Manuscript Number: ic0505246 (Revised manuscript)

Steric Protection of Photosensitizer in a *N,N*-bis[2-(2-pyridyl)ethyl]-2-phenylethylamine-Copper(II) Bowl that Enhances Red Light-induced DNA Cleavage Activity

Shanta Dhar, Munirathinam Nethaji, and Akhil R. Chakravarty*

Department of Inorganic & Physical Chemistry, Indian Institute of Science, Bangalore 560012, India

E-mail: arc@ipc.iisc.ernet.in

Supplementary Material

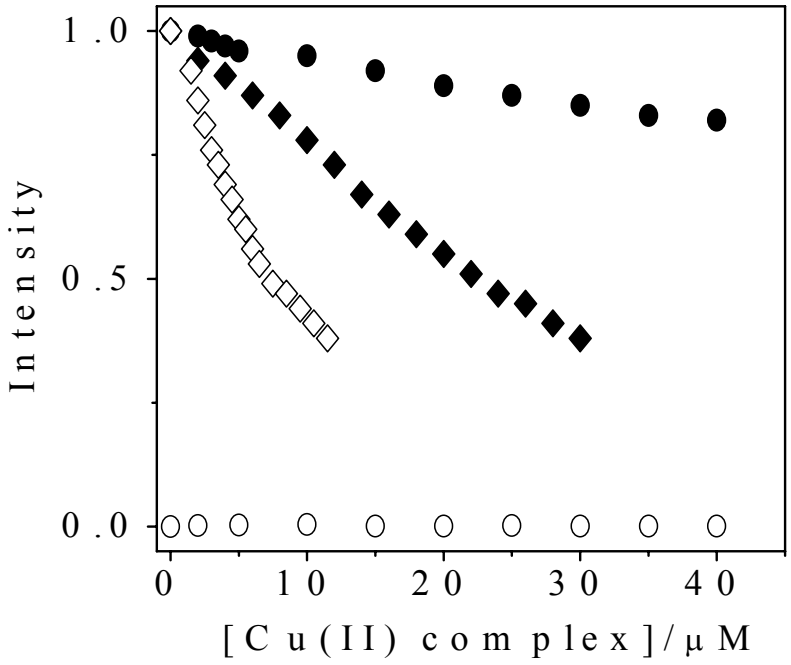

Figure S1. DNA binding plot showing the effect of addition of $[Cu(py_2phe)B](ClO_4)_2$ (B = phen, **1**, ●; dpq, **2**, ♦; dppz, **3**, ◊] to the emission intensity of the 303 μM CT DNA-bound ethidium bromide (1.3 μM) at different complex concentrations (0-40 μM) in a 5 mM Tris-HCl/5mM NaCl buffer (pH 7.2) containing 1% DMF at 25 °C. The emission intensities of EB in absence of CT DNA at various concentrations of **3** are also shown (o).

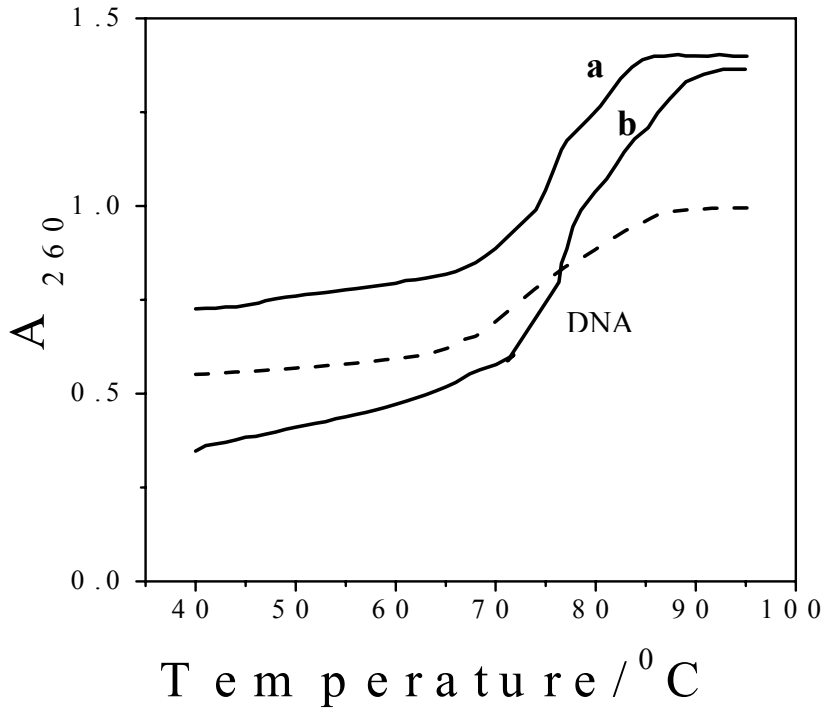

Figure S2. DNA melting curves at 260 nm in the absence (---) and presence of $[Cu(py_2phe)(phen)](ClO_4)_2$ (**1**) (a) and $[Cu(py_2phe)(dpq)](ClO_4)_2$ (**2**) (b)

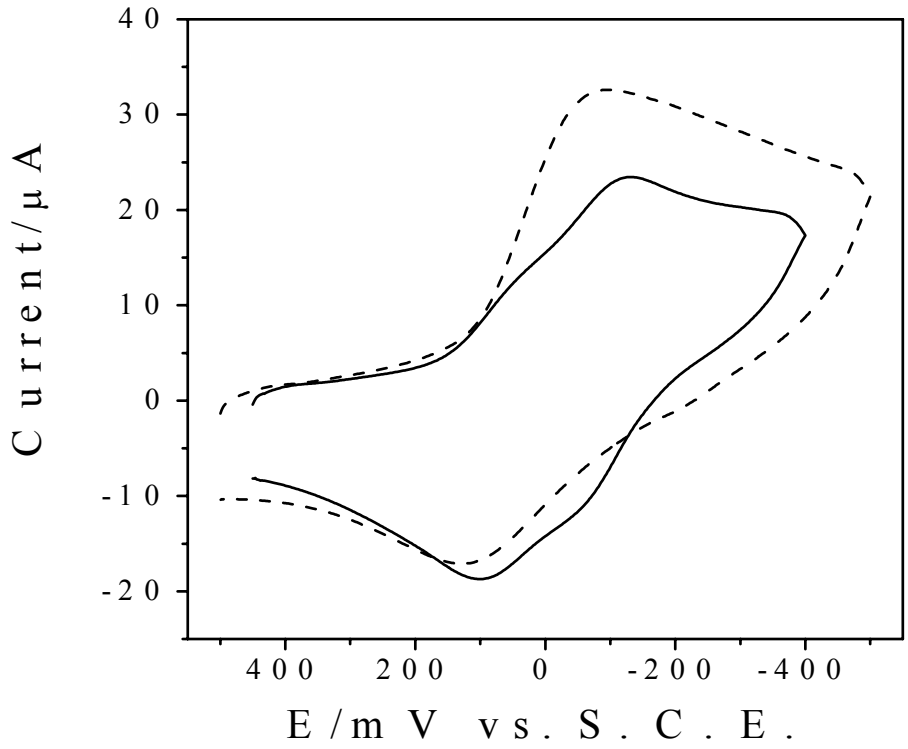

Figure S3. Cyclic Voltamograms of $[Cu(py_2phe)(phen)](ClO_4)_2$ (**1**) (—) and $[Cu(py_2phe)(dpq)](ClO_4)_2$ (**2**) in DMF-Trisbuffer (1:4 v/v)- 0.1 M KCl (---) at 50 mV s^{-1}.

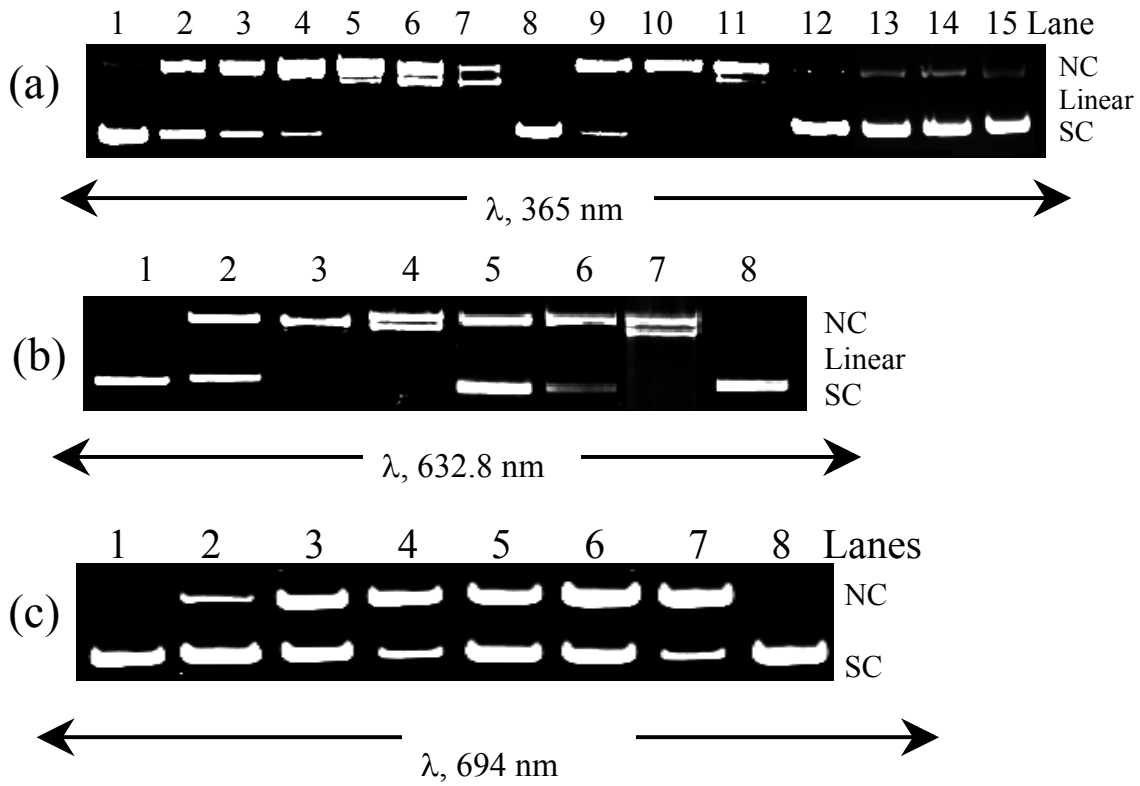

Figure S4.

Lane No.	Conditions	[complex] /μM	t/min	SC/ %	NC/ %	Linear /%
	(a) Light source: UV lamp (12 W), λ = 365 nm					
1.	DNA control	-	60	92	8	-
2.	DNA + $[Cu(py_2phe)(dpq)](ClO_4)_2$ (**2**)	50	5	49	51	-
3.	DNA + $[Cu(py_2phe)(dpq)](ClO_4)_2$ (**2**)	50	10	29	71	-
4.	DNA + $[Cu(py_2phe)(dpq)](ClO_4)_2$ (**2**)	50	15	12	88	-
5.	DNA + $[Cu(py_2phe)(dpq)](ClO_4)_2$ (**2**)	50	30	1	90	9
6.	DNA + $[Cu(py_2phe)(dpq)](ClO_4)_2$ (**2**)	50	45	2	61	37
7.	DNA + $[Cu(py_2phe)(dpq)](ClO_4)_2$ (**2**)	50	60	1	46	53
8.	DNA + $[Cu(py_2phe)(dpq)](ClO_4)_2$ (**2**)	50	dark	92	8	-

9.	DNA + $[Cu(py_2phe)(dppz)](ClO_4)_2$ (**3**)	25	10	22	78	-
10.	DNA + $[Cu(py_2phe)(dppz)](ClO_4)_2$ (**3**)	25	15	1	99	-
11.	DNA + $[Cu(py_2phe)(dppz)](ClO_4)_2$ (**3**)	25	30	1	80	19
12.	DNA + $[Cu(py_2phe)(dppz)](ClO_4)_2$ (**3**)	25	dark	98	2	-
13.	DNA + py_2phe	50	60	99	1	-
14.	DNA + dpq	50	60	96	4	-
15.	DNA + dppz	50	60	94	6	-
	(a) Light source: CW laser (3 mW), λ = 632.8 nm					
1.	DNA control	-	120	98	2	-
2.	DNA + $[Cu(py_2phe)(dpq)](ClO_4)_2$ (**2**)	100 μM	30	41	59	-
3.	DNA + $[Cu(py_2phe)(dpq)](ClO_4)_2$ (**2**)	100 μM	60	2	98	-
4.	DNA + $[Cu(py_2phe)(dpq)](ClO_4)_2$ (**2**)	100 μM	120	1	56	43
5.	DNA + $[Cu(py_2phe)(dppz)](ClO_4)_2$ (**3**)	100 μM	15	56	44	-
6.	DNA + $[Cu(py_2phe)(dppz)](ClO_4)_2$ (**3**)	100 μM	30	34	66	-
7.	DNA + $[Cu(py_2phe)(dppz)](ClO_4)_2$ (**3**)	100 μM	60	2	53	45
8.	DNA + $[Cu(py_2phe)(dppz)](ClO_4)_2$ (**3**)	100 μM	dark	97	3	-
	(a) Light source: Ruby laser (40 mJ/P), λ = 694 nm					
1.	DNA control	-	120	95	5	
2.	DNA + $[Cu(py_2phe)(dpq)](ClO_4)_2$ (**2**)	200	30	71	29	
3.	DNA + $[Cu(py_2phe)(dpq)](ClO_4)_2$ (**2**)	200	60	54	46	
4.	DNA + $[Cu(py_2phe)(dpq)](ClO_4)_2$ (**2**)	200	120	32	68	
5.	DNA + $[Cu(py_2phe)(dppz)](ClO_4)_2$ (**3**)	100	30	52	48	

6.	DNA + $[Cu(py_2phe)(dppz)](ClO_4)_2$ (**3**)	100	60	47	53
7.	DNA + $[Cu(py_2phe)(dppz)](ClO_4)_2$ (**3**)	100	120	28	72
8.	DNA + $[Cu(py_2phe)(dppz)](ClO_4)_2$ (**3**)	100	dark	96	4

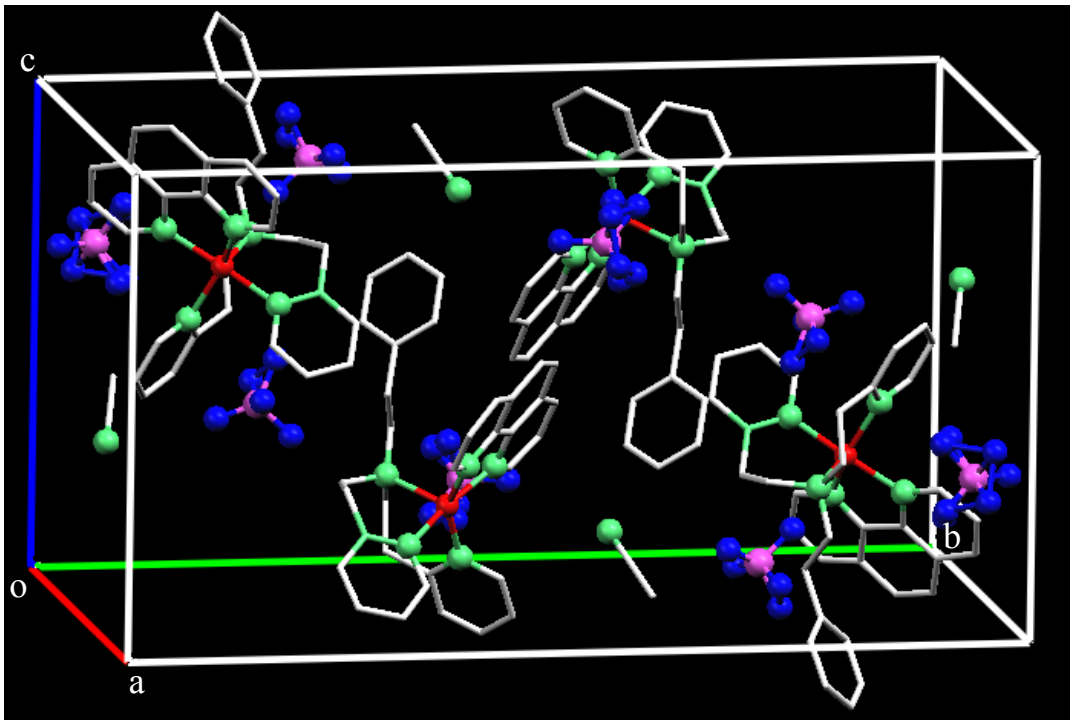

Figure S5. Unit cell packing diagram of [Cu(py$_2$phe)(phen)](ClO$_4$)$_2$.MeCN (**1**.MeCN)