

DNA cleavage behavior of a new *p*-xylyl spaced bisCu(BPA)Cl₂ complex: the steric effect of bulky *p*-xylyl-derived spacer

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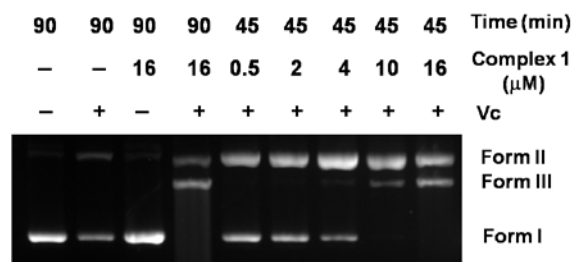


Figure S1. Agarose gel electrophoresis patterns of plasmid pUC19 DNA (0.02 mgmL⁻¹, 30 μM base pair) obtained after at different incubation time when incubated with complex 1 of different concentration in Tris-HCl buffer (50 mM, pH 7.4) at 37 °C in the presence of 100-fold excess of ascorbic acid.

Structural optimization of complex 1

The structure of complex 1 was optimized by density functional theory (DFT) calculations with 6-31G* basis sets using a suite of Gaussian 03 programs.ⁱ Different initial structures of complex 1 were constructed based on the crystal structural data of complex Cu₂(*p*TPXA)Cl₄. Two stable conformations, *anti*-form and *cis*-form, were obtained (Figure S2). The Cu-Cu distance in *cis*-form (11.84 Å) is remarkably larger than the Cu-Cu distance in Cu₂(*p*TPXA)Cl₄ (7.98 Å),ⁱⁱ whose dicopper centers display the internuclear synergic effect in activating O₂ to form ROS, and the two copper centers in *cis*-form are disable to react with the same O₂ molecule in a synergic manner. As to the *anti*-form, the two copper centers located above and below the benzoxadiazole plane respectively, can't react with the same O₂ molecules either, although the Cu-Cu distance is only 8.53 Å. Therefore, the two Cu(BPA)Cl₂ motifs in complex 1 may function solely as a mononuclear copper complex.

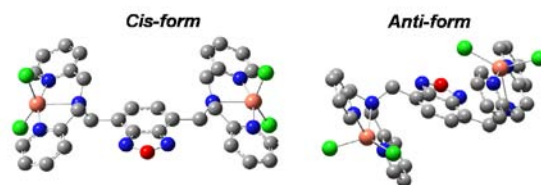


Figure S2. *Cis*- and *anti*-form of complex 1 obtained by theoretical study.

ⁱ M. J. Frisch, G. W. Trucks, H. B. Schlegel, *et al.*, GAUSSIAN 03 (Revision D.02), Gaussian Inc., Pittsburg, PA, 2006.

ⁱⁱ Y. Zhao, J. Zhu, W. He, Z. Yang, Y. Zhu, Y. Li, J. Zhang, Z. Guo, *Chem. Eur. J.* **2006**, *12*, 6621-6629.