Electronic Supplementary Material (ESI) for New Journal of Chemistry. This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2016

## SUPPLEMENTARY INFORMATION

## EFFECTS OF N,N-HETEROCYCLIC LIGANDS ON THE IN VITRO CYTOTOXICITY AND DNA INTERACTIONS OF COPPER(II) CHLORIDE COMPLEXES FROM AMIDINO-O-METHYLUREA LIGANDS

Atittaya Meenongwa,<sup>a</sup> Rosa F. Brissos,<sup>b</sup> Chaiyaporn Soikum,<sup>c</sup> Prapansak Chaveerach,<sup>c</sup> Patrick Gamez,<sup>bd</sup> Yanee Trongpanich<sup>e</sup> and Unchulee Chaveerach<sup>a,\*</sup>

<sup>a</sup> Materials Chemistry Research Center, Department of Chemistry and Center of Excellence for Innovation in Chemistry, Faculty of Science, Khon Kaen University, Khon Kaen 40002, Thailand

<sup>b</sup> Departament de Química Inorgànica, Universitat de Barcelona, Martí I Franqués 1-11, 08028 Barcelona, Spain

<sup>c</sup> Department of Veterinary Public Health, Faculty of Veterinary Medicine, Khon Kaen University, Khon Kaen 40002, Thailand

<sup>d</sup> Institució Catalana de Recerca i Estudis Avançats (ICREA), Passeig Lluís Companys, 23, 08010 Barcelona, Spain

<sup>e</sup> Department of Biochemistry, Faculty of Science, Khon Kaen University, Khon Kaen 40002, Thailand



Fig. S1 ESI+ mass spectra of 1



Fig. S2 ESI+ mass spectra of 2



Fig. S3 ESI+ mass spectra of 3

Fig. S4 ESI+ mass spectra of 4



Fig. S5 Electronic absorption spectra of the copper(II) complexes; (a) 1, (b) 2, (c) 3 and (d) 4 in solid state (----), MeOH (----) and DMSO (....).



Fig. S6 Circular dichroism spectra of free CT-DNA (—) (200  $\mu$ M), free complexes (200  $\mu$ M) (····) and CT-DNA treated by ethidium bromide (a) and 1-4 (b-e) at the [Complex]/[DNA] ratios of 0.5 (—) and 1.0 (—), incubated at 37 °C for 24 h. Arrows indicate direction of the intensity changes of the positive and the negative bands.



Fig. S7 Thermal denaturation profiles of CT-DNA (200  $\mu$ M) in the presence of the complexes 1-4 at different [Complex]/[DNA] ratios of 0.0 (**n**), 0.5 (**•**), 1.0 (**A**), 1.5 (**V**) and 2.0 (**•**) in 3% MeOH/Tris-buffer, pH = 7.2.



Fig. S8 Effect of the complexes 1-4 on the fluorescence emission spectra of the EB-DNA complex in 3% MeOH/Tris-buffer (5 mM Tris-HCl/ 50 mM NaCl at pH = 7.2) at 37 °C. [EB] = 25  $\mu$ M, [DNA] = 50  $\mu$ M, [Complex] = 0–50  $\mu$ M,  $\lambda_{ex}$  = 500 nm and  $\lambda_{em}$  = 593 nm. Insets: the Stern-Volmer plots of fluorescence quenching of the EB-DNA at different complex concentrations.



Fig. S9 Plots of % supercoiled DNA (Form I) (——) and circular nicked DNA (Form II) (—) vs. the concentration of the complexes (a)  $[Cu(L^1)(bipy)]Cl_2$  (1); (b)  $[Cu(L^1)(phen)]Cl_2$  (2); (c)  $[Cu(L^2)(bipy)Cl_2]$  (3) and (d)  $[Cu(L^2)(phen)]Cl_2$  (4). Incubation in HEPES-buffer at 37 °C for 1 h.



Fig. S10 Plots of % supercoiled DNA (Form I) (———), circular nicked DNA (Form II) (——) and linear DNA (Form III) (——) vs. the concentration of the complexes (a)  $[Cu(L^1)(bipy)]Cl_2$  (1); (b)  $[Cu(L^1)(phen)]Cl_2$  (2); (c)  $[Cu(L^2)(bipy)Cl_2]$  (3) and (d)  $[Cu(L^2)(phen)]Cl_2$  (4) in the presence of H<sub>2</sub>ASC (100 µM). Incubation in HEPES-buffer at 37°C for 1 h.