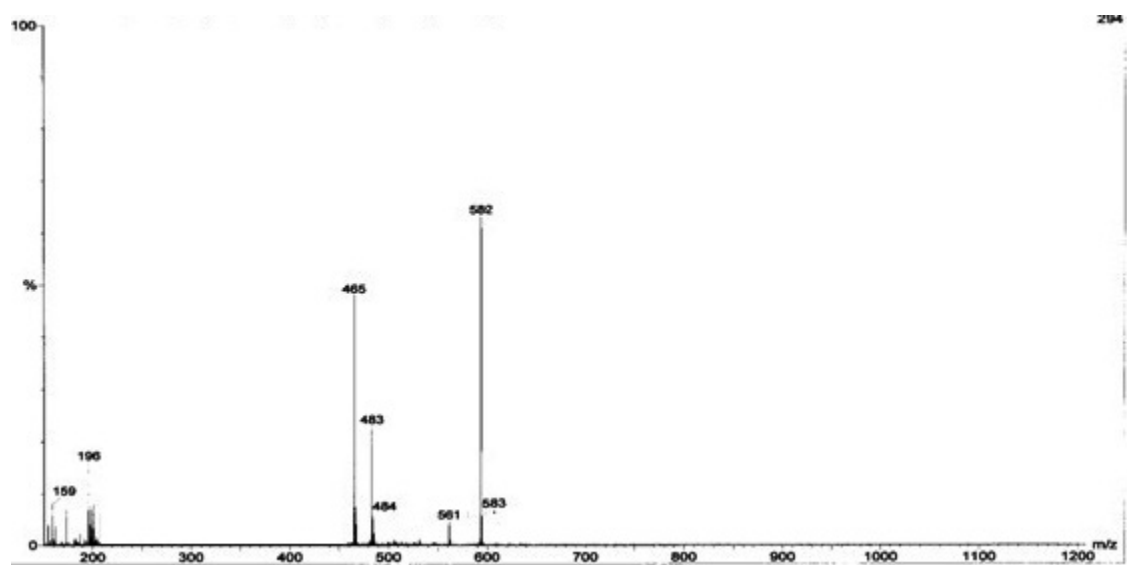
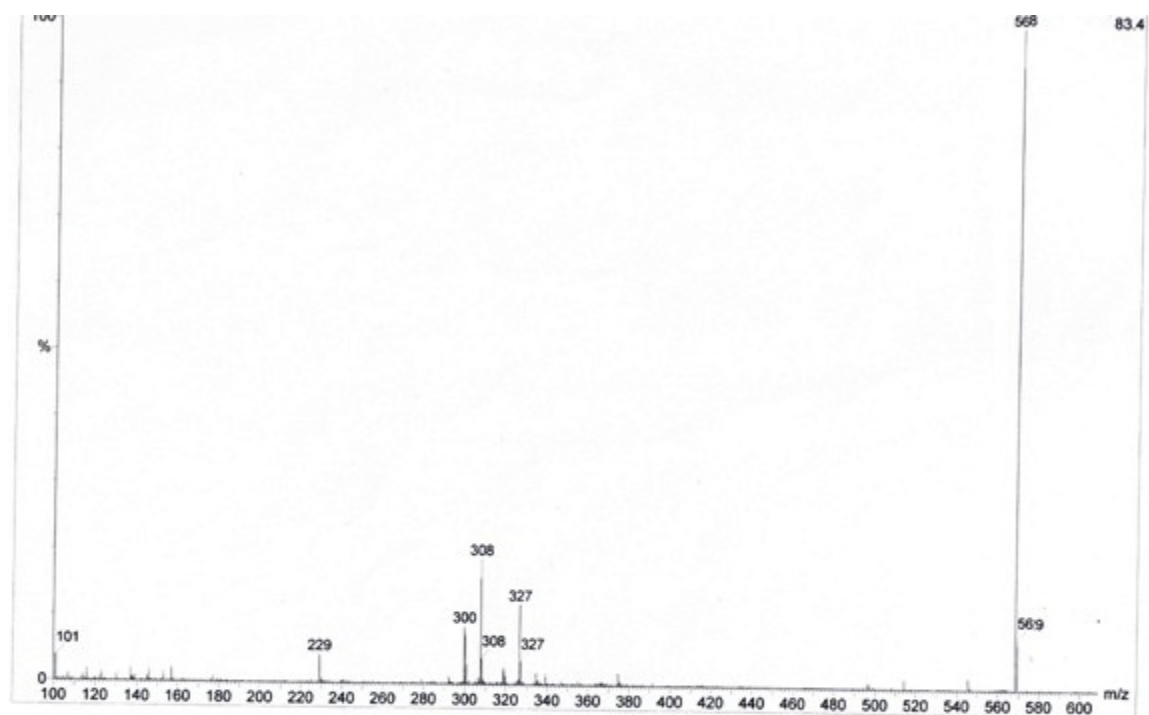


Fig. S1. ESI-MS spectrum of mono nuclear complexes (3) and (5)

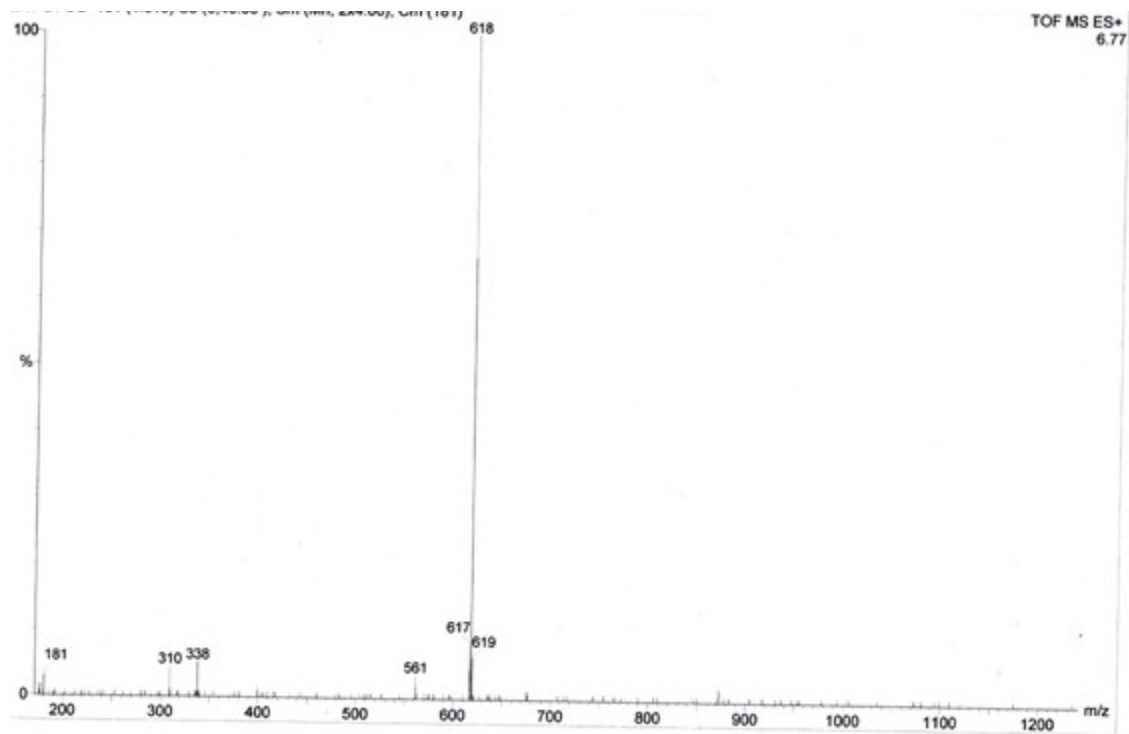


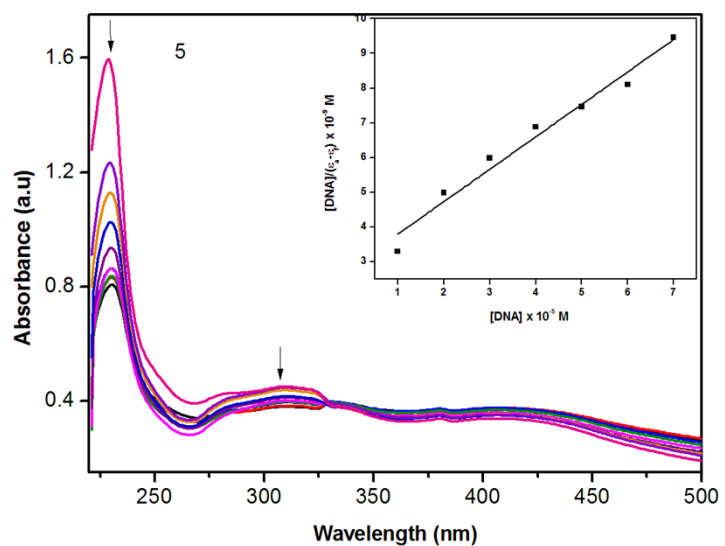
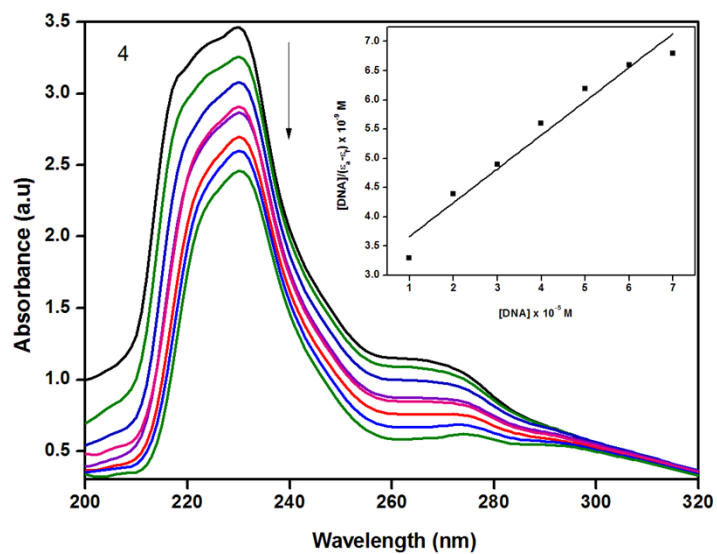
Fig. S1. ESI-MS spectrum of mono nuclear complex (5)

Table S1. Hydrogen bonds for complex 1 [A and deg.].

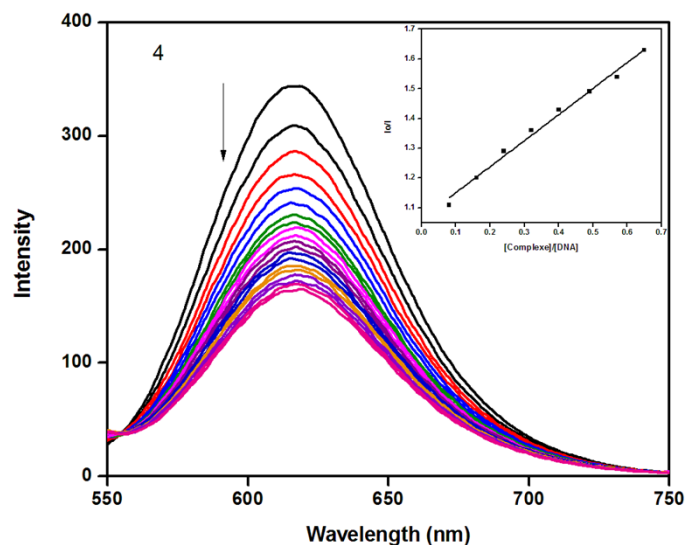
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D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(4)-H(4A)...O(2)	0.849(18)	1.95(3)	2.620(4)	135(3)
C(4)-H(4)...O(6)#1	0.93	2.61	3.261(12)	127.7
C(7)-H(7)...O(4)#2	0.93	2.29	3.218(8)	173.1
C(18)-H(18A)...O(6)#3	0.97	2.75	3.622(14)	149.7
C(14)-H(14)...O(5)#3	0.93	2.49	3.216(9)	135.1
C(17)-H(17A)...O(4)	0.97	2.57	3.470(9)	154.2

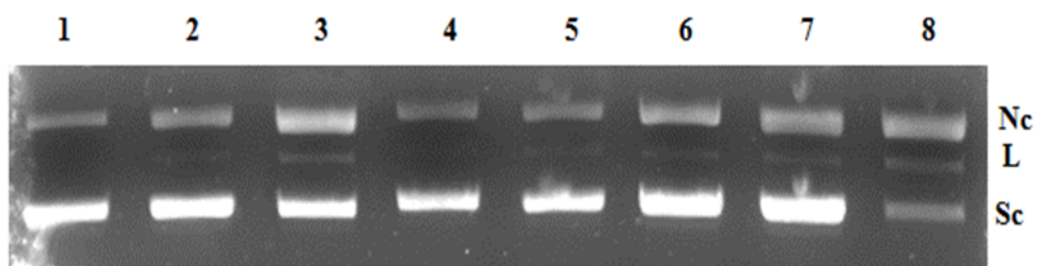
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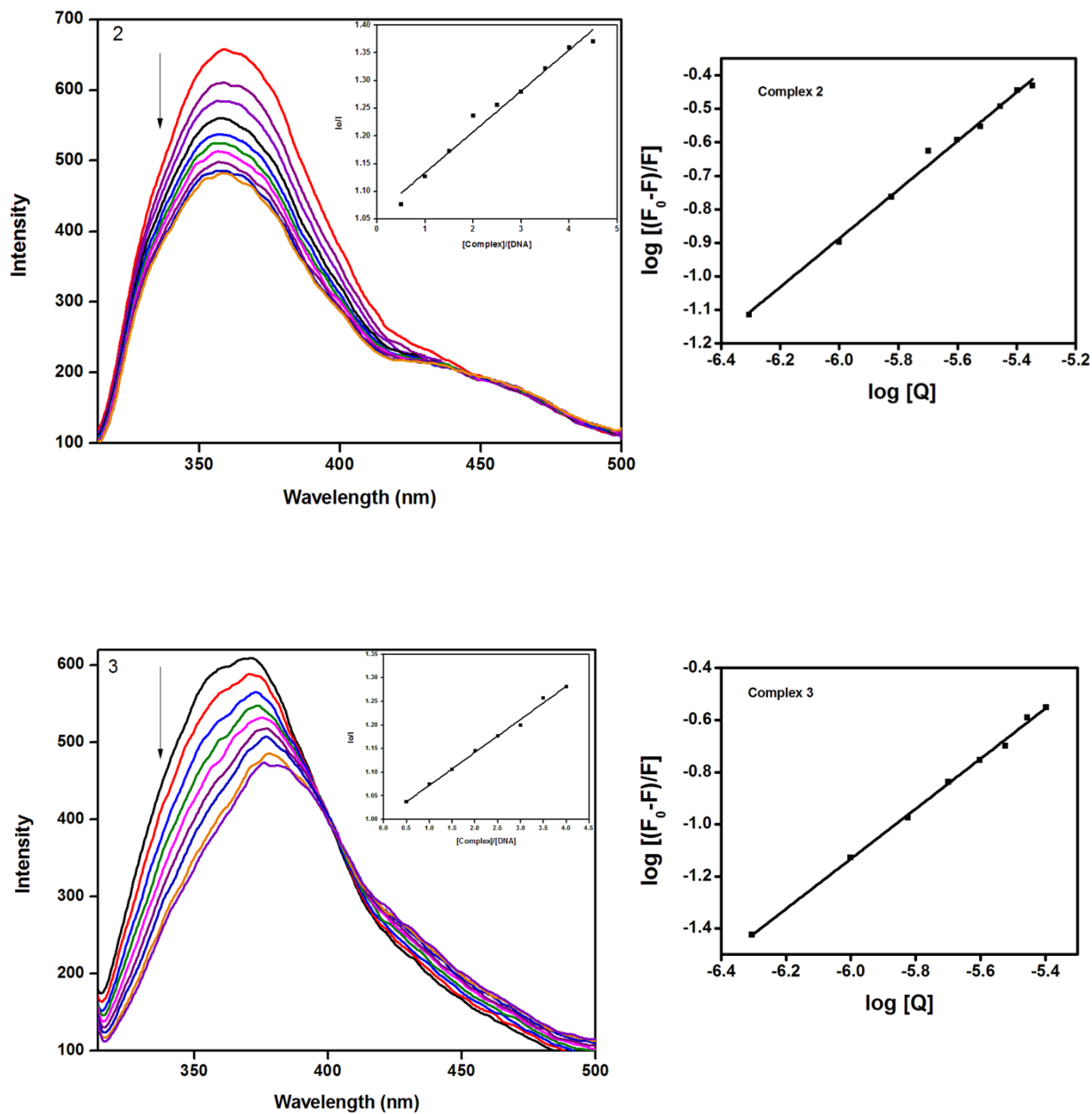
**Fig. S2** Absorption spectra of the complex (4) and (5) in the absence and presence of increasing amounts of CT-DNA (0 – 250  $\mu\text{M}$ ) at 25  $^{\circ}\text{C}$  in 50 mM Tris-HCl (pH = 7.2).



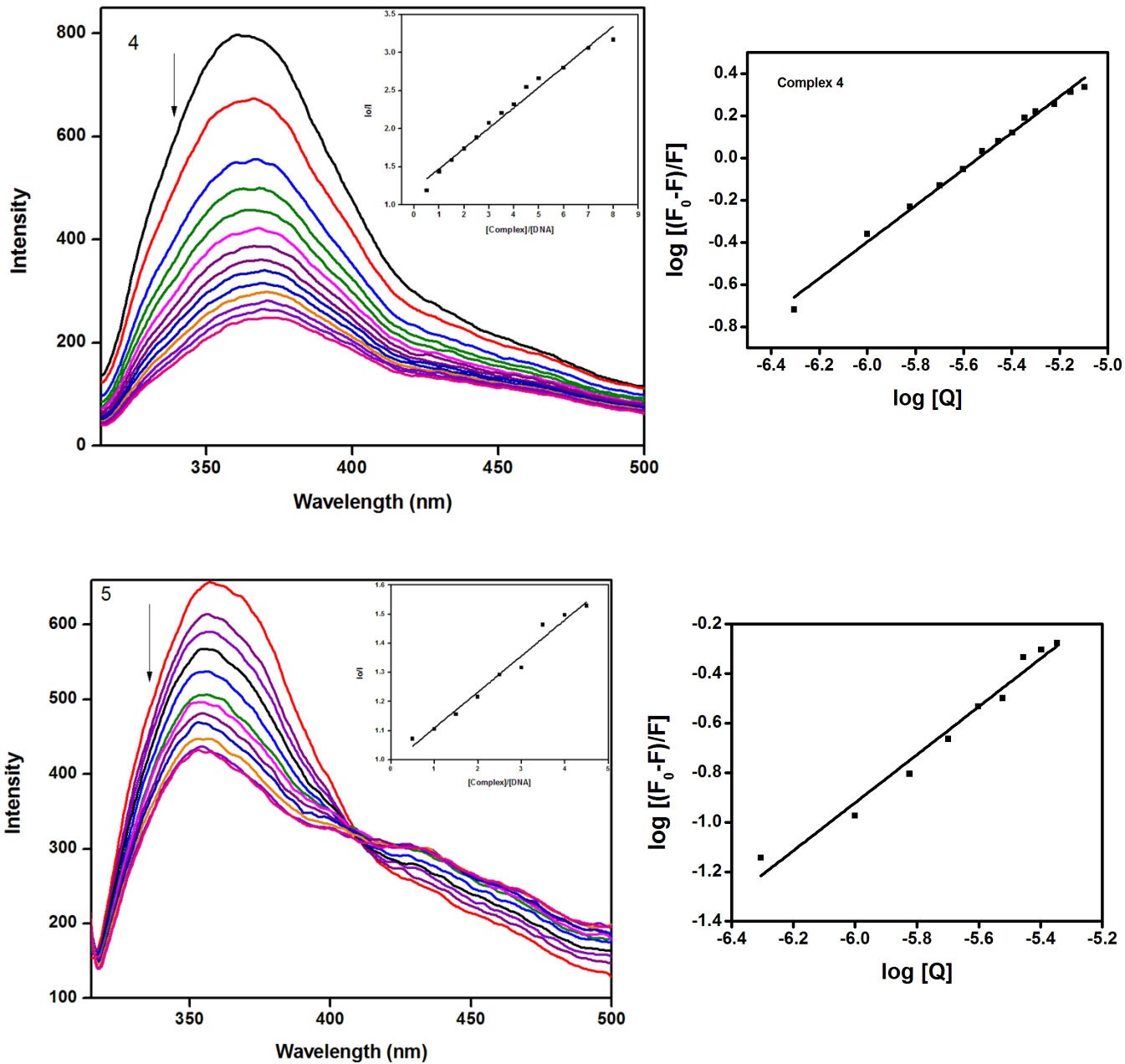
**Fig. S3** Emission spectra ( $\lambda_{\text{ex}} = 520 \text{ nm}$ ) of EB-DNA in Tris-HCl buffer in the absence and presence of the Complex (**4**).  $[\text{EtBr}] = 4 \mu\text{M}$ ,  $[\text{DNA}] = 40 \mu\text{M}$ . Arrow shows the decrease of intensity of EtBr-DNA upon increasing the concentration of complex.



**Fig. S4** Gel electrophoresis diagrams shows the cleavage of supercoiled pBR322 DNA ( $150 \mu\text{g mL}^{-1}$ ) by copper(II) complexes (**3**) ( $0.03 \text{ mM}$ ) in presence of mercaptoethanol (ME) ( $1 \text{ mM}$ ) as reducing agent in ( $50 \text{ mM}$ ) Tris-HCl buffer at pH 7.2 and  $37 \text{ }^\circ\text{C}$  with an incubation time of 3 h and different quenchers. Lane 1, DNA control; Lane 2, DNA + ME +  $\text{Cu}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$ ; Lane 3, DNA + ME + (**3**); Lane 4, DNA + ME + (**3**) +  $\text{NaN}_3$  ( $2 \mu\text{L}$ ); Lane 5, DNA + ME + (**3**) + L-histidine ( $1 \text{ mM}$ ); Lane 6, DNA + ME + (**3**) + DMSO ( $1 \text{ mM}$ ); Lane 7, DNA + ME + (**3**) + KI; Lane 8, DNA + ME + (**3**) + SOD ( $5 \text{ units}$ );



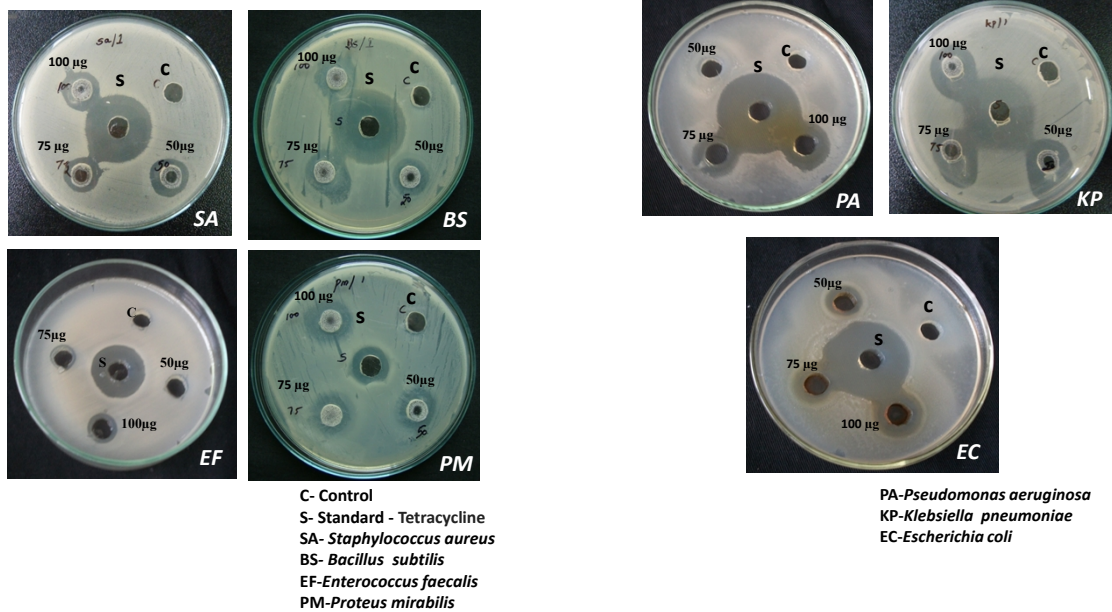
**Fig. S5** Changes in the fluorescence spectra and double-logarithm plot of BSA upon increasing complex (2) and complex (3) concentration at 300 K. The concentration of BSA is 1  $\mu\text{M}$  and complex concentration range from 0.0 to 10  $\mu\text{M}$ , pH = 7.2 and  $\lambda_{\text{ex}} = 280 \text{ nm}$ .



**Fig. S5** Changes in the fluorescence spectra and double-logarithm plot of BSA upon increasing complex (4) and complex (5) concentration at 300 K. The concentration of BSA is 1  $\mu\text{M}$  and complex concentration range from 0.0 to 10  $\mu\text{M}$ , pH = 7.2 and  $\lambda_{\text{ex}} = 280 \text{ nm}$ .



Compound - 5



**Fig. S6** Antimicrobial activity of complex (5) against *S. aureus*, *B. subtilis*, *E. faecalis*, *P. mirabilis*, *P. aeruginosa*, *K. pneumoniae* and *E. coli*.

**Table s2** Antimicrobial activity of complex (5)

	<b>Organisms</b>	<b>Concentration</b>		
		<b>50 µg</b>	<b>75 µg</b>	<b>100 µg</b>
		<b>Zone of inhibition, mm</b>		
<b>(5)</b>	<i>Staphylococcus aureus</i>	12	15	17
	<i>Bacillus subtilis</i>	11	12	16
	<i>Enterococcus faecalis</i>	11	14	15
	<i>Proteus mirabilis</i>	11	12	15
	<i>Pseudomonas aeruginosa</i>	14	18	22
	<i>Klebsiella pneumonia</i>	12	16	16
	<i>Escherichia coli</i>	11	12	17