

## Electronic Supplementary Information

# Synthesis, X-ray structure and *in vitro* cytotoxicity studies of Cu(I/II) complexes of thiosemicarbazone: Special emphasis on their interactions with DNA

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**Fig. S2**  $^1\text{H}$  NMR spectra of complex **1** in DMSO- $d_6$  (a) at time 0 hrs and room temp; (b) at time 24 hrs and room temp; (c) at time 0 hrs and 100  $^\circ\text{C}$ .

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**Fig. S10** Effect of DMF (1%) and ligands on the chemical-induced cleavage of SC pUC19 DNA. 300 ng SC pUC19 DNA was treated with hydrogen peroxide (0.5 mM) in dark for 1 h at 37  $^\circ\text{C}$  in presence of 1 % DMF and various ligands (100  $\mu\text{M}$ ). Lane 1, DNA only; Lane 2, DNA in presence of 1% DMF; Lane 3, DNA +  $\text{HL}^1$ ; Lane 4, DNA +  $\text{HL}^2$ ; Lane 5, DNA +  $\text{HL}^3$ ; Lane 6, DNA +  $\text{H}_2\text{L}^4$ .

**Fig. S11** Gel diagram depicting cleavage of SC pUC19 DNA by **1–4** in presence of various additives in 50 mM Tris-HCl buffer (pH 8.0) containing 1% DMF. SC pUC19 DNA (300 ng) in the presence of various additives was treated with hydrogen peroxide (0.5mM) in dark for 1 h at 37  $^\circ\text{C}$  with **1–4** (100  $\mu\text{M}$ ). The additive concentrations were: sodium azide (0.5 mM), L-histidine (0.5 mM), KI (0.5 mM) and D-mannitol (0.5 mM). Lane 1, DNA + complex; Lane 2, DNA + complex + sodium azide; Lane 3, DNA + complex + L-histidine; Lane 4, DNA + complex + KI; Lane 5, DNA + complex + D-mannitol.

**Fig. S12** Effect of DMF (1%) and ligands on the photo-induced cleavage of SC pUC19 DNA. 300 ng SC pUC19 DNA was photo-irradiated in presence of 1% DMF and various ligands (100  $\mu\text{M}$ ) with UVA at 350 nm for 1 h. Lane 1, DNA only; Lane 2, DNA in presence of 1% DMF; Lane 3, DNA +  $\text{HL}^1$ ; Lane 4, DNA +  $\text{HL}^2$ ; Lane 5, DNA +  $\text{HL}^3$ ; Lane 6, DNA +  $\text{H}_2\text{L}^4$ .

**Fig. S13** Gel diagram depicting cleavage of SC pUC19 DNA by **1–4** in presence of various additives in 50 mM Tris–HCl buffer (pH 8.0) containing 1% DMF. SC pUC19 DNA (300 ng) in the presence of various additives was photo-irradiated at 350 nm for 1 h with **1–4** (100  $\mu$ M). The additive concentrations were: sodium azide (0.5 mM), L-histidine (0.5 mM), KI (0.5 mM) and D-mannitol (0.5 mM). Lane 1, DNA + complex; Lane 2, DNA + complex + sodium azide; Lane 3, DNA + complex + L-histidine; Lane 4, DNA + complex + KI; Lane 5, DNA + complex + D-mannitol.

**Table S1** DNA binding parameters for the ligands

Ligands	Binding Constant ( $K_b$ ) <sup>a</sup> ( $M^{-1}$ )	Stern–Volmer Quenching Constant ( $K_{SV}$ ) ( $M^{-1}$ ) <sup>b</sup>	$K_{app}$ ( $M^{-1}$ ) <sup>c</sup>
<b>HL<sup>1</sup></b>	$5.50 \times 10^3$	$5.01 \times 10^2$	$3.02 \times 10^5$
<b>HL<sup>2</sup></b>	$5.20 \times 10^3$	$5.80 \times 10^2$	$3.60 \times 10^5$
<b>HL<sup>3</sup></b>	$1.80 \times 10^3$	$9.28 \times 10^2$	$6.70 \times 10^5$
<b>H<sub>2</sub>L<sup>4</sup></b>	$7.00 \times 10^3$	$4.50 \times 10^2$	$2.69 \times 10^5$

<sup>a</sup>DNA binding constant by UV–vis spectral method. <sup>b</sup>Stern–Volmer Quenching constant for CT–DNA–EB complex. <sup>c</sup>the apparent DNA binding constant.

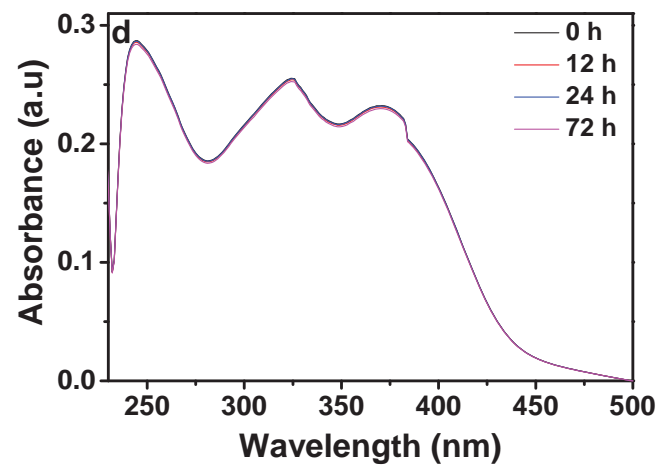
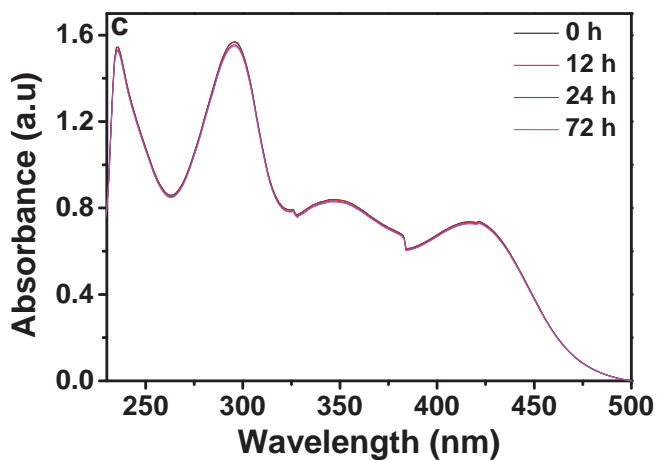
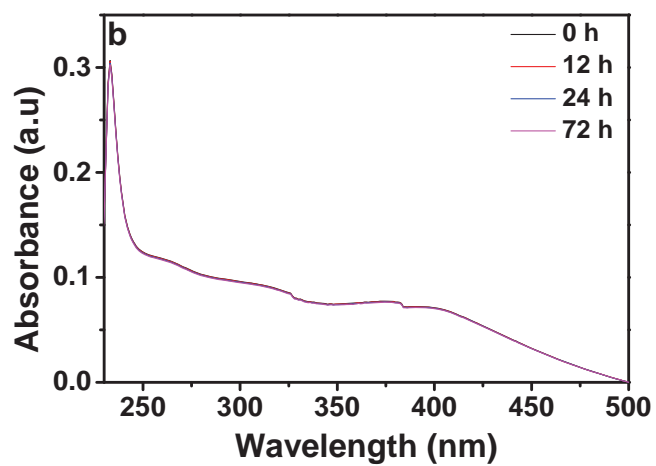
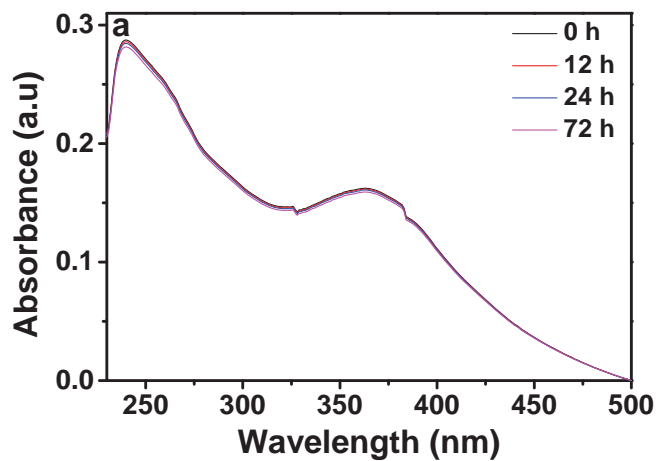


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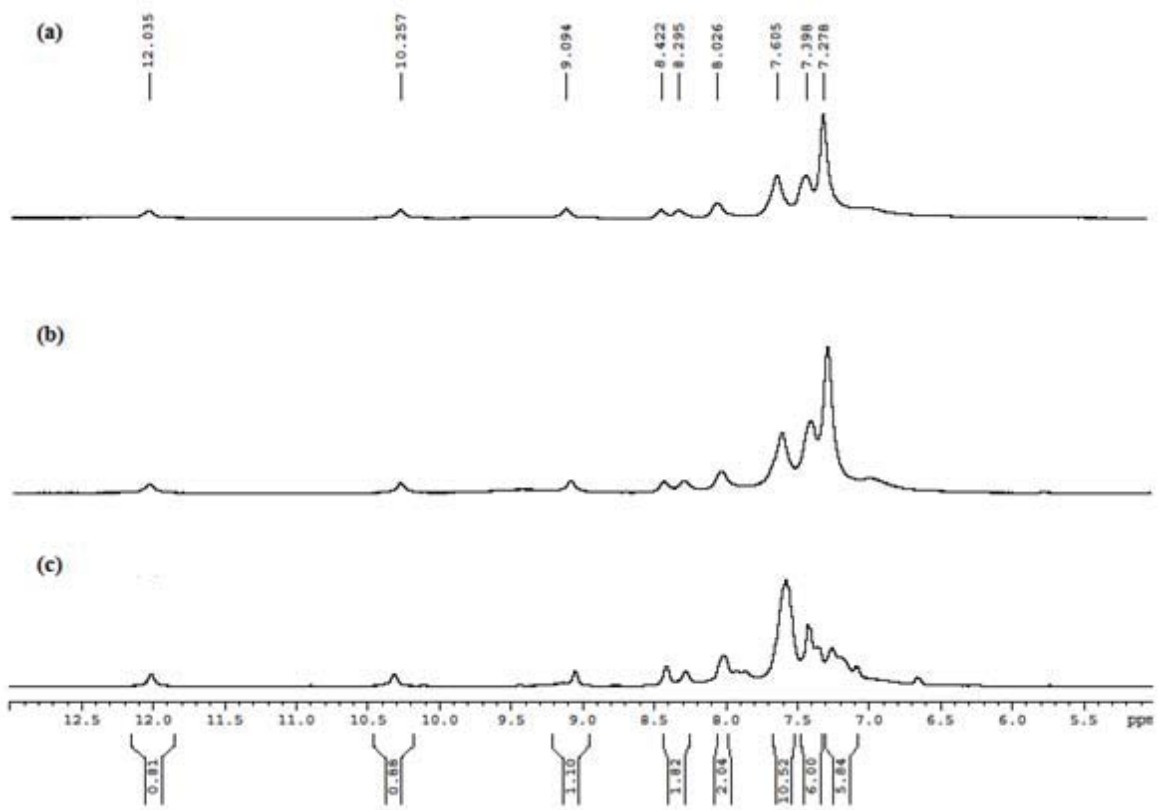


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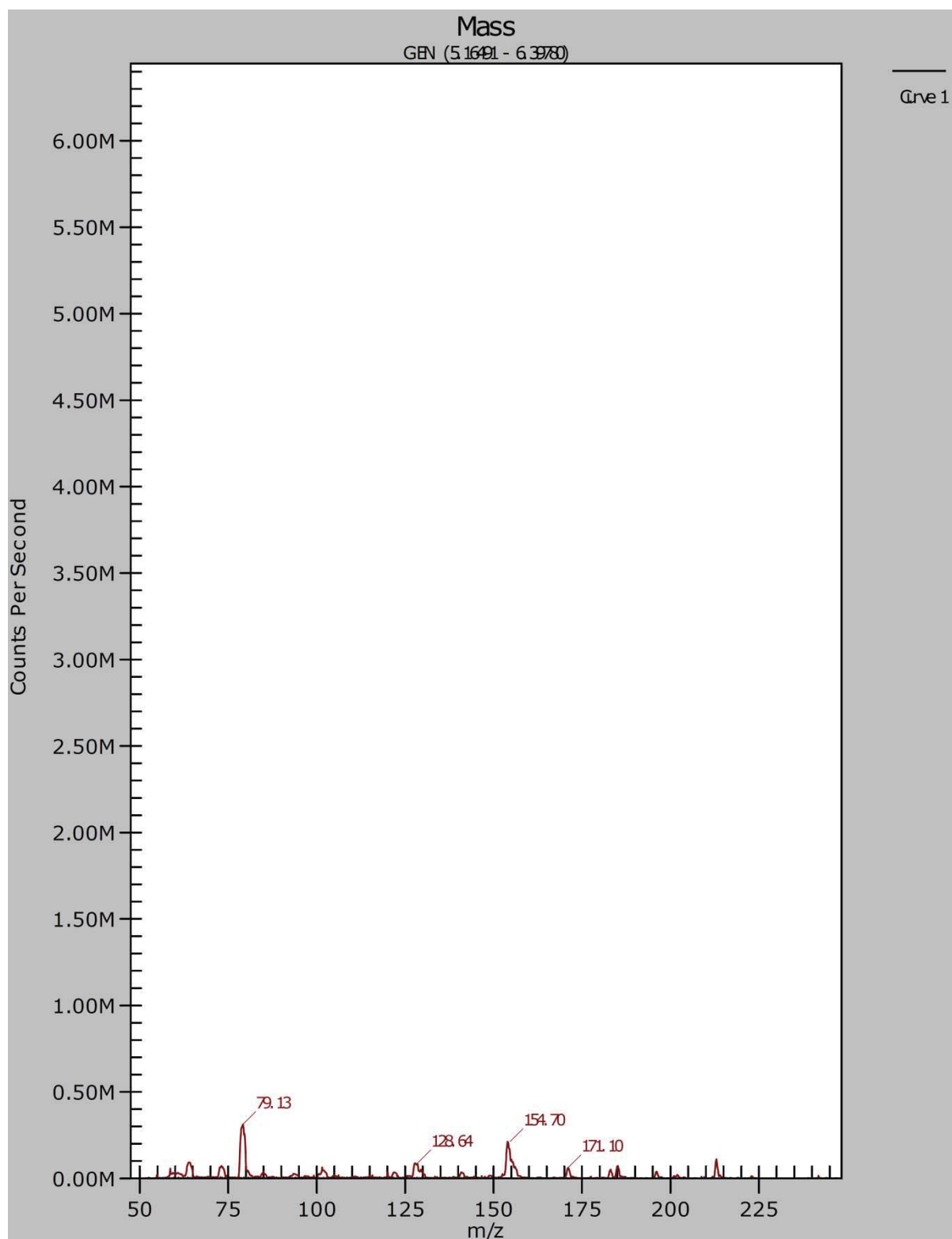


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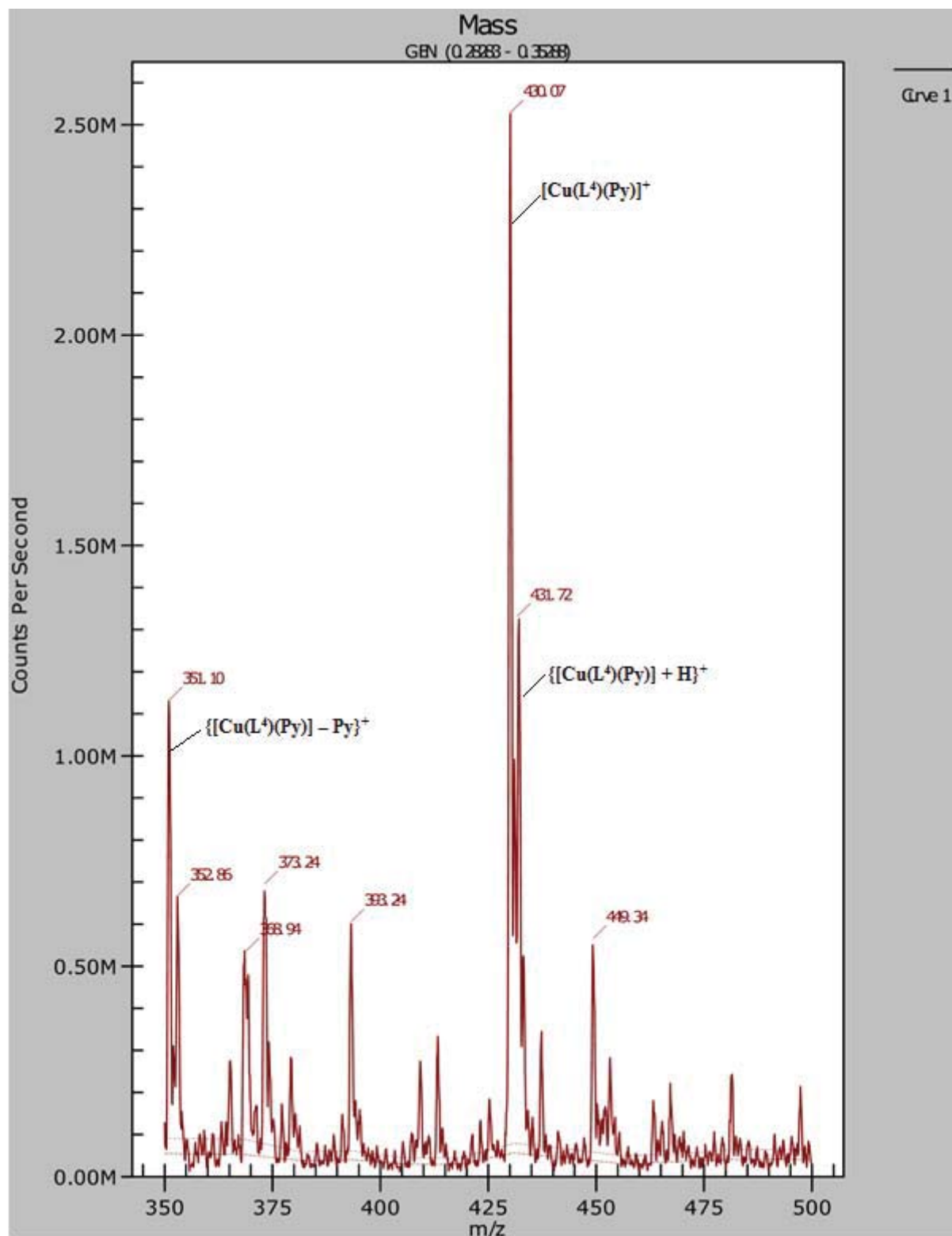


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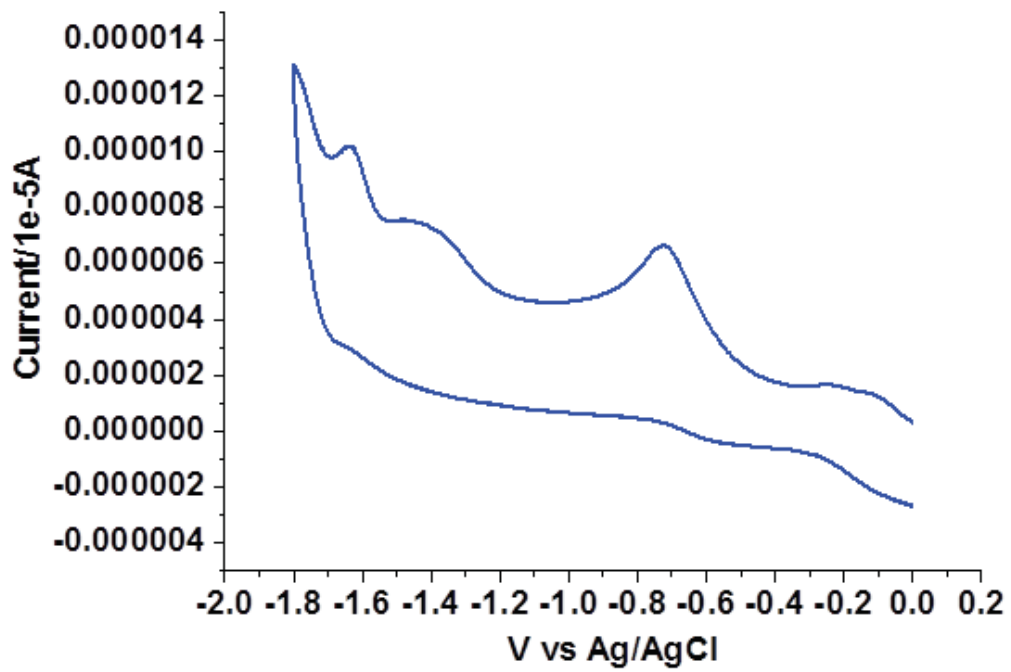


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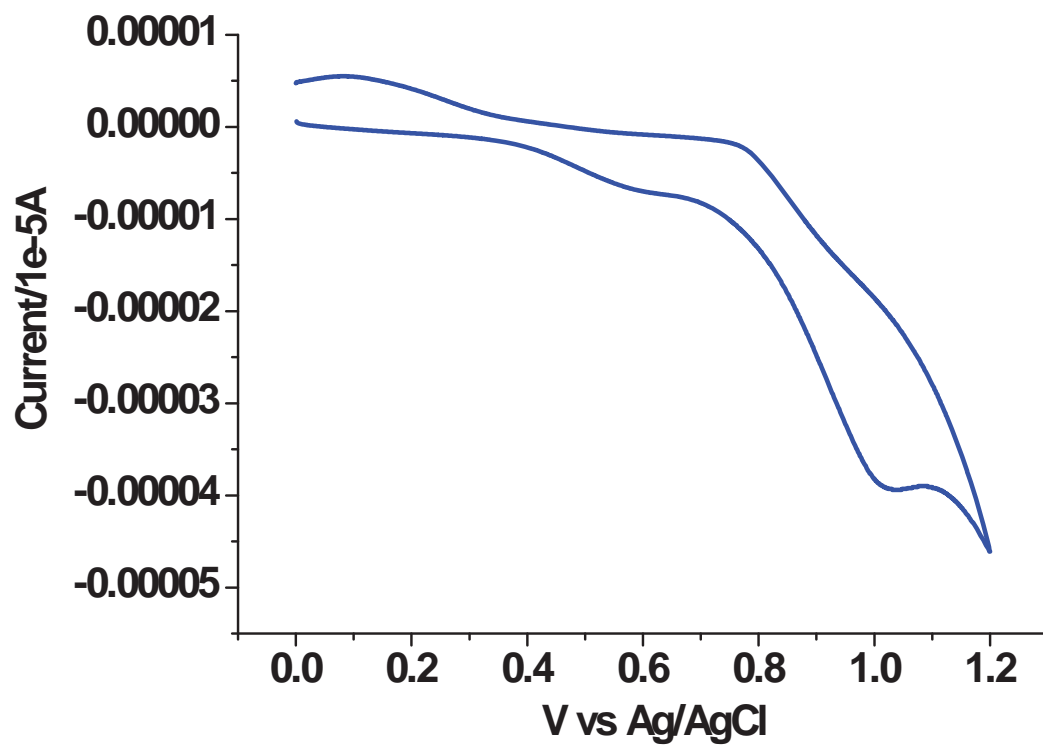


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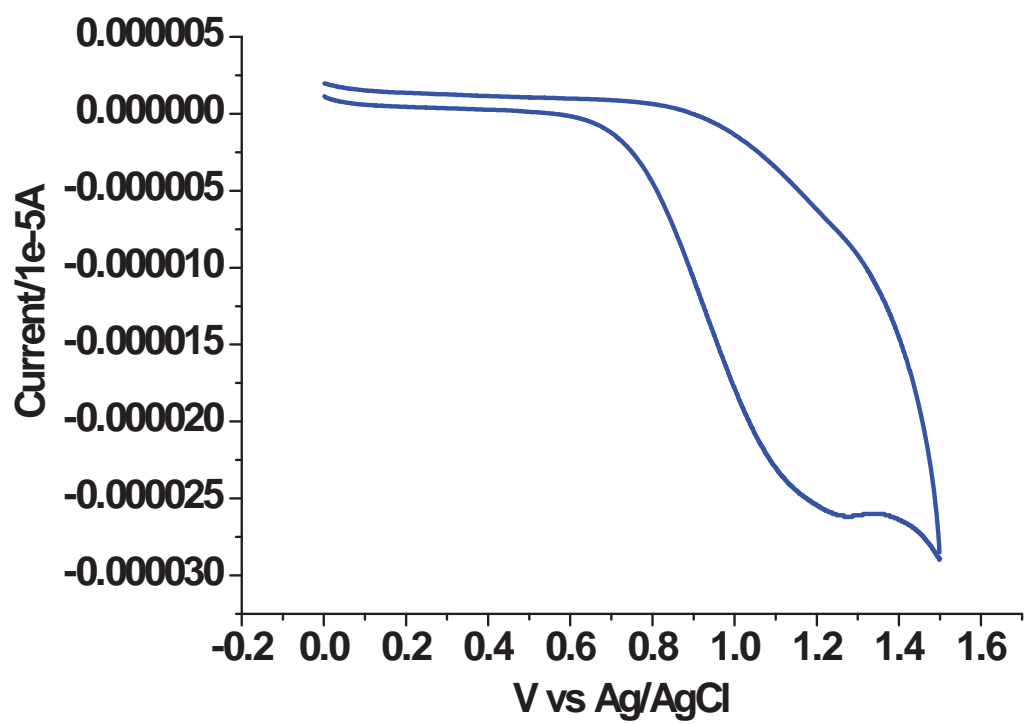


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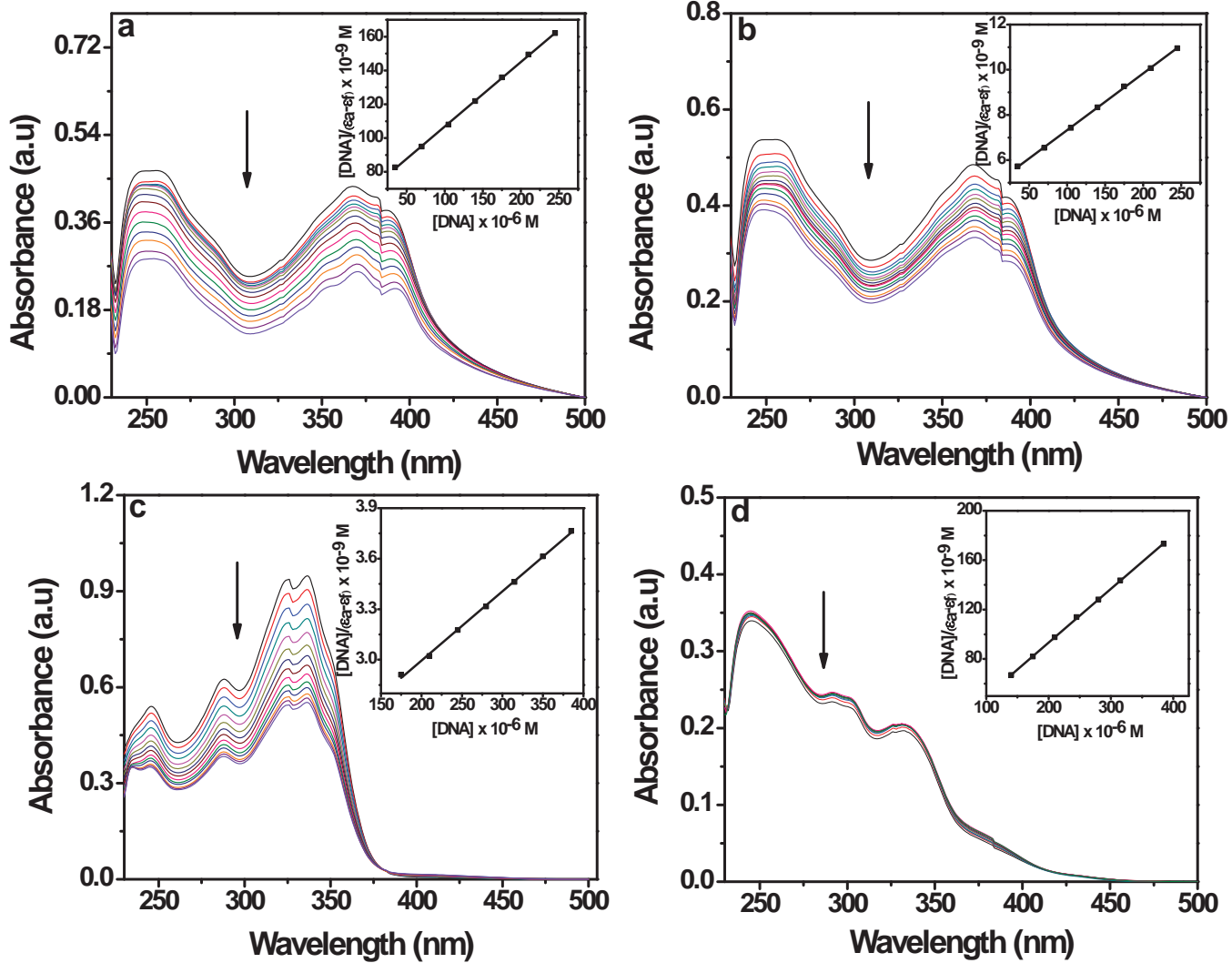


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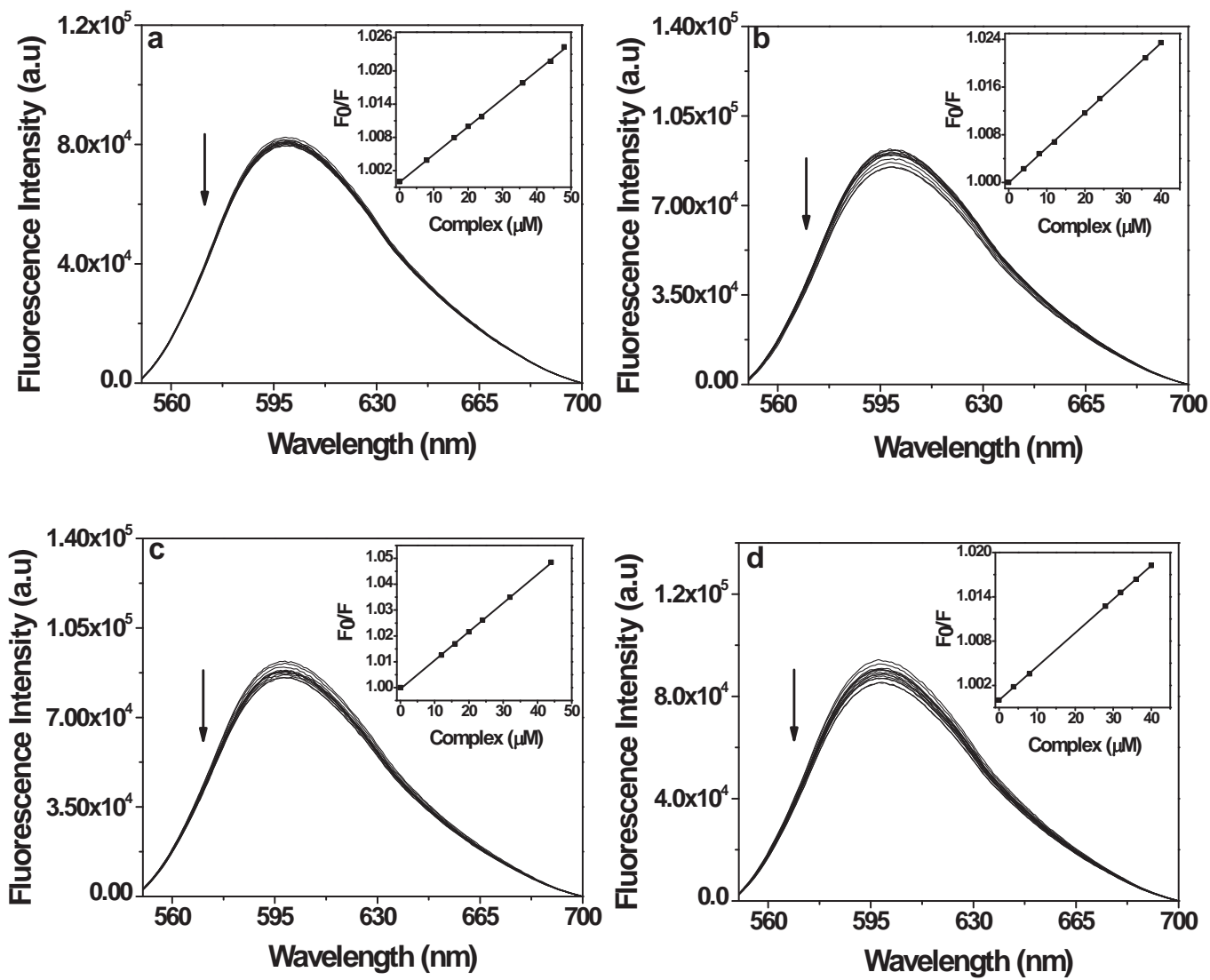


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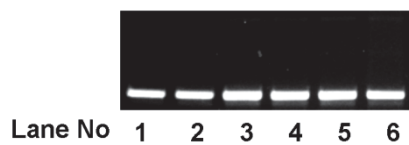


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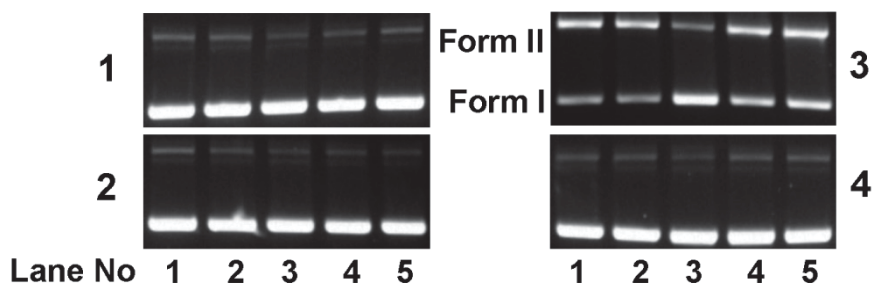


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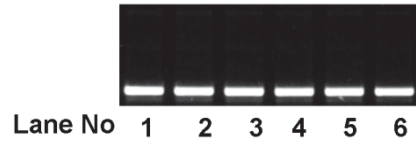


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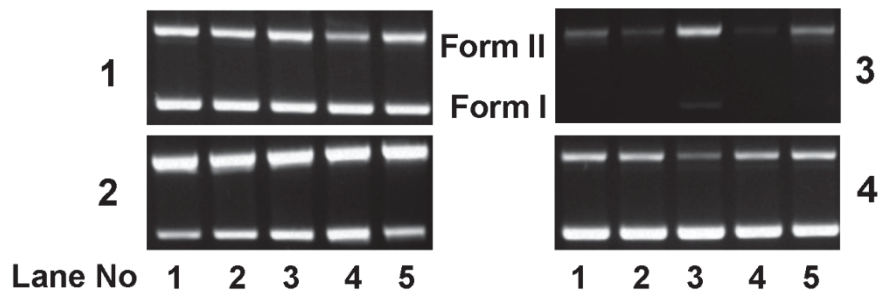


Fig. S13.