

### Supporting Information

#### **Methylene Violet 3RAX-Conjugated Porphyrin for Photodynamic Therapy: Synthesis, DNA Photocleavage and Cell Study**

**Table S1.** Spectral characteristics of compounds **1, 2** interacted with ct-DNA

Compd.	UV-Vis Hypochromicity (H)/ Bathochromicshift ( $\Delta\lambda$ )	Fluorescence emission Hypochromicity (H) / Wavelengthshift ( $\Delta\lambda$ )	CD ( $r=0.01$ )		DNA binding constants ( $M^{-1}$ )
			Positive band (nm)	Negative band (nm)	
1	30.1%/12nm	25.9%/-14nm	-	598	$7.48 \times 10^3$
2	20.1%/3nm	117.6%/-25nm	435	422	$6.48 \times 10^3$

The binding affinities between compound **1, 2** and DNA were expressed by the binding constant ( $K$ ), which was calculated using the equation as follows <sup>1</sup>,

$$[DNA]_{total} / |\varepsilon_A - \varepsilon_F| = [DNA]_{total} / |\varepsilon_B - \varepsilon_F| + 1 / (|\varepsilon_B - \varepsilon_F|K)$$

where  $D$  is the concentration of DNA during the process of titration.  $\varepsilon_A$  is the ratio of  $A_{max}$ / [**1, 2**] during the process of titration.  $\varepsilon_B$  is the ratio of  $A_{max}$ / [**1, 2**] after saturated with DNA and  $\varepsilon_F$  is the ratio of  $A_{max}$ / [**1, 2**] without DNA.

#### **References**

- [1] Z. Xue, A. X. Hou, D. W. J. Kwong and W. K. Wong, *Bioorg. Med. Chem. Lett.*, 2007, **17**, 4266-4270.