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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. 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 μM). 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) [a] (M^{-1})	Stern–Volmer Quenching Constant (K_{SV}) (M^{-1}) [b]	K_{app} (M^{-1})[c]
HL[1]	5.50×10^3	5.01×10^2	3.02×10^5
HL[2]	5.20×10^3	5.80×10^2	3.60×10^5
HL[3]	1.80×10^3	9.28×10^2	6.70×10^5
H_2L[4]	7.00×10^3	4.50×10^2	2.69×10^5

[a]DNA binding constant by UV–vis spectral method. [b]Stern–Volmer Quenching constant for CT–DNA–EB complex. [c]the apparent DNA binding constant.

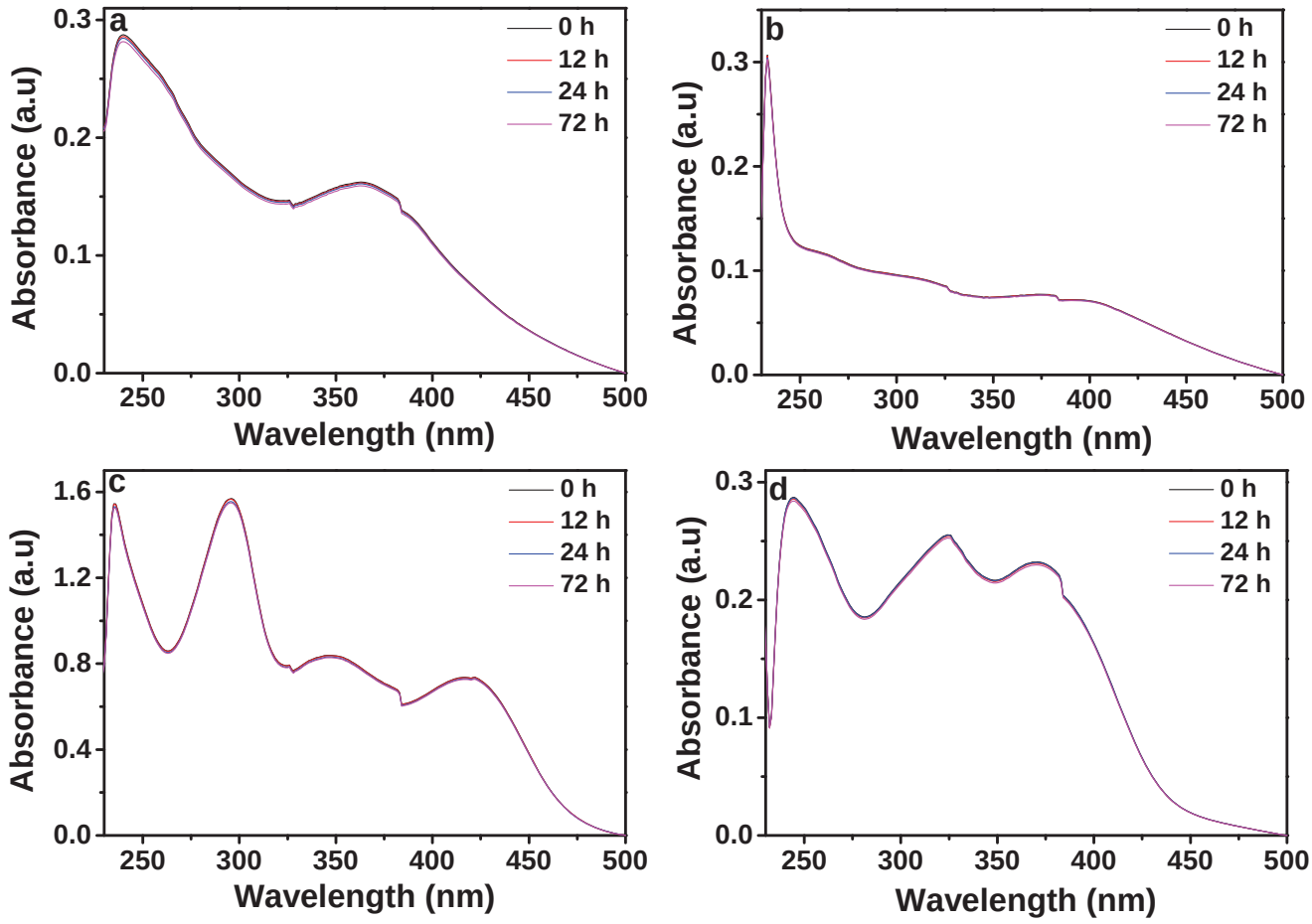
a
b
c
d
0 h
12 h
24 h
72 h
Absorbance (a.u)
Wavelength (nm)
0.0
0.1
0.2
0.3
0.4
0.8
1.2
1.6
250
300
350
400
450
500

Fig. S1.

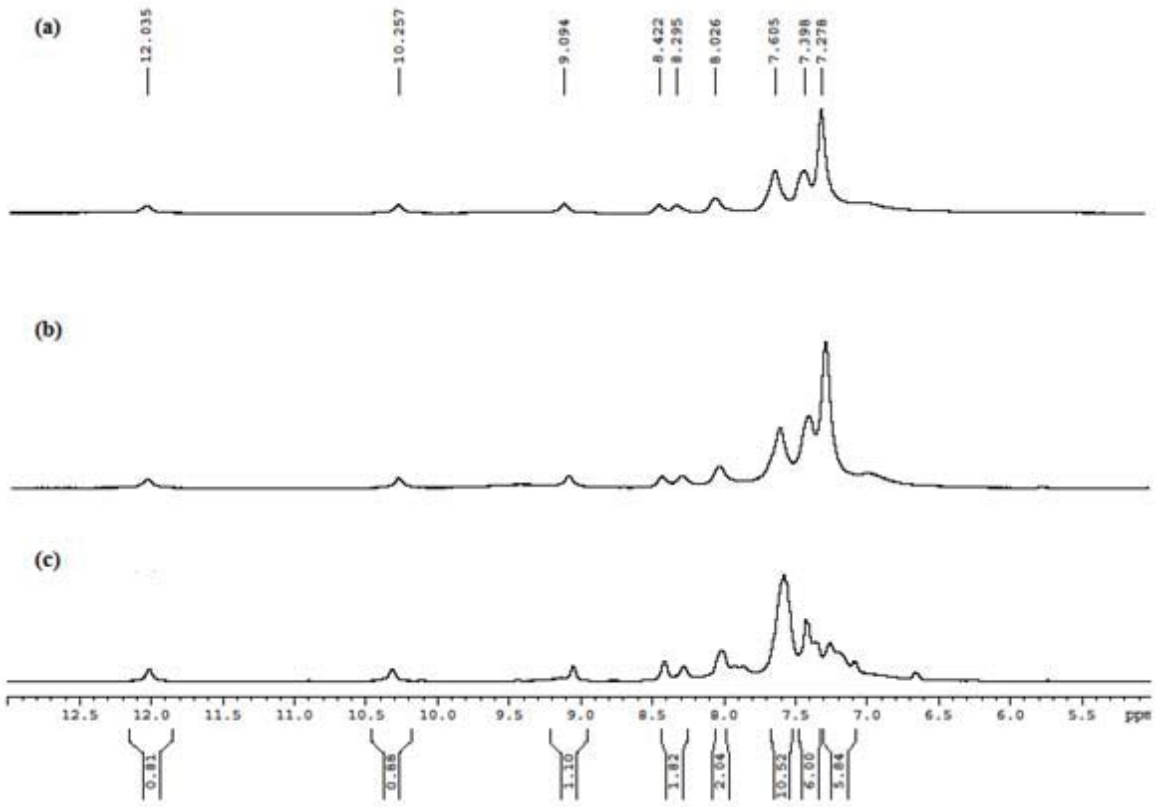
(a)
12.035
10.257
9.094
8.422
8.295
8.026
7.605
7.398
7.278
(b)
(c)
12.5
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
ppm
0.81
0.86
1.10
1.83
2.04
10.52
6.00
5.84

Fig. S2.

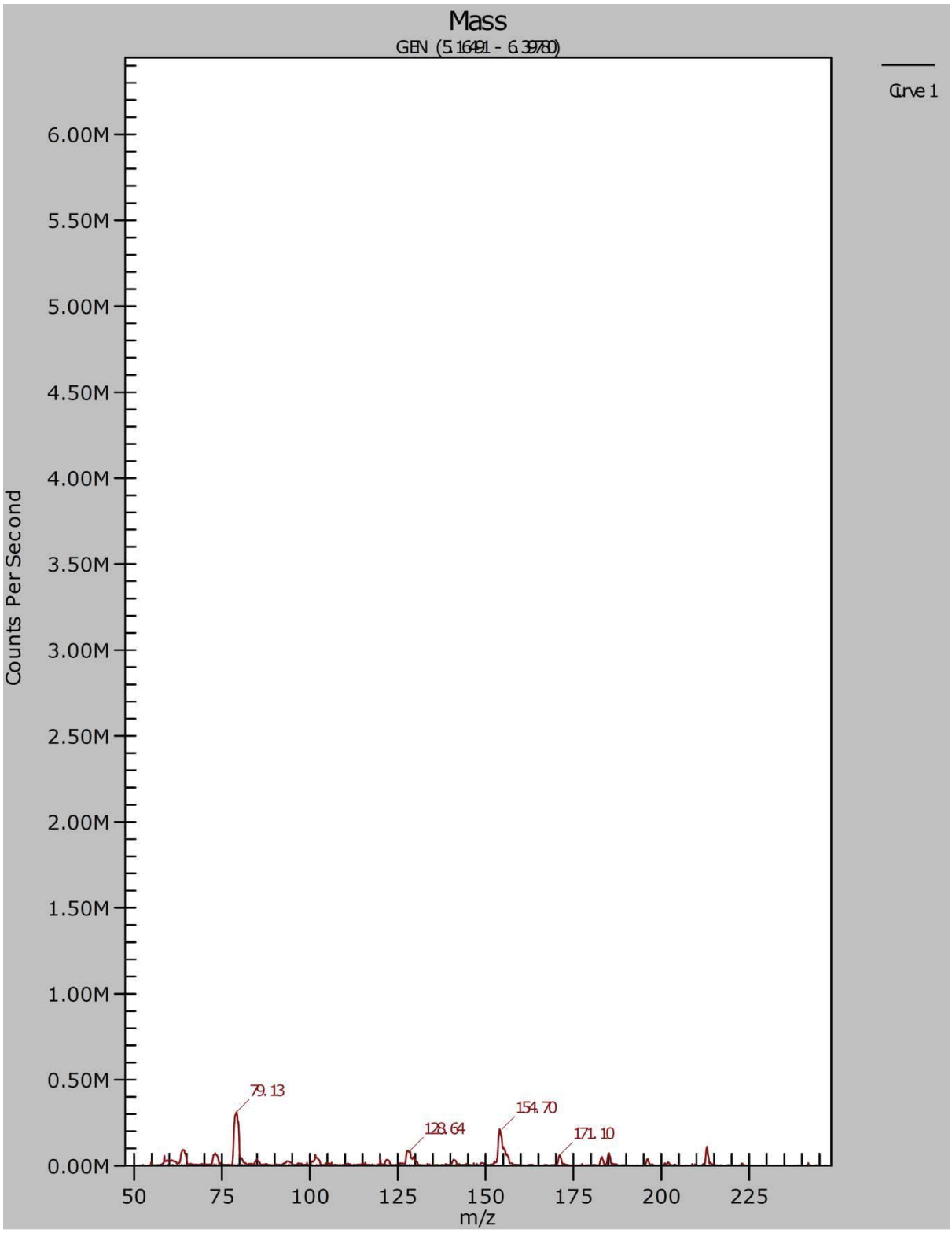
Mass
GEN (5.16491 - 6.39780)
Curve 1
Counts Per Second
6.00M
5.50M
5.00M
4.50M
4.00M
3.50M
3.00M
2.50M
2.00M
1.50M
1.00M
0.50M
0.00M
79.13
128.64
154.70
171.10
50
75
100
125
150
175
200
225
m/z

Fig. S3.

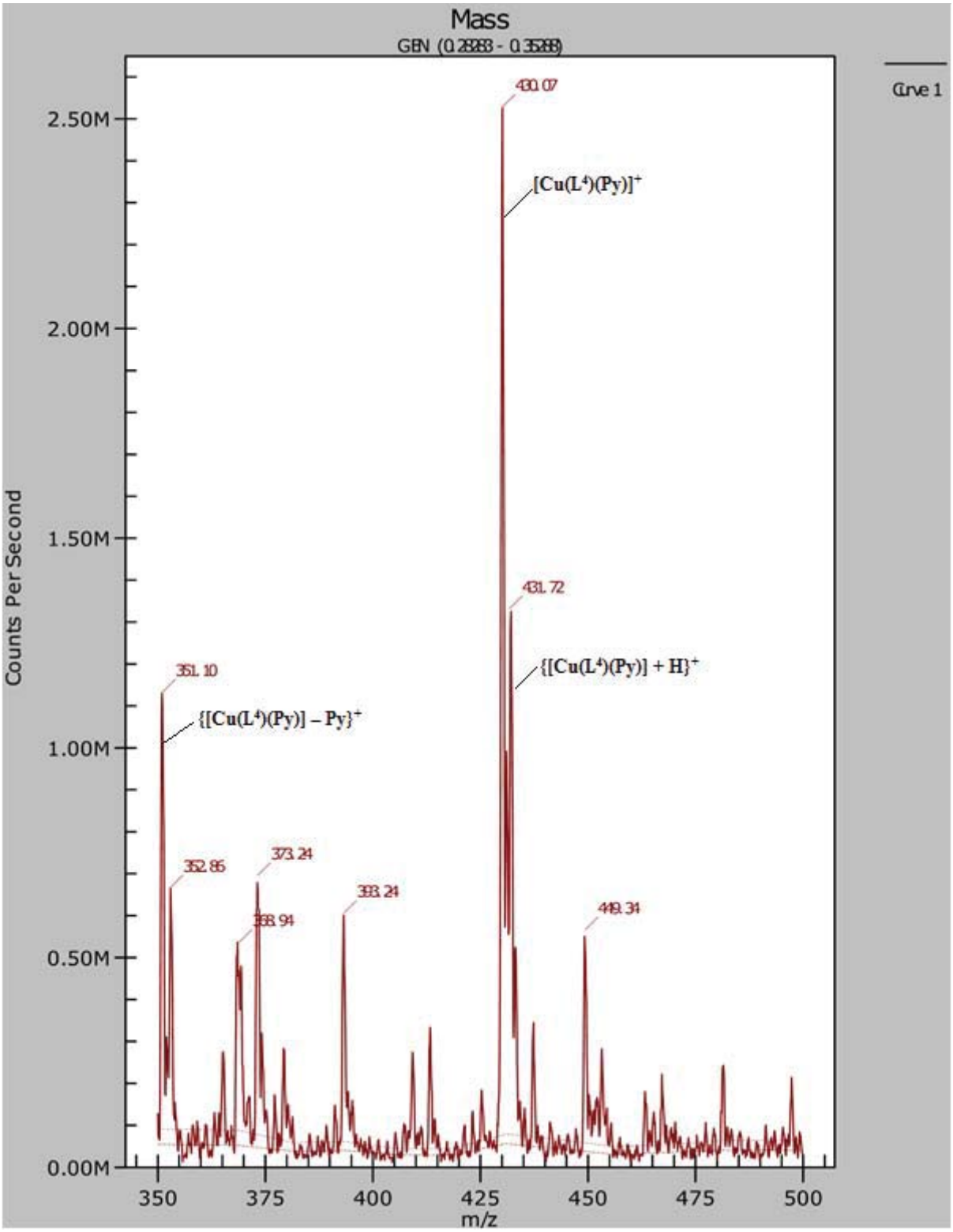
Mass
GEN (0.2883 - 0.3588)
Curve 1
Counts Per Second
2.50M
2.00M
1.50M
1.00M
0.50M
0.00M
350
375
400
425
450
475
500
m/z
430.07
[Cu(L4)(Py)]+
431.72
{[Cu(L4)(Py)] + H}+
351.10
{[Cu(L4)(Py)] – Py}+
352.86
373.24
393.24
368.94
449.34

Fig. S4.

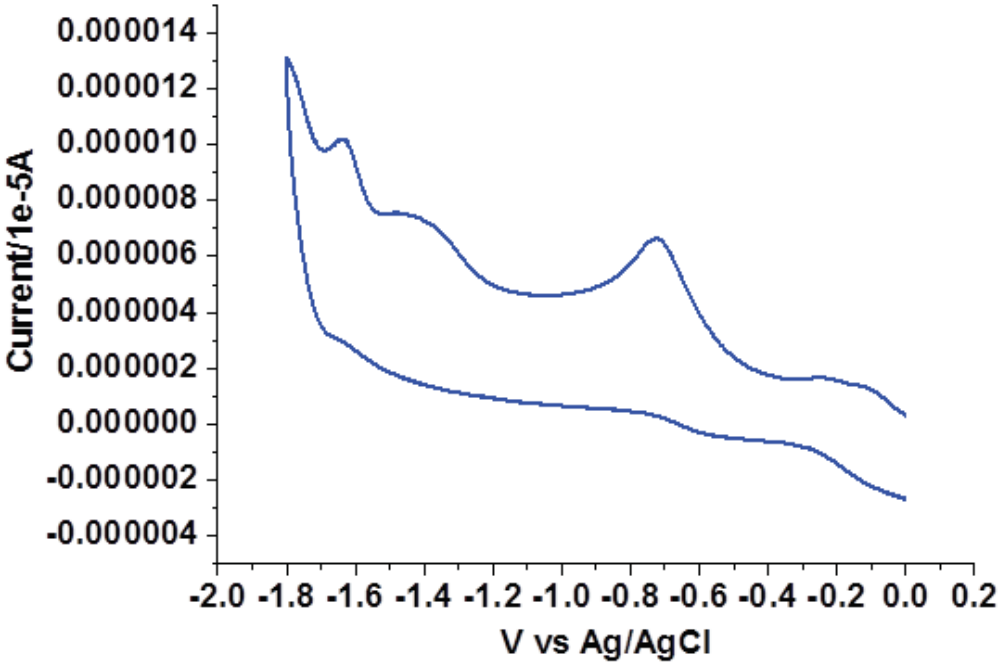
Current/1e-5A
0.000014
0.000012
0.000010
0.000008
0.000006
0.000004
0.000002
0.000000
-0.000002
-0.000004
-2.0 -1.8 -1.6 -1.4 -1.2 -1.0 -0.8 -0.6 -0.4 -0.2 0.0 0.2
V vs Ag/AgCl

Fig. S5.

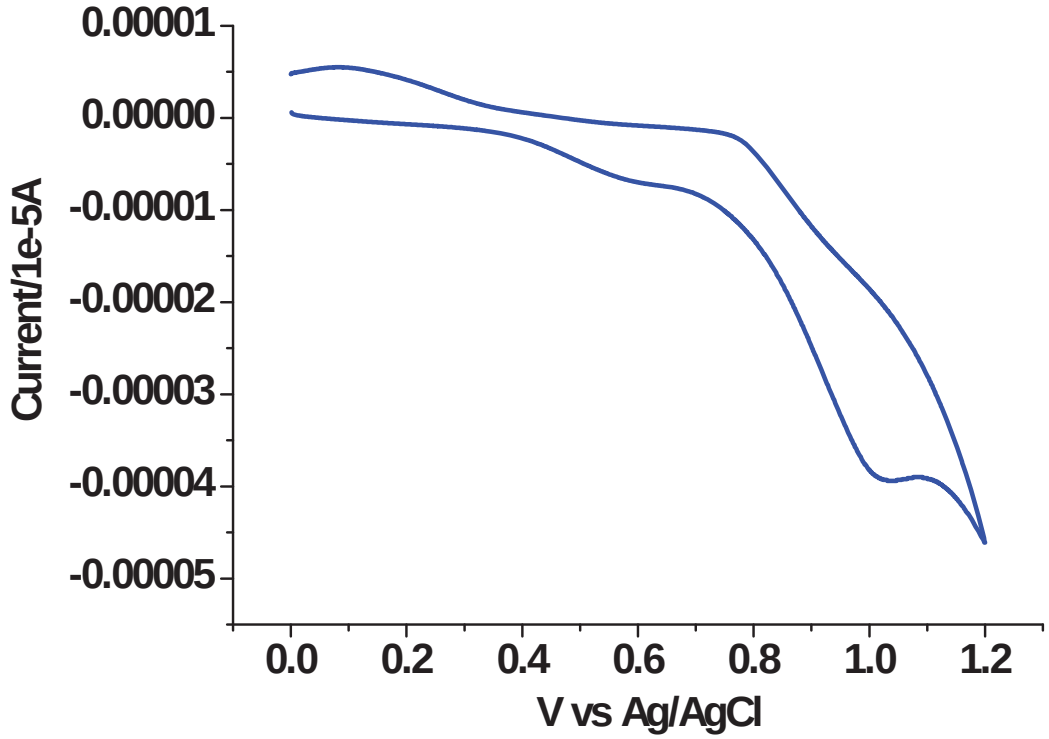
0.00001
0.00000
-0.00001
-0.00002
-0.00003
-0.00004
-0.00005
Current/1e-5A
0.0
0.2
0.4
0.6
0.8
1.0
1.2
V vs Ag/AgCl

Fig. S6.

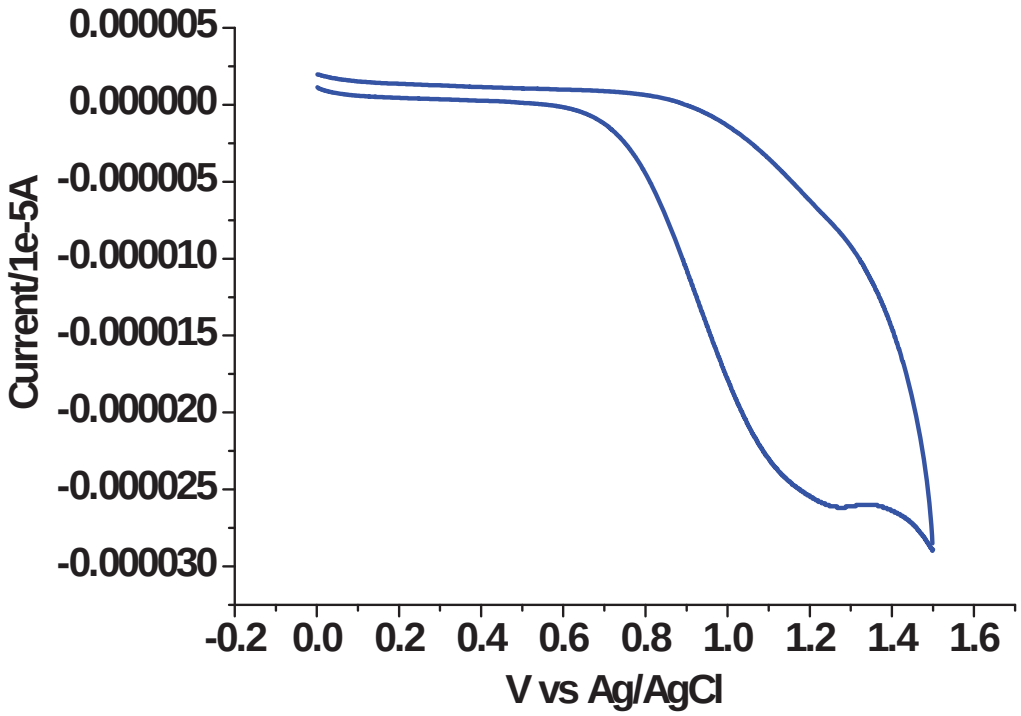
0.000005
0.000000
-0.000005
-0.000010
-0.000015
-0.000020
-0.000025
-0.000030
Current/1e-5A
-0.2
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
V vs Ag/AgCl

Fig. S7.

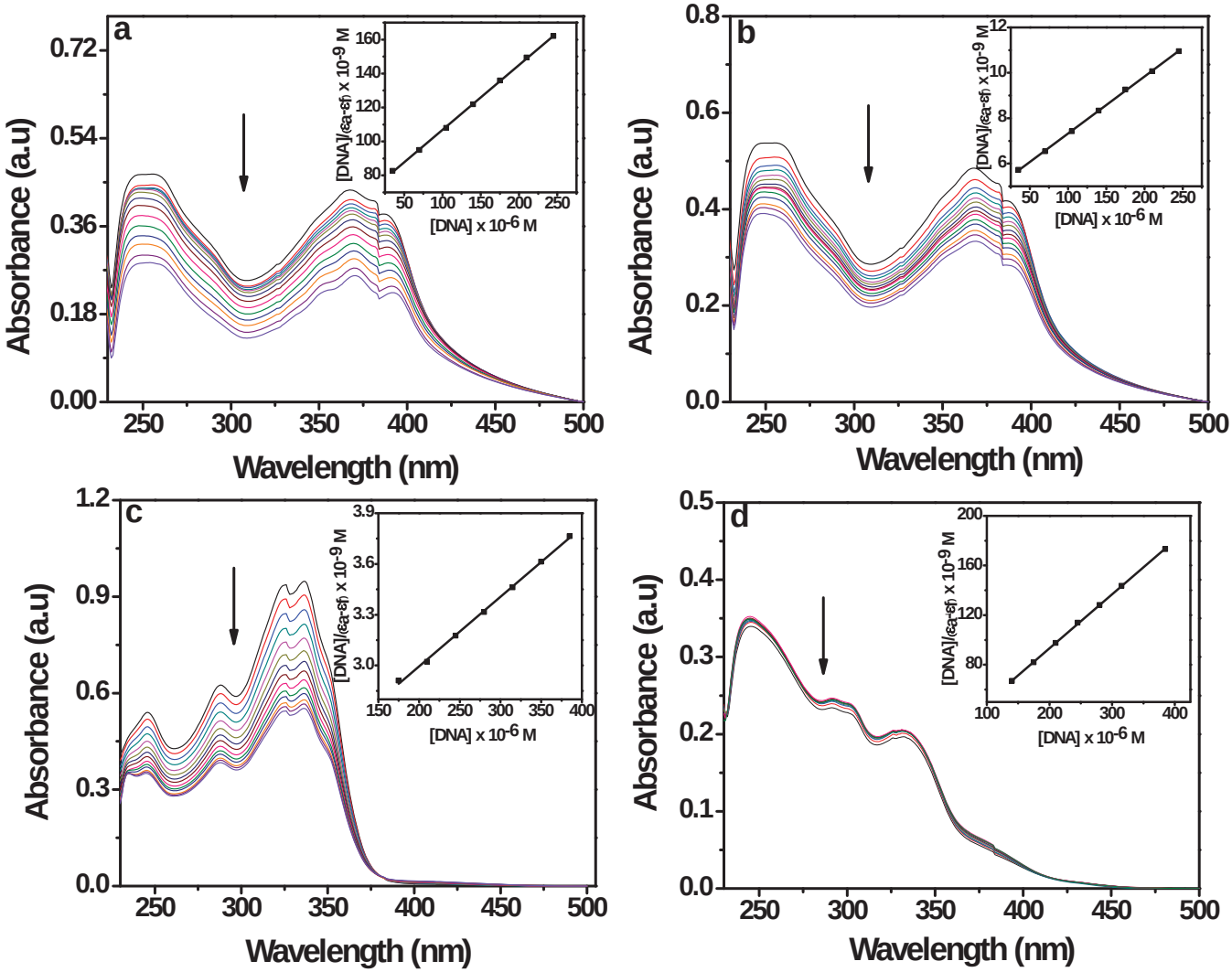
a
Absorbance (a.u)
Wavelength (nm)
[DNA]/(εa-εf) x 10-9 M
[DNA] x 10-6 M
b
Absorbance (a.u)
Wavelength (nm)
[DNA]/(εa-εf) x 10-9 M
[DNA] x 10-6 M
c
Absorbance (a.u)
Wavelength (nm)
[DNA]/(εa-εf) x 10-9 M
[DNA] x 10-6 M
d
Absorbance (a.u)
Wavelength (nm)
[DNA]/(εa-εf) x 10-9 M
[DNA] x 10-6 M

Fig. S8.

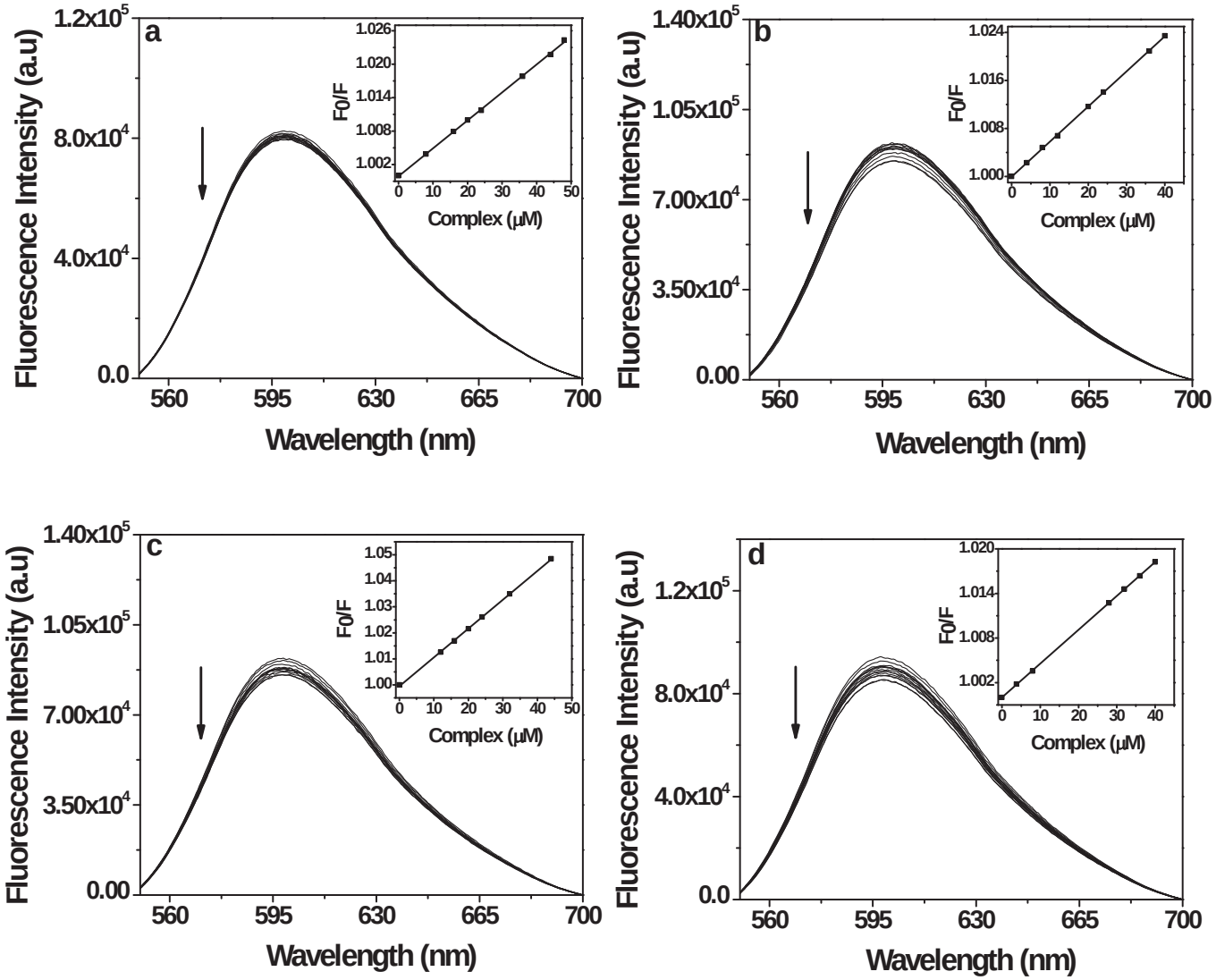
a
b
c
d
Fluorescence Intensity (a.u)
Wavelength (nm)
F0/F
Complex (μM)

Fig. S9.

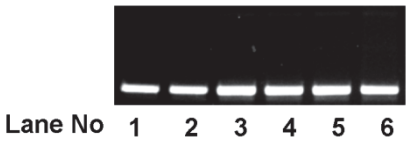

Fig. S10.

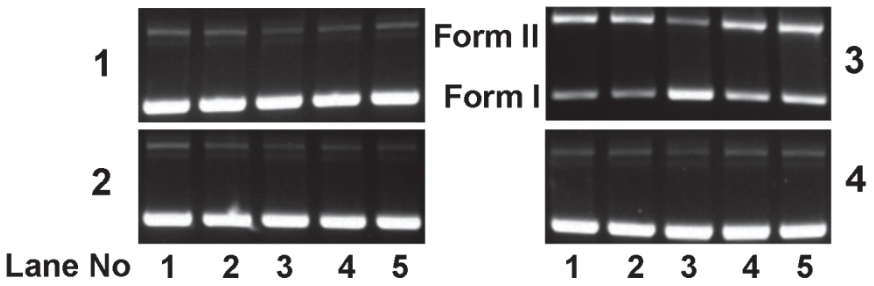

Fig. S11.

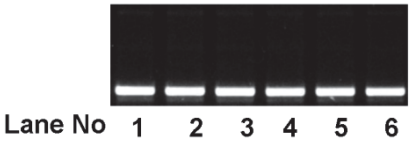

Fig. S12.

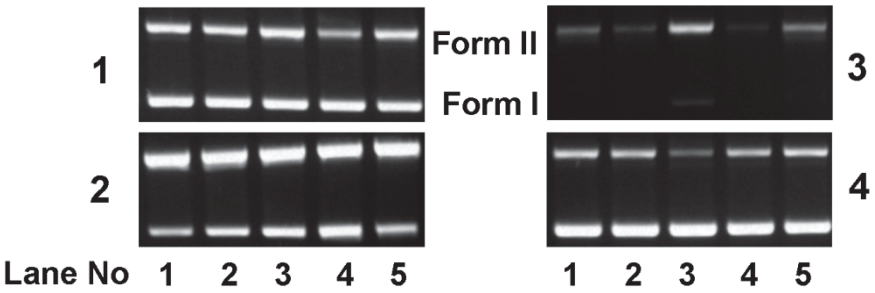

Fig. S13.